Polymers at surfaces, whose modern understanding may be traced back to early work by Sam Edwards 1. Ballroom IV - Gary Grest, Sandia National Laboratories

Surface properties, both as steric stabilizers and as remarkable boundary lubricants, on the coupling between the polyelectrolyte chains and their counterions. The talk will summarize these experiments as well as later work on polymer inter-diffusion across interfaces observed by neutron reflection, where again the tube model is used to interpret the data.

Recent advances with generalized entropy theory of glass-formation in polymers 1, KARL FREED, University of Chicago — The generalized entropy theory (GET) of glass-formation in polymers is a combination of the lattice cluster theory (LCT) for the configurational entropy density with the Adam-Gibbs (AG) theory for the structural relaxation time. A greatly simplified form of the GET (whose expression for the free energy is roughly double that of Flory-Huggins theory) accurately reproduces the four characteristic temperatures of glass-formation (the onset, crossover, glass transition, and Kauzmann temperatures) of the full GET to within 4K for a series of models of polymers composed of semi-flexible chains having the structure of poly(n-alpha olefins). The theory is now simple enough to be used in courses in polymer physics. Although the successes of the GET provide a strong validation of the final form of the AG theory provided the configurational entropy is used, the physical basis of the AG theory has remained an enigma. Hence, we have developed a new, more general, statistical mechanical derivation of AG theory that explains the previously perplexing observations that the string-like elementary excitations have the mass and temperature dependence of systems undergoing equilibrium self-assembly.

The Ordinary-Extraordinary Transition in Dynamics of Solutions of Charged Macromolecules, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — Dynamic light scattering measurements on dilute salt-free polyelectrolyte solutions have shown over the past three decades that there are two distinctive diffusive modes: fast and slow. The diffusion coefficient deduced from the fast mode has been found to be essentially independent of molar mass and polymer concentration and it is merely a factor of four smaller than that of small electrolyte ion such as sodium or potassium ion. The diffusion coefficient deduced from the slow mode is much smaller suggestive of reflection, where again the tube model is used to interpret the data.

Nanotribology of charged polymer brushes, JACOB KLEIN, Weizmann Institute of Science — Polymers at surfaces, whose modern understanding may be traced back to early work by Sam Edwards 1, have become a paradigm for modification of surface properties, both as steric stabilizers and as remarkable boundary lubricants 2. Charged polymer brushes are of particular interest, with both technological implications and especially biological relevance where most macromolecules are charged. In the context of biolubrication, relevant in areas from dry eye syndrome to osteoarthritis, charged polymer surface phases and their complexes with other macromolecules may play a central role. The hydration lubrication paradigm, where tenaciously-held yet fluid hydration shells surrounding ions or zwitterions serve as highly-efficient friction-reducing elements, has been invoked to understand the excellent lubrication provided both by ionized 2 and by zwitterionic 3 brushes. In this talk we describe recent advances in our understanding of the nanotribology of such charged brush systems. We consider interactions between charged end-grafted polymers, and how one may disentangle the steric from the electrostatic surface forces 5. We examine the limits of lubrication by ionized brushes, both synthetic and of biological origins, and how highly-hydrated zwitterionic chains may provide extremely effective boundary lubrication 6. Finally we describe how the lubrication of articular cartilage in the major joints, a tribosystem presenting some of the greatest challenges and opportunities, may be understood in terms of a supramolecular synergy between charged surface-attached polymers and zwitterionic groups 7. 1. Dolan & Edwards, Proc. Roy. Soc. A, 337, 509 (1974). 2. Klein et al., Nature, 370, 634 (1994). 3. Raviv et al., Nature, 425, 163 (2003). 4. Chen et al., Science, 323, 1698 (2009). 5. Peretz et al., to be published. 6. Tairy et al., Macromolecules, 48, 140 (2015). 7. Seror et al., Nature Communications, 6:6497 (2015); Jahn et al., Annual Reviews of Biomedical Engineering (2016)

Self-organization of stress patterns drives state transition in actin cortices, NIKTA FAKHRI, Massachusetts Institute of Technology —
8:36AM A35.00002 Spontaneous actin dynamics in contractile rings1, KARSTEN KRUSE, Theoretical Physics, Saarland University, 66123 Saarbruecken, VIKTORIA WOLLRAUB2, RAGHAVAN THIAGARAJAN, Laboratory of Cell Physics, Institut de Science et d’Ingenieure Supramolaires, 67083 Strasbourg, France, ANNE WALD, Theoretical Physics, Saarland University, 66123 Saarbrucken, DANIEL RIVELINE, Laboratory of Cell Physics, Institut de Science et d’Ingenieure Supramolaires, 67083 Strasbourg, France — Networks of polymerizing actin filaments are known to be capable to self-organize into a variety of structures. For example, spontaneous actin polymerization waves have been observed in living cells in a number of circumstances, notably, in crawling neutrophils and slime molds. During later stages of cell division, they can also spontaneously form a contractile ring that will eventually cleave the cell into two daughter cells. We present a framework for describing networks of polymerizing actin filaments, where assembly is regulated by various proteins. It can also include the effects of molecular motors. We show that the molecular processes driven by these proteins can generate various structures that have been observed in contractile rings of fission yeast and mammalian cells. We discuss a possible functional role of each of these patterns.

1The work was supported by Agence Nationale de la Recherche, France, (ANR-10-LABX-0030-INRT) and by Deutsche Forschungsgemeinschaft through SFB1027.
2Present address: FOM Institute AMOLF, 1098 XG Amsterdam, The Netherlands.

8:48AM A35.00003 Fluctuations and nematic order in collective motion of filamentous bacteria1, DAIKI NISHIGUCHI, The University of Tokyo, KEN H. NAGAI, JAIST, MASAKI SANO, The University of Tokyo — Although there are many numerical and theoretical studies on Vicsek-like models, there have been no convincing experiments that clearly observe predicted properties of collective motion such as giant number fluctuations. To realize such experiments with a biological system, we used filamentous bacteria, which are 20 times as long as usual bacteria. Due to strong alignment interactions arising from their elongated shapes, these bacteria exhibit a nematic state when their dense suspensions are confined in a quasi-two-dimensional plane. We have quantitatively evaluated the nematic order parameter in this ordered state and concluded that it has a true long-range order, and we have obtained giant number fluctuations in this true long-range ordered state. All the obtained experimental results are consistent with a Vicsek-like model with the same symmetry as our experiments, namely, the Vicsek-like self-propelled rods model, in which each particle has polarity and their interactions are nematic.

1Supported by a Grant-in-Aid for Japan Society for Promotion of Science (JSPS) Fellows (Grant No. 26-9915) and KAKENHI (No. 25103004, Fluctuation & Structure) from MEXT, Japan.

9:00AM A35.00004 Modeling flexible active nematics1, MICHAEL VARGA, ROBIN SELINGER, Liquid Crystal Institute, Kent State University — We study active nematic phases of self-propelled flexible chains in two dimensions using computer simulation, to investigate effects of chain flexibility. In a “dry” phase of self-propelled flexible chains, we find that increasing chain stiffness enhances orientational order and correlation length, narrows the distribution of turning angles, increases persistence length, and increases the magnitude of giant density fluctuations. We further adapt the simulation model to describe behavior of microtubules driven by kinesin molecular motors in two different environments: on a rigid substrate with kinesin immobilized on the surface; and on a lipid membrane where kinesin is bonded to lipid head groups and can diffuse. Results are compared to experiments by L. Hirst and J. Xu. Lastly, we consider active nematics of flexible particles enclosed in soft, deformable encapsulation in two dimensions, and demonstrate novel mechanisms of pattern formation that are fundamentally different from those observed in bulk.

1Supported by NSF-DMR 1409658.

9:12AM A35.00005 Active nematics confined within a shell2, RUI ZHANG, YE ZHOU, MOHAMMAD RAHIMI, JUAN DE PABLO, University of Chicago. DEPABLO TEAM — Active fluids exhibit many striking flow patterns when confined within complex geometries. For example, recent work has demonstrated that a thin film of extensile microtubules is confined within a vesicle, the four +1/2 defects periodically oscillate between a tetrahedral and a planar configuration (Keber, et al. Science (2014)). Here we employ hybrid lattice Boltzmann simulations to study the dynamics of active nematics confined between two concentric spherical surfaces. We find that in both extensile and contractile systems, the four defects are coupled with noticeable macroscopic velocities and they move along their symmetry axes, even though in different patterns. We observe that in extensile systems with moderate activity, defects repel each other due to elastic forces, and their collective motion leads to the same patterned dynamics as observed in the above experiment. We further show that this periodic dynamics is accompanied by oscillations of the defect velocity, system’s elastic energy, and the emergence and annihilation of vortices. We also observe that with stronger activity, the extensile system evolves to chaos. In contrast, the contractile system remains passive for the entire activity range, with defects being attracted to each other in pairs.

9:24AM A35.00006 Active Cellular Nematics, GUILLAUME DUCLOS, CHRISTOPH ERLENKAEMPER, SIMON GARCIA, HANNAH YEVICK, JEAN-FRANCOIS JOANNY, PASCAL SILBERZAN, Physico-Chimie Curie, UMR 168, UPMC, Institut Curie, BIOLOGY INSPIRED PHYSICS AT MESOSCALES TEAM, PHYSICAL APPROACH OF BIOLOGICAL PROBLEMS TEAM — We study the emergence of a nematic order in a two-dimensional tissue of apolar elongated fibroblast cells. Initially, these cells are very motile and the monolayer is characterized by giant density fluctuations, a signature of far-from-equilibrium systems. As the cell density increases because of proliferation, the cells align with each other forming large perfectly oriented domains while the cellular movements slow down and eventually freeze. Therefore topological defects characteristic of nematic phases remain trapped at long times, preventing the development of infinite domains. By analogy with classical non-active nematics, we have investigated the role of boundaries and we have shown that cells confined in stripes of width smaller than typically 500 m are perfectly aligned in the stripe direction. Experiments performed in crossed-patterns show that both the number of cells and the degree of alignment impact the final orientation. Reference: Duclos G., Garcia S., Yevick H.G. and Silberzan P., “Perfect nematic order in confined monolayers of spindle-shaped cells”, Soft Matter, 10, 14, 2014

9:36AM A35.00007 Defect dynamics and ordering in compressible active nematics,1, PRASHANT MISHRA, Department of Physics, Syracuse University, PRAGYA SRIVASTAVA, The Francis Crick Institute, M. CRISTINA MARCHETTI, Department of Physics, Syracuse University — Active nematics, such as suspensions of biopolymers activated by molecular motors or bacteria swimming in passive liquid crystals, exhibit complex self-sustained flow, excitability and defect generation. Activity renders the defect themselves self-propelled particles, capable of organizing in emergent ordered structures. We have developed a minimal model of compressible active nematics on a substrate. We eliminate the flow velocity in favor of the nematic order parameter via the balance of frictional dissipation and active driving to obtain a dynamical description entirely in terms of the nematic alignment order parameter. Activity renormalizes the bend and splay elastic constants rendering them anisotropic and driving them to zero or even negative, resulting in the appearance of modulated states and defective structures. Using linear stability analysis and numerics we organize the various regimes into a phase diagram and discuss the relation to experiments.

1This work was supported by NSF-DMR-1305184.
Directed and persistent movement arises from mechanochemistry of the ParA/ParB system. Longhua Hu, National Heart, Lung, and Blood Institute, National Institutes of Health, Anthony G. Vecchietti, Kiyoji Mizuuchi, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Keir C. Newman, Jian Liu, National Heart, Lung, and Blood Institute, National Institutes of Health — The segregation of DNA prior to cell division is essential for faithful genetic inheritance. In many bacteria, segregation of the low-copy-number plasmids involves an active partition system composed of ParA ATPase and its stimulator protein ParB. Recent experiments suggest that ParA/ParB system motility is driven by a diffusion-ratchet mechanism in which ParB-coated plasmid both creates and follows a ParA gradient on the nucleoid surface. However, the detailed mechanism of ParA/ParB-mediated directed and persistent movement remains unknown. We develop a theoretical model describing ParA/ParB-mediated motility. We show that the ParA/ParB system can work as a Brownian ratchet, which effectively couples the ATPase-dependent cycling of ParA-nucleoid affinity to the motion of the ParB bound cargo. Paradoxically, the resulting processive motion relies on quenching diffusive plasmid motion through a large number of transient ParA/ParB-mediated tethers to the nucleoid surface. Our work sheds light on a new emergent phenomenon in which non-motor proteins work collectively via mechanochemical coupling to propel cargos — an ingenious solution shaped by evolution to cope with the lack of processive motor proteins in bacteria.

10:00AM A35.00009 Decoupling tissue and cell scale stresses using embedded oil microdroplets1, Elijah Shelton, Friedhelm Serwane, Alessandro Mongera, Adam Lucio, Otger Camps, University of California Santa Barbara — Embryonic development and organ morphogenesis require mechanical stresses to be patterned in space and time over length scales ranging from cellular to tissue level. While several approaches use 4D live-imaging to infer forces from the observed flow fields, few techniques allow direct measurements of stresses two and in cellular. We use a microdroplet approach in between cell scale and tissue scale to measure the local stress distribution within living tissue. Imaging and custom software for high resolution 3D droplet surface reconstruction, we can directly measure the patterns of stress by looking at the deformations of the drop. This analysis allows us to decouple the stresses at the tissue scale from those generated at cellular scales by disentangling ellipsoidal droop deformation modes from higher order deformation modes using this technique we measure both tissue and cell scale stresses within aggregates of mesenchymal cells as well as within developing zebrafish embryonic tissues. The decoupling of mechanical stresses at cell and tissue scales makes our technique uniquely suited for understanding how tissue scale reorganizations emerge from cell scale interactions.

1This material is based upon work supported by the National Science Foundation Graduate Research Fellowship

10:12AM A35.00100 Volume Changes During Active Shape Fluctuations in Cells, Caterina A. M. La Porta, Alessandro Taloni, University of Milan, Elena Kardash, University of Geneve, Oguz Umut Salman, CNRS, Paris, Lev Truskinovsky, CNRS, Ecole Polytechnique, Palaiseau, Stefano Zapperi, University of Milan — Cells modify their volume in response to changes in osmotic pressure but it is usually assumed that other active shape variations do not involve significant volume fluctuations. Here we report experiments demonstrating that water transport in and out of the cell is needed for the formation of blebs, commonly observed protrusions in the plasma membrane driven by cortex contractions. We develop a model of fluid-mediated membrane-cortex deformations and show that a permeable membrane is necessary for bleb formation which is otherwise impaired. Taken together, our experimental and theoretical results emphasize the subtle balance between hydrodynamics and elasticity in actively driven cell morphological changes[2].


10:24AM A35.00110 Probing the Dynamics of the Cellular Actomyosin Network with Magnetic Microposts, Yu Shi, Department of Physics and Astronomy, Johns Hopkins University, Steven Henry, John Crocker, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Daniel Reich, Department of Physics and Astronomy, Johns Hopkins University — The actomyosin network in living cells is commonly accepted as an archetypal example of an active matter system. To characterize the dynamic properties and the effects of non-thermal motion of such a system requires simultaneously measuring the fluctuation spectrum of internal stresses as well as its local viscoelasticity. Via use of PDMS micropost arrays with magnetic nanowires embedded in selected posts, we measure the local complex modulus of cells through mechanical actuation of the magnetic microposts using a dual magnetic tweezer system. The microposts are also used as passive probes to measure the force fluctuations inside the cytoskeleton. The active and passive responses of fibroblasts will be presented, together with measurements of correlations between different subcellular regions, and the influence of cytoskeleton and myosin inhibitors. Results on the anisotropy of internal stress fluctuations and their response to chemical perturbations will also be discussed.

10:36AM A35.00120 Active Contraction of Microtubule Networks, Peter Foster, John A. Paulson School of Engineering and Applied Sciences and FAS Center For Systems Biology, Harvard University, Sebastien Firthauer, Courant Institute of Mathematical Science, New York University and Department of Molecular and Cellular Biology, Harvard University, Michael Shelley, Courant Institute of Mathematical Science, New York University, Daniel Needleman, John A. Paulson School of Engineering and Applied Sciences, FAS Center For Systems Biology, Harvard University — Many cellular processes are driven by cytoskeletal assemblies. While processes involving cytoskeletal components affect the large scale behaviors of these systems, here, we investigate the self-organization of stabilized microtubules in Xenopus oocyte extracts and find that they can form macroscopic networks that spontaneously contract. We propose that these contractions are driven by the clustering of microtubule minus ends by dynein. Based on this idea, we construct an active fluid theory of network contractions which predicts a dependence of the timescale of contraction on initial network geometry, a development of density inhomogeneities during contraction, a constant final network density, and a strong influence of dynein inhibition on the rate of contraction, all in quantitative agreement with experiments. These results demonstrate that the motor-driven clustering of filament ends is a generic mechanism leading to contraction.

10:48AM A35.00130 Collective dynamics during cell division, Stefano Zapperi, University of Milan, Zsolt Bertalan, Zoe Budrikis, ISI Foundation, Caterina A. M. La Porta, University of Milan — In order to correctly divide, cells have to move all their chromosomes at the center, a process known as congression. This task is performed by the combined action of molecular motors and randomly growing and shrinking microtubules. Chromosomes are captured by growing microtubules and transported by motors using the same microtubules as track. Coherent motion occurs as a result of a large collection of random and deterministic dynamical events. Understanding this process is important since a failure in chromosome segregation can lead to chromosomal instability one of the hallmarks of cancer. We describe this complex process in a three dimensional computational model involving thousands of microtubules. The results show that coherent and robust chromosome congression can only happen if the total number of microtubules is neither too small, nor too large. Our results allow for a coherent interpretation of a variety of biological factors already associated in the past with chromosomal instability and related pathological conditions[1].


2Z. Bertalan et al. Role of the Number of Microtubules in Chromosome Segregation during Cell Division, PLoS One, 10 e0141305 (2015)
8:00AM A40.00001 Jarzynski equality for non-Hamiltonian dynamics\textsuperscript{1}, DIBYENDU MANDAL, Department of Physics, University of California Berkeley,\textsuperscript{2} MICHAEL R. DEWEÉSE, Department of Physics, Redwood Center for Theoretical Neuroscience, and Helen Wills Neuroscience Institute, University of California Berkeley — Recent years have witnessed major advances in our understanding of nonequilibrium processes. The Jarzynski equality, for example, provides a link between equilibrium free energy differences and finite-time, nonequilibrium dynamics. We propose a generalization of this relation to non-Hamiltonian dynamics, relevant for active matter systems, continuous feedback, and computer simulation. Surprisingly, this relation allows us to calculate the free energy difference between the desired initial and final states using arbitrary dynamics. As a practical matter, this dissociation between the dynamics and the initial and final states promises to facilitate a range of techniques for free energy estimation in a single, universal expression.

\textsuperscript{1}This material is based upon work supported in part by the U.S. Army Research Laboratory and the U.S. Army Research Office under contract number W911NF-13-1-0390.

8:12AM A40.00002 Field Theoretic Description of Nonequilibrium Work Relations, BENJAMIN VOLLMAYR-LEE, Bucknell University, ANDREW BAISH, UC Santa Barbara — We develop Doi-Peliti field theory for driven, interacting particles coupled to a thermal bath. This mapping of classical particles to a field theory does not require any assumption of large particle numbers or slow modes. As an application we consider nonequilibrium work relations. With the introduction of an auxiliary complex field, the Jarzynski relation emerges from the field theory as direct consequence of time reversal.

8:24AM A40.00003 Extending Landauer’s Bound from Bit Erasure to Arbitrary Computation, DAVID WOLPERT, Santa Fe Institute — Recent analyses have calculated the minimal thermodynamic work required to perform any computation \( \sigma \) whose output is independent of its input, e.g., bit erasure. First I extend these analyses to calculate the work required even if the output of \( \sigma \) depends on its input. Next I show that if a physical computer \( C \) implementing a computation \( \pi \) will be re-used, then the work required depends only on the dynamics of the logical variables under \( \pi \), independent of the physical details of \( C \). This establishes a formal identity between the thermodynamics of (re-usable) computers and theoretical computer science. To illustrate this identity, I prove that the minimal work required to compute a bit string \( \sigma \) on a (physical) Turing machine \( M \) is \( k_B T \ln(2) \) [kolmogorov complexity(\( \sigma \)) + \( \log \) (Bernoulli measure of the set of strings that compute \( \sigma \)) + \( \log \) (halting probability of \( M \))]. I also prove that uncertainty about the inputs over which the computer increases the minimal work required to run the computer. I end by using these results to relate the free energy flux incident on an organism / robot / biosphere to the maximal amount of computation that the organism / robot / biosphere can do per unit time.

8:36AM A40.00004 Average work measurement below the Landauer limit for memory erasure\textsuperscript{1}, MOMČILO GAVRILOV, JOHN BECHHOEFER, Simon Fraser University — Landauer’s Principle states that erasing a one-bit memory requires an average work of at least \( k_B T \ln 2 \). Recent experiments have confirmed this prediction for a one-bit memory represented by a symmetric double well potential. However, if a memory is represented by a non-equilibrium state in an asymmetric double-well potential, theoretical studies predict that one can measure work below \( k_B T \ln 2 \). Using a feedback trap, we have confirmed this prediction. Surprisingly, we found that two different erasure protocols give two different values for the asymptotic work. We can explain this result by noting that one protocol is symmetric with the respect to time reversal and the other is not.

\textsuperscript{1}This work was supported by NSERC (Canada).

8:48AM A40.00005 Dynamics and thermodynamics of open chemical networks, MASSIMILIANO ESPOSITO, University of Luxembourg — Open chemical networks (OCN) are large sets of coupled chemical reactions where some of the species are chemostated (i.e. continuously restored from the environment). Cell metabolism is a notable example of OCN. Two results will be presented. First, dissipation in OCN operating in nonequilibrium steady-states strongly depends on the network topology (algebraic properties of the stoichiometric matrix)\textsuperscript{1} An application to oligosaccharides exchange dynamics performed by so-called D-enzymes will be provided\textsuperscript{2} Second, at low concentration the dissipation of OCN is in general inaccurately predicted by deterministic dynamics (i.e. nonlinear rate equations for the species concentrations). In this case a description in terms of the chemical master equation is necessary. A notable exception is provided by so-called deficiency zero networks, i.e. chemical networks with no hidden cycles present in the graph of reactant complexes\textsuperscript{3}.

\textsuperscript{1}M. Polettini and M. Esposito, J. Chem. Phys. 141, 024117 (2014)
\textsuperscript{2}R. Yao, D. Lacoste and M. Esposito, arxiv:1509.07436
\textsuperscript{3}M. Polettini, A. Wachtel and M. Esposito, arxiv:1507.00058

9:00AM A40.00006 Cost and consequences of breaking the fluctuation dissipation relation in biochemical networks\textsuperscript{1}, YUHAI TU, IBM — Living systems need to be highly responsive, and also to keep fluctuations low. These goals are incompatible in equilibrium systems due to the Fluctuation Dissipation Theorem (FDT). Here, we show that biological sensory systems, driven far from equilibrium by free energy consumption, can reduce their intrinsic fluctuations while maintaining high responsiveness. By developing a continuum theory of the E. coli chemotaxis pathway, we demonstrate that adaptation can be understood as a non-equilibrium phase transition controlled by free energy dissipation, and it is characterized by a breaking of the FDT\textsuperscript{1}. We show that the maximum response at short time is enhanced by free energy dissipation. At the same time, the low frequency fluctuations and the adaptation error decrease with the free energy dissipation algebraically and exponentially, respectively.\textsuperscript{1} “Free Energy Cost of Reducing Noise while Maintaining a High Sensitivity”, Pablo Sartori and Yuhui Tu, Phys. Rev. Lett. 2015. 115: 118102.

\textsuperscript{1}This work is partly supported by a NIH grant (R01GM081747 to YT)

9:12AM A40.00007 Mimicking Nonequilibrium Steady States with Time-Periodic Driving, OREN RAZ, YIGIT SUBASI, CHRISTOPHER JARZYNSKI, Univ of Maryland-College Park — Under static conditions, a system satisfying detailed balance generically relaxes to an equilibrium state in which there are no currents: to generate persistent currents, either detailed balance must be broken or the system must be driven in a time-dependent manner. A stationary system that violates detailed balance evolves to a nonequilibrium steady state (NESS) characterized by fixed currents. Conversely, a system that satisfies instantaneous detailed balance but is driven by the time-periodic variation of external parameters - also known as a stochastic pump (SP) - reaches a periodic state with non-vanishing currents. In both cases, these currents are maintained at the cost of entropy production. Are these two paradigmatic scenarios effectively equivalent? For discrete-state systems we establish a mapping between NESS and SP. Given a NESS characterized by a particular set of stationary probabilities, currents and entropy production rates, we show how to construct a SP with exactly the same (time-averaged) values. The mapping works in the opposite direction as well. These results establish a proof of principle: they show that SP are able to mimic the behavior of NESS, and vice-versa, within the theoretical framework of discrete-state stochastic thermodynamics.
9:24AM A40.00008 The thermal vacuum for non-equilibrium steady state, RYOSUKE IMAI, YUKIRO KUWAHARA, YUSUKE NAKAMURA, YOSHIYA YAMANAKA, Waseda Univ — Our purpose is to construct a theoretical description of non-equilibrium steady state (NESS), employing thermo field dynamics (TFD). TFD is the operator-based formalism of thermal quantum field theory, where every degree of freedom is doubled and thermal averages are given by expectation values of the thermal vacuum. To specify the thermal vacuum for NESS, a non-trivial issue, and we attempt it on the analogy between the superoperator formalism and TFD. Using the thermal vacuum thus obtained, we analyze the NESS which is realized in the two-reservoir model. It will be shown that the NESS vacuum of the model coincides with the fixed point solutions of the quantum transport equation derived by the self-consistent renormalization of the self-energy in non-equilibrium TFD.

1. H. Umewaza, Thermo Field Dynamics and Condensed States (Elsevier Science Ltd, 1982).


9:36AM A40.00009 Closed hierarchies and non-equilibrium steady states of driven systems, ISRAEL KLICH, University of Virginia — We present a class of tractable non-equilibrium dynamical quantum systems which includes combinations of injection, detection and extraction of particles interspersed by unitary evolution. We show how such operations generate a hierarchy of equations tying lower correlation functions with higher order ones. The hierarchy closes for particular choices of measurements and leads to a rich class of evolutions whose long time behavior can be simulated efficiently. In particular, we use the method to describe the dynamics of current generation through a generalized quantum exclusion process, and exhibit an explicit formula for the long time energy distribution in the limit of weak driving.

9:48AM A40.00010 Mechanical autonomous stochastic heat engines, MARC SERRA-GARCIA, ANDRE FOEHR, MIGUEL MOLERON, Swiss Federal Institute of Technology (ETH), JOSEPH LYDON, jlydon@ethz.ch, CHRISTOPHER CHONG, Bowdoin College, CHIARA DAVICO, Swiss Federal Institute of Technology (ETH), TEAM — Stochastic heat engines extract work from the Brownian motion of a set of particles out of equilibrium. So far, experimental demonstrations of stochastic heat engines have required extreme operating conditions or nonautonomous external control systems. In this talk, we will present a simple, purely classical, autonomous stochastic heat engine that uses the well-known tension induced nonlinearity in a string. Our engine operates between two heat baths out of equilibrium, and transfers energy from the hot bath to a work reservoir. This energy transfer occurs even if the work reservoir is at a higher temperature than the hot reservoir. The talk will cover a theoretical investigation and experimental results on a macroscopic setup subject to external noise excitations. This system presents an opportunity for the study of non-equilibrium thermodynamics and is an interesting candidate for innovative energy conversion devices.

10:00AM A40.00011 A dissipation bound for thermodynamic control, BENJAMIN MACHTA, Princeton Univ — Biological and engineered systems operate by coupling function to the transfer of heat and/or particles down a thermal or chemical gradient. In idealized deterministically driven systems, thermodynamic control can be exerted reversibly, with no entropy production, as long as the rate of the protocol is made slow compared to the equilibration time of the system. Here we consider fully realizable, entropically driven systems where the control parameters themselves obey rules that are reversible and that acquire directionality in time solely through dissipation. We show that when such a system moves in a directed way through thermodynamic space, it must produce entropy that is on average larger than its generalized displacement as measured by the Fisher information metric. This distance measure is sub-extensive but cannot be made small by slowing the rate of the protocol.

10:12AM A40.00012 Thermodynamic second law in a feedback process with time delay, JAEJONG UM, Korea Institute for Advanced Study, CHULAN KWON, Myongji University, HYUNGGYU PARK, Korea Institute for Advanced Study — We investigate a realistic feedback protocol repeated in multiple steps where a feedback protocol from measurement is applied with delay and maintains for a finite duration until next step. Unlike a feedback without delay, a composite system consists of the system and two memories where previous and present measurement outcomes are stored, leading to the 3-state Shannon entropy for the composite system. Then according to the thermodynamic second law, the change of the 3-state Shannon entropy provides the upper bound for heat flow from reservoir to system during the feedback and relaxation process. However, if the feedback protocol is depending on memory states sequentially, it turns out that the tighter bound for heat production can be obtained by integrating out the irrelevant memory states. We exemplify a cold damping case where a velocity of a particle is measured and a dissipative protocol is applied by feedback, and it is confirmed that the Shannon-entropy change of the reduced composite system gives the tighter bound for heat production.

10:24AM A40.00013 Direct measurement of the Einstein relation in a macroscopic, non-equilibrium system of chaotic surface waves, KYLIE WELCH, ALEXANDER LIEBMAN-PELAEZ, ERIC CORWIN, University of Oregon — Equilibrium statistical mechanics is traditionally limited to thermal systems. Can it be applied to athermal, non-equilibrium systems that nonetheless satisfy the basic criteria of steady-state chaos and isotropy? We answer this question using a macroscopic system of chaotic surface waves which is, by all measures, non-equilibrium. The waves are generated in a dish of water that is vertically oscillated above a critical amplitude. We have constructed a rheometer that actively measures the drag imparted by the waves on a buoyant particle, a quantity entirely divorced in origin from the drag imparted by the fluid in which the particle floats. We also perform a separate, passive measurement, extracting a diffusion constant and effective temperature. Having directly measured all three properties (temperature, diffusion constant, and drag coefficient) we go on to show that our macroscopic, non-equilibrium case is wholly consistent with the Einstein relation, a classic result for equilibrium thermal systems.

10:36AM A40.00014 Least action and entropy considerations of self-organization in Benard cells, GEORGI GEORGIEV, VPI and Assumption College, GERMANO IANNACCIONE, VPI — We study self-organization in complex systems using first principles in physics. Our approach involves the principle of least action and the second law of thermodynamics. In far from equilibrium systems, energy gradients cause internal ordering to facilitate the dissipation of energy in the environment. This internal ordering decreases their internal entropy in order to obey the principle of least action, minimizing the product of time and energy for transport through the system. We are considering the connection between action and entropy decrease inside Benard cells in order to derive some general features of self-organization. We are developing mathematical treatment of this coupling and comparing it to results from experiments and simulations.

10:48AM A40.00015 Dissipation and irreversibility for models of mecanochemical machines, AIDAN BROWN, DAVID SIVAK, Simon Fraser University — For biological systems to maintain order and achieve directed progress, they must overcome fluctuations so that reactions and processes proceed forwards more than they go in reverse. It is well known that some free energy dissipation is required to achieve irreversible forward progress, but the quantitative relationship between irreversibility and free energy dissipation is not well understood. Previous studies focused on either abstract calculations or detailed simulations that are difficult to generalize. We present results for mecanochemical models of molecular machines, exploring a range of model characteristics and behaviours. Our results describe how irreversibility and dissipation trade off in various situations, and how this trade-off can depend on details of the model. The irreversibility-dissipation trade-off points towards general principles of microscopic machine operation or process design. Our analysis identifies system parameters which can be controlled to bring performance to the Pareto frontier.
We find that large events result from stored elastic energy in the plates in this coupled granular-continuum system. Earthquakes and avalanches. We further explore the high-speed dynamics of system events and also discuss the effective granular friction of the sheared layer.

Of quasistatic shear, disordered solids demonstrate non-equilibrium critical behavior including power-law distributions of avalanches. The gel may either display transient shear banding towards complete fluidization, or steady-state shear banding. In the former case, we unravel the relationship between shear rate and shear stress during shear startup experiments. In practice, after being rejuvenated by a preshear, the gel is left to age during a time \( t_{\text{conv}} \). We investigate in detail the effects of both \( t_{\text{conv}} \) and \( \gamma \) on the fluidization dynamics and build a detailed state diagram of the gel response to shear startup flows. The gel may either display transient shear banding towards complete fluidization, or steady-state shear banding. In the former case, we unravel that the progressive fluidization occurs by successive steps that appear as peaks on the gel stress relaxation signal, which diverges as \( t_{\text{conv}} \sim |\theta - \theta_c|^{-\alpha/2} \).

Using molecular dynamics simulations of 2D and 3D overdamped binary LJ glasses, we explore the critical behavior in the limit of finite strain rate. We use finite-size scaling to find the critical exponents characterizing shear stress, kinetic energy, and measures of temporal and spatial correlations. The shear stress of the system rises as a power \( \beta \) of the strain rate. Larger system sizes extend this power law to lower rates. This behavior is governed by a power law drop of the dynamic correlation length with increasing shear stress defined by the exponent \( \nu \). This finite-size scaling affects the scaling of the RMS kinetic energy with strain rate as avalanches begin nucleating simultaneously leading to continuous deformation of the solid. As system size increases, avalanches begin overlapping at lower rates. The correlation function of non-affine displacement exhibits novel anisotropic power law scaling with the magnitude of the wave vector. Its strain rate dependence is used to determine the scaling of the dynamic correlation length.

Using dynamic analysis, we report on the fluidization dynamics of an attractive gel composed of non-Brownian particles made of fused silica. We investigate the effects of both \( t_{\text{conv}} \) and \( \gamma \) on the fluidization dynamics and build a detailed state diagram of the gel response to shear startup flows. The gel may either display transient shear banding towards complete fluidization, or steady-state shear banding. In the former case, we unravel that the progressive fluidization occurs by successive steps that appear as peaks on the gel stress relaxation signal. Flow imaging reveals that the shear band grows up to complete fluidization of the material by sudden avalanche-like events which are distributed heterogeneously along the vorticity direction and correlated to large peaks in the slip velocity at the moving wall.

Using renormalization group methods, quasibrittle or disordered brittle materials like concrete evade usual fracture analysis because of strong finite-size effects connected to the tip of quasibrittle cracks, a process that is not well understood. Recently, a scaling crossover theory was developed by Sethna and Shekhawat to explain the influence of finite size on the fracture mechanism and avalanche precursors. We extend this theory to model the scaling of stress and distribution of microcracking in the process zone.

Using numerical simulation, we try to understand the flow of particles and evolution of force chains inside the media and during avalanches. We directly determine the spatial and temporal distributions of strain displacements of the quasi-two-dimensional granular material (bi-dispersed nylon rods). We analyze the power spectrum of the force signal to understand the effect of the loading speed and of the tip of quasibrittle cracks, a process that is not well understood. Recently, a scaling crossover theory was developed by Sethna and Shekhawat to explain the influence of finite size on the fracture mechanism and avalanche precursors. We extend this theory to model the scaling of stress and distribution of microcracking in the process zone.

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9:36AM A43.00007 Tuning Parameters and Scaling For Avalanches On A Slowly-Driven Conical Bead Pile with Cohesion1. SUSAN LEHMAN, D. T. JACOBS, PAROMA PALCHOUKDURU, AVI VAJPEYI, JUSTINE WALKER, College of Wooster, KARIN DAHMEN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, JONATHAN UHL, Retired — Slip avalanches on a slowly driven pile are investigated experimentally using a 3D conical pile built from uniform 3 mm steel beads. Beads are added to the pile by dropping them onto the apex one at a time; avalanches are measured through changes in pile mass. We investigate the dynamic response of the pile by recording avalanches from the pile over the course of tens of thousands of bead drops. The statistical properties of the avalanches, including probability of particular avalanche sizes and the time between avalanches of given size, are well-characterized by universal power laws and scaling functions. By adding a uniform magnetic field, we may systematically vary the cohesion between the beads and tune the critical behavior of the system. As the cohesion increases we observe an increase in both size and number for very large avalanches and decreases in the mid-size avalanches, causing a deviation from the power law. A full study of the effect of cohesion on the size and time distributions is in process, combining the experimental results with predictions from an analytical mean-field model [Dahmen, Nat Phys 7, 554 (2011)].

9:48AM A43.00008 Universality and depinning models for plastic yield in amorphous materials. ZOE BUDRIKIS, ISI Foundation, via Alassio 11/c 10126 Torino, Italy, DAVID FERNANDEZ CASTELLANO, STEFAN SANDFIELD, MICHAEL ZAIZER, 8-Materials Simulation, FAU University of Erlangen-Nuremberg, Germany, STEFANO ZAPPERI, Dipartimento di Fisica, Universita di Milano, Italy — Plastic yield in amorphous materials occurs as a result of complex collective dynamics of local reorganizations, which gives rise to rich phenomena such as strain localization, intermittent dynamics and power-law distributed avalanches. While such systems have received considerable attention, both theoretical and experimental, controversy remains over the nature of the yielding transition. We present a new fully-tensorial coarsegrained model in 2D and 3D, and demonstrate that the exponents describing avalanche distributions are universal under a variety of loading conditions, system dimensionality and size, and boundary conditions. Our results show that while depinning-type models in general are apt to describe the system, mean field depinning models are not.

10:00AM A43.00009 Atomic-scale reversibility in sheared glasses, MENG FAN, MINGLEI WANG, YANHUI LIU, JAN SCHROERS, Department of Mechanical Engineering and Materials Science, Yale University, MARK SHATTUCK, Department of Physics and Benjamin Levich Institute, The City College of the City University of New York, New York, COREY O’HERN, Department of Mechanical Engineering and Materials Science, Yale University — Systems become irreversible on a macroscopic scale when they are sheared beyond the yield strain and begin flowing. Using computer simulations of oscillatory shear, we investigate atomic scale reversibility. We employ molecular dynamics simulations to cool binary Lennard-Jones liquids to zero temperature over a wide range of cooling rates. We then apply oscillatory quasistatic shear at constant pressure to the zero-temperature glasses and identify neighbor-switching atomic rearrangement events. We determine the critical strain $\gamma^*$, beyond which atoms in the system do not return to their original positions upon reversing the strain. We show that for more slowly cooled glasses, the average potential energy is lower and the typical size of atomic rearrangements is smaller, which correlates with larger $\gamma^*$. Finally, we connect atomic- and macro-scale reversibility by determining the number of and correlations between the atomic rearrangements that occur as the system reaches the yield strain.

10:12AM A43.00010 Multiscale minimal modeling of microscale crystal plasticity: Finite-size scaling and stochastic plastic flow, STEFANOS PAPANIKOLAOU, Johns Hopkins University, PETER ISPANOVITY, Etvs University — We investigate the multiscale description from continuum to discrete modeling of crystal plasticity in the context of a minimal model. We develop a continuum plasticity description of discrete edge dislocations moving athermally in a single slip system; Our continuum modeling not only matches the statistical behavior of the model, but also the onset of emergent length scales as load increases. We perform quasistatic stress-controlled simulations of our continuum model and compare it with the corresponding discrete dislocation dynamics model, which describes crystal plasticity at a smaller spatiotemporal discretization scale. We investigate the properties of strain bursts (dislocation avalanches) occurring during plastic deformation, as well as the onset of a dislocation patterning lengthscale, and compare in detail the continuum and discrete descriptions. Our approach provides a pathway to multiscale modeling of complex, multi-slip and three dimensional crystal plasticity.

10:24AM A43.00011 The effectiveness of mean-field theory for avalanche distributions, EDWARD LEE, ARCHISHMAN RAJU, JAMES SETHNA, Cornell University — We explore the mean-field theory of the pseudogap found in avalanche systems with long-range antiferromagnetic interactions using analytical and numerical tools. The pseudogap in the density of low-stability states emerges from the competition between stabilizing interactions between spins in an avalanche and the destabilizing random movement towards the threshold caused by anisotropic couplings. Pazmandi et al. have shown that for the Sherrington-Kirkpatrick model, the pseudogap scales linearly and produces a distribution of avalanche sizes with exponent $\tau=1$ in contrast with that predicted from RFIM $\tau=3/2$. Lin et al. have argued that the scaling exponent $\gamma$ of the pseudogap depends on the tail of the distribution of couplings and on non-universal values like the strain rate and the magnitude of the coupling strength. Yet others have argued that the relationship between the pseudogap scaling and the distribution of avalanche sizes is dependent on dynamical details. Despite the theoretical arguments, the class of RFIM mean-field models is surprisingly good at predicting the distribution of avalanche sizes in a variety of different magnetic systems. We investigate these differences with a combination of theory and simulation.

10:36AM A43.00012 Elasto-plastic automata with realistic near field interactions: avalanches and diffusion, CRAIG MALONEY, Northeastern, BOTOND TYUKODI, DAMIEN VANDEMBRUCQ, ESPCI — We present results on an elasto-plastic automaton model of an athermal amorphous solid under shear. We study four different variants of the model with two different loading geometries and two different stochastic prescriptions (random yield thresholds or random strain amplitudes). We perform a finite size scaling analysis for the avalanche size distribution and single-site displacement and strain statistics. The avalanche size distribution in all four cases is inconsistent with mean-field depinning results. For three of the four variants, the distribution differs from the predictions with previous results from atomistic simulations and other related elasto-plastic models. The fourth variant shows that different scaling properties and may lie in a different universality class. The mean-sized distribution exhibits a pronounced dependence on the microscopic ingredients of the model and is completely non-universal. These results show that while certain microscopic ingredients of the model may be irrelevant for the individual avalanches, they may exhibit a profound impact on long-time correlations and long-lived shear localization.

10:48AM A43.00013 Rearrangements in deformed foams near jamming, MERLIJN VAN DEEN, VERA JANSSSEN, ALEXANDER SIEMENS, MARTIN VAN HECKE, Huygens-Kamerlingh Onnes Lab, Leiden University — We deform two-dimensional foams at different densities and show there are two distinct regimes: a high density regime where bubbles deform affinely until the built up stress is released in rapid events (shear transformation zones), and a low density regime where bubbles are continuously in motion and rapid events are rare.
11:15AM B2.00001 Numerical calculation of granular entropy: counting the uncountable. , DAAN FRENKEL, U. Cambridge — In 1989, Sir Sam Edwards introduced the concept of ‘granular entropy’, defined as the logarithm of the number of distinct packings of $N$ granular particles in a fixed volume $V$. The proposal was rather controversial but much of the debate was sterile because the granular entropy could not even be computed for systems as small as 20 particles - hardly a good approximation of the thermodynamic limit. In my talk I will describe how granular entropies of much larger systems can now be computed, using a novel algorithm. Interestingly, it turns out the definition of granular entropy will have to be modified to guarantee that granular entropy is extensive.

11:51AM B2.00002 Granular statistical mechanics – Building on the legacy of Sir Sam Edwards\(^1\), RAPHAEL BLUMENFELD, National University of Defense Technology, Changsha and Imperial College London, UK, Co-Author, Shahar Amital, Imperial College London, UK — When Sir Sam Edwards laid down the foundations for the statistical mechanics of jammed granular materials he opened a new field in soft condensed matter and many followed. In this presentation we review briefly the Edwards formalism and some of its less discussed consequences. We point out that the formalism is useful for other classes of systems - cellular and porous materials. A certain shortcoming of the original formalism is then discussed and a modification to overcome it is proposed. Finally, a derivation of an equation of state with the new formalism is presented; the equation of state is analogous to the PVT relation for thermal gases, relating the volume, the boundary stress and measures of the structural and stress fluctuations.

12:27PM B2.00003 Unifying Suspensions and Inertial Granular flows near Jamming , WYART MATTIEU, Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne — Observations support that the fluid to solid transition in granular materials is a continuous transition, with diverging length scales and singular flow curves. I will introduce a framework that predict quantitatively scaling exponents near this transition when particles are frictionless. This framework captures both aerial granular flows and over-damped suspensions, phenomena traditionally studied by two distinct communities.

In this description, the dearth fluid phase can be thought as a gas of excitations of the solid phase. Key aspects of the solid entering the description can be obtained by dynamical argument, and imply that the solid is marginally stable. Recent calculations in infinite spatial dimension support however that thermodynamics arguments a la Edwards also capture this marginality.

1:03PM B2.00004 Soft active matter : a contemporary example of Edwardsian statistical mechanics\(^1\), TANNIEMOLA LIVERPOOL, University of Bristol — Colonies of swimming bacteria, algae or spermatozoa are examples of active systems composed of interacting units that consume energy and collectively generate motion and mechanical stresses. Due to the anisotropy of their interactions, these active particles can exhibit orientational order at high concentrations and have been called living liquid crystals\(^2\). Biology at the cellular and multicellular scale provides numerous examples of these active systems. They provide a novel class of experimentally accessible system far from equilibrium. Their rich collective behaviour includes non-equilibrium phase transitions and pattern formation on mesoscopic scales. Interestingly however, some of the theoretical insights gained from field theories applied to equilibrium soft matter systems can be used to explain aspects of their behaviour, but with a number of surprising new twists. I will describe and summarise recent theoretical results characterising the behaviour of such soft active systems highlighting in particular the effects of their internal dynamics on their macroscopic behaviour.

1:39PM B2.00005 Thinking Outside the Sandbox , JASN JASNA BRUJIC, New York Univ NYU — Theoretical approaches for inherently out-of-equilibrium systems, from granular to live matter, are at the forefront of soft condensed matter physics. Edwards pioneered a statistical mechanics framework to describe jammed particulate materials, which explains the slow compaction of granular materials towards a given density, the reversibility of such experiments, and the equilibrium between shaken powders of different types. During my PhD, Edwards’s theoretical work inspired me to develop a transparent emulation system to test the microscopic distributions underlying granular thermodynamics. I will talk about what it was like to have Sir Sam as a PhD adviser and how he uniquely inspired my curiosity to design and build novel materials, which are not random, but assemble via mobile, multiflavored bonds that respond to environmental queues. I will give an overview of this kind of experimentally guided assembly: these results call for new theories of emulsions with programmable architectures.

\(^1\) with support of the EPSRC Grant No. EP/G026440/1

\(^2\) supported by the EPSRC Grant No. EP/I00786X/1

Monday, March 14, 2016 11:15AM - 2:15PM – Session B40 GSNP DFD: Fluids and Elasticity 343 - Doug Holmes, Boston University

11:15AM B40.00001 Direct measurement of surface stress of stretched soft solids. , QIN XU, ERIC DUFRESNE, Mechanical Engineering and Materials Science, Yale University — The wetting profile of liquid droplets on soft solids is determined by the competition between elasticity and solid surface stress. Near the contact point, the bulk elasticity becomes negligible such that Neumann’s classic analysis nicely captures the wetting geometry and provides us an effective approach to directly measure the solid surface stress. Here, we report our experiments using confocal microscopy in studying the wetting of liquids on soft PDMS gels. While the droplets are sitting on the top, the substrates are biaxially strained. We observe that the wetting profiles and the three-phase contact angles are changing dramatically as the substrate is stretched. With Neumann’s principle, we obtain the quantitative relation between surface stress of the PDMS and the applied strain. These results suggest a significant strain-dependence of surface energy and surface stress for our PDMS.

11:27AM B40.00002 A numerical modeling capability for the interplay between surface energy and elasticity in soft materials , DAVID HENANN, YUHAO WANG, Brown University — Surface energy is an important factor in the deformation of fluids but is typically a minimal or negligible effect in solids. However, when a solid is soft and its characteristic dimension is small, forces due to surface energy can become important and induce significant elastic deformation. The interplay between surface energy and elasticity can lead to interesting elastico-capillary phenomena. We have developed a finite-element formulation for problems involving these effects in both 2D and 3D settings and will demonstrate the simulation capability by examining two elastico-capillary problems. (1) The Rayleigh-Plateau instability in an elastic material – In a fluid, this instability causes fluid jets to break up into droplets; however, as shown in recent experiments (Mora et al., PRL, 2010), break-up is prohibited in an elastic material, resulting in a stable undulatory configuration. (2) The effect of fluid-filled droplet inclusions on a soft solid – When the matrix material is stiff, the presence of fluid-filled droplets leads to stiffening. In this talk, we will show that our simulation capability predicts all experimentally observed phenomena and provides a straightforward route for describing nonlinear aspects of elastico-capillarity, which are difficult to address via analytics.
11:39 AM B40.00003 Elastocapillary Deformations and Fracture of Soft Gels, KAREN DANIELS, NC State University, MARION GRZELKA, ENS-Cachan, JOSHUA BOSTWICK, Clemson University — When a droplet is placed on the surface of a soft gel, the surface deforms by an amount proportional to the elastocapillary length calculated from the ratio of surface tension and elastic modulus. For sufficiently large deformations, the gel can fracture due to the forces generated under the liquid-gel contact line. We observe that a starburst of channel fractures forms on the surface of the gel, driven by fluid propagating away from the central droplet. To understand the initiation of these cracks, we model the substrate as an incompressible, linear-elastic solid and quantify the elastic response. This provides quantitative agreement with experimental measurements of the number of fracture arms as a function of material properties and geometric parameters. In addition, we find that the initiation process is thermally-activated, with delay time that decreases as a function of the elastocapillary length.

11:51 AM B40.00004 Surface tension and deformation in soft adhesion, KATHARINE JENSEN, Yale University — Modern contact mechanics was originally developed to account for the competition between adhesion and elasticity for relatively stiff deformable materials like rubber, but much softer sticky materials are ubiquitous in biology, engineering, and everyday consumer products. In such soft materials, the solid surface tension is an important force resisting shape change, and significantly moderates the platelet contact with soft materials. We report indentation and pull-off experiments that bring small, rigid spheres into adhesive contact with compliant silicone gel substrates, varying both the surface functionalization of the spheres and the bulk elastic properties of the gels. We map the resulting deformation profiles using optical microscopy and image analysis. We examine the substrate geometry in light of capillary and elastic theories in order to explore the interplay of surface tension and bulk elasticity in governing soft adhesion.

12:27 PM B40.00005 Elastocapillary Swelling: When coalesced structures curl apart, DOUGLAS HOLMES, Boston University, PIERRE-THOMAS BRUN, MIT, ANUPAM PANDEY, University of Twente, SUZIE PROTIERE, Institut Jean Le Rond d’Alembert — We consider the elastocapillary rise between swellable structures using a favorable solvent. We study the elastocapillary rise and subsequent swelling-induced bending, and characterize the dynamic deformations and resulting equilibrium configurations for various beam geometries. Our analysis highlights the importance of two characteristic length scales, and uses these lengths to predict both the elastocapillary rise and the critical curvature for peeling. We predict the transition between coalescence dominated beams and bending dominated beams using a balance of bending, stretching, and surface energies, and use a relaxed constraint on Euler’s elastica to describe the fluid ratcheting.

12:39 PM B40.00006 Effects of elastocapillarity on periodic films folding and unfolding, OSAMA BILAL, ANDRE FOEHR, JINUWONG CHA, CHIARA DARAIIO, Department of Mechanical and Process Engineering, ETH-Zurich — Thin films interact with liquid surfaces through elastocapillary forces. These forces can control structural deformations of wetted thin films. Deformations arise from the interplay between the elastic strain energy in bulk of the films, and the energy on the surface. In this work, we study the interplay between the surface tension of water and periodic patterns on different thin films. Our analysis explores the utilization of these periodically patterned films for the deployability of micro and nano-systems. The main attention is paid to the experimental results of this phenomenon and the results are supported by numerical analysis.

12:51 PM B40.00007 Wrinkles and folds in a compressed granular raft, ETIENNE JAMBON-PUILLET, CHRISTOPHE JOSSE RAND, SUZIE PROTIERE, Institut Jean le Rond d’Alembert, Univ Paris 6 UPMC, CNRS UMR 7190, France — Wrinkles and folds occur in a wide variety of situations, we find them in Nature but also in man-made products. They typically appear when a thin sheet bound to a foundation is compressed. Here we demonstrate that particle lattice interfaces, despite being made of discrete very hard particles, can form wrinkles and folds like a soft elastic solid. We call granular raft a close packed monolayer of heavy, athermal particles at the interface between two fluids. We use beads of different materials with diameters ranging from 30 µm to 0.8 mm dispersed at a planar oil/water interface. Upon uniaxial compression the raft buckles out of plane like a soft elastic solid and forms a periodic wrinkling pattern, then the deformation localizes in a large unique fold/crease. This behavior is reminiscent of a compressed elastic sheet floating on water. We will highlight similarities and differences between the mechanical properties of our discrete heavy granular raft and a continuous elastic floating film. Finally we will show how elasticity and gravity contribute to rationalize the original shape of the fold we observe.

1:03 PM B40.00088 Wrapping with a splash, DEEPAK KUMAR, University of Massachusetts Amherst, JOSEPH PAULSEN, Syracuse University, THOMAS RUSSELL, NARAYANAN MENON, University of Massachusetts Amherst — Ultrathin sheets have been used to encapsulate droplets of thin fluid in another. When the sheet is thin enough that bending energies are much smaller than interfacial energies, experiment and theory show that optimal wrappings are achieved without any special sheet design [1]. Here we study wrappings generated by the impact of an oil droplet onto a planar thinnest film (30-200 nm) polystyrene film floating on water. Depending on the energy of impact, a large deformation of the air-water interface is followed by formation of an oil phase wrapped around the polymer film, submerging in the water. Even though the energetic cost of bending of the polymer film is very small, we find that successful wrapping requires an impact energy much larger than the energy difference between the initial and final configurations. We explore the dynamics of the fluid and the sheet in this process with a view to devising an efficient method to create optimal wrappings. [1] J.D. Paulsen, V. Dmery, C.D. Santangelo, T.P. Russell, B. Davidvitch, and N. Menon, doi:10.1038/nmat4397 (2015).

1:15 PM B40.00009 Deformation of flexible micro helices under flow, MARINE DAI EFF, ANKE LIN D NER, OLIVIA DU ROURE, PIMHH-ESPCI, Paris, France, ALEXANDER MOROZOV, University of Edinburgh, United Kingdom, JONATHAN PHAM, ALFRED CROSBY, University of Massachusetts, Amherst, USA — The interaction of small helices with fluids is important because of its relevance to both fundamental science and technological applications, such as swimming micro-robots or microflow sensors. Helically shaped flagella are also exploited by swimming microorganisms to move through their surrounding fluids. Here we study experimentally the deformation of flexible helical ribbons under flow in a microfluidic channel. This analysis of the helical ribbon geometry and dynamics allows us to characterize the bending and viscosity. We focus on two different aspects: the bending stiffness of the helix and the viscous frictional properties. The frictional coefficients determined by our experiments are consistent with calculated values in the context of resistive force theory. Deformation of helices by viscous flow is well-described by non-linear finite extensibility. Due to the non-uniform distribution of the pitch under distributed loading, we identify both linear and nonlinear behavior along the contour length of a single helix. Utilizing our system, we explore the impact of non-Newtonian fluid properties on the mechanics of helix-fluid interactions.

1:27 PM B40.00010 Dynamics and propulsion of a rotating flexible helical rod near a no-slip rigid boundary, MOHAMMAD JAWED, HUSSAIN KARIMI, PEDRO REIS, Massachusetts Institute of Technology — We study the effect of a no-slip rigid boundary on the locomotion of uni-flagellar bacteria in a viscous fluid at low Reynolds number conditions, through a combination of computer simulations and experiments. In our analogue model experiments, we exploit the prominence of geometry in this class of problems to rescale the original micron-scale system onto the desktop-scale. We manufacture elastomeric filaments with fully customizable geometric and material properties, and rotate them in a glycerin bath at a finite distance away from a rigid boundary. The experimental results are compared against numerical simulations that combine the Discrete Elastic Rods method in conjunction with Lighthill Slender Body Theory. The no-slip boundary condition on the wall is implemented by the method of images. We first show that the filament buckles above a critical rotation frequency due to fluid loading, and then quantify the dependence of this critical threshold on the distance from the boundary. Excellent agreement is found between experiments and simulations, with no fitting parameters. Moreover, we find that the generated propulsion force is strongly affected by the presence of a nearby boundary.
1:39PM B40.00011 Fluid-structure interaction of reticulated porous wings. ELIZABETH STRONG, MOHAMMAD JAWED, PEDRO REIS, MIT — Insects of the orders Neuroptera and Hymenoptera locomote via flapping flight with reticulated wings that have porous structures that confers them with remarkable lightweight characteristics. Yet these porous wings still perform as contiguious plates to provide the necessary aerodynamic lift and drag required for flight. Even though the fluid flow past the bulk of these insects may be in high Reynolds conditions, viscosity can dominate over inertia in the flow through the porous sub-features. Further considering the flexibility of these reticulated wings yields a highly nonlinear fluid-structure interaction problem. We perform a series of dynamically-scaled precision model experiments to gain physical insight into this system. Our experiments are complemented with computer simulations that combine the Discrete Elastic Rods method and a model for the fluid loading that takes into account the 'leakiness' through the porous structure. Results are anticipated to find applications in micro-air vehicle aerodynamics.

1:51PM B40.00012 Switchable and Tunable Aerodynamic Drag on Cylinders. MARK GUTTAG, FRANCISCO LOPZ JIMNET, MIT, PRIYANK UPADHYAYA, SHANMUGAM KUMAR, Masdar Institute, PEDRO REIS, MIT — We report results on the performance of Smart Morphable Surfaces (Smorphs) that can be mounted onto cylindrical structures to actively reduce their aerodynamic drag. Our system comprises of an elastomeric thin shell with a series of carefully designed subsurface cavities that, once depressurized, lead to a dramatic deformation of the surface topography, on demand. Our design is inspired by the morphology of the giant cactus (Carnegiea gigantea) which possesses an array of axial grooves, thought to help reduce aerodynamic drag, thereby enhancing the structural robustness of the plant under wind loading. We perform systematic wind tunnel tests on cylinders covered with our Smorphs and characterize their aerodynamic performance. The switchable and tunable nature of our system offers substantial advantages for aerodynamic performance when compared to static topographies, due to their operation over a wider range of flow conditions.

2:03PM B40.00013 Fanning the Optimal Breeze with an Abanico. GRACE GOON, JOEL MARTHELOT, PEDRO REIS, MIT, MIT EGS LAB TEAM — Flexible hand-held fans, or abanicos, are universally employed as cooling devices that are both portable and sustainable. Their to and fro axial motion about one's hand generates an airflow that increases the evaporation rate near the skin and refreshes. We study this problem in the context of fluid-structure interaction, through precision model experiments. We first characterize the elastic properties of a semi-circular thin plates with various thickness and evaluate their aerodynamic performance in a custom built apparatus. The air velocity profile that results from the flapping motion of the fan is characterized for different driving conditions. A systematic variation of the geometric and elastic parameters, along with an exploration of the parameter space of the periodic driving motion (amplitude and frequency), allows us to establish optimal design and operational conditions for maximal output of the generated airflow, while minimizing the input power.

Monday, March 14, 2016 11:15AM - 2:03PM — Session B43 GSNP GSOFT: Avalanches in Granular and Other Particle-based Materials II 346

- Bob Behringer, Duke University

11:15AM B43.00001 Global and local avalanches in cohesive and non cohesive granular material: cracking and seismicity. JONATHAN BARES, LMGC Montpellier, France — Commonly, granular materials yield or flow if sufficiently large stress is applied, leading to avalanche-like behavior. For experimentally wedge split cohesive granular material and sheared 2D and 3D grains, we seek to understand the dynamics of these burst of activity from the local to the global scale. Whether the system rearranges locally like in the case of a fracture front propagating in a cohesive material or in the whole system like in the case of sheared granular medium, similar free scale statistics are observed for the intensity of the rearrangements. We present first an experimental setup that allows growing well-controlled tensile cracks in brittle heterogeneous solids of tunable microstructure. Also, force networks and displacement fields are measured both on two- and three-dimensional sheared material for cyclically sheared photoelastic and hydrogel particles. Avalanches, their size, location and duration are extracted at the global scale from the rapid variation of the stored energy whereas at the local scale they are measured form the energy drop, displacement and acoustic activity. Statistics of those different quantities are computed and correlated to test their intrinsic entanglement and analyze their universal dynamics.

11:51AM B43.00002 Experimental Avalanches in a Rotating Drum.1. ALINE HUBARD, Levich Institute of City College of New York, COREY O’HERN, Department of Mechanical Engineering & Materials Science, Department of Applied Physics, and Department of Physics, Yale University, MARK SHATTUCK, Levich Institute and Physics Department of The City College of New York and CUNY Graduate Center — We address the question of universality in granular avalanches and the system size effects on it. We set up an experiment made from a quasi-two-dimensional rotating drum half-filled with a monolayer of stainless-steel spheres. We measure the size of the avalanches created by the increased gravitational stress on the pile as we quasi-statically rotate the drum. We find two kinds of avalanches determined by the drum size. The size and duration distributions of the avalanches that do not span the whole system follow a power law and the avalanche shapes are self-similar and nearly parabolic. The distributions of the avalanches that span the whole system are limited by the maximal amount of potential energy stored in the system at the moment of the avalanche.

1NSF CMMI-1462439, CMMI-1463455

12:03PM B43.00003 Stability of Granular Packings Jammed under Gravity: Avalanches and Unjamming. CARL MERRIGAN, Brandeis University, SUMIT BIRWA, TIFR Hyderabad, SHUBHA TEWARI, UMass Amherst, BUL-BUL CHAKRABORTY, Brandeis University — Granular avalanches indicate the sudden destabilization of a jammed state due to a perturbation. We propose that the perturbation needed depends on the entire force network of the jammed configuration. Some networks are stable, while others are fragile, leading to the unpredictability of avalanches. To test this claim, we simulated an ensemble of jammed states in a hopper using LAMMPS. These simulations were motivated by experiments with vibrated hoppers where the unjamming times followed power-law distributions. We compare the force networks for these simulated states with respect to their overall stability. The states are classified by how long they remain stable when subject to continuous vibrations. We characterize the force networks through both their real space geometry and representations in the associated force-tile space extending this tool to jammed states with body forces.

1Supported by NSF Grant DMR1409093 and DGE1068620
et al. MAGHSOODI, ERIK LUIJTEN, Northwestern University — Although common in nature and industry, the jamming transition has long eluded a concrete, calibrate the non-local rheology over the whole range of stresses in the system. In this perspective, we complement the experimental results with 2D simulations profiles in the depth with an asymptotic solution of the non-local equation. However, the boundary condition at the free surface needs to be selected in order to Coulomb yield threshold. A correction for the local rheology was proposed. To test further this non-local constitutive relation, we built an inclined narrow a rather good prediction of the flowing regime but does not foresee the existence of a creep regime as observed by Komatsu et al. (PRL 2001). In the context of CLEMENT, BRUNO ANDREOTTI, ESPCI — A local constitutive relation was proposed to describe dense granular flows (GDR MiDi, EPJE 2004). It provides a rather good prediction of the flowing regime but does not foresee the existence of a creep regime as observed by Komatsu et al. (PRL 2001). In the context of a 2D shear cell, a relaxation length for the velocity profile was measured (Bouzid et al., PRL 2013) which confirmed the existence of a flow below the standard Coulomb yield threshold. A correction for the local rheology was proposed. To test further this non-local constitutive relation, we built an inclined narrow channel within which we monitor the flow from the side. We managed to observe the creep regime over five orders of magnitude in velocity and fit the velocity profiles in the depth with an asymptotic solution of the non-local equation. However, the boundary condition at the free surface needs to be selected in order to calibrate the non-local rheology over the whole range of stresses in the system. In this perspective, we complement the experimental results with 2D simulations of hard and frictional discs on an inclined plane in which we introduce a surface friction force proportional to the effective pressure in the granular. We analyze these results in the light of the non-local rheology.

12:27PM B43.00005 Intermittent Flow of Granular Matter in an Annular Geometry. TED BRZINSKI, KAREN E. DANIELS, NC State University — Granular solids can be subjected to a finite stress below which the response is elastic. Above this yield stress, however, the material fails catastrophically, undergoing a rapid plastic deformation. In the case of a monotonically increasing stress the material exhibits a characteristic stick-slip response. We investigate the statistics of this intermittent failure in an annular shear geometry, driven with a linear-ramp torque in order to generate the stick-slip behavior. The apparatus is designed to allow visual access to particle trajectories and inter-particle forces (through the use of photelastic materials). Additionally, twelve piezoelectric sensors at the outer wall measure acoustic emissions due to the plastic deformation of the material. We vary volume fraction, and use both fixed and deformable boundaries. We measure how the distribution of slip size and duration are related to the bulk properties of the packing, and compare to systems with similar governing statistics.

12:39PM B43.00006 Effect of interstitial fluid on event-size distribution for granular hoppers. JUHA KOIVISTO, DOUGLAS DURIAN, Univ of Pennsylvania — The discharge of granular hoppers is avalanche-like in that flow proceeds until probabilistically interrupted by the formation of a stable arch over the hole. The average event size appears to diverge at a critical hole size, thus defining a putative clogging transition. However, we now believe that instead it grows exponentially as a power of the hole diameter, so in fact all hoppers are susceptible to clogging. To investigate the influence of grain dynamics on arch formation, we conducted a series of experiments where the event size distribution was measured for a system that was totally submerged in water. We find that the distribution is exponential, just as for dry non-cohesive grains in air. However, for a given hole the number of grains in the average event decreases roughly with a factor of two, and the critical hole size increases by 10%. Thus, submerged hoppers are more susceptible to clogging and dynamics play a role. In air, the “effective temperature” set by rms grain speed helps to prevent arch formation.

12:51PM B43.00007 Non-local rheology for dense granular flows in avalanches. ADRIEN IZZET, ERIC CLEMENT, BRUNO ANDREOTTI, ESPCI — A local constitutive relation was proposed to describe dense granular flows (GDR MiDi, EPJE 2004). It provides a rather good prediction of the flowing regime but does not foresee the existence of a creep regime as observed by Komatsu et al. (PRL 2001). In the context of a 2D shear cell, a relaxation length for the velocity profile was measured (Bouzid et al., PRL 2013) which confirmed the existence of a flow below the standard Coulomb yield threshold. A correction for the local rheology was proposed. To test further this non-local constitutive relation, we built an inclined narrow channel within which we monitor the flow from the side. We managed to observe the creep regime over five orders of magnitude in velocity and fit the velocity profiles in the depth with an asymptotic solution of the non-local equation. However, the boundary condition at the free surface needs to be selected in order to calibrate the non-local rheology over the whole range of stresses in the system. In this perspective, we complement the experimental results with 2D simulations of hard and frictional discs on an inclined plane in which we introduce a surface friction force proportional to the effective pressure in the granular. We analyze these results in the light of the non-local rheology.

1:03PM B43.00008 Jamming and chaotic dynamics in different granular systems. HOMAYOON MAGHSOODI, ERIK LUIJTEN, Northwestern University — Although common in nature and industry, the jamming transition has long eluded a concrete, mechanistic explanation. Recently, Banigan et al. (Nat. Phys. 9, 288–292, 2013) proposed a method for characterizing this transition in a granular system in terms of the system’s chaotic properties, as quantified by the largest Lyapunov exponent. They demonstrated that in a two-dimensional shear cell the jamming transition coincides with the bulk density at which the system’s largest Lyapunov exponent changes sign, indicating a transition between chaotic and non-chaotic regimes. To examine the applicability of this observation to realistic granular systems, we study a model that includes frictional forces within an expanded phase space. Furthermore, we test the generality of the relation between chaotic and jamming by investigating the relationship between jamming and the chaotic properties of several other granular systems, notably sheared systems (Howell, D., Behringer R. P., Veje C., Phys. Rev. Lett. 82, 5241–5244, 1999) and systems with free boundaries (Woolley, D. C. et al., Nat. Phys. 9, 174–178, 2013). In this work, we develop a model that describes the competition between the largest Lyapunov vector and collective rearrangements of the system to demonstrate the predictive capabilities enabled by adopting this perspective of jamming.

1:15PM B43.00009 3D imaging of particle-scale rotational motion in cyclically driven granular flows. MATT HARRINGTON, University of Pennsylvania, DYLAN POWERS, University of Maryland, ERIC COOPER, Pomona College, WOLFGANG LOSERT, University of Maryland — Recent experimental advances have enabled three-dimensional (3D) imaging of motion, structure, and failure within granular systems. 3D imaging allows researchers to directly characterize bulk behaviors that arise from particle- and meso-scale features. For instance, segregation of a bidisperse system of spheres under cyclic shear can originate from microscopic irreversibilities and the development of convective secondary flows. Rotational motion and frictional rotational coupling, meanwhile, have been less explored in such experimental 3D systems, especially under cyclic forcing. In particular, relative amounts of sliding and/or rolling between pairs of contacting grains could influence the reversibility of both trajectories, in terms of both position and orientation. In this work, we directly observe rotational motion of individual grains by combining confocal microscopy with a technique that is cyclically driven and measure both translational and rotational motion of individual grains. We relate measured rotational motion to resulting shear bands and convective flows, further indicating the degree to which pairs and neighborhoods of grains collectively rotate.

1:27PM B43.00010 Characterizing local forces and rearrangements inside a gravity-driven granular flow. EMMA THACKRAY, KERSTIN NORDSTROM, Mount Holyoke College — While the gravity-driven flow of a granular material in a silo geometry can be modeled by the Beverloo equation, the mesoscale-level particle rearrangements and interactions that drive this flow are not well-understood. We have constructed a quasi-two-dimensional system of bidisperse, millimeter-scale disks with photoelastic properties that make force networks within the material visible. The system is contained in an acrylic box with an adjustable bottom opening. We can approach the clogging transition by adjusting this opening and by adding external forcing to the top of the flowing pile. By placing the system between cross-polarizers, we can obtain high-speed video of this system during flow, and extract intensity signals that can be used to identify and quantify localized, otherwise indeterminate forces. We can simultaneously track individual particle motions, which can be used to identify shear transformation zones in the system. We are therefore able to correlate local forces with rearrangements within the system, and characterize the evolution of this interplay on the approach to the clogging transition.
Anderson localization and related phenomena in such systems. Specifically, we treat particles as network nodes, and pressure-dependent forces between particles as layer-specific network edges. Then, we use a generalization of community detection methods to multilayer networks, and develop quantitative measures that characterize changes in the architecture of the force network as a function of pressure. We observe that branchlike domains reminiscent of force chains evolve differentially as pressure is applied: topological characteristics of these domains at rest predict their coalescence or dispersion under pressure. Our methods allow us to study the dynamics of mesoscale structure in granular systems, and provide a direct way to compare data from systems under different external conditions or with different physical makeup.

Monday, March 14, 2016 2:30PM - 5:30PM –
Session C12 GSNP GSOFT: Intrinsic Localized Modes: Recent Developments and Future Perspectives 308 - David Campbell, Boston University

2:30PM C12.00001 From Discrete Breathers to Many Body Localization and Flatbands, SERGEJ FLACH1. Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon, South Korea — Discrete breathers (DB) and intrinsic localized modes (ILM) are synonymic dynamical states on nonlinear lattices - periodic in time and localized in space, and widely observed in many applications. I will discuss the connections between DBs and many-body localization (MBL) and the properties of DBs on flatband networks. A dense quantized gas of strongly excited DBs can lead to a MBL phase in a variety of different lattice models. Its classical counterpart corresponds to a ‘nonergodic metal’ in the MBL language, or to a nonGibbsian selftrapped state in the language of nonlinear dynamics. Flatband networks are lattices with small amplitude waves exhibiting macroscopic degeneracy in their band structure due to local symmetries, destructive interference, compact localized eigenstates and horizontal flat bands. DBs can preserve the compactness of localization in the presence of nonlinearity with properly tuned internal phase relationships, making them promising tools for control of the phase coherence of waves.

3:06PM C12.00002 Recent advances in the physics of localized states, YURI KIVSHAR1, Nonlinear Physics Center, Australian National University, Canberra, Australia — We will review several examples of the existence and generation of localized states in optics and metamaterials including weakly coupled optical waveguides and arrays of nonlinear “meta-atoms” in metamaterials. We will also mention some recent studies on an interplay of nonlinearity-induced energy localization and edge states in discrete systems appeared in the systems with nontrivial topology.

3:42PM C12.00003 Shepherding intrinsic localized modes in micro-mechanical arrays, ALBERT SIEVERS, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853 — The energy profiles of intrinsic localized modes (ILMs) in periodic physical lattices with nonlinear forces resemble those of localized vibrational modes at defects of a harmonic lattice but, like solitons, they can propagate; however, in contrast with solitons they lose energy as they move through the lattice - the more localized the excitation the faster the energy loss. One of our experimental studies with micro-mechanical arrays involves steady state locking of ILMs, and their interactions with impurities. By measuring the linear response spectra of a driven array containing an ILM both the dynamics of bifurcation transitions and the hopping of vibrational energy have been connected to the transition properties of soft modes. Recently the search for a completely mobile ILM has focused attention on minimizing the resonance interaction that occurs between the localized excitation and small amplitude plane wave modes. Via simulations we demonstrate that when more than one type of nonlinear force is present their Fourier components can often be designed to cancel against each other in the k-space region of the plane wave dispersion curve, removing the resonance. The end result is super-transmission for an ILM in a discrete physical lattice. Such an engineered, intrinsic, low loss channel may prove to be a useful property for other physical systems treated within a tight binding approximation. In collaboration with M. Sato.

4:18PM C12.00004 Localized Modes in Granular Chains, MASON PORTER, University of Oxford — Granular crystals are tightly-packed lattices (or more disordered arrangements) of solid particles that deform elastically when they contact each other. In the presence of precompression, they can exhibit breather solutions in the form of intrinsic localized modes and defect modes. I’ll give an introduction to granular crystals and will then examine breathers in one-dimensional granular crystals (i.e., granular chains) in both models and experiments. I will give examples using both diatomic configurations and homogeneous configurations with defect particles. I will also consider disordered granular chains and discuss recent work on nonlinear Anderson localization and related phenomena in such systems.
Intrinsic Localized Modes in Optical Photonic Lattices and Arrays

Monday, March 14, 2016 2:30PM - 5:06PM –
Session C35 DBIO GSOFT GSNP: Active Matter: Collective Phenomena in Living Systems II
1

2:30PM C35.00001 Using a stochastic field theory to understand group behavior in microswimmer suspensions, PATRICK UNDERHILL, YUZHOU QIAN, PETER KRAMER, Rensselaer Polytech Inst — Active suspensions of microswimmers appear both in natural biological systems (e.g. bacteria or algae) and in synthetic systems. Even without external forcing they are out of equilibrium, which gives rise to interesting properties in both small and large concentrations of the particles. These properties have been observed in experiments as well as simulation/modeling approaches. It is important to understand how hydrodynamic interactions between active swimmers cause and/or alter the suspension properties including enhanced transport and mixing. One of the most successful approaches has been a mean field theory. However, in some situations the mean field theory makes predictions that differ significantly from experiments and direct (agent or particle based) simulations. There are also some quantities that cannot be calculated by the mean field theory. In this talk, we will describe our new approach which uses a stochastic field to overcome the limitations of the mean field assumption. It allows us to calculate how interactions between organisms alter the correlations and mixing in conditions where the mean field theory cannot.

2:42PM C35.00002 ABSTRACT WITHDRAWN —

2:54PM C35.00003 Geometry and mechanics of growing bacterial colonies, ZHIHONG YOU, DANIEL PEARCE, Univ of Leiden, ANUPAM SENGUPTA, ETH Zurich, LUCA GIOMI, Univ of Leiden — Bacterial colonies are abundant on living and non-living surfaces, and are known to mediate a broad range of processes in ecology, medicine and industry. Although extensively researched from single cells up to the population levels a comprehensive biophysical picture, highlighting the cell-to-colony dynamics, is still lacking. Here, using numerical and analytical models, we study the mechanics of self-organization leading to the colony morphology of cells growing on a substrate with free boundary. We consider hard rods to mimic the growth of rod-shaped non-motile cells, and show that the colony, as a whole, does not form an ordered nematic phase, nor does it result in a purely disordered (isotropic) phase. Instead, different sizes of domains, in which cells are highly aligned at specific orientations, are found. The distribution of the domain sizes follows an exponential relation indicating the existence of a characteristic length scale that determines the domain size relative to that of the colony. A continuum theory, based on the hydrodynamics of liquid crystals, is built to account for these phenomena, and is applied to describe the buckling transition from a planar to three-dimensional (3D) colony. The theory supports preliminary experiments conducted with different strains of rod shaped bacterial cells, and reveals that the buckling transition can be regulated by varying the cell stiffness and aspect ratio. This work proposes that, in addition to biochemical pathways, the spatio-temporal organization in microbial colonies is significantly tuned by the biomechanical and geometric properties of the microbes in consideration.

3:06PM C35.00004 Cell-cell interactions impacts on the rate of swarm expansion and the edge shape of a colony swarming Pseudomonas aeruginosa, ABOUTALEB AMIRI, University of Notre Dame, Physics Deptment, GIORDANO TIERRA, Charles University in Prague, Mathematical Institute, ZHILIANG XU, University of Notre Dame, Applied computational Mathematics and Statistics, JOSHUA SHROUT, University of Notre Dame, Department of Civil and Environmental Engineering, MARK ALBER, University of Notre Dame, Physics Department, Department of Applied Computational Mathematics and Statistics — Collective motion has been observed by several bacterial species including the pathogenic bacterium P. aeruginosa. A flagellum at the pole is known to generate a self-propulsion motion. However, the role of type IV pili (TFP), distributed on the cell membrane, during swarming needs to be investigated in more details. In this work we introduce a model that combines the hydrodynamic and biophysical interactions in order to study the impact of the TFP interactions on swarming behavior of the colony. The model describes the motion and interactions of rod-shaped self propelled bacteria inside a thin liquid film. It also includes the equations describing the production and diffusion of surfactant rhamnolipids that is responsible for extraction of water from substrate, and Marangoni driven expansion of the thin liquid film by altering the surface tension. We show that TFP interactions are responsible for slower expansion rate of colonies of TFP deficient mutants compared to wild type. Experimental observations were used to calibrate the model and verify the model assumptions and predictions.
3:18PM C35.00005 The 3-D spatial structure of multicellular aggregates can give them a competition-dependent growth advantage in early biofilm development. VERNITA GORDON, U. Texas, Austin, KASPER KRACH, U. Copenhagen, JAIME HUTCHISON, U. Texas, Austin, GAVIN MELAUGH, U. Edinburgh, CHRIS RODESNEY, U. Texas, Austin, ALED ROBERTS, U. Nottingham, YASUHIKO IRIE, U. Bath, PETER JENSEN, U. Copenhagen, STEPHEN DIGGLE, U. Nottingham, ROSALIND ALLEN, U. Edinburgh, THOMAS BJARNSHOLT, U. Copenhagen — Biofilms are structured communities of sessile microbes. Traditional models of biofilm development begin with single bacteria seeding a surface. However, biofilms can also be seeded by multicellular aggregates. How the three-dimensional structure of aggregates impacts the initiation and development of biofilms is not known. Here we use a combination of experiments and simulations to determine the impact of the seeding structure. We find that whether aggregates or single cells grow better depends on the density of single cells initially seeded. The density of single cells, which we take as our measure of the level of competition, impacts per-cell access to growth resource. The overall biomass accumulation arising from an aggregate is a combination of slow growth in the resource-limited interior, and faster growth on the sides and top. When competition is low, aggregates are disadvantaged, compared with single cells. However, when competition is high, aggregates are fitter than single cells, because the cells at the top of the aggregates have better access to growth resources than do high-density single cells on the surface.

3:30PM C35.00006 Mechanical signaling coordinates the embryonic heart. KEVIN CHIOU, JASON ROCKS, Department of Physics and Astronomy, University of Pennsylvania, BENJAMIN PROSSER, Department of Physiology, Penn Muscle Institute, University of Pennsylvania Perelman School of Medicine, DENNIS DISCHER, Molecular & Cell Biophysics Lab, University of Pennsylvania, ANDREA LIU, Department of Physics and Astronomy, University of Pennsylvania — The heart is an active material which relies on robust signaling mechanisms between cells in order to produce well-timed, coordinated beats. Heart tissue is composed primarily of active heart muscle cells (cardiomyocytes) embedded in a passive extracellular matrix. During a heartbeat, cardiomyocyte contractions are coordinated across the heart to form a waveform that propagates through the tissue to pump blood. In the adult heart, this contractile wave is coordinated via intercellular electrical signaling. Here we present theoretical and experimental evidence for mechanical coordination of embryonic heartbeats. We model cardiomyocytes as mechanically excitable Eshelby inclusions embedded in an overcompressed elastic-fluid biphasic medium. For physiological parameters, this model replicates recent experimental measurements of the contractile waveform which are not captured by electrical signaling models. We additionally challenge our model by pharmacologically blocking gap junctions, inhibiting electrical signaling between myocytes. We find that while the functional properties of the heart are modified after gap junction blockage, embryonic hearts continue beating even at significantly higher concentrations, providing strong support for a mechanical signaling mechanism.

3:42PM C35.00007 Jamming and Localization of Interacting Run-and-Tumble Particles, RICHARD BLYTHE, MARTIN EVANS, ALEXANDER SLOWMAN, University of Edinburgh — Certain species of bacteria, notably Escherichia coli, exhibit a characteristic run-and-tumble motion comprising a sequence of straight-line runs at constant velocity interspersed with tumble events that randomize the direction of motion. In a many-body setting, this nonequilibrium dynamics can generate the phenomenon of motility-induced phase separation, which is also seen for a wide variety of self-propelled particles more generally. Whilst the propensity of self-propelled particles to phase separate is understood at a mesoscopic level, the origin of this behaviour in the inelastic collisions between particles implies that the microscopic dynamics is not. Here we present exact results for run-and-tumble particles in one dimension that reveal a richly-structured stationary state that comprises a superposition of three distinct physical states whose relative weights vary with the run and tumble rates, namely a jammed state, a localized state and a delocalized state.

3:54PM C35.00008 Wing attachment position of fruit fly minimizes flight cost. ROBERT NOEST, JANE WANG, Cornell University — Flight is energetically costly which means insects need to find ways to reduce their energy expenditure during sustained flight. Previous work has shown that insect muscles can recover some of the energy used for producing flapping motion. Moreover the form of flapping motions are efficient for generating the required force to balance the weight. In this talk, we show that one of the morphological parameters, the wing attachment point on a fly, is suitably located to further reduce the cost for flight, while allowing the fly to be close to stable. We investigate why this is the case and attempt to find a general rule for the optimal location of the wing hinge. Our analysis is based on computations of flapping free flight together with the Floquet stability analysis of periodic flight for descending, hovering and ascending cases.

4:06PM C35.00009 Noise regulation and symmetry breaking during vertebrate body elongation. THIERRY EMONET, DIPJYOTI DAS, SCOTT A. HOLLEY, Yale University — Elongation of the vertebrate body axis is driven by collective cell migration and cell proliferation at the posteriorly advancing embryonic tailbud. Within the Zebrafish tailbud an ordered stream of cells symmetrically bifurcates to produce well-timed, coordinated beats. However, when competition is high, aggregates are fitter than single cells, because the cells at the top of the aggregates have better access to growth resources than do high-density single cells on the surface.

4:18PM C35.00010 Spontaneous Planar Chiral Symmetry Breaking in Cells. JEREMY HADIDJOJO, DAVID LUBENSKY, Univ of Michigan — Recent progress in animal development has highlighted the central role played by planar cell polarity (PCP) in epithelial tissue morphogenesis. Through PCP, cells have the ability to collectively polarize in the plane of the epithelium by localizing morphogenetic proteins along a certain axis. This allows direction-dependent modulation of tissue mechanical properties that can translate into the formation of complex, non-rotationally invariant shapes. Recent experimental observations show that cells, in addition to being planar-polarized, can also spontaneously develop planar chirality, perhaps in the effort of making yet more complex shapes that are reflection non-invariant. In this talk, we will present our work in characterizing general mechanisms that can lead to spontaneous chiral symmetry breaking in cells. We decompose interfacial concentration of polarity proteins in a hexagonal cell packing into irreducible representations. We find that in the case of polar concentration distributions, a chiral state can only be reached from a secondary transition can send the system from disorder directly to a chiral state. In addition, we find that perturbing the system by stretching the hexagonal packing enables direct (supercritical, or "first-order") chiral transition in the nematic case. Finally, we do a Landau expansion to study competition between stretch-induced chirality and the tendency towards a non-chiral state in packings that have retained the full 6-fold symmetry. [1] K. Taniguchi et al., Science (2011)

4:30PM C35.00011 Epithelial Proliferation on Curved Toroidal Surfaces. YA-WEN CHANG, RICARDO CRUZ, ALEXANDROS FRAGKOPoulos, Georgia Institute of Technology, SAMANTHA MARQUEZ, Yale University, ANDRES GARCIA, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Cellular environment influences a multitude of cellular functions by providing chemical and physical signals that modulate cell behavior, dynamics, development, and eventually survival. In strongly interacting epithelial cells, cells coordinate their behavior to respond to mechanical constraints in 3D. Local differences in tissue tension has also been shown to impact cell reproduction within an epithelial-cell sheet. Much less is known about how cells respond to out-of-plane curvatures. Here, we describe the proliferation of MDCK on toroidal hydrogel substrates, which unlike spheres or planes, have regions of both positive and negative Gaussian curvature. Additionally, the range of curvatures can be controlled by varying the size and aspect ratio of the torus, allowing us to quantify the relation between substrate curvature and cell proliferation.
4:42PM C35.00012 Brownian microswimmer in a Poiseuille Flow, LEONARDO APAZA-PILCO, Universidad Mayor de San Andres, MARIO SANDOVAL, Metropolitan Autonomous University — We study the two and three dimensional dynamics of a microswimmer at low-Reynolds-number in a Poiseuille flow and subject to thermal fluctuations. A deterministic analysis is also performed, and we find that under certain conditions the swimmer becomes hydrodynamically trapped thus performing periodic orbits. We provide an analytical expression where this trapping occurs.

A numerical solution for the coupled system of stochastic differential equations based on two parameters, the Peclet number and the ratio of the swimming velocity and the flow velocity, is also obtained. Based on this parameter space, it is found that the mean-square displacement (MSD) along the longitudinal axis (flow direction) is always quadratic in time, whereas along the transversal direction the mean-square displacement achieves a constant value due to the presence of physical boundaries. A comparison among the 2D and 3D MSD results are also discussed. Finally, the effect of the Poiseuille flow on the angular probability distribution for the two-dimensional motion is also computationally shown.

4:54PM C35.00013 Synthetic electrophysiology: optically controlled oscillators in an engineered bioelectric tissue, HAROLD MCNAMARA, HONGKANG ZHANG, CHRISTOPHER WERLEY, Harvard University, ADAM COHEN, Harvard University and HHMI — Multicellular electrical dynamics underlie crucial physiological functions, but the complexity of natural bioelectricity can obscure the relation of individual components (proteins, cells) to emergent system-level dynamics. Here we introduce optopatch-spiking HEK(OS-HEK) tissue, a minimal synthetic bioelectric tissue with 4 transgenic components that supports optical initiation of propagating electrical waves as well direct optical voltage readout. In conjunction with a home-built inverted microscope capable of patterned illumination, we use this tissue to probe the biophysical attributes of this excitable bioelectric medium, including dispersion relations, curvature-dependent wavefront propagation, electrotonic coupling, and effects of boundaries. We then used chemical patterning to define cellular circuits that support controllable oscillations and which retain memory for more than 2 hours (corresponding to 10^4 oscillations), constituting a substrate for binary bioelectric data storage. Finally, we use optical patterning of boundary conditions in a physically homogeneous tissue to design dynamically reconfigurable oscillators.


2:30PM C40.00001 Hydraulic fracture and toughening of a brittle layer bonded to a hydrogel, ALESSANDRO LUCANTONIO, GIOVANNI NOSELLI, SISSA - International School for Advanced Studies, XAVIER TREPAT, IBEC - Institute for Bioengineering of Catalonia, ANTONIO DESIMONE, SISSA - International School for Advanced Studies, MARINO ARROYO, UPC - Universitat Politècnica de Catalunya — Brittle materials fracture under tensile or shear stress. When stress attains a critical threshold, crack propagation becomes unstable and proceeds dynamically. In the presence of several precracks, a brittle material always propagates only the weakest crack, leading to catastrophic failure [1]. Here, we show that all these features of brittle fracture are radically modified when the material susceptible to cracking is bonded to a porous medium, such as a hydrogel, a common situation in biological tissues [2]. In particular, we show that the brittle material can fracture in compression and can resist cracking in tension, thanks to the hydraulic coupling with the hydrogel. In the case of multiple cracks, we find that localized fracture occurs when the permeability of the hydrogel is high, whereas increased permeability leads to toughening by promoting multiple cracking. Our results [3] may contribute to the understanding of fracture in biological tissues and provide inspiration for the design of tough, biomimetic materials.


2:42PM C40.00002 Geometry and Mechanics of Thin Growing Bilayers¹, MATTEO PEZZULLA, GABRIEL SMITH, Boston University, PAOLA NARDINOCCHI, Sapienza Universit di Roma, DOUGLAS HOLMES, Boston University — We investigate how thin sheets of arbitrary shapes morph under the isotropic in-plane expansion of their top surface, which may represent several stimuli such as nonuniform heating, local swelling and differential growth. Inspired by geometry, an analytical model is presented that rationalizes how the shape of the disk influences morphing, from the initial spherical bending to the final isometric limit. We introduce a new measure of slenderness that describes a sheet in terms of both thickness and plate shape. We find that the mean curvature of the isometric state is three fourths the natural curvature, which we verify by numerical and experiments. We finally investigate the emergence of a preferred direction of bending in the isometric state, guided by numerical analyses. The scalability of our model suggests that it is suitable to describe the morphing of sheets spanning several orders of magnitude.

¹ NSF grant CMMI1308860

2:54PM C40.00003 Buckling, driven by constrained phase separation, of toroidal-shaped hydrogels, MICHAEL S. DIMITRIYEV, YA-WEN CHANG, Georgia Institute of Technology, ANTON SOUSLOV, Universiteit Leiden, ALBERTO FERNANDEZ- nieves, PAUL M. GOLDBART, Georgia Institute of Technology — We investigate the buckling process observed in connection with the temperature-induced shrinking of an elastic toroid composed of hydrogel. Hydrogels are polymeric network media that become swollen when mixed with water, provided the temperature is low enough. As the temperature is increased beyond a certain point, such gels undergo a first-order de-swelling transition to a de-mixed state, in which the network segregates from the water, resulting in a shrunk phase. It is known that the rapid heating of swollen hydrogels beyond the de-swelling transition results in the formation of a shrunk-phase boundary region, or shell. This shell hinders the expulsion of fluid associated with the equilibration of the sample interior, and gives rise to a prolonged period of coexistence between shrunk and swollen domains in the interior of the sample. In contrast with the spherical case, toroidal samples have been observed to undergo a constrained phase separation that is accompanied by a global buckling (or “Pringling”) deformation of the sample shape. We present a model of hydrogel toroid Pringling in which such deformations are driven by this phase separation process.

3:06PM C40.00004 Modeling and design of the self-twisting of hydrogel bilayer strips, Authors: Jiayu Liu, Jingkai Guo, Tanvi Shroff, ChangKyu Yoon, David Gracias & Thao D Nguyen, JIAYU LIU, JINGKAI GUO, TANVI SHROFF, CHANGKYU YOON, DAVID GRACIAS, THAO NGUYEN, Johns Hopkins University — Self-folding of hydrogels via heterogeneous swelling can be used to create complex, 3D structures. A bilayer structure with a thermo-responsive hydrogel layer, that swells with decreasing temperature, and a non-swelling layer can respond to a temperature change by either bending into a ring or twisting into a helix. The equilibrium structure depends on the thickness ratio of the two layers, the ratio of the width to thickness of the bilayer, as well as the stiffness of the two layers and equilibrium swelling ratio of the hydrogel. These parameters can be controlled using lithographic photopatterning and multilayer deposition techniques. To guide the design of the bilayer structures, we developed a finite element model of the bilayer structure. The constitutive model of the hydrogel is described by a free energy density that includes a quasi-incompressible Neo-Hookean component for the strain energy density of the polymer network and a Flory-Huggins component for the free-energy density of mixing of the polymer and solvent. We discussed how variations in the layer thickness, slenderness, stiffness, and equilibrium swelling ratio can be used to design self-folded rings of different curvatures and helices with different helix angle and diameters.
3:18PM C40.00005 Mechanics of a leaf detaching from tree, TIM ZEHNBAUER, SUNGHWAN JUNG, Virginia Tech — Deciduous trees shed their leaves through an abscission process. The abscission zone is formed at the base of the petiole, and consists of a top layer with weak walls and a bottom layer that expands and breaks the walls of the cells in the top layer. Although this process is well understood biologically, the mechanical principles underlying this shedding have received little attention. In the present study, we characterize the stress-strain relation of the petiole-branch connection failure over the seasons. The testing is done with a 1kN load cell, where the stem is pulled directly from the branch to make a stress-strain curve. The slope of the stress-strain curve, Youngs modulus, is obtained using least squares linear regression of the curve. We show that Youngs modulus stays constant from spring to late fall, while the maximum tensile strength falls. We are investigating the role of the shape of a leaves petiole in this behavior.

3:30PM C40.00006 ABSTRACT WITHDRAWN —

3:42PM C40.00007 The role of deformable structured surfaces on viscous forces during peeling, CHARLES DHONG, JOELLE FRECHETTE, Johns Hopkins University — It is known that tree frogs are able to adhere well in flooded environments, presumably due to their interconnected network of drainage channels formed by hexagonal epithelial cells in their toe pads. To investigate this effect, a patterned surface of hexagonally arranged cylindrical posts was brought close to a stationary substrate in a submerged, viscous fluid via a normal load, and then peeled off to measure a retraction force. Because these structured surfaces were made from PDMS, they are able to deform throughout the process. We find that these deformable surfaces further reduce the work required to peel apart the two surfaces, even when compared to previous studies in the same system with rigid structures, and we isolated these contributions independent of conservative forces. We then conducted experiments to compare the effect of deformation on the viscous forces and conservative forces. We find that there are several regimes where deformation either increases or decreases the retraction force since we have found that elasticity decreases retraction forces when considering viscous contributions but is also known to increase adhesion in the context of conservative forces.

1Office of Naval Research, National Science Foundation, Hopkins Extreme Materials Institute

3:54PM C40.00008 Bio-inspired microfluidics: The case of the velvet worm, ANDRES CONCHA, PAULA MELLADO, Adolfo Ibanez university, BERNAL MORERA-BREÑES, Laboratorio de Genética Evolutiva, Universidad Nacional de Costa Rica, CRISTIANO SAMPAIO-COSTA, University of Sao Paulo, L. MAHADEVAN, School of Engineering and Sciences, Harvard University, JULIAN MONGE-NAJERA, Tropical Biology, University of Costa Rica. — The rapid squirt of a proteinaceous slime jet endow velvet worms (Onychophora) with a unique mechanism for defense from predators and for capturing prey by entangling them in a disordered web that immobilizes their target. However, to date neither qualitative nor quantitative descriptions have been provided for this unique adaptation. We have investigated the mechanism that allows velvet worms the fast oscillatory motion of their oral papillae and the exiting liquid jet that oscillates with frequencies f ~ 30 – 60 Hz. Using anatomical images and high speed videography, we show that even without fast muscular action of the papilla, a strong contraction of the slime reservoir and the geometry of the reservoir-papilla system suffices to accelerate the slime to speeds up to v ~ 5 m/s in about Δt ~ 60 ms. A theoretical analysis and a physical simulacrum allow us to infer that this fast oscillatory motion is the result of an elastohydrodynamic instability driven by the interplay between the elasticity of oral papille and the fast unsteady flow during squiring. We propose several applications that can be implemented using this instability, ranging from high-throughput droplet production, printing, and micro-nanofiber production among others.

3 A.C was partially supported by Fondecyt grant 11130075.

4:06PM C40.00009 Nonlinear adhesion dynamics of confined lipid membranes, TUNG TO, THOMAS LE GOFF, OLIVIER PIERRE-LOUIS, Univ Lyon 1 UA 442 CNRS — Lipid membranes, which are ubiquitous objects in biological environments are often confined. For example, vesicles are formed between a substrate and the cytoskeleton between cell adhesion, or between other membranes in stacks, or in the Golgi apparatus. We present a study of the nonlinear dynamics of membranes in a model system, where the membrane is confined between two flat walls. The dynamics derived from the lubrication approximation is highly nonlinear and nonlocal. The solution of this model in one dimension exhibits frozen states due to oscillatory interactions between membranes caused by the bending rigidity. We develop a kink model for these phenomena based on the historical work of Kawasaki and Otha. In two dimensions, the dynamics is more complex, and depends strongly on the amount of excess area in the system. We discuss the relevance of our findings for experiments on model membranes, and for biological systems.

1Supported by the grand ANR Biolub
2T. Le Goff, P. Politi and O. Pierre-Louis, PRE 90, 032114 (2014).
5T. B. T. To, T. Le Goff, O. Pierre-Louis, preprint.

4:18PM C40.00010 Statistical Mechanics of Sliced Graphene Ribbons, MARK BOWICK, Syracuse University, EMILY RUSSELL, Google, RASTIKO SKNEPNEK, University of Dundee, DAVID NELSON, Harvard University — Two-dimensional crystalline membranes have recently been realized experimentally in such systems as graphene and molybdenum disulphide, sparking a resurgence in interest in their statistical properties. These fluctuations can significantly change the effective mechanical properties of these membranes, renormalizing both bending rigidity and elastic moduli so that thermal membranes are stiffer to bending than their bare bending rigidity would suggest. We use molecular dynamics simulations to examine the further effect of topology and geometry on the properties of thermal membranes, and find that the introduction of a slit suppresses the scale of thermal fluctuations.

4:30PM C40.00011 Statistical mechanics of thin spherical shells, ANDREJ KOSMRLJ, Princeton University, DAVID R. NELSON, Harvard University — We explore how thermal fluctuations affect the mechanics of thin amorphous spherical shells via renormalization group calculations. It is well known that for flat solid membranes thermal fluctuations effectively increase the bending rigidity and reduce the bulk and shear moduli. This is still true for spherical shells. However, the additional coupling between the shell curvature, the local in-plane stretching modes and the local out-of-plane undulations leads to novel phenomena. In spherical shells thermal fluctuations effectively produce negative surface tension, which is equivalent to applying external pressure. We find that small spherical shells are stable, but for sufficiently large shells this thermally generated pressure becomes big enough to crush spherical shells. Such shells can be reinitialized by increasing internal pressure, where the effective shell size grows non-linearly as a function of internal pressure with a power law exponent characteristic for thermally fluctuating flat membranes under uniform tension.

4:42PM C40.00012 Phyllotactic transformations as plastic deformations of tubular crystals with defects, DANIEL BELLER, DAVID NELSON, Harvard University — Tubular crystals are 2D lattices in cylindrical topologies, which could be realized as assemblies of colloidal particles, and occur naturally in biological microtubules and in single-walled carbon nanotubes. Their geometry can be understood in the language of phyllotaxis borrowed from botany. We study the mechanics of plastic deformations in tubular crystals in response to tensile stress, as mediated by the formation and separation of dislocation pairs in a triangular lattice. Dislocation motion allows the growth of one phyllotactic arrangement at the expense of another, offering a low-energy, stepwise mode of plastic deformation in response to external stresses. Through theory and simulation, we examine how the tube’s radius and helicity affects, and is in turn altered by, dislocation glide. The crystal’s bending modulus is found to produce simple but important corrections to the tube’s deformation mechanics.
4:54PM C40.00013 Defect-driven shape instabilities in cohesive filament bundles, ISAAC BRUSS, University of Michigan, GREGORY GRASON, University of Massachusetts — When defects are incorporated into the lattice of a flexible 2D crystalline membrane, it buckles into a new configuration. Specifically, 5- and 7-fold disclinations produce conical- and saddle-like geometries respectively. For bundles composed of a crystalline array of cohesive flexible filaments, we propose a similar phenomena of defect-induced buckling. This revelation is fueled by a recently discovered mapping between the metric properties of a curved surface, and the inter-filament spacing within a deformed bundle. Using a combination of continuum elasticity theory and numerical simulations, we investigate the effects of defects in the cross section on a bundle's global structure. We find that positive disclinations promote the twisting of filaments around a central axis within the bundle, while negative disclinations promote twisting around two parallel axes simultaneously. Both instabilities are interpreted by means of their equivalent Gaussian curvature, and map appropriately to the the corresponding membrane responses. Additionally, for 5-fold disclinations we uncover a new equilibria structure, torsional wrinkling, with the intriguing ability to focus gradients in filament tilt much like curvature-focusing for the analogous membrane.

1 NSF (CAREER) DMR-0955760

5:06PM C40.00014 Ring Correlations in Two-Dimensional (2D) Random Networks, MAHDI SAD-JADI, M. F., THORPE, Arizona State Univ — Amorphous materials can be characterized by their ring structure. Recently, two experimental groups imaged bilayers of vitreous silica at atomic resolution which provides a direct access to the ring structure of a 2D glass. It has been shown that experimental samples have various ring statistics, obey Aboav-Weaire law and have a distinct area law. In this work, we study correlations between rings as a function of their size and topological separation. We show that correlation is medium-range and vanishes when the separation is about three rings apart. We also present a generalization of the Aboav-Weaire law.


5:18PM C40.00015 The Effect of Loops in Connectivity Percolation, VARD'A F. HAGH, Arizona State University, M. F. THORPE, Arizona State University - Rudolf Peierls Centre for Theoretical Physics, University of Oxford — We introduce a new method that employs the concepts of redundancy and stress from rigidity theory to study the effect of loops in connectivity percolation. In the rigidity percolation redundant bonds are not necessary to maintain the rigidity of a network. These redundant bonds cause internal stress in some regions and as a result those regions carry finite forces that characterize them as over-constrained. In connectivity percolation the bonds that cause a loop correspond to redundant bonds in rigidity and all the bonds that are part of a loop are equivalent to over-constrained bonds in rigidity. To illustrate this we start with a network in 2D where all the bonds are present and remove the bonds randomly. Then using renormalization groups and numerical simulations we study the behavior of loops near percolation transition in hierarchical networks and lattices.


- Mark Shattuck, CCNY

2:30PM C43.00001 Onset of erosion and sediment transport by a fluid flow over a granular bed, ARSHAD KUDROLLI, Clark Univ — Erosion and deposition of grains by a fluid flowing past the surface of a granular bed occurs in many natural and industrial processes. While considerable number of empirical studies has been conducted, very little is in fact known in detail on conditions which lead to erosion and deposition of sediments and their transport coefficients. We discuss a series of laboratory experiments to develop the physics of erosion starting with a single particle resting on a surface in a fluid flow. Fluorescent fluid-particle index matching techniques allow us to visualize not only the particles at the surface of a granular bed but also the flow within the bed and the individual particles within the bed. We will discuss the conditions governing the onset of particle motion under simple shear and their transport as a function of bed and fluid flow properties.

1Supported by the U.S. DOE Office of Science and Office of BES program under DE-FG02-13ER16401, and NSF Grant No. CBET-1335928.

3:06PM C43.00002 The cessation threshold of continuous sediment transport in Newtonian fluid, THOMAS PHTZ, Ocean College, Zhejiang University, ORECINIO DURAN, MARUM-Center for Marine Environmental Sciences, University of Bremen — One of the classical problems in sediment transport science is to predict the threshold Shields number below which a bed of loose sediment particles sheared by a homogeneous fluid flow ceases to move continuously. Depending on the particle-fluid density ratio \( s \), it has been believed for many decades that this threshold is a consequence of either fluid forces being just strong enough to dislodge particles resting on the bed (small \( s \), e.g., water) or of particle-bed impacts being just strong enough to eject sufficient bed particles (large \( s \), e.g., air). However, here we find from state-of-the-art numerical simulations that particle-bed impacts play an important role in sustaining sediment transport regardless of \( s \). Guided by these simulations, we propose a simple, unified analytical model of the cessation of continuous sediment transport, which is quantitatively consistent with measurements in water (the famous “Shields diagram”) and air on Earth and Mars. This model predicts that sediment transport on Pluto (transport of nitrogen ice particles in a very thin nitrogen atmosphere) can be sustained under surface winds comparable to those on Earth and Mars. This might explain wind streaks on Pluto’s surface which have puzzled the lead researchers of the New Horizons mission.

1We acknowledge support from grants National Natural Science Foundation of China (Nos. 1151101041 and 41376095) and Natural Science Foundation of Zhejiang Province (No. LR16E090001).

3:18PM C43.00003 Rod Climbing of Suspensions, YOUJING GUO, XIAORONG WANG, Chemical Engineering, Tongji University, Shanghai — We wish to report an unexpected effect observed for particle suspensions sucked to pass through a vertical pipe. Above a critical concentration, the suspension on the outside of the pipe may climb along the outside wall of the pipe and then display a surprising rod-climbing effect. Our study shows that the phenomenon is influenced mainly by the suspension composition, the pipe dimension and the suction speed. The effects of the pipe materials of different kinds are negligible. Increasing the suction force and the concentration increases the climbing height. Increasing the pipe diameter and wall thickness reduces the climbing effect. This behavior may be relevant to that the suspensions of the type described are all displaying markedly shear-thickening.

3:30PM C43.00004 Laboratory investigations of granular and hydrodynamic processes in tidewater glacial fjords

Accelerated warming in the past few decades has led to a dramatic increase in glacial activity. This is perhaps most apparent in tidewater glacial fjords, where gravitational flows from ice sheets are focused into narrow channels of thick, fast-flowing ice which terminate into the ocean. The result is a complex system involving both melting and iceberg calving which has a direct impact on the Earth’s climate and sea level rise. However, there are numerous inherent difficulties in collecting field data from remote, ice-choked fjords. To address this, we use a laboratory scale model to measure aspects of tidewater glaciers which are not observable in nature. Our model has helped to uncover the source of glacial earthquakes, where floating, cubic-kilometer scaled icebergs capsize due to gravitational instability, and temporarily reverse the velocity of the glacier. In addition, we use our model to address two important components of tidewater glaciers involving a granular ice mélangé which applies stresses on the glacier, and the role of iceberg capsize in disrupting the stratified heat transport at the glacier’s terminus.

1We acknowledge support from NSF DMR-1506446

3:42PM C43.00005 A phase diagram for fluid-driven sediment trasport

When a fluid flows laterally over a granular bed, grains may be transported with the flow. This process shapes much of the natural world. The boundary between states with and without grain motion has been studied for decades. However, this boundary is not well understood, since the process whereby grains are transported involves the coupling of several complex phenomena: turbulent fluid flow near a rough boundary, Darcy flow through the pore structure of the granular bed, the yield strength of granular beds comprised of frictional grains with irregular shape, and inertial effects of grains that become entrained in the flow. In order to clarify the essential physics that governs the onset of granular motion, we study this process computationally by including only the minimal features and then adding complexities one by one. We start with a simple numerical model that includes only gravity, grain-grain interactions that are repulsive and frictionless, and a purely horizontal viscous fluid flow. By varying the fluid flow rate and the effective viscosity, we find behavior that is qualitatively consistent with a large collection of experimental data known as the Shields curve. Thus, our results suggest that the main features of this curve result from a competition between grain inertia and viscous damping. We find this phase diagram to be qualitatively insensitive to secondary effects, such as friction, irregular grain shape, and restitution losses.

1Funded by U.S. Army Research Office under Grant No. W911NF-14-1-0005

4:18PM C43.00006 The drag mechanics of an intruder moving in sheared granular medium

We perform an experimental study on an intruder dragged at a constant force in a quasi-statically cyclic-sheared granular medium. A Teflon disk is embedded in a layer of bidisperse photoelastic disks. The granular medium is contained in a horizontal square cell, which can be deformed into a parallelogram with the same area, to produce simple shear. To explain the mechanism of intruder motion, we analyze the motion under cyclic shear of multiple properties: coordination number, density, affine and non-affine motion of disk-granular system. We find that the motion of the intruder is strongly dependent on the fore-and-aft jam state of the intruder. The intruder can move along the drag force or opposite to the drag force, which is determined by the value of the drag force and the packing fraction of the granular system.

1We acknowledge support from NSF Grant No. DMR1206351, NASA Grant No. NNX15AD38G and the W.M. Keck Foundation

4:30PM C43.00007 Dynamics of pull out in a granular material

When an object is pulled out from a granular material, some striking phenomena can be observed. To visualize the pull out process in an experiment, we use grains composed of 2D photoelastic disks, from which circular intruders of different sizes are pulled out. We apply forces that are close to the minimum to initiate intruder motion. Then we find that the velocities of intruders depend exponentially on time, and equivalently the accelerations linearly vary with displacement. To better understand this dynamic system, we compute the drag force caused by the granular disks from the acceleration of the intruder. The result shows that the drag force depends linearly on the thickness of disks above the intruder. However, the drag force is much bigger than the weight of particles above the intruder. Additionally, we visualize the force chains formed inside the photoelastic disks and calculate the space-time evolution and curvature of those force chains. It is shown that curvatures obey the same distribution for circular intruders of different sizes.

1We would like to acknowledge NSF-DMR1206351 and the W.M.Keck Foundation.

4:42PM C43.00008 How does particle shape affect the near jamming properties of granular materials? Pentagons vs. disks

Understanding the role of particle shape in system-scale properties is a fundamental challenge in granular physics. We investigated the difference between the response of systems made of pentagons vs. more traditional disks. We performed isotropic compression experiments on 2D photoelastic pentagons and disks near the jamming transition. These experiments show qualitative and quantitative differences in the macroscopic responses of the two systems, such as shifts in the packing fraction at jamming onset and differences in the contact number evolution. Some of these differences are due to a reduction of packing order and the appearance of side-side contacts for the pentagons. We also examined the stress relaxation and dynamical heterogeneity of pentagon particles by performing cyclic compression to allow the system explore phase diagram. We contrast disk and pentagon evolution using four-point-susceptibility and G² techniques.

1Work supported by NSF-DMR1206351, DMS1248071, NASA NNX15AD38G, and the W.M. Keck Foundation

4:54PM C43.00009 The evolution of orientational order in sheared, 2D granular media of convex and concave elongated particles

The evolution of orientational order in sheared, 2D granular media of convex and concave elongated particles

1This work is supported by NSF grant DMRPD-09-1765
We investigate the micro-mechanisms underpinning dense granular flow behaviour from a series of DEM simulations of pure shear flows of dry grains. We observe the development of transient clusters of jammed particles within the flow. Typical size of such clusters is found to scale with the inertial number with a power law that is similar to the scaling of shear-rate profile relaxation lengths observed previously. Based on the simple argument that transient clusters of size ℓ exist in the dense flow regime, the formulation of steady state condition for non-homogeneous shear flow results in a general non-local relation, which is similar in form to the non-local relation conjectured for soft glassy flows. These findings suggest the formation of jammed clusters to be the key micro-mechanism underpinning non-local behaviour in dense granular flows.
9:12AM E34.00005 Modeling Shear Banding in Amorphous Solids, from Atomic to Continuum

Our proposal provides an unambiguous link between discrete-particle models and continuum mechanics at the nanoscale. We exemplify these facts in local stress calculations of defective graphene, lipid bilayers, and fibrous proteins. Furthermore, we propose a new physical and mathematical description of shear banding in amorphous solids, from atomistic to continuum scales. We show that, within our model, friction between grains produces stick-slip behavior at intermediate shear rates, even if the material is rate strengthening at larger rates. In addition, externally generated acoustic vibrations alter the stick-slip amplitude, or suppress stick-slip altogether, depending on the pressure and shear rate. We construct a phase diagram that indicates the regimes for stick-slip behavior in amorphous solids.

9:24AM E34.00006 Identifying shear transformation zones in amorphous solids via a virtual strain method

MICHAEL FALK, Johns Hopkins University — Molecular dynamics simulations of strain localization are carried out using different materials, systems, and interatomic potentials including CuZr modeled via the embedded-atom method (EAM), amorphous Si modeled using Stillinger-Weber (SW) and a binary Lennard-Jones (LJ) system. Quench schedules and strain rates are varied. Different systems exhibit marked similarities in plastic behavior. Systematic differences between systems are analyzed in the context of shear transformation zone (STZ) theory in the effort to develop a generalized constitutive framework for plasticity in glasses. Effective temperature inferred from the potential energy is explored as a local coarse-grained measure of the degree of disorder.

9:36AM E34.00007 Stick-slip instabilities in sheared granular flow: The role of friction and acoustic vibrations

CHARLES K. C. LIEOU, Los Alamos National Laboratory and University of California, Santa Barbara, AHMED E. ELBANNA, University of Illinois at Urbana-Champaign, JAMES S. LANGER, JEAN M. CARLSON, University of California, Santa Barbara — We propose a theory of shear flow in dense granular materials. A key ingredient of the theory is an effective temperature that determines how the material responds to external driving forces such as shear stresses and vibrations. We show that, within our model, friction between grains produces stick-slip behavior at intermediate shear rates, even if the material is rate strengthening at larger rates. In addition, externally generated acoustic vibrations alter the stick-slip amplitude, or suppress stick-slip altogether, depending on the pressure and shear rate. We construct a phase diagram that indicates the regimes for stick-slip behavior in amorphous solids.

9:48AM E34.00008 A microstructural description of shear thickening in dense suspensions

ABHINENDRA SINGH, Levich Institute, City College of New York, ROMAIN MARI, DAMTP, University of Cambridge, RYOHEI SETO, Mathematical Soft Matter Unit, Okinawa Institute of Science and Technology, JEFF MORRIS, MORTON DENN, Chemical Engineering Department, City College of New York — The mechanism of shear thickening in dense suspensions has been recently linked to a transition from a lubricated “frictionless” to an unlubricated “frictional” rheology. Recent simulations indicate that the transition is successful to quantitatively reproduce both the continuous and discontinuous shear thickening as observed experimentally. However, a microstructural description of these suspensions is still lacking, which would aid in understanding and predicting the flow behavior of shear thickening suspensions. To tackle this challenging issue, we explore various microscopic properties, like the inter-particle force distribution, the particle motion correlations, and the anisotropy (in both contact and force network). Further, we also attempt to link the observed rheological behavior observed at the macro scale to mean displacement and fluctuations at the particle scale.

10:00AM E34.00009 Deformation in Metallic Glass: Connecting Atoms to Continua

ADAM R. HINKLE, MICHAEL L. FALK, Johns Hopkins University, CHRIS R. RYCRIOFT, Harvard University, MICHAEL D. SHIELDS, Johns Hopkins University — Metallic glasses like other amorphous solids experience strain localization as the primary mode of failure. However, the development of continuum constitutive laws which provide a quantitative description of disorder and mechanical deformation remains an open challenge. Recent progress has shown the necessity of accurately capturing fluctuations in material structure, in particular the statistical changes in potential energy of the atomic constituents during the non-equilibrium process of applied shear. Here we directly cross-compare molecular dynamics simulations of a ZrCu glass with continuum shear transformation zone (STZ) theory representations. We present preliminary results for a methodology to coarse-grain detailed molecular dynamics data with the goal of initializing a continuum representation in the STZ theory.

1 NSF Grants Awards 1107838, 1408685, and 0801471
2 NSF IGERT Fellowship Award Number 0801471
10:12AM E34.00010 Size effects and internal length scales in the elasticity of random fiber networks

CATALIN PICU, Rensselaer Polytechnic Institute, KAMEL BERKACHE, EPSTA Alger, Algeria, ALI SHAHSAVARI, Rensselaer Polytechnic Institute, JEAN-FRANCOIS GANGHOFFER, Universite de Lorraine, Nancy, France — Random fiber networks are the structural element of many biological and man-made materials, including connective tissue, various consumer products and packaging materials. In all cases of practical interest the scale at which the material is used and the scale of the fiber diameter or the mean segment length of the network are separated by several orders of magnitude. This precludes solving boundary value problems defined on the scale of the application while resolving every fiber in the system, and mandates the development of continuum constitutive models which provide a quantitative description of disorder and mechanical deformation remains an open challenge. Recent progress has shown the necessity of accurately capturing fluctuations in material structure, in particular the statistical changes in potential energy of the atomic constituents during the non-equilibrium process of applied shear. Here we directly cross-compare molecular dynamics simulations of a ZrCu glass with continuum shear transformation zone (STZ) theory representations. We present preliminary results for a methodology to coarse-grain detailed molecular dynamics data with the goal of initializing a continuum representation in the STZ theory.

10:24AM E34.00011 Is the microscopic stress computed from molecular simulations in mechanical equilibrium?

ALEJANDRO TORRES-SANCHEZ, Universitat Politècnica de Catalunya, JUAN M. VANEGAS, Sandia National Laboratories, MARINO ARROYO, Universitat Politècnica de Catalunya — The microscopic stress field connects atomistic simulations with the mechanics of materials at the nano-scale through statistical mechanics. However, its definition remains ambiguous. In a recent work [1,2] we showed that this is not only a theoretical problem, but rather that it greatly affects local stress calculations from molecular simulations. We find that popular definitions of the local stress, which are commonly used to calculate the mechanical properties of materials, do not correctly capture the stress field at the nano-scale. In this work, we study the microscopic length scales of the network and the size effect associated with them. We consider both Cauchy and micropolar continuum models and calibrate them based on the discrete network behavior. We develop a method to predict the characteristic length scales of the problem and the minimum size of a representative element of the network based on network structural parameters and on fiber properties.

10:36AM E34.00012 Extending two-phase theories of soft composite solids to the non-dilute regime. FRANCESCO MANCARELLA, Nordic Institute of Theoretical Physics (NORDITA), ROBERT STYLE, University of Oxford, JOHN WETTLAUFER, Yale University and Nordic Institute of Theoretical Physics (NORDITA) — Composite materials are ubiquitous in the natural environment and in engineered materials and hence capture the interest of a wide audience. Eshelby’s 1957 theory treats the interaction of macroscopic stress fields with isolated inclusions within an elastic solid, and it has been widely used to treat the mechanics of composite materials. However, due to its neglect of interface stress, which is a particularly key effect in soft materials, the theory breaks down whenever the typical inclusion size $R$ is of order or less than the elastocapillary lengthscale $L$. In this regime, under external stress, the effect of inclusion shape becomes strongly size-dependent. Here, we develop two new non-dilute theories, estimate the elastic moduli of composites comprised of an isotropic, compressible, linear-elastic compliant solid hosting a non-dilute spatially-random distribution of identical liquid droplets. The composite stiffness depends on a single dimensionless parameter $L/R$, and we find significant elastic moduli corrections for inclusions sizes $R$ as large as $100 L$. By generalizing the exact theory recently developed for the corresponding dilute case, we find that when $R < 3L/2$ ($R = 3L/2$) liquid inclusions stiffen (cloak the far-field signature of) of the host solid.

1Swedish Research Council Grant No. 638-2013-9243.

10:48AM E34.00013 Continuum modeling of dense granular flow down heaps. DAVID HENANN, DAREN LIU, Brown University — Dense, dry granular flows display many manifestations of grain-size dependence, or nonlocality, in which the finite-size of grains has an observable impact on flow phenomenology. Such behaviors make the formulation of an accurate continuum model for dense granular flow particularly difficult, since local continuum models are not equipped to describe size-effects. One example of grain-size dependence is seen when avalanches occur on a granular heap — a situation which is frequently encountered in industry, as in rotating drums, as well as in nature, such as in landslides. In this case, flow separates into a thin, quickly flowing surface layer and a slowly creeping bulk. While existing local granular flow models are capable of capturing aspects of the flowing surface layer, they fail to even predict the existence of creeping flow beneath, much less being able to quantitatively describe the flow fields. Recently, we have proposed a new, scale-dependent continuum model — the nonlocal granular fluidity (NGF) model — that successfully predicted steady, slow granular flow fields, including grain-size-dependent shear-band widths in a variety of flow configurations. In this talk, we extend our model to the rapid flow regime and show that the model is capable of quantitatively predicting all aspects of gravity-driven heap flow. In particular, the model predicts the coexistence of a rapidly flowing, rate-dependent top surface layer and a rate-independent, slowly creeping bulk — a feature which is beyond local continuum approaches.

Tuesday, March 15, 2016 8:00AM - 11:00AM — Session E35 DBIO GSNP: Population and Evolutionary Dynamics I 338 - Michael Pleimling, Virginia Tech

8:00AM E35.00001 A non-classical phase diagram for virus-bacterial co-evolution mediated by CRISPR. , PU HAN, MICHAEL DEEM, Rice University — CRISPR is a newly discovered prokaryotic immune system. Bacteria and archaea with this system incorporate genetic material from invading viruses into their genomes, providing protection against future infection by similar viruses. Due to the cost of CRISPR, bacteria can lose the acquired immunity. We will show an intriguing phase diagram of the virus extinction probability, which when the rate of losing the acquired immunity is small, is more complex than that of the classic predator-prey model. As the CRISPR incorporates genetic material, viruses are under pressure to evolve to escape the recognition by CRISPR, and this co-evolution leads to a non-trivial phase structure that cannot be explained by the classical predator-prey model.

8:12AM E35.00002 Bacterial Invasion Dynamics in Zebrafish Gut Microbial Communities. SAVANNAH LOGAN, MATTHEW JEMIELITA, Department of Physics, University of Oregon, TRAVIS WILES, Institute of Molecular Biology, University of Oregon, BRANDON SCHLOMANN, Department of Physics, University of Oregon, BRIAN HAMMER, School of Biology, Georgia Institute of Technology, KAREN GUILLEMIN, Institute of Molecular Biology, University of Oregon, RAGHUVEER PARTHASARATHY, Department of Physics, University of Oregon — Microbial communities residing in the vertebrate intestine play an important role in host development and health. These communities must be in part shaped by interactions between microbial species as they compete for resources in a physically constrained system. To better understand these interactions, we use light sheet microscopy and zebrafish as a model organism to image established gut microbial communities as they are invaded by robustly-colonizing challengers. We demonstrate that features of the challenger, including motility and spatial distribution, impact success in invasion and in outcompeting the original community. We also show that physical characteristics of the host, such as the motility of the gut, play important roles in mediating inter-species competition. Finally, we examine the influence of the contact-dependent type VI secretion system (T6SS), which is used by specific bacteria to cause cell lysis by injecting toxic effector proteins into competitors. Our findings provide insights into the determinants of microbial success in the complex ecosystems found in the gut.

8:24AM E35.00003 Multiple Cancer Cell Population Dynamics in a Complex Ecology. KE-CHIH LIN, Princeton University, GONZALO TARGA, KENNETH PIENTA, Johns Hopkins Medical Institute, JAMES STURM, ROBERT AUSTIN, Princeton University — We have developed a technology for study of complex ecology cancer population dynamics. The technology includes complex drug gradients, full bright field/dark field/fluorescence imaging of areas of several square millimeters and thin gas-permable membranes which allow single cell extraction and analysis. We will present results of studies of prostate cancer cell dynamics.

8:36AM E35.00004 Migration in asymmetric, random environments. MICHAEL DEEM, DONG WANG, Rice University — Migration is a key mechanism for expansion of communities. As a population migrates, it experiences a changing environment. In heterogeneous environments, rapid adaption is key to the evolutionary success of the population. In the case of human migration, environmental heterogeneity is naturally asymmetric in the North-South and East-West directions. We here consider migration in random, asymmetric, modularly correlated environments. Knowledge about the environment determines the fitness of each individual. We find that the speed of migration is proportional to the inverse of environmental change, as asymmetric in the North-South and East-West directions. We here consider migration in random, asymmetric, modularly correlated environments. Knowledge about the environment determines the fitness of each individual. We find that the speed of migration is proportional to the inverse of environmental change, and in particular we find that North-South migration rates are lower than East-West migration rates. Fast communication within the population of pieces of knowledge between individuals, similar to horizontal gene transfer in genetic systems, can help to spread beneficial knowledge among individuals. We show that increased modularity of the relation between knowledge and fitness enhances the rate of evolution. We investigate the relation between optimal information exchange rate and modularity of the dependence of fitness on knowledge. These results for the dependence of migration rate on heterogeneity, asymmetry, and modularity are consistent with existing archaeological facts.
8:48AM E35.00005 Velocity locking and pulsed invasions of fragmented habitats with seasonal growth, KIRILL KOROLEV, CHING-HAO WANG, Boston University — From crystal growth to epidemics, spatial spreading is a common mechanism of change in nature. Typically, spreading results from two processes: growth and dispersal in ecology or chemical reactions and diffusion in physics. These two processes combine to produce a reaction-diffusion wave, an invasion front advancing at a constant velocity. We show that the properties of these waves are remarkably different depending whether space and time are continuous, as they are for a chemical reaction, or discrete, as they are for a pest invading a patchy habitat in seasonal climates. For discrete space and time, we report a new type of expansions with velocities that can lock into specific values and become insensitive to changes in dispersal and growth, i.e., the dependence of the velocity on model parameters exhibits plateaus or pauses. As a result, the evolution and response to perturbations in locked expansions can be markedly different compared to the expectations based on continuous models. The phenomenon of velocity locking requires cooperative growth and does not occur when per capita growth rate decline monotonically with population density. We obtain both numerical and analytical results describing highly non-analytic properties of locked expansions.

9:00AM E35.00006 Spatial organization of cooperation, NICOLAS DESPRAT, LPS - Ecole Normale Superieure (Paris) — The structure of the environment spatially confines bacteria inside groups where they live and evolve with their siblings. This population structure may not only select for individual abilities but also for group properties that would eventually enhance the fitness of the colony. In poor media, we might think that maximizing the contact with the environment would maximize the fitness of individual cells. However, we will show that the microcolony of P. aeruginosa adapts its morphogenesis to maximize cell-cell contacts rather than cell-environment interactions when iron becomes scarce in the environment. In this case, reducing the surface of exchange with the environment allows to limit the loss of secreted molecules required to efficiently fetch extracellular iron at very low concentration.

9:36AM E35.00007 Non-equilibrium relaxation in a two-dimensional stochastic lattice Lotka-Volterra model, SHENG CHEN, UWE C. TAUBER, Department of Physics, Virginia Tech — We employ Monte Carlo simulations to study a stochastic Lotka-Volterra model on a two-dimensional square lattice with periodic boundary conditions. There are stable states when the predators and prey coexist. If the local prey carrying capacity is finite, there emerges an extinction threshold for the predator population at a critical value of the predation rate. We investigate the non-equilibrium relaxation of the predator density in the vicinity of this critical point. The expected power law dependence between the relaxation time and predation rate is observed (critical slowing down). The numerically determined associated critical exponents are in accord with the directed percolation universality class. Following a sudden predation rate change to its critical value, one observes critical aging for the predator density autocorrelation function with a universal scaling exponent. This aging scaling signature of the absorbing state phase transition emerges at significantly earlier times than stationary critical power laws, and could thus serve as an advanced indicator of the population's proximity to its extinction threshold.

9:48AM E35.00008 The effects of sudden changes in environmental conditions on the non-equilibrium relaxation of ecological systems, SHADI ESMAEILI, MICHEL PLEIMLING, Virginia Tech — We study the responses of predator-prey systems to temporary changes in environmental conditions. Such changes can cause a variation in species’ predatory preferences which in our model appears as a perturbation in a many-species system. The type of perturbation that we consider in this study is a sudden change in the interaction scheme. We focus on systems evolving on a two-dimensional lattice and discuss the way the systems transition from one steady state to another. Using Monte Carlo simulations we monitor these transitions via the space-time correlation function and the derived correlation length.

10:00AM E35.00009 Effect of flow and active mixing on bacterial growth in a colon-like geometry, JONAS CREMER, IGOR SEGOTA, MARKUS ARNOLDINI, ALEX GROISMAN, TERENCE HWA, Department of Physics, U.C. San Diego — The large intestine harbors bacteria from hundreds of species, with bacterial densities reaching up to \(10^{12}\) cells per gram. Many different factors influence bacterial growth dynamics and thus bacterial density and microbiota composition. One dominant force is flow which can in principle lead to a washout of bacteria from the proximal colon. Active flow by contractions of the colonic wall together with bacterial growth might counteract such flow-forces and allow high bacterial densities to occur. As a step towards understanding bacterial growth in the presence of mixing and flow, we constructed an in-vitro setup where controlled wall-deformations of a channel emulate contractions. We investigate growth along the channel under a steady nutrient inflow. In the limits of no or very frequent contractions, the device behaves like a plug-flow reactor and a chemostat respectively. Depending on mixing and flow, we observe varying spatial gradients in bacterial density along the channel. Active mixing by deformations of the channel wall is shown to be crucial in maintaining a steady-state bacterial population in the presence of flow. The growth-dynamics is quantitatively captured by a simple mathematical model, with the effect of mixing described by an effective diffusion term.

10:12AM E35.00010 Predicting community composition from pairwise interactions, JONATHAN FRIEDMAN, Physics, MIT, LOGAN HIGGINS, Microbiology, MIT, JEFF GORE, Physics, MIT — The ability to predict the structure of complex, multiplex communities is crucial for understanding the impact of species extinction and invasion on natural communities, as well as for engineering novel, synthetic communities. Communities are often modeled using phenomenological models, such as the classical generalized LotkaVolterra (gLV) model. While a lot of our intuition comes from such models, their predictive power has rarely been tested experimentally. To directly assess the predictive power of this approach, we constructed synthetic communities comprised of up to 8 soil bacteria. We measured the outcome of competition between all species pairs, and used these measurements to predict the composition of communities composed of more than 2 species. The pairwise competitions resulted in a diverse set of outcomes, including coexistence, exclusion, and bistability, and displayed evidence for both interference and facilitation. Most pair-outcomes could be captured by the gLV framework, and the composition of multispaces communities could be predicted for communities composed solely of such pairs. Our results demonstrate the predictive ability and utility of simple phenomenology, which enables accurate predictions in the absence of mechanistic details.

10:24AM E35.00011 A field-theoretic approach to the May-Leonard cyclic population dynamics model, SHANNON SERRAO, UWE TÄUBER, Virginia Tech — Spatially extended stochastic population dynamics models with cyclic predation interactions display intriguing time evolution and spontaneous structure formation. We study a version of the May-Leonard cyclic competition model in d dimensions with diffusive particle propagation. We use the second-quantized Doi-Peliti formalism and ensuing coherent-state path integral representation to construct its continuum representation and explore its collective dynamics. Expanding the resulting action about the mean-field species concentrations enables us to compute the diagonalized harmonic propagators and hence ‘masses’, i.e., relaxation rates and eigenfrequencies of the fundamental modes. Furthermore, operating near the Hopf bifurcation point, we identify the validity range for the necessary time scale separation that allows us to project out the purely relaxing eigenmode. The remaining oscillating fields obey the complex Ginzburg-Landau equation, which is consistent with spiral pattern formation.
10:36AM E35.00012 Range expansions transition from pulled to pushed waves with increasing cooperativity in an experimental microbial population, SAURABH GANDHI, EUGENE YURTSEV, Massachusetts Inst of Tech-MIT, KIRILL KOROLEV, Boston University, JEFF CORE, Massachusetts Inst of Tech-MIT — Range expansions are becoming more frequent due to environmental changes and rare long distance dispersal, often facilitated by anthropogenic activities. Simple models in theoretical ecology explain many emergent properties of range expansions, such as a constant expansion velocity, in terms of organism-level properties such as growth and dispersal rates. Testing these quantitative predictions in natural populations is difficult because of large environmental variability. Here, we used a controlled microbial model system to study range expansions of populations with and without intra-specific cooperativity. For non-cooperative growth, the expansion dynamics were dominated by population growth at the low-density front, which pulled the expansion forward. We found these expansions to be in close quantitative agreement with the classical theory of pulled waves by Fisher and Skellam, suitably adapted to our experimental system. However, as cooperativity increased, the expansions transitioned to being pushed, i.e. controlled by growth in the bulk as well as in the front. Although both pulled and pushed waves expand at a constant velocity and appear otherwise similar, their distinct dynamics leads to very different evolutionary consequences. Given the prevalence of cooperative growth in nature, understanding the effects of cooperativity is essential to managing invading species and understanding their evolution.

10:48AM E35.00013 Selection of Cooperation in Spatially Structured Populations, HYUNMO YANG, Ulsan National Institute of Science and Technology, CHEOL-MIN GHIM, Biomedical Engineering, Ulsan National Institute of Science and Technology — The social dilemma games give rise to an emergence of cooperation in which altruistic individuals survive the natural selection at higher rate than random chance. We try to extend our understanding of this spatial reciprocity by including the impact of degree-degree correlation on the propensity toward prosocial behaviour in an otherwise well-mixed population. In a stochastic death-birth process with weak selection, we find that the disassortative degree mixing, or negative correlation between the degrees of neighbouring nodes significantly promotes the fixation of cooperators whereas the assortative mixing acts to suppress it. This is consistent with the fact that the spatial heterogeneity weakens the average tendency of a population to cooperate, which we describe in a unified scheme of the effective isothermality in coarse-grained networks. We also discuss the individual-level incentives that indirectly foster restructuring the social networks toward the more cooperative topologies.

Tuesday, March 15, 2016 8:00AM - 11:00AM
Session E40 GSNP GPC: Leo Kadanoff Session I 343 - Sidney Nagel, University of Chicago

8:00AM E40.00001 Droplet formation and neck rupture in granular streams and dense suspensions, HEINRICH JAEGER, University of Chicago — When a pendant drop of liquid breaks off, the final stages of neck formation before the singular event of separation are well described by a power law with an exponent that characterizes the liquid. Specifically, a linear decrease of the neck width with time to breakup implies a highly viscous liquid, while sublinear behavior with exponent 2/3 signals the inviscid limit. It therefore has come as a complete surprise that droplet neck formation in dry granular streams as well as concentrated suspensions, both systems with high apparent viscosity, exhibits the same scaling as the inviscid case. I will discuss some of the experimental evidence for this behavior and attempt an explanation that explicitly considers an aspect unique to the presence of the particles: the feedback between the ability of a (nearly) jammed state to deform and the Gaussian curvature introduced by the neck.

8:12AM E40.00002 Particle Laden Flows from Theory to Experiment1, ANDREA BERTOZZI, Univ of California - Los Angeles — Leo Kadanoff inspired a generation of collaboration across the boundaries of applied mathematics, theoretical physics, engineering, an experimental physics. His influence is seen in laboratories, classrooms, PhD theses, and even undergraduate research across the world. In this talk I review a body of research at UCLA spanning the past ten years in which we have worked to understand the basic physics of particle laden flow by comparing experiments with mathematical models. The project was inspired by some initial experiments and models developed by A. Hosoi’s group at MIT. We derive and analyze systems of conservation laws with rich behavior that includes multiple shocks, rarefactions, and singular shocks - and study these along side laboratory experiments. Our work includes both basic physics problems and industrial applications such as spiral separators used in the mining industry.

1Supported by NSF grants DMS-1312543 and DMS-1045536

8:24AM E40.00003 Surface tension models for particle laden thin films1, JEFFREY WONG, LI WANG, ANDREA BERTOZZI, Univ of California - Los Angeles — We study viscous slurries on an incline spanning the past ten years in which we have worked to understand the basic physics of particle laden flow by comparing experiments with mathematical models. The project was inspired by some initial experiments and models developed by A. Hosoi’s group at MIT. We derive and analyze systems of conservation laws with rich behavior that includes multiple shocks, rarefactions, and singular shocks - and study these along side laboratory experiments. Our work includes both basic physics problems and industrial applications such as spiral separators used in the mining industry.

1This work is supported by NSF grants DMS-1312543 and DMS-1045536.

8:36AM E40.00004 Plastic flow of polycrystalline materials, JAMES LANGER1, University of California, Santa Barbara — Leo Kadanoff had a long interest in fluid flows, especially fingering instabilities. This interest was one example of his insatiable curiosity about simple, fundamentally important, and often multidisciplinary phenomena. Here is an example of another class of such phenomena that I had hoped to show him this year. The experts in polycrystalline solid mechanics have insisted for decades that their central problem – dislocation-mediated strain hardening – is intrinsically unsolvable. I think they’re wrong. My colleagues and I have made progress recently in theories of both amorphous and polycrystalline plasticity by introducing an effective disorder temperature as a dynamical variable in our equations of motion. In this way, we have been able to describe how the densities of flow defects or dislocations evolve in response to external forcing, and thus to develop theories that promise to become as predictive, and full of surprises, as the laws of fluid flow.

1For Kadanoff session

8:48AM E40.00005 Scaling theory of the jamming transition1, ANDREA LIU, University of Pennsylvania, Department of Physics and Astronomy, CARL GOODRICH, SEAS, Harvard University, JAMES SETHNA, Cornell University; Department of Physics, SIDNEY NAGEL, University of Chicago — James Franck Institute — The concept of jamming was first introduced at the University of Chicago by Sid Nagel and Yoram Wolf. By now we know that there is a zero-temperature critical jamming transition that marks the onset of rigidity in packings of soft repulsive spheres. In contrast to the perfect fcc crystal state, which is the maximally stable state for such systems, the jammed state is only marginally stable mechanically, and thus represents an opposite extreme to the perfect crystal. This marginal stability gives rise to power law scalings and diverging length scales at the transition. Here I will discuss recent developments that put the jamming transition in the same place that the Ising transition was when Leo Kadanoff introduced the ideas of coarse-graining and rescaling into critical phenomena.

1Supported by DOE-DE-FG02-05ER46199
9:00AM E40.00006 Thermal Boundary Layer Equation for Turbulent Rayleigh-Bénard Convection

EMILY SC CHING, Department of Physics, The Chinese University of Hong Kong, OLGA SHISHKINA, Max Planck Institute for Dynamics and Self-Organization, SUSANNE HORN, Department of Mathematics, Imperial College, SEBASTIAN WAGNER, Max Planck Institute for Dynamics and Self-Organization — Turbulent Rayleigh-Bénard convection, consisting of a fluid confined between two horizontal plates, heated from below and cooled from above, is a paradigm system for studying turbulent thermal convection, which is ubiquitous in nature. In turbulent Rayleigh-Bénard convection, there are viscous boundary layers near all rigid walls and two thermal boundary layers, one above the bottom plate and one below the top plate. The classical Prandtl-Blasius-Pohlhausen theory has often been used to describe the mean velocity and temperature boundary layer profiles but systematic deviations are known to exist. These deviations are due to turbulent fluctuations. In this talk, we report a new thermal boundary layer equation for turbulent Rayleigh-Bénard convection derived for Prandtl number (Pr) greater than 1, which takes into account the effects of turbulent fluctuations by using the idea of an eddy thermal diffusivity. Solving this equation, we have obtained two analytical mean temperature profiles for Pr ~ 1 and Pr ≥ 1. These two theoretical predictions are shown to be in excellent agreement with the results of our direct numerical simulations for Pr=4.38 (water) and Pr=2547.9 (glycerol).

Work of ESCC was supported by the Hong Kong Research Grants Council under Grant No. CUHK-400311.

9:12AM E40.00007 Leo Kadanoff’s legacy for turbulent thermal convection

DETLEF LOHSE, University of Twente — Rayleigh-Bénard (RB) convection... (Rayleigh, Chandrasekhar) and had been paradigmatic in pattern formation and in the study of spatial-temporal chaos (Ahlers, Libchaber, and many others). It was Leo Kadanoff and his associates in Chicago who, in the 1980s and 1990s, propagated the RB system as paradigmatic for the physics of fully developed turbulence and contributed tremendously to today’s understanding of thermally driven turbulence. He and his experimental coworkers (Libchaber et al.) revealed the importance of the thermal plumes and the large-scale wind, and elucidated the interplay between thermal boundary layers and bulk. His scaling analysis laid the basis for our present understanding of turbulent convection, which I will review in this talk, highlighting Leo’s trailblazing contributions.

1 Kadanoff session

9:24AM E40.00008 Control and large deformations of marginal disordered structures

ARVIND MURUGAN, MATTHEW PINSON, University of Chicago, ELIZABETH CHEN, Harvard University — Designed origami patterns, such as origami structures, provide a way to make easily controlled mechanical metamaterials with tailored responses to external forces. We focus on an often overlooked regime of origami - non-linear deformations of large disordered origami patterns with no symmetries. We find that practical questions of control in origami have counterintuitive answers, because of intimate connections to spin glasses and neural networks. For example, 1 degree of freedom origami structures are actually difficult to control about the flat state with a single actuator; the actuator is thrown off by an exponential number of 'red herring' zero modes for small deformations, all but one of which disappear at larger deformations. Conversely, structures with multiple programmed motions are much easier to control than expected - in fact, they are as easy to control as a dedicated single-motion structure if the number of programmed motions is below a threshold ('memory capacity').

9:36AM E40.00009 Planarity of Force Tilings in Jammed Packings of Disks

KABIR RAMOLA, BULBUL CHAKRABORTY, Brandeis University — We propose a new order parameter for load induced jamming transitions in disk packings based on the planarity of force tilings. Contact forces between disks in mechanical equilibrium can be arranged in a dual space to form a network (tiling) represented by a set of vertices and edges G = (V, E). A Delaunay triangulation of these vertices then forms a related network G_D = (V, E_D). We define a planarity order parameter ψ as the overlap of these two graphs ψ = ⟨G_D,G⟩. We use this parameter to characterize jamming transitions in two dimensional granular systems. We find clear signatures of the existence of non-planar and planar phases as a function of external load. We study this behaviour using simulation data of frictionless soft disks and experimental data of frictional disk packings.

This work has been supported by NSF-DMR 1409093 and the W. M. Keck Foundation.

9:48AM E40.00010 Consolidation by adiabatic jamming fronts

DOUGLAS DURIAN, CARLOS ORTIZ, TED BRZINSKI, University of Pennsylvania — We formulate a nonlinear partial differential equation to describe changes in packing fraction for sedimenting particles at low Reynolds number. It is based on two key fluid-mediated forces. One is the viscous interaction of a particle with the surrounding suspension, which causes the settling speed to decrease with increasing packing fraction according to a hindered settling function; we constrain its form by a comprehensive data compilation. The other ingredient is a lubrication force that resists change in separation between neighboring particles; it diverges at low Reynolds number. It is based on two key fluid-mediated forces. One is the viscous interaction of a particle with the surrounding suspension, which causes the settling speed to decrease with increasing packing fraction according to a hindered settling function; we constrain its form by a comprehensive data compilation. The other ingredient is a lubrication force that resists change in separation between neighboring particles; it diverges at low Reynolds number. It is based on two key fluid-mediated forces. One is the viscous interaction of a particle with the surrounding suspension, which causes the settling speed to decrease with increasing packing fraction according to a hindered settling function; we constrain its form by a comprehensive data compilation. The other ingredient is a lubrication force that resists change in separation between neighboring particles; it diverges at low Reynolds number. It is based on two key fluid-mediated forces. One is the viscous interaction of a particle with the surrounding suspension, which causes the settling speed to decrease with increasing packing fraction according to a hindered settling function; we constrain its form by a comprehensive data compilation. The other ingredient is a lubrication force that resists change in separation between neighboring particles; it diverges at low Reynolds number.

10:00AM E40.00011 What are the microscopic origins of shear jamming?

BOB BEHRINGER, DONG WANG, Duke University, JIE REM, Merck & Co., JONATHAN BARES, Duke University, BULBUL CHAKRABORTY, Brandeis University, LENKA KOVALCINOVA, LOU KONDIC, NJIT — Granular materials can jam by shear: shear strain applied to a stress-free state in a packing fraction range φ < φ_c < φ_J, leads to mechanically stable (jammed) anisotropic states (Bi et al. Nature, 2011). φ_J is the lowest φ for which an isotropic state is jammed, and shear jamming ceases below φ_c. The process of shear jamming involves the formation of strong force networks that are initially highly anisotropic ‘force chains’, then become more isotropic with increasing shear. The mechanisms that lead to shear jamming are also presumably similar to those that lead to Reynolds dilatancy.

What microscopic processes can account for shear jamming? Force chains, roughly linear sequences of particles experiencing average or above forces are not stable by themselves. Hence, force chain particles must form additional ‘non-chain’ contacts. Here, we propose micro-scale structures and their response to shear that serves as a basis to understand the formation of stable force networks and shear jamming. We identify these structures in experimental and numerical data, and track their response to shear.

Work supported by NSF-DMR1206351, DMS1248071, NASA NNX15AD38G, and the W.M. Keck Foundation.
10:12AM E40.00012 Itokawa: a case for ballistic segregation\textsuperscript{1}, TROY SHINBROT, Rutgers University, TAPAN SABAWULA, Okinawa Institute for Science and Technology, THEO SIU, MIGUEL VIVAR LAZO, Rutgers University, PINAKI CHAKRABORTY, Okinawa Institute for Science and Technology — Recent photographs of the asteroid Itokawa have revealed strong separation between regions populated almost entirely by small pebbles and other regions consisting only of larger boulders. This size separation has been attributed to the Brazil Nut Effect (BNE), however we point out here that the BNE depends on conditions such as isotropic gravity, parallel sidewalls and periodic vertical shaking that are wholly absent on asteroids. On the other hand, surface areas of boulders and pebbles appear to be comparable on Itokawa, and in this situation it follows that the asteroid must have suffered many orders of magnitude more collisions with pebbles than with boulders. We observe that a pebble will tend to bounce off of a boulder but will sink into a sea of similar pebbles, and so we predict that seas of pebbles must grow on such asteroids. We carry out experiments and simulations to evaluate this and related predictions, and we demonstrate that this new mechanism of segregation based on simple counting of grains can produce the strong separation of sizes reported.

\textsuperscript{1}Support provided by NSF grant 1404792

10:24AM E40.00013 A trans-phase granular continuum relation and its use in simulation, KEN KAMRIN, SACHITH DUNATUNGA, HESAM ASKARI, MIT — The ability to model a large granular system as a continuum would offer tremendous benefits in computation time compared to discrete particle methods. However, two infamous problems arise in the pursuit of this vision: (i) the constitutive relation for granular materials is still unclear and hotly debated, and (ii) a model and corresponding numerical method must wear "many hats" as, in general circumstances, it must be able to capture and accurately represent the material as it crosses through its collisional, dense-flowing, and solid-like states. Here we present a minimal trans-phase model, merging an elastic response beneath a fictional yield criterion, a mu(I) rheology for liquid-like flow above the static yield criterion, and a disconnection rule to model separation of the grains into a low-temperature gas. We simulate our model with a meshless method (in high strain/mixing cases) and the finite-element method. It is able to match experimental data in many geometries, including collapsing columns, impact on granular beds, draining silos, and granular drag problems.

10:36AM E40.00014 A Hierarchy of Dynamic Equilibria and a View of a Fly’s Equilibrium Reflex, Z. JANE WANG\textsuperscript{2}, Cornell University — Understanding structures within a structure is a topic that has fascinated Leo throughout his life, and we are now benefiting from his fundamental insights when we think about living organisms. A living organism is far from statistical equilibrium and it does not have a single critical parameter. However, each organism has a hierarchical structure within itself. Recently, asking how often a fly must sense its orientation in order to balance in air has led us to suggest one of the fly’s 17 steering muscles, the first basalar muscle, is responsible for maintaining flight stability. Here I suggest that the chain of events associated with flight equilibrium reflex can be viewed as a succession of local linear transformation about a set of dynamic equilibria\textsuperscript{1}. Each of the functionally different parts, the sensors, motor neurons, muscles, wing-hinges, flapping wings, and the thorax, operate near its own dynamic equilibrium, often close to the boundary between stability and instability. Locomotion rises as an organism responds to a small perturbation from these equilibria. \textsuperscript{1}JZ Wang, Ann. Rev. Cond. Matter Physics, Vol 7, 2016

\textsuperscript{2}Kadanoff session

10:48AM E40.00015 The life of vortex knots and the flow of helicity, WILLIAM IRVINE, University of Chicago — What happens if you take a vortex loop - akin to a smoke ring in air - and tie it into a knot or a link? The knottness (Helicity) of a fluid is a conserved quantity in many idealized situations (such as Euler fluids) offering the potential for fundamental insights into fluid flow. In real fluids, progress has been hindered by lack of accessible experimental systems. I will tell of how to make a vortex knot and link in water, in the wave function of a superfluid (on a computer) and of what happens thence, with an emphasis on universal aspects of the dynamics and the flow of helicity.

Tuesday, March 15, 2016 8:00AM - 11:00AM – Session E43 GSNP GSOFT: Jamming and the Glass Transition I

8:00AM E43.00001 ABSTRACT WITHDRAWN –

8:12AM E43.00002 A system for granular crosses\textsuperscript{1}, ZEGAN SHANG, Duke University, HU ZHENG, Hohai University, DONG WANG, JONATHAN BARES, ROBERT BEHRINGER, Duke University — A disordered stress-free granular packing can be turned into a rigid structure, which is called jammed state, by increasing the density of particles per unit volume or by applying shear deformation. The jamming behavior of systems made of 2D circular discs have been investigated in detail, but very little is known about the special geometry particles, particularly non-convex particles like crosses. Here, we perform an experimental study on the jamming of a system of quasi-2D granular crosses. In the present experiments, we measure the pressure, and coordinate number evolution of a 2D packing of photo-elastic cross discs. This talk will present results from a simple shear experiment for stresses and for the order parameter associated with the cross orientation and its correlation.

\textsuperscript{1}We acknowledge support from NSF Grant No. DMR1206351, NASA Grant No. NNX15AD38G and the W.M. Keck Foundation

8:24AM E43.00003 Experimental studies of contact networks in jammed colloidal systems, ERU KYEYUNE-YONOMI, LANE GILCHRIST, HERNN MAKSE, City College of New York — Recent theoretical advances in the statistical mechanics of jamming have provided a new outlook for thermodynamically characterizing packings of granular matter. Packing density, spatial ordering metrics, and the number of inter-particle contacts are a few fundamental parameters used in various theoretical models. However, experimental measurements of inter-particle forces have been illusive. Here, fluorescent molecular probes are used to identify inter-particle contacts in high resolution confocal images of jammed colloidal systems.

8:36AM E43.00004 Experimental Study of Athermal Elastic Network Mechanics, JONATHAN MICHEL, PETER YUNKER, Georgia Institute of Technology — Recently, significant theoretical effort has been directed towards understanding the mechanics of networks. Elastic networks are of inherent fundamental interest\textsuperscript{1} and serve as useful analogs for describing other physical systems. Recent applications include modeling of collagen\textsuperscript{2} and descriptions of jamming in granular media and glass formation\textsuperscript{3}. I propose to discuss ongoing experimental efforts to study mechanical properties of elastic networks, such as Youngs modulus and ultimate strength, in the athermal limit. I will begin with the simple case of regular, isostatic crystalline lattices and proceed to studies of random, connected elastic networks of varying bond number for a given number of lattice sites, including both isostatic and sub-isostatic networks.

\textsuperscript{1}Mao, X., Stenull, O. and Lubensky, T.C., “Elasticity of a filamentous kagome lattice”, Physical Review E, 87:042604
\textsuperscript{2}Licup, J. et al., “Stress Controls the mechanics of collagen networks”, PNAS, 2015, 112:9573-9578
8:48AM E43.00005 Interparticle contact networks of granular packings below jamming, BHASKAR SEN GUPTA, THIBAULT BERTRAND, COREY O’HERN, Yale University, MARK D. SHATTUCK, City College of New York — We employ computer simulations to investigate the structural properties of interparticle contact networks in granular packings of bidisperse disks below jamming onset at which the system becomes solid-like. We show that the properties of the contact networks are highly sensitive to changes in the packing-generation protocol and its numerical implementation. Thus, we formulate an analytical method to implement steepest descent of hard, athermal particles undergoing isotropic compression, which allows us to calculate the number of contacts as a function of packing fraction. These results represent an important first step in developing a theoretical description of shear- and compression-induced jamming in frictional granular media.

9:00AM E43.00006 Contact breaking in frictionless granular packings1, QIKAI WU, THIBAULT BERTRAND, COREY O’HERN, Yale University, MARK SHATTUCK, City College of the City University of New York — We numerically study the breaking of interparticle contact networks in static granular packings of frictionless bidisperse disks that are subjected to vibrations. The packings are created using an isotropic compression protocol at different values of the total potential energy per particle $E_p$. We first add displacements along a single vibrational mode $i$ of the dynamical matrix to a given packing and calculate the minimum amplitude $A_i$ of the perturbation at which the first interparticle contact breaks. We then identify the minimum amplitude $A_{\min}$ over all perturbations along each mode and study the distribution of $A_{\min}$ from an ensemble of packings at each $E_p$. We then study two-, three-, and multi-mode excitations and determine the dependence of $A_{\min}$ on the number of modes that are included in the perturbation.

9:12AM E43.00007 Echoes of the glass transition in athermal soft spheres, PETER MORSE, ERIC CORWIN, University of Oregon — The glass transition and the athermal jamming transition are both transitions from one disordered state to another marked by a sudden increase in rigidity. Before the onset of rigidity, thermally hard spheres and athermal soft spheres both share the same configuration space. Is there a signature of the glass transition in the topology of the allowed configuration space, and is this same signature present for athermal spheres? I will answer these questions by introducing the concept of local rigidity, and in doing so, I will demonstrate the existence of a pre-jamming phase transition precisely at the glass transition density.

9:24AM E43.00008 Structural Signatures of the glass transition, CHI ZHANG, Department of Physics, Université de Fribourg, CH-1700 Fribourg, Switzerland, NICOLETTA GNAN, EMANUELA ZACCARELLI, CNR-ISC, UOS Sapienza, P.le A. Moro 2, Roma I-00185, Italy, Dipartimento di Fisica, Sapienza Università di Roma, P.le A. Moro 2, Roma I-00185, Ital, FRANK SCHEFFOLD, Department of Physics, Université de Fribourg, CH-1700 Fribourg, Switzerland. — The nature of colloidal glasses and the glass transition remains a topic of scientific interest. Scientists often focus on the study of dynamical properties since major structural changes have not been found to date in the vicinity of the glass transition. In this work we study both structural and dynamic signatures of the glass and jamming transition. Confocal microscopy measurements and molecular dynamic simulations are conducted on buoyancy and index matched microscale emulsion droplets with polydispersity of 12%, where crystallization is avoided. We find that the glass transition of such system is associated with detailed structural signatures on both global and local scales. At the global level, the peak amplitude of the radial distribution function shows a nonmonotonic evolution around a volume fraction of 59%. At the individual particle level, some local parameters such as the configuration of the nearest neighbors and the locally favoured structures also evolve differently across a volume fraction of about 59% whereas the jamming transition if observed at higher densities 64%. Our results reveal clear structural signatures of the glass transition, which could help the further understanding of the underlying physical mechanism leading to dynamical arrest.

9:36AM E43.00009 Casimir forces in systems near jamming1, JUSTIN BURTON, JUAN-JOSÉ LIETOR-SANTOS, Department of Physics, Emory University — Casimir forces arise when long-range fluctuations are geometrically confined between two surfaces. In most cases these fluctuations are quantum or thermal in nature, such as those near a classical critical point, yet this is not a requirement. The $T = 0$ jamming transition in frictionless, granular systems shares many properties with classical critical points, such as a diverging correlation length, although it has recently been identified as a unique example of a random first-order transition (RFOT). Here we show the existence of Casimir forces between two pinned particles immersed in systems near the frictionless jamming transition. We observe two components to the total force: a short-ranged, depletion force and a long-ranged, repulsive Casimir force. The Casimir force dominates when the pinned particles are much larger than the ambient jammed particles. In this case, we find that particles with the largest forces have the least number of contacts, and that these particles are clustered between the pinned particles, giving rise to a repulsive force which is independent of system preparation and inter-particle potential.

1We acknowledge support from NSF DMR-1455086

9:48AM E43.00010 Rearrangements in Sheared Disordered Solids: Low and High Pressure Regimes, SVEN WIJTMANS, Syracuse University, MERLIJN VAN DEEN, MARTIN VAN HECKE, Universiteit Leiden, M. LISA MANNING, Syracuse University — We study contact changes and rearrangements in quasistatic shear of disordered jammed packings at a range of pressures. We distinguish rearrangements where particle positions are discontinuous, leading to energy and stress discontinuities, from more frequent network events where contacts change but particle positions remain continuous. Moreover, we introduce two distinct protocols to unambiguously distinguish line reversible, loop reversible and irreversible events. The prevalence and spatial extension of five distinct event types (there are no loop reversible network events) evidence two distinct regimes: a low pressure regime dominated by irreversible extended events and a high pressure regime dominated by reversible localized ones. These trends indicate a crossover in the qualitative nature of plastic behavior in disordered solids near and far from jamming.

10:00AM E43.00011 ABSTRACT WITHDRAWN

10:12AM E43.00012 Rheological Transition of Sheared Frictionless Disks with Rotational Motion1, PETER OLSSON, Ume University, STEVE TEITEL, University of Rochester — We consider the massive Durian bubble model for sheared bidisperse disks, but modified so as to include the rotational motion of particles due to dissipative collisional torques. In such a model, particles possess a viscous tangential dissipation, though no elastic tangential friction. As the packing fraction is increased, we find a discontinuous transition from Bagnoldian to Newtonian rheology, at a packing fraction that lies below the jamming transition. At this transition we find a region of coexisting shear bands of Bagnoldian and Newtonian rheology, and suggestions of discontinuous shear thickening upon increasing the shear strain rate.

1This work has been supported by NSF Grant No. DMR-1205800.
10:24AM E43.00013 Critical Scaling of Bagndold Rheology at the Jamming Transition of Frictionless Disks1, STEPHEN TEITEL, University of Rochester, DANIEL VÄGGER, Delft Univ of Tech, PETER OLSSON, Umed University — We simulate shear-driven, frictionless, bidisperse disks in two dimensions, as a function of applied shear strain rate and packing fraction, for a model with a normal viscous dissipation that results in Bagndoldian rheology for all control parameters. Carrying out a critical scaling analysis of the pressure and shear stress near the jamming transition we find values of the critical exponents that disagree with theoretical predictions of Otsuki and Hayakawa[1] but are closer to more recent theoretical results by DeGiuli et al[2], as well as earlier simulations by Peyneau and Roux[3]. We find that it is essential to include leading corrections-to-scaling to arrive at self-consistent results.

1 This work has been supported by NSF Grant No. DMR-1205800, Swedish Research Council Grant No. 2010-3725, and the Dutch Organization for Scientific Research (NWO).

10:36AM E43.00014 Single Particle Jumps in Sheared SiO21, SEAN MCAHON, KATHARINA VOLLMAYR-LEE, Bucknell University, JONATHAN COOKMEYER, Haverford College, JUERGEN HORBACH, Heinrich-Heine-University Duesseldorf, Germany — We study the dynamics of a sheared glass via molecular dynamics simulations. Using the BKS potential we simulate the strong glass former SiO2. The system is initially well equilibrated at a high temperature, then quenched to a temperature below the glass transition, and, after a waiting time at the desired low temperature, sheared with constant strain rate. We present preliminary results of an analysis of single particle trajectories of the sheared glass.

2We acknowledge the support via NSF REU grant PHY-1156964, DoD ASSURE program, and NSF-MRI CHE-1229354 as part of the MERCURY high-performance computer consortium. We thank G.P. Shrivastav, Ch. Scherer and B. Temelso.

10:48AM E43.00015 Increasing the maximally randomly jammed density with electric field to reduce the fat level in chocolate. R. TAO1, H. TANG, Temple Univ — Chocolate is one of the most popular food types and flavors in the world. Unfortunately, at present, chocolate products contain too much fat, leading to obesity. For example, a typical molding chocolate has various fat up to 40% in total and chocolate for covering ice cream has fat 50 -60%. Especially, as children are the leading chocolate consumers, reducing the fat level in chocolate products to make them healthier is important and urgent. While this issue was called into attention and elaborated in articles and books decades ago and led to some patent applications, no actual solution was found unfortunately. Why is reducing fat in chocolate so difficult? What is the underlying physical mechanism? We have found that this issue is deeply related to the basic science of soft matters, especially to their viscosity and maximally random jammed (MRJ) density ϕ_{r}. All chocolate productions are handling liquid chocolate, a suspension with cocoa solid particles in melted fat, mainly cocoa butter. The fat level cannot be lower than 1-ϕ_{r} in order to have liquid chocolate to flow. Here we show that with application of an electric field to liquid chocolate, we can aggregate the suspended particles into prolate spheroids. This microstructure change reduces liquid chocolate’s viscosity along the flow direction and increases its MRJ density significantly. Hence the fat level in chocolate can be effectively reduced. We are looking forward to a new class of healthier and tasteful chocolate coming to the market soon.

1Dept. of Physics, Temple Univ, Philadelphia, PA 19122

Tuesday, March 15, 2016 11:15AM - 1:39PM — Session F1 DCMP GSNP: Pattern Formation Ballroom I - Sidney Nagel, University of Chicago

11:15AM F1.00001 Fingers, toes and tongues: the anatomy of interfacial instabilities in viscous fluids. IRMGARD BISCHOFBERGER, Massachusetts Institute of Technology — The invasion of one fluid into another of higher viscosity is unstable and produces complex patterns in a quasi-two dimensional geometry. This viscous-fingering instability, a bedrock of our understanding of pattern formation, has been characterized by a most-unstable wavelength that sets the characteristic length of the fingers. We have shown that a second, previously overlooked, parameter governs the length of the fingers and characterizes the dominant global features of the patterns. Because interfacial tension suppresses short-wavelength fluctuations, its elimination would suggest an instability producing highly ramified singular structures. Our experimental investigations using miscible fluids show the opposite behavior – the interface becomes more stable even as the stabilizing effect of interfacial tension is removed. This is accompanied by slender structures, tongues, that form in the narrow thickness of the fluid. Among the rich variety of global patterns that emerge is a regime of blunt structures, “toes”, that exhibit the unusual features characteristic of proportionate growth. This type of pattern formation, while quite common in mammalian biology, was hitherto unknown in physical systems.

11:51AM F1.00002 Pattern formation with proportionate growth1, DEEPAK DHAR, Tata Institute of Fundamental Research, Mumbai — It is a common observation that as baby animals grow, different body parts grow approximately at same rate. This property, called proportionate growth is remarkable in that it is not encountered easily outside biology. The models of growth that have been studied in Physics so far, e.g diffusion –limited aggregation, surface deposition, growth of crystals from melt etc. involve only growth at the surface, with the inner structure remaining frozen. Interestingly, patterns formed in growing sandpiles provide a very wide variety of patterns that show proportionate growth. One finds patterns with different features, with sharply defined boundaries. In particular, even with very simple rules, one can produce patterns that show striking resemblance to those seen in nature. We can characterize the asymptotic pattern exactly in some special cases. I will discuss in particular the patterns grown on noisy backgrounds.

1supported by J. C. Bose fellowship from DST ( India)

12:27PM F1.00003 Patterns in Active Nematics, JULIA M YEMANS, University of Oxford — Active systems, from bacterial suspensions to cellular monolayers, are continuously driven out of equilibrium by local injection of energy from their constituent elements and exhibit turbulent-like, chaotic patterns. We describe how active systems can be stabilised by tuning a physical feature of the system, friction. We demonstrate how the crossover between wet active systems, whose behaviour is dominated by hydrodynamics, and dry active matter where any flow is screened, can be achieved by using friction as a control parameter and demonstrate vortex ordering at the wet-dry crossover. We show that the self organisation of vortices into lattices is accompanied by the spatial ordering of topological defects leading to active crystal-like structures. The emergence of vortex lattices which leads to the positional ordering of topological defects may be a useful step towards the design and control of active materials.
1:03PM F12.00004 Instabilities and pattern formation on the pore scale, ANNE JUEL, University of Manchester — What links a baby's first breath to adhesion debonding, enhanced oil recovery, or even drop-on-demand devices? All these processes involve moving or expanding bubbles displacing fluid in a confined space, bounded by either rigid or elastic walls. In this talk, we show how spatial confinement may either induce or suppress interfacial instabilities and pattern formation in such flows. We demonstrate that a simple change in the bounding geometry can radically alter the behaviour of a fluid-displacing air finger both in rigid and elastic vessels. A rich array of propagation modes, including steady and oscillatory fingers, is uncovered when air displaces oil from axially uniform tubes that have local variations in flow resistance within their cross-sections. Moreover, we show that the experimentally observed states can all be captured by a two-dimensional depth-averaged model for bubble propagation through wide channels. Viscous fingering in Hele-Shaw cells is a classical and widely studied fluid-mechanical instability: when air is injected into the narrow, liquid-filled gap between parallel rigid plates, the axisymmetrically expanding air-liquid interface tends to be unstable to non-axisymmetric disturbances. We show how the introduction of wall elasticity (via the replacement of the upper bounding plate by an elastic membrane) can weaken or even suppress the fingering instability by allowing changes in cell confinement through the flow-induced deflection of the boundary. The presence of a deformable boundary also makes the system prone to additional solid-mechanical instabilities, and these wrinkling instabilities can in turn enhance viscous fingering.

1The financial support of EPSRC and the Leverhulme Trust is gratefully acknowledged.

Tuesday, March 15, 2016 11:15AM - 2:15PM –
Session F12 GPC DFD GSNP: Climate Science Frontier: Cloud and Precipitation Physics

11:15AM F12.00001 Precipitation and atmospheric moisture transport responses to increased infrared opacity, ELISABETH MOYER, University of Chicago — No abstract available.

11:51AM F12.00002 Prototypes for the dynamics underlying precipitation and temperature extremes, J DAVID NEELIN, UCLA — Projecting changes in precipitation and temperature extreme events can be aided by a deeper understanding of the dynamics underlying such variations. For precipitation, this is closely connected to the interaction of fast, small-scale motions with variability of large-scale climate. Simple prototype models from the physics and applied math literature can point to analysis methods, connections among related quantities, and hypotheses for the dynamics, especially when the prototype models can be derived from climate-model equations. An overview will be provided including recent work with a number of collaborators. For distributions of precipitation-related variables, prototypes including Fokker-Planck solutions and first-passage problems for variations across an onset threshold yield insights into the form of present-day observed distributions and predictions for the form of the global warming change to evaluate in climate models. In distributions of water vapor and temperature, the widespread occurrence of non-Gaussian tails is likely explained in part by prototypes for tracer advection across a maintained gradient. The shape of these tails can have substantial implications for regional changes in probabilities of precipitation and temperature extremes with large-scale warming.

1Supported in part by the National Science Foundation.

12:27PM F12.00003 The physics of atmospheric instability, lightning, and global warming, DAVID ROMPS, University of California, Berkeley — No abstract available.

1:03PM F12.00004 Thermodynamic analysis of atmospheric convection, OLIVIER PAULUIS, Courant Institute of Mathematical Sciences — No abstract available.

1:39PM F12.00005 Aerosols, Clouds, and Precipitation as Scale Interactions in the Climate System and Controls on Climate Change, LEO DONNER, Geophysical Fluid Dynamics Laboratory/NOAA — Clouds are major regulators of atmospheric energy flows. Their character depends on atmospheric composition, dynamics, and thermodynamic state. Clouds can assume organized structures whose scales are planetary, while processes important for determining basic properties occur on the scale of microns. The range of processes, scales, and interactions among them has precluded the development of concise theories for the role of clouds in climate, and limitations in modeling clouds in complex climate models remain among the key uncertainties in understanding and projecting climate change. The distribution function of vertical velocities (updraft speeds) in clouds is an important control on climate forcing by clouds and possibly a strong correlate with climate sensitivity. (Climate forcing refers to the change in Earth’s energy balance as atmospheric composition changes, in particular, due to human activity. Climate sensitivity is defined here as the equilibrium change in globally averaged annual surface temperature as a result of doubled carbon dioxide.) Vertical velocities are central because they determine the thermodynamic environment governing phase changes of water, with both equilibrium and non-equilibrium phenomena important. The spatial and temporal spectra of relevant vertical velocities includes scales both numerically resolved by climate models and below their resolution limit. The latter implies a requirement to parameterize these smaller scale motions in models. The scale dependence of vertical velocities emerging observational constraints on their distribution provide new opportunities for representing aerosols, clouds, and precipitation in climate models. Success in doing so could provide important breakthroughs in understanding both climate forcing and sensitivity.

Tuesday, March 15, 2016 11:15AM - 2:15PM –
Session F35 DBIO GSNP: Population and Evolutionary Dynamics II

11:15AM F35.00001 The effect of extrinsic noise on the dynamics of simple gene network motifs, MICHAEL ASSAF, Hebrew University of Jerusalem — Cellular processes do not follow deterministic rules; even in identical environments genetically identical cells can make random choices leading to different phenotypes. This randomness originates from fluctuations present in the biomolecular interaction networks. Most previous work has been focused on the intrinsic noise of these networks. Yet, especially for high-copy-number biomolecules, extrinsic or environmental noise has been experimentally shown to dominate the variation. Here we develop an analytical formalism that allows for calculation of the combined effect of intrinsic and extrinsic noise on gene expression motifs. We introduce a new and generic method for modeling bounded extrinsic noise as an auxiliary species in the master equation. We focus our study on motifs that can be viewed as the building blocks of genetic switches: a non-regulated gene, a self-inhibiting gene, and a self-promoting gene. The role of the extrinsic noise properties (magnitude, correlation time, and distribution) on the statistics of interest are systematically investigated, and the effect of fluctuations in different reaction rates is compared. Due to its analytical nature, our formalism can be used to quantify the effect of extrinsic noise on the dynamics of biochemical networks and can also be used to improve the interpretation of data from single-cell gene expression experiments.
11:51AM F35.00002 Backward evolution from gene network dynamics, MERZU BELETE, University of Houston and Laufer Center for Physical and Quantitative Biology, Stony Brook University, Stony Brook, New York, United States of America, DANIEL CHARLEBOIS, GABOR BALAZSI, Laufer Center for Physical and Quantitative Biology, Stony Brook University, Stony Brook, New York, United States of America — Gene expression is often controlled by regulator genes that form gene regulatory network cascades. How mutation in the genes comprising regulatory cascades influences cell populations dynamics has not been adequately investigated. In this study, we developed a model to study how a mutation in a regulator gene that reaches the effector gene with a time delay affects short-term and long-term population growth. We find a paradoxical outcome of evolution, where a mutation in a regulator gene leads to an interaction between gene regulatory network dynamics and population dynamics, causing in certain cases a permanent decrease in population fitness.

12:03PM F35.00003 Collective evolution of cyanobacteria and cyanophages mediated by horizontal gene transfer, HONG-YAN SHIH, Department of Physics and Weose Institute for Genomic Biology, University of Illinois at Urbana-Champaign, TIM ROGERS, Department of Mathematical Sciences, University of Bath, NIGEL GOLDFELD, Department of Physics and Weose Institute for Genomic Biology, University of Illinois at Urbana-Champaign — We describe a model for how antagonistic predator-prey coevolution can lead to mutualistic adaptation to an environment, as a result of horizontal gene transfer. Our model is a simple description of ecosystems such as marine cyanobacteria and their predator cyanophages, which carry photosynthesis genes. These genes evolve more rapidly in the virosphere than the bacterial pan-genome, and thus the bacterial canopy competitor. By exploiting the competition between the two species, we study this balance between individual sacrifice and collective benefits. The outcome is an emergent mutualistic coevolution of improved photosynthesis capability, benefiting both bacteria and phage. This form of multi-level selection can contribute to niche stratification in the cyanobacteria-phage ecosystem. This work is supported in part by a cooperative agreement with NASA, grant NNA13AA91A/A0018.

12:15PM F35.00004 Environmental quality modulates the cooperative and competitive nature of a microbial cross-feeding mutualism, TIM HOEK, CsD Master Program, University Utrecht, Utrecht, The Netherlands, KEVIN AXELROD, Biophysics PhD Program, Harvard University, Cambridge, MA, EUGENE YURTSEV, JEFF GORE, Physics of Living Systems, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA — Mutualisms are essential for ecosystem function and stability. However, in some environments the competitive aspects of an interaction may dominate the mutualistic aspects. Although these transitions could have far-reaching implications, it has been difficult to study the causes and consequences of this mutualistic-competitive transition in experimentally tractable systems. Here we experimentally study a microbial cross-feeding mutualism in which each yeast strain supplies an essential amino acid for its partner strain. We find that, depending upon the amino acid concentration, this pair of strains can exhibit any of: obligatory mutualism, facultative mutualism, competition, parasitism, competitive exclusion, or failed mutualism leading to extinction of one of the populations. A simple model capturing the essential features of this interaction predicts that environmental quality specifies the outcome and provides a “phase diagram” of net interactions in this mutualism. In addition, the model accurately predicts that changes in the dynamics of the mutualism in deteriorating environments can predict that population collapse is imminent. Our results provide a general framework for how mutualisms may transition between qualitatively different regimes of interaction.

12:27PM F35.00005 Predicting evolutionary dynamics, GABOR BALAZSI, Laufer Center for Physical and Quantitative Biology, Stony Brook University — We developed an ordinary differential equation-based model to predict the evolutionary dynamics of yeast cells carrying a synthetic gene circuit. The predicted aspects included the speed at which the ancestral genotype disappears from the population, as well as the types of mutant alleles that establish in each environmental condition. We validated these predictions by experimental evolution. The agreement between our predictions and experimental findings suggests that cellular and population fitness landscapes can be useful to predict short-term evolutionary dynamics.

12:39PM F35.00006 Complex dynamics of selection and cellular memory in adaptation to a changing environment, EDO KUSSELL, WEI-HSIANG LIN, New York University — We study a synthetic evolutionary system in bacteria in which an antibiotic resistance gene is controlled by a stochastic on/off switching promoter. At the population level, this system displays all the basic ingredients for evolutionary selection, including diversity, fitness differences, and heritability. At the single cell level, physiological processes can modulate the ability of selection to act. We expose the stochastic switching strains to pulses of antibiotics of different durations in periodically changing environments using microfluidics. Small populations are tracked over a large number of periods at single cell resolution, allowing the visualization and quantification of selective sweeps and counter-sweeps at the population level, as well as detailed single cell analysis. A simple model is introduced to predict long-term population growth rates from single cell measurements, and reveals unexpected aspects of population dynamics, including cellular memory that acts on a fast timescale to modulate growth rates.

This work is supported by NIH grant no. R01-GM097356.

12:51PM F35.00007 Exploiting temporal gradients of antibiotic concentration against the emergence of resistance, MARIANNE BAUER, Ludwig-Maximilians-Universität Munich, VUDTIWAT NGAMPRUETIKORN, Okinawa Institute of Science and Technology, ERWIN FREY, Ludwig-Maximilians-Universität Munich, GREG STEPHENS, Vrije Universiteit Amsterdam and Okinawa Institute of Science and Technology — A very simple model for antibiotic resistance - involving one normal and one more resistant species interacting indirectly through a carrying capacity - shows that the temporal variation of the antibiotic can affect the effect of the antibiotic. For a single antibiotic pulse, we find that for different minimal inhibitory concentrations of the two species an optimal pulse shape may exist, which increases the likelihood of bacterial extinction. For a long series of pulses, efficiency does not vary monotonically with the length of the gap between two individual pulses, but instead, the gap length can be optimised by exploiting the competition between the two species. Finally, a series of pulses is not always more efficient than a single pulse. Shorter pulses may be more efficient in an initial time window without risking population level resistance. We elucidate this behaviour with a phase diagram, and discuss the meaning of this work for current experiments.

1:03PM F35.00008 Emergence of elevated levels of multiple infections in spatial host-virus dynamics, BRADFORD TAYLOR, Georgia Inst of Tech, CATHERINE PENINGTON, Queensland Univ of Tech, JOSHUA WEITZ, Georgia Inst of Tech — Bacteria are subject to infection and potentially to multiple simultaneous infections by viruses. Multiply infected hosts have altered life-history traits (e.g., viral burst size) and evolutionary rates (e.g., viral recombination). Yet our understanding of multiple infections of microbes is limited to lab settings where the ratio of inoculant viruses to hosts is controlled. In contrast, rates of multiple infection in natural environments are unknown. Here, we develop an individual based model to quantify rates of multiple infections by a single viral type. We explore different dispersal regimes by varying the viral adsorption rate. High dispersal regimes lead to spatial dynamics and rates of multiple infection equivalent to predictions from mean field models. Local clustering of bacterial hosts occurs for low dispersal. Comparing to mean field, the clustering leads to increased rates of multiple infection and faster tails in the distribution of the number of internal viruses. The emergence of individual colocalization of viruses with infected hosts leads to these deviations. We show these deviations result from the wave-like spread of viruses when invading clusters of bacteria. Our work represents a key step in understanding the population-level effects of multiple infections.
MICHAEL BRENNER, Harvard University, SAHAND HORMOZ, California Institute of Technology, ALAIN PUMIR, ENS Lyon — We describe a potential mechanism for a singular solution of the Euler equation. The mechanism involves the interaction of vortex filaments, but occurs sufficiently quickly and at small enough scales that it could have plausibly evaded experimental and computational detection. Scaling estimates for the characteristics of this solution will be presented, as well as numerical simulations of the initial stages. This implies a new step toward an effective vaccine against rapidly mutating complex pathogens.

BUTLER, Massachusetts Inst of Tech-MIT, BRUCE WALKER, Ragon Institute of MGH, MIT & Harvard, ANDREW MCMICHAEL, University of Oxford, ARUP CHAKRABORTY, Massachusetts Institute of Technology — Pathogens are complex and evolving fast. They have developed full ranges of disguises to divert immune responses and often manage to escape recognition and thereby outcome natural immunity. A prominent example is the scarce and staggered development of broadly neutralizing antibodies against highly mutable viruses. It remains unclear under what evolutionary conditions these exceptional antibodies could emerge and dominate the response. To address this challenge, we construct an individual-based stochastic model of the Darwinian evolution of antibody-producing immune cells. We consider complexity of viral epitopes, varying diversity of the immune cell population, and allow a time varying population size and extinction — new aspects essential for designing a realistic vaccine. We show that various temporal statistics of antigenic environments would select distinct evolutionary paths that lead to predominantly non-neutralizing, strain-specific or broadly neutralizing antibody responses. We suggest strategies to focus antibody responses on the targeted vulnerability of the virus and confer selective advantage to cross-reactive lineages.

1:27PM F35.00010 Modeling the interactions between pathogenic bacteria, bacteriophage and immune response, CHUNG YIN (JOEY) LEUNG, JOSHUA S. WEITZ, School of Biology and School of Physics, Georgia Institute of Technology — The prevalence of antibiotic-resistant strains of pathogenic bacteria has led to renewed interest in the use of bacteriophage (phage), or virus that infects bacteria, as a therapeutic agent against antibiotic infections [1]. However, little is known about the theoretical mechanism by which phage therapy may work. In particular, interactions between the bacteria, the phage and the host immune response crucially influence the outcome of the therapy. Few models of phage therapy have incorporated all these three components, and existing models [2] suffer from unrealistic assumptions such as unbounded growth of the immune response. We propose a model of phage therapy with an emphasis on nonlinear feedback arising from interactions with bacteria and the immune response. Our model shows a synergistic effect between the phage and the immune response which underlies a possible mechanism for phage to catalyze the elimination of bacteria even when neither the immune response nor phage could do so alone. We study the significance of this effect for different parameters of infection and immune response, and discuss its implications for phage therapy. References: [1] C. Potera, Environ. Health Perspect. 121, A48 (2013). [2] B. R. Levin and J. J. Bull, Nature Rev. Microbiol. 2, 166 (2004).

1:39PM F35.00011 Modeling HIV Cure, ALAN PERELSON, Los Alamos National Laboratory. JESSICA CONWAY, Pennsylvania State University, YOUFANG CAO, Los Alamos National Laboratory — A large effort is being made to find a means to cure HIV infection. I will present a dynamical model of post-treatment control (PTC) or functional cure of HIV infection. Some patients treated with suppressive antiviral therapy have been taken off of therapy and then spontaneously control HIV infection such that the amount of virus in the circulation is maintained undetectable by clinical assays for years. The model explains PTC occurring in some patients by having a partner regime in which the model exhibits bistability, with both a low and high steady state viral load being stable. The model makes a number of predictions about how to attain the low PTC steady state. Bistability in this model depends upon the immune response becoming exhausted when over stimulated. I will also present a generalization of the model in which immunotherapy can be used to reverse immune exhaustion and compare model predictions with experiments in SIV infected macaques given immunotherapy and then taken off of antiretroviral therapy. Lastly, if time permits, I will discuss one of the hurdles to true HIV eradication, latently infected cells, and present clinical trial data and a new model addressing pharmacological means of flushing out the latent reservoir.

1:51PM F35.00012 The kinetics and location of intra-host HIV evolution to evade cellular immunity are predictable, JOHN BARTON, Massachusetts Inst of Tech-MIT, NILU GOONETILLEKE, University of North Carolina, THOMAS BUTLER, Massachusetts Inst of Tech-MIT, BRUCE WALKER, Ragon Institute of MGH, MIT & Harvard, ANDREW MCMICHAEL, University of Oxford, ARUP CHAKRABORTY, Massachusetts Inst of Tech-MIT — Human immunodeficiency virus (HIV) evolves within infected persons to escape targeting and clearance by the host immune system, thereby preventing effective immune control of infection. Knowledge of the timing and pathways of escape that result in loss of control of the virus could aid in the design of effective strategies to overcome the challenge of viral diversification and immune escape. We combined methods from statistical physics and evolutionary dynamics to predict the course of in vivo viral sequence evolution in response to T cell-mediated immune pressure in a cohort of 17 persons with acute HIV infection. Our predictions agree well with both the location of documented escape mutations and the clinically observed time to escape. We also find that the mutational pathways to escape depend on the viral sequence background due to epistatic interactions. The ability to predict escape pathways, and the duration over which control is maintained by specific immune responses prior to escape, could be exploited for the rational design of immunotherapeutic strategies that may enable long-term control of HIV infection.

2:03PM F35.00013 Outbreak and Extinction Dynamics in a Stochastic Ebola Model, GARRETT NIEDDU, Montclair State University, SIMONE BIANCO, IBM Almaden Research Center, LORA BILLINGS, Montclair State University and National Science Foundation, ERIC FORGOSTON, Montclair State University, JAMES KAUFMAN, IBM Almaden Research Center — A zoonotic disease is a disease that can be passed between animals and humans. In many cases zoonotic diseases can persist in the animal population even if there are no infections in the human population. In this case we call the infected animal population the reservoir for the disease. Ebola virus disease (EVD) and SARS are both notable examples of such diseases. There is little work devoted to understanding stochastic disease extinction and reintroduction in the presence of a reservoir. Here we build a stochastic model for EVD and explicitly consider the presence of an animal reservoir. Using a master equation approach and a WKB ansatz, we determine the associated Hamiltonian of the system. Hamilton’s equations are then used to numerically compute the 12-dimensional optimal path to extinction, which is then used to estimate mean extinction times. We also numerically investigate the behavior of the model for dynamic population size. Our results provide an improved understanding of outbreak and extinction dynamics in diseases like EVD.

Tuesday, March 15, 2016 11:15AM - 2:03PM – Session F40 GS NP DCMP: Leo Kadanoff Session II / GS NP Student Awards 343 - Susan Coppersmith, Bulbul Chakraborty, University of Wisconsin, Brandeis University

11:15AM F40.00001 Fractions, trees and unfinished business, BORIS SHRAIMAN, KITP, UC Santa Barbara — In this talk, mourning the loss of a teacher and a dear friend, I would like to share some unfinished thoughts loosely connecting – via Farey fraction trees – statistical physics and evolutionary dynamics to predict the course of viral sequence evolution in response to T cell-mediated immune pressure in a cohort of 17 persons with acute HIV infection.

11:27AM F40.00002 A potential mechanism for a singular solution of the Euler Equations, MICHAEL BRENNER, Harvard University, SAHAND HORMOZ, California Institute of Technology, ALAIN PUMIR, ENS Lyon — We describe a potential mechanism for a singular solution of the Euler equation. The mechanism involves the interaction of vortex filaments, but occurs sufficiently quickly and at small enough scales that it could have plausibly evaded experimental and computational detection. Scaling estimates for the characteristics of this solution will be presented, as well as numerical simulations of the initial stages.
11:39AM F40.00003 Nonlinear dynamics of a strongly driven single spin solid state qubit. S. N. COPPERSMITH, University of Wisconsin-Madison, Madison, WI 53706, USA, THIBAUT JULLIEN, P. SCARLINO, E. KAWAKAMI, QuTech and Kavli Institute of Nanoscience, TU Delft, Lorentzweg 1, 2628 CJ Delft, The Netherlands — This talk will discuss how dynamical systems theory can yield new insight into some exotic behavior found in experiments on strongly driven quantum spins in silicon/silicon-germanium heterostructures. Spin resonance experiments were performed by using ac voltages to drive an electron wavefunction in a strong magnetic field gradient. Nontrivial dependence of the resonance frequency on applied power, including the observation of multiple resonant frequencies at one power, are shown to be consistent with frequency-dependent attenuation in the high-frequency lines. The method of analysis is very similar to that presented in the course on nonlinear dynamics that Leo Kadanoff developed at the University of Chicago in the early 1990’s.

1This work was supported in part by ARO (W911NF-12-0607). Development and maintenance of the growth facilities used for fabricating samples is supported by DOE (DE-FG02-03ER46028). This research utilized NSF-supported shared facilities at UW-Madison.

11:51AM F40.00004 Learning in a noisy environment: a Lyapunov equation approach. SARA A SOLLA, Northwestern University, YARDEN COHEN, Weizmann Institute of Science, PREDRAG CVITANOVIC, Georgia Institute of Technology — Consider a behavioral task described as a finite state time through a d-dimensional space, segmented in K time steps, and thus fully specified by a vector \( X \) in the \( n = d \times K \) dimensional state space of possible trajectories. Consider the dynamics of learning a desired target trajectory \( X^* \). In the vicinity of \( X^* \), the learning dynamics at the t-th discrete learning time step can be linearized to \( Y_{t+1} = MY_t + \xi_t \), where, \( Y_t = X_t - X^* \) and \( \xi \) is an independent Gaussian noise of zero mean and covariance \( \Delta \). The balance between contracting dynamics and noise leads to an asymptotic covariance \( Q \) that obeys the Lyapunov equation \( Q = MQM^* + \Delta \). Given \( Q \), how can the unknown deterministic component \( M \) be estimated? How can we use the use of systematic target perturbations \( X^* \rightarrow X^* + \epsilon V_j \), with unit vectors \( V_j \), \( 1 \leq j \leq n \) that span the space \( X \). We argue, convincingly if not rigorously, that the linear response to these perturbations fully characterizes the asymptotic dynamics of the learning process. We illustrate the method by analyzing networks of neurons with either intrinsic or extrinsic noise, at time resolutions that span from spike timing to spiking rates.

12:03PM F40.00005 ABSTRACT WITHDRAWN –

12:15PM F40.00006 Nonlinear dynamics, Waddington landscape and stem cells. CHAO TANG, Peking University — There are hundreds of different cell types (skin, neuron, muscle, etc.) in human body, all derived from the stem cell and all have the same genetic information. About 60 years ago, Waddington speculated that the different cell types correspond to different minima in a landscape emerged from genetic interactions. Recently, biologists succeeded in transforming one cell type to another by perturbing the genetic interactions in a cell. I will discuss the experiments and a mathematical model of a set of such cell type transformations in mice, in which we can see an actual example of the Waddington landscape and ways to it to facilitate cell type transformation – in particular, to reprogram a differentiated cell back into a stem cell.

12:27PM F40.00007 From Glaciers to Icebergs. WENDY ZHANG, University of Chicago — I will describe works from a collaboration between physics and glaciology that grew out of interactions at the Computations in Science seminar Leo Kadanoff organized at the University of Chicago. The first project considers the interaction between ocean waves and Antarctic ice shelves, large floating portions of ice formed by glacial outflows. Back-of-envelope calculation and seismic sensor data suggest that crevasses may be distributed within an ice shelf to shield it from wave energy. We also examine numerical scenarios in which changes in environmental forcing causes the ice shelf to fail catastrophically. The second project investigates the aftermath of iceberg calving off glacier terminus in Greenland using data recorded via time-lapse camera and terrestrial radar. Our observations indicate that the melting of icebergs within the fjord experiences widespread jamming during a calving event and therefore is always close to being in a jammed state during periods of terminus quiescence. Joint work with Jason Amundson, Ivo R. Peters, Julian Freed Brown, Nicholas Guttenberg, Justin C Burton, L. Mac Cathles, Ryan Cassotto, Mark Fahnestock, Kristopher Darnell, Martin Truffer, Dorian S. Abbot and Douglas MacAyeal.

1Kadanoff Session DCMP

12:39PM F40.00008 Multifractals, random walks and Arctic sea ice. SAHIL AGARWAL, Yale University, JOHN WETTLAUFER, Yale University and Nordic Institute of Theoretical Physics (NORDITA) — We examine the long-term correlations and multifractal properties of daily satellite retrievals of Arctic sea ice albedo, extent, and ice velocity for decadal periods. The approach harnesses a recent development called Multifractal Temporally Weighted Detrended Fluctuation Analysis (MF-TWDFA), which exploits the intuition that points closer in time are more likely to exhibit related than distant points. In both data sets we extract multiple crossover times, as characterized by generalized Hurst exponents, ranging from synoptic to decadal. The method goes beyond treatments that assume a single decay scale process, such as a first-order autoregression, which cannot be justifiably fit to these observations. The ice extent data exhibits white noise behavior from seasonal to bi-seasonal time scales, whereas the clear fingerprints of the short (weather) and long (~7 and 9 year) time scales remain, the latter associated with the recent decay in the ice cover. Thus, long term persistence is reemergent beyond the seasonal scale and it is not possible to distinguish whether a given ice extent minimum/maximum will be followed by a minimum/maximum that is larger or smaller in magnitude. The ice velocity data show long term persistence in auto covariance.

1NASA Grant NNN13ZDA001N-CRYO and Swedish Research Council Grant No. 638-2013-9243

12:51PM F40.00009 Phase transition to turbulence in a pipe. NIGEL GOLDENFELD, University of Illinois at Urbana-Champaign — Leo Kadanoff taught us much about phase transitions, turbulence and collective behavior. Here I explore the transition to turbulence in a pipe, showing how a collective mode suppresses the universality class. Near the transition, turbulent breakfasts either directly or through splitting, with characteristic time-scales that exhibit a super-exponential dependence on Reynolds number. Direct numerical simulations reveal that a collective mode, a so-called zonal flow emerges at large scales, activated by anisotropic turbulent fluctuations, as represented by Reynolds stress. This zonal flow imposes a shear on the turbulent fluctuations that tends to suppress their anisotropy, leading to a Landau theory of predator-prey type, in the directed percolation universality class. Stochastic simulations of this model reproduce the functional form and phenomenology of pipe flow experiments. Talk based on work performed with Hong-Yan Shih and Tsung-Lin Hsieh.

1This work was partially supported by the National Science Foundation through grant NSF-DMR-1044901.

2Kadanoff Session

1:03PM F40.00010 Material Flows in an Active Nematic Liquid Crystal. STEPHEN DECAMP, Brandeis University —

MQM = \frac{Q}{\sqrt{1 - \frac{Q}{\sqrt{1 - Q^2}}}} = \frac{Q}{\sqrt{1 - Q^2}}

MQM = \frac{Q}{\sqrt{1 - Q^2}}
1:15PM F40.00011 Lie Algebraic Analysis of Thin Film Marangoni Flows: Multiplicity of Self-Similar Solutions, ZACHARY NICOLAOU, Nicolaou —

1:27PM F40.00012 Order-to-chaos transition in the hardness of random Boolean satisfiability problems, MELINDA VARGA, University of Notre Dame —.

1:39PM F40.00013 Hamiltonian-Based Model to Describe the Nonlinear Physics of Cascading Failures in Power-Grid Networks, YANG YANG, Northwestern University —

1:51PM F40.00014 Cell fate reprogramming by control of intracellular network dynamics, JORGE G.T. ZANUDO, Pennsylvania State University —

Tuesday, March 15, 2016 11:15AM - 2:15PM —

Session F41 DBIO GSNP GSOFT: Maximum Entropy Models: A Promising Link Between Statistical Physics, Inference, and Biology 344 - Gasper Tkacik, IST Austria

11:15AM F40.00001 Learning probabilities from random observables in high dimensions: the maximum entropy distribution and others, TOMOYUKI OBUCHI, Tokyo Institute of Technology, SIMONA COCCO, Laboratoire de Physique Statistique de l'Ecole Normale Superieure, REMI MONASSON, Laboratoire de Physique Theorique de l'Ecole Normale Superieure — We consider the problem of learning a target probability distribution over a set of N binary variables from the knowledge of the expectation values (with this target distribution) of M observables, drawn uniformly at random. The space of all probability distributions compatible with these M expectation values within some fixed accuracy, called version space, is studied. We introduce a biased measure over the version space, which gives a boost with the entropy of the distributions and with an arbitrary ‘temperature’. The choice of the temperature allows us to interpolate between the flat measure over all the distributions and the pointwise measure concentrated at the maximum entropy distribution. Using the replica method we compute the volume of the version space and other quantities of interest, such as the distance R between the target distribution and the center-of-mass distribution over the version space. Some phase transitions are found, corresponding to qualitative improvements in the learning of the target distribution and to the decrease of the distance R. However, the distance R does not vary with the temperature, meaning that the maximum entropy distribution is not closer to the target distribution than any others.

11:27AM F40.00002 Semiparametric energy-based models of systems exhibiting criticality, JAN HUMPLIK, GASPER TKACIK, Institute of Science and Technology Austria — Over the last decade, several empirical studies have found evidence that many biological and natural systems exhibit critical fluctuations analogous to those observed during second-order phase transitions in equilibrium systems. In many cases, these fluctuations were shown to be equivalent to a thermodynamic version of Zipf’s law–if the system is sufficiently large, then a log-log plot of the probability of a state vs. its rank yields a straight line with slope −1. Because the origin of critical fluctuations cannot be traced to a unique mechanism, it is important that data-driven phenomenological models of natural systems are flexible enough so as to easily capture any kind of criticality. Here we study a class of models with exactly this property. This class consists of energy-based models in which the exponential Boltzmann factor is replaced by an arbitrary nonlinear function. We demonstrate the usefulness of our method by modeling the spiking activity of a population of retinal neurons, and the distribution of light intensities in small patches of natural images. In light of recent work on models with hidden variables, the proposed method can separate interactions induced by an unknown fluctuating environment from interactions intrinsic to the system.

11:39AM F40.00003 From Maximum Entropy Models to Non-Stationarity and Irreversibility, RODRIGO COFRE, Department of Theoretical Physics, University of Geneva, BRUNO CEISSAC, Inria, Neuramathcomp team, CESAR MALDONADO, Centro de Modelamiento Matematico, Universidad de Chile —

The maximum entropy distribution can be obtained from a variational principle. This is important as a matter of principle and for the purpose of finding approximate solutions. One can exploit this fact to obtain relevant information about the underlying stochastic process. We report here in recent progress in three aspects to this approach.
1- Biological systems are expected to show some degree of irreversibility in time. Based on the transfer matrix technique to find the spatio-temporal maximum entropy distribution, we build a framework to quantify the degree of irreversibility of any maximum entropy distribution.
2- The maximum entropy solution is characterized by a functional called Gibbs free energy (solution of the variational principle). The Legendre transformation of this functional is the rate function, which controls the speed of convergence of empirical averages to their ergodic mean. We show how the correct description of this functional is determinant for a more rigorous characterization of first and higher order phase transitions.
3- We assess the impact of a weak time-dependent external stimulus on the collective statistics of spiking neuronal networks. We show how to evaluate this impact on any higher order spatio-temporal correlation.

RC supported by ERC advanced grant "Bridges", BC: KEOPS ANR-CONICYT, Renvision and CM: CONICYT-FONDECYT No. 3140572

11:51AM F40.00004 Learning Maximal Entropy Models from finite size datasets: a fast Data-Driven algorithm allows to sample from the posterior distribution, ULISSE FERRARI, Institut de la Vision, Sorbonne Universités, UPMC, INSERM U968, CNRS, UMR709, Paris, F-75012, France. — A maximal entropy model provides the least constrained probability distribution that reproduces experimental averages of an observable set. In this work we characterize the learning dynamics that maximizes the log-likelihood in the case of large but finite datasets. We first show how the steepest descent dynamics is not optimal as it is slowed down by the inhomogeneous curvature of the model parameters space. We then provide a way for rectifying this space which relies only on dataset properties and does not require large computational efforts. We conclude by solving the long-time limit of the parameters dynamics including the randomness generated by the systematic use of Gibbs sampling. In this stochastic framework, rather than converging to a fixed point, the dynamics reaches a stationary distribution, which for the rectified dynamics reproduces the posterior distribution of the parameters. We sum up all these insights in a “rectified” Data-Driven algorithm that is fast and by sampling from the parameters posterior avoids both under- and over-fitting along all the directions of the parameters space. Through the learning of pairwise Ising models from the recording of a large population of retina neurons, we show how our algorithm outperforms the steepest descent method.

This research was supported by a grant from the Human Brain Project (HBP CLAP)
12:03PM F41.00005 UniEnt: uniform entropy model for the dynamics of a neuronal population1, DAMIAN HERNANDEZ LAHME, Department of Physics, Emory University, ILYA NEMENMAN, Department of Physics and Department of Biology, Emory University — Sensory information and motor responses are encoded in the brain in a collective spiking activity of a large number of neurons. Understanding the neural code requires inferring statistical properties of such collective dynamics from multicellular neurophysiological recordings. Questions of whether synchronous activity or silence of multiple neurons carries information about the stimuli or the motor responses are especially interesting. Unfortunately, detection of such high order statistical interactions from data is especially challenging due to the exponentially large dimensionality of the state space of neural activity. Here we present UniEnt, a method for the inference of strengths of multivariate neural interaction patterns. The method is based on the Bayesian prior that makes no assumptions (uniform a priori expectations) about the value of the entropy of the observed multivariate neural activity, in contrast to popular approaches that maximize this entropy. We then study previously published multi-electrode recordings data from salamander retina, exposing the relevance of higher order neural interaction patterns for information encoding in this system.

1This work was supported in part by grants JSMF/220020321 and NSF/IOS/1208126.

12:15PM F41.00006 Modeling the Mass Action Dynamics of Metabolism with Fluctuation Theorems and Maximum Entropy. , WILLIAM CANNON, DENNIS THOMAS, DOUGLAS BAXTER, JEREMY ZUCKER, GARRETT GOH, Pacific Northwest National Laboratory — The laws of thermodynamics dictate the behavior of biotic and abiotic systems. Simulation methods based on statistical thermodynamics can provide a fundamental understanding of how biological systems function and are coupled to their environment. While mass action kinetic simulations are based on solving ordinary differential equations using rate parameters, analogous thermodynamic simulations of mass action dynamics are based on models that are defined through the chemical potential. The latter have the advantage that standard free energies of formation/reaction and metabolite levels are much easier to determine than rate parameters, allowing one to model across a large range of scales. Bridging theory and experiment, statistical thermodynamics simulations allow us to both predict activities of metabolites and enzymes and use experimental measurements of metabolites and proteins as input data. Even if metabolite levels are not available experimentally, it is shown that a maximum entropy assumption is quite reasonable and in many cases results in both the most energetically efficient process and the highest material flux.

12:27PM F41.00007 On the sufficiency of pairwise interactions in maximum entropy models of networks1, ILYA NEMENMAN, Emory University, LINA MERCHANT, Savannah State University — Biological information processing networks consist of many components, which are coupled by an even larger number of complex multivariate interactions. However, analyses of data sets from fields as diverse as neuroscience, molecular biology, and physics have reported that observed statistics of states of some biological networks can be approximated well by maximum entropy models with only pairwise interactions among the components. Based on simulations of random Ising spin networks with p-spin (p ≤ 2) interactions, here we argue that this reduction in complexity can be thought of as a natural property of some densely interacting networks in certain regimes, and not necessarily as a special property of living systems.

1This work was supported in part by James S. McDonell Foundation grant No. 220020321.

12:39PM F41.00008 Insights in connecting phenotypes in bacteria to coevolutionary information.1, , RYAN CHENG, Rice University, FARUCK MORCOS, University of Texas at Dallas, RYAN HAYES, University of Michigan, RODNEY HELM, University of Houston, HERBERT LEVINE, JOSÉ ONUCHIC, Rice University — It has long been known that protein sequences are far from random. These sequences have been evolutionarily selected to maintain their structure to fold into stable, three-dimensional folded structures as well as their ability to form macromolecular assemblies, perform catalytic functions, etc. For these reasons, there exist quantifiable mutational patterns in the collection of sequence data for a protein family arising from the need to maintain favorable residue-residue interactions to facilitate folding as well as cellular function. Here, we focus on studying the correlated mutational patterns that give rise to interaction specificity in bacterial two-component signaling (TCS) systems. TCS proteins have evolved to be preferentially bind and transfer a phosphate group to their signaling partner while avoiding phosphotransfer with non-partners. We infer a Potts model Hamiltonian governing the correlated mutational patterns that are observed in the sequence data of TCS partners and apply this model to recently published in vivo mutational data. Our findings further support the notion that statistical models built from sequence data can be used to predict bacterial phenotypes as well as engineer interaction specificity between non-partner TCS proteins.

1This research has been supported by the NSF INSPIRE award (MCB-1241332) and by the CBTP sponsored by the NSF (Grant PHY-1427654).

12:51PM F41.00009 Computational Amide I Spectroscopy for Refinement of Disordered Peptide Ensembles — Maximum Entropy and Related Approaches, MICHAEL REPPERT, Massachusetts Inst of Tech-MIT, ANDREI TOKMAKOFF, University of Chicago — The structural characterization of intrinsically disordered peptides (IDPs) presents a challenging biophysical problem. Extreme heterogeneity and rapid conformational interconversion make traditional methods difficult to interpret. Due to its ultrafast (ps) shutter speed, Amide I vibrational spectroscopy has received considerable interest as a novel technique to probe IDP structure and dynamics. Historically, Amide I spectroscopy has been limited to investigating secondary structural information. More recently, however, the method has been adapted to study structure at the local level through incorporation of isotope labels into the protein backbone at specific amide bonds. Thanks to the acute sensitivity of Amide I frequencies to local electrostatic interactions—particularly hydrogen bonds—spectroscopic data on isotope labeled residues directly reports on local peptide conformation. Quantitative information can be extracted using electrostatic frequency maps which translate molecular dynamics trajectories into Amide I spectra for comparison with experiment. Here we report on the development of a rigorous approach to incorporating Amide I spectroscopic restraints into refined molecular dynamics structural ensembles using maximum entropy and related approaches. By combining force field predictions with experimental spectroscopic data, we construct refined structural ensembles for a family of short, strongly disordered, elastin-like peptides in aqueous solution.

1:39PM F41.00011 Phase transitions in Hidden Markov Models\textsuperscript{1}. JOHN BECHHOEFER, EMMA LATHOUWERS, Simon Fraser Univ — In Hidden Markov Models (HMMs), a Markov process is not directly accessible. In the simplest case, a two-state Markov model emits one of two symbols at each time step. We can think of these symbols as noisy measurements of the underlying state. With some probability, the symbol implies that the system is in one state when it is actually in the other. The ability to judge which state the system is in sets the efficiency of a Maxwell demon that observes state fluctuations in order to extract heat from a coupled reservoir. The state-inference problem is to infer the underlying state from such noisy measurements at each time step. We show that there can be a phase transition in such measurements for measurement error rates below a certain threshold, the inferred state always matches the observation. For higher error rates, there can be continuous or discontinuous transitions to situations where keeping a memory of past observations improves the state estimate. We can partly understand this behavior by mapping the HMM onto a 1d random-field Ising model at zero temperature. We also present more recent work that explores a larger parameter space and more states.

\textsuperscript{1}Research funded by NSERC, Canada

1:51PM F41.00012 Distinguishing cell type using epigenotype\textsuperscript{2}. THOMAS WYLOCK, ADILSON E MOTTER, Dept. Physics and Astronomy, Northwestern University — Recently, researchers have proposed that unique cell types are attractors of their epigenetic dynamics including gene expression and chromatin conformation patterns. Traditionally, cell types have been classified by their function, morphology, cytochemistry, and other macroscopically observable properties. Because these properties are the result of many proteins working together, it should be possible to predict cell types from gene expression or chromatin conformation profiles. In this talk, I present a maximum entropy approach to identify and distinguish cell type attractors on the basis of correlations within these profiles. I will demonstrate the flexibility of this method through its separate application to gene expression and chromatin conformation datasets. I show that our method out-performs other machine-learning techniques and uncorrelated benchmarks. We adapt our method to predict growth rate from gene expression in E. coli and S. cerevisiae and compare our predictions with those from metabolic models. In addition, our method identifies a nearly convex region of state-space associated with each cell type attractor basin. Estimates of the growth rate and attractor basin make it possible to rationally control gene regulatory networks independent of a model.

\textsuperscript{2}This research was supported by NSF-GRFP, NSF-GK12, GAANN, and Northwestern’s NIH-NIGMS Molecular Biophysics Training Grant

Tuesday, March 15, 2016 11:15AM - 1:51PM – Session F43 GSNP GSOFT: Jamming and the Glass Transition II 346 - Paolo Sibani

11:15AM F43.00001 Jamming vs Caging in Three Dimensional Jamming Percolation, YAIR SHOKEF, NIMROD SEGALL, EIAL TEOMY, Tel Aviv University — We study a three-dimensional kinetically-constrained lattice-gas model [1], in which the ability of a particle to move depends on the occupation of neighboring sites in an orientational manner. The kinetic rules are constructed such that chains of permanently-frozen particles reach an infinite length at the critical density of directed percolation. Thus at this critical density the system undergoes a jamming transition, above which there is a finite fraction of jammed particles. We demonstrate that the three-dimensional mesh-like structure of the one-dimensional jammed chains enables the free particles to propagate through the holes in this mesh. This diffusive motion is terminated at a second critical density above which all particles are caged. The largest and second largest clusters of dynamically-connected sites exhibit singularities at both densities. Thus our model, which models constrained activity rates and interactions between pairs of neurons, is well fit to the activity ‘states’ in the hippocampus and cortex of mice performing cognitive tasks while navigating in a virtual reality environment.

11:27AM F43.00002 Relation between structure of blocked clusters and relaxation dynamics in kinetically constrained models, EIAL TEOMY, YAIR SHOKEF, Tel Aviv University — In a liquid all the particles are mobile, while in a glass only some of them are mobile at any given time. Although overall the structure is amorphous in both cases, the difference is that in glasses there are local structures that inhibit the movement of particles inside them. We investigate the size of these structures by considering the minimum number of particles that need to move before a specific particle can move. In kinetically-constrained models this structural property, the mean culling time, is easy to find by iteratively culling mobile particles from a snapshot of the system. We use the Kob-Andersen, Fredrickson-Andersen, and the spiral models, which are either lattice gases in which a particle may hop to a nearby site if its local environment satisfies some constraint, or Ising-like models in which a spin, representing regions of high and low mobility, can flip if its environment satisfies some constraint. We compare these structural properties to the dynamics in these models by measuring the persistence time, which is the average time it takes a particle to move for the first time. We find an algebraic relation between the mean culling time and the persistence time, with a model-dependent exponent.

11:39AM F43.00003 Growing Hyperuniformity of Bidisperse Soft Discs on Approach to Jamming, ANTHONY CHIECO, CARL GOODRICH, ANDREA LIU, DOUGLAS DURIAN, University of Pennsylvania — We study the development of hyperuniformity in simulated systems of bidisperse soft discs as the packing fraction $\phi$ is increased from below to above jamming, using the real-space spectrum of hyperuniformity disorder lengths, $h(L)$. For a set of randomly placed $L \times L$ measuring windows, $h(L)$ specifies the distance from the window boundaries over which fluctuations are important; for liquid-like systems, $h(L)$ scales like $L$; but for strongly hyperuniform systems, $h(L) \approx \lambda_c$ is constant. We use two preparation protocols, one rapidly-quenches a system by immediately minimizing particle overlap and the other allows particles to move under low temperature thermal driving. Above jamming, both systems become strongly hyperuniform as defined by $h(L) \rightarrow R_{mam} / \sqrt{5}$ at large $L$. Below jamming, but near the transition, the behavior of $h(L)$ at small $L$ is just like above jamming. But for larger $L$, $h(L)$ breaks away and grows in a protocol-dependent fashion. In general, thermal systems are more uniform than quenched systems, as signified by smaller hyperuniformity disorder lengths. And the development of hyperuniformity happens simultaneously with the onset of jamming.
11:51 AM F43.00004 Crossover from facilitation to hopping in a colloidal glass-former, SHREYAS GOKHALE, Indian Inst of Science, RAJESH GANAPATHY, K HIMA NAGAMANASA, Jawaharlal Nehru Centre for Advanced Scientific Research, A K SOOD, Indian Inst of Science. Despite extensive research, it remains to be established whether glass formation is a fundamentally thermodynamic or dynamic phenomenon. In particular, it is not yet clear whether structural relaxation is dominated by the correlated motion of localized excitations, as postulated by the dynamical fluctuation (DF) theory, or by the collective hopping of groups of particles, as envisioned by various thermodynamic approaches. Here, by analyzing data from experiments on dense colloidal suspensions, we critically compare the role of facilitation and hopping in governing structural relaxation in glass-forming liquids. In particular, we investigate the spatial organization of localized excitations within clusters of most mobile particles as well as their partitioning into shell-like and core-like regions. Our study reveals the existence of a dynamical crossover from a facilitation dominated regime at low area fractions to one dominated by collective hopping close to the glass transition. Our findings strongly suggest that glass formation is thermodynamic in origin.

1 Currently at the Center for Soft and Living Matter, UNIST, Republic of Korea

12:03PM F43.00005 Measuring Temperature-like State Variables in History-Dependent Jammed Granular Systems, EPHRAIM BILLIGN, KAREN DANIELS, North Carolina State University. Granular systems are athermal, thus a complete statistical mechanics framework must be based on a set of macroscopic state variables which excludes temperature. One leading theory incorporates a stress-based ensemble, and predicts a Boltzmann-like distribution of the force–moment tensor with respect to the conjugate, temperature-like variable, angoricity. We experimentally test this theory on a static, bispersive, two-dimensional packing of discs. Basal friction is eliminated by floating the discs on a sub-fluidizing upflow of air, and the packings are subjected to either uniaxial compression or simple shear. We simultaneously measure the contact forces acting on each disc using photoelasticity. These measurements are repeated over many configurations of discs by dilating and rearranging the system, and the angoricity is computed as a function of the confining pressure. In particular, we test the predicted linear relationship between angoricity and pressure. Comparison to prior results and numerical simulations also suggests a history-dependent angoricity, an undesirable feature in the proposed state variable.

12:15PM F43.00006 Universal, non-Debye scaling in the density of states for jammed amorphous systems, ERIC CORWIN, Univ of Oregon, ALEXIS PONCET, cole Normale Supérieure. The presence of anomalous modes in amorphous packings close to jamming is well known: the density of states of packings close to jamming goes to a constant at low frequency. But the scaling at higher densities is still unclear. Naïvely, one might expect to find simple Debye scaling. However, recently available theories for systems thought to belong to the same universality class predict a logarithmic scaling which is applicable to the infinite dimensional case. Do these (mean–field) predictions bring some information about finite-dimensional systems? Here we study packings of soft spheres in dimensions 3 through 7 and show that indeed, from jamming, we find a universal non-Debye scaling in the density of states, consistent with the mean-field predictions.

12:27PM F43.00007 Nonconvex optimization and jamming, YOAV KALLUS, Santa Fe Institute. Recent work on the jamming transition of particles with short-range interactions has drawn connections with models based on minimization problems with linear inequality constraints and a concave objective. These properties reduce the continuous optimization problem to a discrete search among the corners of the feasible polytope. I will discuss results from simulations of models with and without quenched disorder, exhibiting critical power laws, scaling collapse, and protocol dependence. These models are also well-suited for study using tools of algebraic topology, which I will discuss briefly.

1 Supported by an Omidyar Fellowship at the Santa Fe Institute

12:39PM F43.00008 Configurational entropy of glass-forming systems from graph isomorphism, YUXING ZHOU, SCOTT MILTER, The Pennsylvania State University. The configurational entropy plays a central role in the thermodynamic scenario of glass transition, such as Adam-Gibbs theory and random first-order transition theory. By definition, the configurational entropy $S_C$ is the difference between the entropy of liquid and the vibrational entropy with structural rearrangement restricted, both of which can be obtained by means of thermodynamic integration. On the other hand, $S_C$ is essentially a measure of the number of basins in the energy landscape, and therefore it can also be estimated by explicitly enumerating the basins. Naïvely, one might expect to predict the glass transition by simply enumerating the basins. But this is inapplicable to the infinite-dimensional case. The Voronoi graph entropy is calculated as $S_{V} \approx -\sum N_i \log(N_i)$, where $N_i$ is the probability of finding the $i$th distinct graph. We find that $S_{V}(n)$ scales linearly with $n$, and $S_C$ can be estimated from the slope.

12:51PM F43.00009 Suppression of the threshold of a granular solid by mechanical fluctuations, AXELLE AMON, Université Rennes 1, ADELINE PONS, THIERRY DARNIGE, PMMH, ESPCI, Université Paris 6 & 7; JÉRÔME CRASSOUS, Université Rennes 1, ERIC CLÉMENT, PMMH, ESPCI, Université Paris 6 & 7. For a granular material, when the ratio between the shear stress and the confining pressure is smaller than the Mohr-Coulomb threshold, the system can be considered as a solid. Nevertheless, a long-term creep is observed in this solid phase in stress imposed experiments. We present recent experimental and theoretical results demonstrating that the superposition of tiny modulations to the imposed stress are sufficient to change the response of the system from a logarithmic creep to a linear one even deep in the jammed phase. We give a theoretical interpretation of this fluidization without invoking an effective temperature due to a mechanical noise. We interpret our observations as a secular effect, i.e. a ratcheting process which is revealed only on very long times. We show that a local fluidity model is sufficient to interpret fully our experimental observations.

1:03PM F43.00010 Fast magnetic resonance imaging of the internal impact response of dense granular suspensions, CHRISTOPH MILLER, Laboratory for Energy Science and Engineering, ETH Zurich, ALEXANDER PENN, Laboratory for Energy Science and Engineering, ETH Zurich and Institute for Biomedical Engineering, University and ETH Zurich, KLAAS P. PRIEÜSSMANN, Institute for Biomedical Engineering, University and ETH Zurich. Dense granular suspensions exhibit a number of intriguing properties such as discontinuous shear-thickening and the formation of dynamic jamming fronts when impacted by a solid. Probing non-intrusively these phenomena experimentally in full three-dimensional systems is, however, highly challenging as suspensions are commonly opaque and thus, not accessible optically. Here we report the development and implementation of a non-magnetic, thus a complete statistical mechanics framework must be based on a set of macroscopic state variables which excludes temperature. One leading theory incorporates a stress-based ensemble, and predicts a Boltzmann-like distribution of the force–moment tensor with respect to the conjugate, temperature-like variable, angoricity. We experimentally test this theory on a static, bispersive, two-dimensional packing of discs. Basal friction is eliminated by floating the discs on a sub-fluidizing upflow of air, and the packings are subjected to either uniaxial compression or simple shear. We simultaneously measure the contact forces acting on each disc using photoelasticity. These measurements are repeated over many configurations of discs by dilating and rearranging the system, and the angoricity is computed as a function of the confining pressure. In particular, we test the predicted linear relationship between angoricity and pressure. Comparison to prior results and numerical simulations also suggests a history-dependent angoricity, an undesirable feature in the proposed state variable.

1:15PM F43.00011 Local fluctuations in the relaxation rate in a glassy system, RAJIB PANDIT, Ohio University, ELIJAH FLENNER, Colorado State University, HORACIO E. CASTILLO, Ohio University. We numerically study the equilibrium dynamics of a glass-forming hard-disk/sphere fluids, and gradually decreases to a value below 2 as the glass transition is approached. We conclude that a description of fluctuations in terms of local relaxation rates is only applicable at long times and for packing fractions close to the glass transition.
1:27PM F43.00012 Finite temperature mechanical instability in disordered lattices, LEYOU ZHANG, XIAOMING MAO, Univ of Michigan – Ann Arbor — Mechanical instability takes different forms in various ordered and disordered systems, and little is known about how thermal fluctuations affect different classes of mechanical instabilities. We develop an analytic theory involving renormalization of rigidity and coherent potential approximation that can be used to understand finite-temperature mechanical instabilities in various disordered systems. We used this theory to study two disordered lattices: randomly diluted triangular lattice and randomly braced square lattice. These two lattices belong to two different universality classes as they approach mechanical instability at \( T = 0 \). We show that thermal fluctuations stabilize both lattices. In particular, the triangular lattice displays a critical regime in which the shear modulus scales as \( G \sim T^{1/2} \), whereas the square lattice shows \( G \sim T^{2/3} \). We discuss generic scaling laws for finite \( T \) mechanical instabilities and relate to experimental systems including jamming and glass transitions.

1:39PM F43.00013 Scaling theory for the jamming transition, CARL GOODRICH, Harvard University, ANDREA LIU, University of Pennsylvania, JAMES SETHNA, Cornell University — We propose a scaling ansatz for the elastic energy of a system near the critical jamming transition in terms of three relevant fields: the compressive strain \( \Delta \phi \) relative to the critical jammed state, the shear strain \( \epsilon \), and the inverse system size \( 1/N \). We also use \( \Delta Z \), the number of contacts relative to the minimum required at jamming, as an underlying control parameter. Our scaling theory predicts new exponents, exponent equalities and scaling collapses for energy, pressure and shear stress that we verify with numerical simulations of jammed packings of soft spheres. It also yields new insight into why the shear and bulk moduli exhibit different scalings: the difference arises because the shear stress vanishes as \( 1/\sqrt{N} \) while the pressure approaches a constant in the thermodynamic limit. The success of the scaling ansatz implies that the jamming transition exhibits an emergent scale invariance, and that it should be possible to develop a renormalization-group theory for jamming.

Tuesday, March 15, 2016 2:30PM - 5:30PM –
Session H35 DBIO GSNP: Population and Evolutionary Dynamics III 338 - Robert Austin, Princeton University

2:30PM H35.00001 Standing variation in spatially growing populations, DIANA FUSCO, MATTI GRALKA, JONA KAYSER, OSKAR HALLATSCHEK, Univ of California - Berkeley — Patterns of genetic diversity not only reflect the evolutionary history of a species but they can also determine the evolutionary response to environmental change. For instance, the standing genetic diversity of a microbial population can be key to rescue in the face of an antibiotic attack. While genetic diversity is in general shaped by both demography and evolution, very little is understood when both factors matter, as e.g. for biofilms with pronounced spatial organization. Here, we quantitatively explore patterns of genetic diversity by using microbial colonies and well-mixed test tube populations as antipodal model systems with extreme and very little spatial structure, respectively. We find that Eden model simulations and KPZ theory can remarkably reproduce the genetic diversity in microbial colonies obtained via population sequencing. The excellent agreement allows to draw conclusions on the resilience of spatially-organized populations and to uncover new strategies to contain antibiotic resistance.

2:42PM H35.00002 Crowds as an Excitable Medium for Spiral Wave Dynamics\(^1\), ANDREA WELSH, EDWIN GRECO, FLAVIO FENTON, Georgia Institute of Technology — Spiral wave (SW) patterns are studied in many physical, biological, and chemical excitable systems. Of particular importance are SW of electrical activity that develop in the heart and give rise to arrhythmias such as tachycardia (single SW) and fibrillation (multiple SWs). We investigate if a crowd of people given simple rules for activation and deactivation, modeled on cardiac cells, can act as a living simulation for SW dynamics. For group sizes ranging from 50 to 650 people we demonstrate, experimentally, the existence of stable spiral waves and of spiral wave breakup leading to chaotic dynamics. Numerical simulation predicts the simple rules lead to well define wave fronts. People, however, respond with various degrees of anticipation and misinformation. This human behavior can lead to smoothed fronts or even lead to spiral wave breakup and chaos. We present a new cell model that includes variations in reaction to account for the observed behavior in crowds. This model may be useful in the study of coupling and decoupling of cardiac cells that lead to arrhythmic behavior.

\(^1\)Supported by NSF

2:54PM H35.00003 Adapting populations in space: clonal interference and genetic diversity, DANIEL WEISSMAN, Emory University, NICK BARTON, IST Austria — Most species inhabit ranges much larger than the scales over which individuals interact. How does this spatial structure interact with adaptive evolution? We consider a simple model of a spatially-extended, adapting population and show that, while clonal interference severely limits the adaptation of purely asexual populations, even rare recombination is enough to allow adaptation at rates approaching those of well-mixed populations. We also find that the genetic hitchhiking produced by the adaptive alleles sweeping through the population has strong effects on the patterns of genetic diversity. In large spatial ranges, even low rates of adaptation cause all individuals in the population to rapidly trace their ancestry back to individuals living in a small region in the center of the range. The probability of fixation of an allele is thus strongly dependent on the alleles spatial location, with alleles from the center favored. Surprisingly, these effects are seen genome-wide (instead of being localized to the regions of the genome undergoing the sweeps). The spatial concentration of ancestry produces a power-law dependence of relatedness on distance, so that even individuals sampled far apart are likely to be fairly closely related, masking the underlying spatial structure.

3:06PM H35.00004 3-D Technology Approaches for Biological Ecologies\(^1\), LIYU LIU, Chongqing University/Institute of Physics, Chinese Academy of Sciences, ROBERT AUSTIN, Princeton University, U.S.-CHINA PHYSICAL-ONCOLOGY SCIENCES ALLIANCE (PS-OA) TEAM — Constructing three dimensional (3-D) landscapes is an inevitable issue in deep study of biological ecologies, because in whatever scales in nature, all of the ecosystems are composed by complex 3-D environments and biological behaviors. Just imagine if a 3-D technology could help complex ecosystems be built easily and mimic in vivo microenvironment realistically with flexible environmental controls, it will be a fantastic and powerful thrust to assist researchers for explorations. For years, we have been utilizing and developing different technologies for constructing 3-D micro landscapes for biophysics studies in vitro. Here, I will review our past efforts, including probing cancer cell invasiveness with 3-D silicon based Tepuis, constructing 3-D microenvironment for cell invasion and metastasis through polydimethylsiloxane (PDMS) soft lithography, as well as explorations of optimized stenting positions for coronary bifurcation disease with 3-D wax printing and the latest home designed 3-D bio-printer. Although 3-D technologies is currently considered not mature enough for arbitrary 3-D micro-ecological models with easy design and fabrication, I hope through my talk, the audiences will be able to sense its significance and predictable breakthroughs in the near future.

\(^1\)This work was supported by the State Key Development Program for Basic Research of China (Grant No 2013CB837200), the National Natural Science Foundation of China (Grant No 11474345) and the Beijing Natural Science Foundation (Grant No 7154221).
3:42PM H35.00005 Population Dynamics of Viral Inactivation\textsuperscript{1}, KRISTA FREEMAN, DONG LI, Carnegie Mellon University, MANJA BEHRENS, Lund University, KIRIL STRELETZKY, Cleveland State University, ULF OLSSON, Lund University, ALEX EVILEVITCH, Carnegie Mellon University — We have investigated the population dynamics of viral inactivation in vitro using time-resolved cryo electron microscopy combined with light and X-ray scattering techniques. Using bacteriophage λ as a model system for pressurized double-stranded DNA viruses, we found that virions incubated with their cell receptor eject their genome in a stochastic triggering process. The triggering of DNA ejection occurs in a non-synchronized manner after the receptor addition, resulting in an exponential decay of the number of genome-filled virions with time. We have explored the characteristic time constant of this triggering process at different temperatures, salt conditions, and packaged genome lengths. Furthermore, using the temperature dependence we determined an activation energy for DNA ejections. The dependencies of the time constant and activation energy on internal DNA pressure, affected by salt conditions and encapsidated genome length, suggest that the triggering process is directly dependent on the conformational state of the encapsidated DNA. The results of this work provide insight into how the in vivo kinetics of the spread of viral infection are influenced by intra- and extra cellular environmental conditions.

\textsuperscript{1}This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1252522

3:54PM H35.00006 Coalescent Theory Analysis of Population Collapse and Recovery in a Neutral Evolution Model\textsuperscript{1}, DAWN KING, SONYA BAHAR, University of Missouri at Saint Louis — As we move through the Anthropocene Epoch, human-driven climate change is predicted to accelerate extinction risk in the near future. Therefore, understanding basic underlying mechanisms of population loss and recovery could be paramount to saving key species in changing ecosystems. Here, we present an evolutionary model that investigates the dynamics of population collapse and recovery following a simulated mass extinction. Previously, we have shown that nonequilibrium, continuous phase transitions of the directed percolation universality class occur as a function of two different control parameters: the mutability, \( \mu \), which dictates how phenotypically different an offspring can be from its parent, and the death probability, \( \delta \), which probabilistically removes organisms within each generation. Here, we characterize the phylogenetic tree structures at two levels of biological organization—the organism and species level. Using methods from coalescent theory, we examine the phylogenetic tree structures at, and above, criticality, by considering common descent. The times to most recent common ancestor show phase transition behavior, as well as scale-free branching behavior at both levels of organization. We further examine these genealogical structures pre- and post-extinction.

\textsuperscript{1}This research was supported by funding from the James S. McDonnell Foundation

4:06PM H35.00007 Confirming Time-reversal Symmetry of a Directed Percolation Phase Transition in a Model of Neutral Evolutionary Dynamics\textsuperscript{1}, STEPHEN ORDWAY, DAWN KING, SONYA BAHAR, University of Missouri at Saint Louis — Reaction-diffusion processes, such as branching-coalescing random walks, can be used to describe the underlying dynamics of nonequilibrium phase transitions. In an agent-based, neutral model of evolutionary dynamics, we have previously shown that our system undergoes a continuous, nonequilibrium phase transition, from extinction to survival, as various system parameters were tuned. This model was shown to belong to the directed percolation (DP) universality class, by measuring the critical exponents corresponding to correlation length \( \xi_L \), correlation time \( \tau \), and particle density \( \beta \). The fourth critical exponent that defines the DP universality class is \( \beta' \), which measures the survival probability of growth from a single seed organism. Since DP universality is theorized to have time-reversal symmetry, it is assumed that \( \beta = \beta' \). Here, we confirm the existence of time-reversal symmetry in our model, we evaluate the system growth from a single asexually reproducing organism. Importantly, the critical exponent \( \beta' \) could be useful for comparison to experimental studies of phase transitions in biological systems, since observing growth of microbial populations is significantly easier than observing death.

\textsuperscript{1}This research was supported by funding from the James S. McDonnell Foundation

4:18PM H35.00008 Holes influence the mutation spectrum of human mitochondrial DNA.

MARTHA VILLAGRAN, JOHN MILLER, University of Houston, Dept. of Physics & Texas Ctr. for Superconductivity — Mutations drive evolution and disease, showing highly non-random patterns of mutation frequency vs. nucleotide position. We use computational DNA hole spectroscopy [M.Y. Suarez-Villagran & J.H. Miller, Sci. Rep. 5, 13571 (2015)] to reveal sites of enhanced hole probability in selected regions of human mitochondrial DNA. A hole is a mobile site of positive charge created when an electron is removed, for example by radiation or contact with a mutagenic agent. The hole spectra are quantum mechanically computed using a two-stranded tight binding model of DNA. We observe significant correlation between spectra of hole probabilities and of genetic variation frequencies from the MITOMAP database. These results suggest that hole-enhanced mutation mechanisms exert a substantial, perhaps dominant, influence on mutation patterns in DNA. One example is where a trapped hole induces a hydrogen bond shift, known as tautomerization, which then triggers a base-pair mismatch during replication. Our results deepen overall understanding of sequence specific mutation rates, encompassing both hotspots and cold spots, which drive molecular evolution.

4:30PM H35.00009 A kinetic theory for age-structured stochastic birth-death processes\textsuperscript{1}, TOM CHOU, Univ of California - Los Angeles, CHRIS GREENMAN, University of East Anglia — Classical age-structured mass-action models such as the McKendrick-von Foerster equation have been extensively used but they are structurally unable to describe stochastic fluctuations or population-size-dependent birth and death rates. Conversely, current theories that include size-dependent population dynamics (e.g., carrying capacity) cannot be easily extended to take into account age-dependent birth and death rates. In this paper, we present a systematic derivation of a new fully stochastic kinetic theory for interacting age-structured populations. By defining multiparticle probability density functions, we derive a hierarchy of kinetic equations for the stochastic evolution of an aging population undergoing birth and death. We show that the fully stochastic age-dependent birth-death process precludes factorization of the corresponding probability densities, which then must be solved by using a BBGKY-like hierarchy. Our results generalize both deterministic models and existing master equation approaches by providing an intuitive and efficient way to simultaneously model age- and population-dependent stochastic dynamics applicable to the study of demography, stem cell dynamics, and disease evolution.

\textsuperscript{1}NSF

4:42PM H35.00010 Theoretical ecology without species, MIKHAIL TIKHONOV, Harvard University — The sequencing-driven revolution in microbial ecology demonstrated that discrete ‘species’ are an inadequate description of the vast majority of life on our planet. Developing a new theoretical language that, unlike classical ecology, would not require postulating the existence of species, is a challenge of tremendous medical and environmental significance, and an exciting direction for theoretical physics. Here, it is proposed that community dynamics can be described in a naturally hierarchical way in terms of population fluctuation eigenmodes. The approach is applied to a simple model of division of labor in a multi-species community. In one regime, effective species with a core and accessory genome are shown to naturally appear as emergent concepts. However, the same model allows a transition into a regime where the species formalism becomes inadequate, but the eigenmode description remains well-defined. Treating a community as a black box that expresses enzymes in response to resources reveals mathematically exact parallels between a community and a single coherent organism with its own fitness function. This coherence is a generic consequence of division of labor, requires no cooperative interactions, and can be expected to be widespread in microbial ecosystems.

\textsuperscript{1}Harvard Center of Mathematical Sciences and Applications; John A. Paulson School of Engineering and Applied Sciences
A new model for biological effects of radiation and the driven force of molecular evolution. TAKAHIRO WADA, Department of Pure and Applied Physics, Kansai University, YUICHIRO MANABE, Division of Sustainable Energy and Environmental Engineering, Osaka University, HIROO NAKAJIMA, Department of Radiation Biology and Medical Genetics, Osaka University, YUCHI TSUYOYAMA, Radiisotope Research Center, Kyoto University, MASAKO BANDO, RCNP, Osaka University — We proposed a new mathematical model to estimate biological effects of radiation, which we call Whack-A-Mole (WAM) model. A special feature of WAM model is that it involves the dose rate of radiation as a key ingredient. We succeeded to reproduce the experimental data of various species concerning the radiation induced mutation frequencies. As a result, the analysis of the mega-mouse experiments, we obtained the mutation rate per base-pair per year of mice which is consistent with several orders of magnitude. We also analyzed Drosophila data and obtained essentially the same numbers. This clearly indicates that the natural radiation is not the dominant driving force of the molecular evolution, but we should look for other factors, such as miscopy of DNA in duplication process. We believe this is the first quantitative proof of the small contribution of the natural radiation in the molecular evolution.

5:06PM H35.0012 Scaling of expected survival time in a stochastic harvesting model. HAROLD HASTINGS, Hofstra University and Bard College at Simon’s Rock, MICHAEL RADIN, TAMAS WIANDT, Rochester Institute of Technology — We explore the dynamics of modified version of a standard fishery model (Gordon-Schafer-Munro), with additive and multiplicative noise, under a quota-based harvest. A harvest quota induces an effective strong Allee effect (a positive unstable steady state population level, below which populations die out), with expected survival time following generalized Ornstein-Uhlenbeck dynamics. In particular, for additive noise, the expected survival time is exponential in $\sigma^2/\beta$, where $\sigma$ is the difference between stable and unstable steady state populations and $\beta$ is the noise level. Thus survival time depends sensitively upon harvest quota (which determines steady state population), perhaps a warning to avoid future collapses such as that of the Atlantic cod fishery. 1. Gordon HS. J Fisheries Board Canada 10, 442 (1953); Schaefer MB. ibid 14, 669 (1957); Clark, CW. Munro GR. J Environ Econ and Management 2, 92 (1975). 2. Beale PD. Phys Rev A 40, 3998 (1989). 3. c.f. www.millenniumassessment.org/

5:18PM H35.0013 Computational design of hepatitis C vaccines using maximum entropy models and population dynamics. GREGORY HART, ANDREW FERGUSON, Univ of Illinois - Urbana — Hepatitis C virus (HCV) afflicts 170 million people and kills 350,000 annually. Vaccination offers the most realistic and cost effective hope of controlling this epidemic. Despite 20 years of research, no vaccine is available. A major obstacle is the virus' extreme genetic variability and rapid mutational escape from immune pressure. Improvements in the vaccine design process are urgently needed. We propose a new computational framework for rational design which exploits the properties of structural and dynamic responses to multiplicative and additive noise. Computationally designed vaccines with broad sero-protective activity have been obtained.

Tuesday, March 15, 2016 2:30PM - 5:30PM – Session H40 GSNP GSOFT: Mechanical Metamaterials and Origami I 343 - Chris Santangelo, University of Massachusetts Amherst

2:30PM H40.00001 Wave Manipulation in Metamaterials: A LEGO® Bricks Enabled Platform1, PAOLO CELLI, STEFANO GONELLA, University of Minnesota — In this work, we show how simple, reconfigurable arrangements of LEGO® bricks can be turned into the building blocks of an experimental platform for the investigation of wave phenomena in metamaterial architectures. The approach involves the assembly of reconfigurable specimens consisting of patterns of bricks on a baseplate and the use of a 3D laser vibrometer to reconstruct global and local wave features. The ability to seamlessly transition between different topologies makes this an effective approach for rapid experimental verification and proof of concept in the arena of mechanical metamaterials engineering. The intuitive nature of the brick-and-baseplate assembly paradigm can also be leveraged to implement families of intuitive lab demonstrations with significant didactic and scientific outreach potential. The versatility of the platform is tested through a series of experiments that illustrate a variety of wave manipulation effects, such as waveguiding and seismic isolation, both in periodic and disordered topologies.

1 We acknowledge the support of the National Science Foundation (grant CMMI-1266089)

2:42PM H40.00002 Transformable topological mechanical metamaterials1, D. ZEB ROCKLIN, SHANGNAN ZHOU, KAI SUN, XIAOMING MAO, University of Michigan, Department of Physics — We present a class of mechanical metamaterials characterized by a uniform soft deformation—a large, zero-energy homogeneous elastic deformation mode of the structure—that may be used to induce topological transitions and dramatically change mechanical and acoustic properties of the structure. We show that the existence of such a mode determines certain exotic mechanical and acoustic properties of the structure and its activation can reversibly alter and tune these properties. This serves as the basis for a design principle for mechanical metamaterials with tunable properties. When the structure’s uniform mode is primarily dilational (shearing) its surface (bulk) possesses phonon modes with vanishing speed of sound. Maxwell lattices comprise a subclass of such material which, owing to their critical coordination number (four, in 2D), necessarily possess such a uniform zero mode, often termed a Guest mode, and which may be topologically polarized, such that zero modes are moved from one edge to another. We show that activating such a mode can alter the shear/dilational character of the mode and topologically polarize the structure, thereby altering the bulk and surface properties at no significant energy cost. arXiv:1510.06389 [cond-mat.soft]

1NWO, Delta Institute of Physics, ICAM fellowship (DZR) and NSF grant PHY-1402971 at University of Michigan (KS)

2:54PM H40.00003 Tuning the Response in Disordered Networks, NIDHI PASHINE, Department of Physics, The University of Chicago, Chicago, IL, JASON W. ROCKS, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA, IRMGARD BISCHOFBERGER, Department of Physics, The University of Chicago, Chicago, IL, CARL P. GOODRICH, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, SIDNEY R. NAGELE, Department of Physics, The University of Chicago, Chicago, IL, ANDREA J. LIU, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA — The fact that amorphous materials are structurally different from crystals has important consequences for how the properties of a disordered structure can be tuned. We have used jamming as a method to create spring networks in both two and three dimensions. By selectively removing a small percentage of bonds, we can tune the network to have a desired response. For example, we can tune the network’s Poisson ratio anywhere between the auxetic and incompressible limits. We can also produce a targeted response at a local scale; by perturbing the positions of pairs of particles at one point we can tune in a desired response a large distance away. This response is similar to the allosteric regulation in proteins where a reaction at one site activates another site of the protein molecule. Experimentally, we have successfully demonstrated such mechanical networks in 2D (by laser cutting) or in 3D (3D printing).
3:06PM H40.00004 The breakdown of breathers in the Fermi-Pasta-Ulam-Tsingou system¹ , ALEXANDRA WESTLEY, RAHUL KASHYAP, SURAJIT SEN, State Univ of NY - Buffalo — It is well known that in many nonlinear lattices, remarkably stable and localized disturbances known as breathers may form. Here we discuss in short the properties of these objects in the context of the Fermi-Pasta-Ulam-Tsingou (FP'T) system which consists of a mass-spring chain, with spring potentials containing both quadratic and quartic terms. These breathers, though long-lasting, inevitably decay and eventually break apart with sudden violence. This talk in particular will focus on recent numerical work studying the lead-up to the breakdown in which the breather emits at (seemingly) random intervals solitary and anti-solitary waves in the highly nonlinear limit. Furthermore, a possible method to predict the times at which these waves are emitted by examining the frequency structure of the breather will be discussed.

¹Partially supported by US Army Research Office

3:18PM H40.00005 Multifunctional Lattices with Low Thermal Expansion and Low Thermal Conductivity, HANG XU, LU LIU, DAMIANO PASINI², Mechanical Engineering, McGill University — Systems in space are vulnerable to large temperature changes when travelling into and out of the Earth’s shadow. Variations in temperature can lead to undesired geometric changes in susceptible applications requiring very fine precision. In addition, temperature-sensitive electronic equipment hosted in a satellite needs adequate thermal-control to guarantee a moderate ambient temperature. To address these specifications, materials with low coefficient of thermal expansion (CTE) and low coefficient of thermal conductivity (CTC) over a wide range of temperatures are often sought, especially for bearing components in satellites. Besides low CTE and low CTC, these materials should also provide desirable stiffness, strength and extraordinarily low mass. This work presents ultralightweight bi-material lattices with tunable CTE and CTC, besides high stiffness and strength. We show that the compensation of the thermal expansion and joint rotation at the lattice joints can be used as an effective strategy to tailor thermomechanical performance. Proof-of-concept lattices are fabricated from Al and Ti alloy sheets via a simple snap-fit technique and vacuum brazing, and their CTE and CTC are assessed via a combination of experiments and theory.

²Corresponding Author

3:30PM H40.00006 Finite-temperature twisted-untwisted transition of the kagome lattice, DESHPREET BEDI, D. ZEB ROCKLIN, XIAOMING MAO, University of Michigan — Mechanical instability governs many fascinating phenomena in nature, including jamming, glass transitions, and structural phase transitions. Although mechanical instability in athermal systems is well understood, how thermal fluctuations modify such transitions remains largely unexplored. Recent studies reveal that, due to the large number of floppy modes that emerge at mechanical instability, intriguing new phenomena occur, such as fluctuation-driven first-order transitions and order-by-order. In this talk, we present an analytic study of the finite-temperature rigidity transition for the kagome lattice. Our model exhibits a zero-temperature continuous twisted-untwisted transition as the sign of the next-nearest-neighbor spring constant changes. At finite temperature, we show that the divergent contribution of floppy modes to the vibrational entropy renormalizes this spring constant, resulting in a first-order transition. We also propose an experimental manifestation of this transition in the system of self-assembling triblock Janus particles.

3:42PM H40.00007 Topological design of torsional metamaterials, VINCENZO VITELLI, JAYSON PAULOSE, ANNE MEEUSSEN, Institute Lorentz for Theoretical Physics, Leiden, TOPOLOGICAL MECHANICS LAB TEAM — Frameworks – stiff elements with freely hinged joints – model the mechanics of a wide range of natural and artificial structures, including mechanical metamaterials with auxetic and topological properties. The unusual properties of the structure depend crucially on the balance between degrees of freedom associated with the nodes, and the constraints imposed upon them by the connecting elements. Whereas networks of featureless nodes connected by central-force springs have been well-studied, many real-world systems such as frictional granular packings, gear assemblies, and flexible beam meshes incorporate torsional degrees of freedom on the nodes, coupled together with transverse shear forces exerted by the connecting elements. We study the consequences of such torsional constraints on the mechanics of periodic isostatic networks as a foundation for mechanical metamaterials. We demonstrate the existence of soft modes of topological origin, that are protected against disorder or small perturbations of the structure analogously to their counterparts in electronic topological insulators. We have built a lattice of gears connected by rigid beams that provides a real-world demonstration of a torsional metamaterial with topological edge modes and mechanical Weyl modes.

3:54PM H40.00008 Surface morphology of pre-stressed bilayer shells for tunable optical transmittance, RASHED AL-RASHED, FRANCISCO LPEZ JIMNEZ, JOEL MARTHELOT, ANNA LEE, PEDRO REIS, Massachusetts Institute of Technology — We introduce a new class of pre-stressed bilayer shells, whose surface morphology can be used to smoothly tune their optical transmittance by pneumatic actuation. Each sample is fabricated by pressurizing a disk made out of an optically clear silicone-based rubber to bulge it into a nearly hemispherical pre-stressed shell. The surface of this shell is then taken as a substrate and coated with a thin layer of a polymer suspension with black micron-sized dye particles, which, upon curing, can make the samples opaque. The sample becomes planar when it is depressurized to remove the pre-strain, and its surface develops a complex shell. The surface of this shell is then taken as a substrate and coated with a thin layer of a polymer suspension with black micron-sized dye particles, which, upon curing, can make the samples opaque. The sample becomes planar when it is depressurized to remove the pre-strain, and its surface develops a complex topography that significantly affects its optical transmittance (i.e. the amount of light that passes through the sample). Re-pressureurization of the samples allow for their transmittance to be smoothly tuned in a reversible manner. We explore the parameter space of the system by systematically varying its geometric and material properties. A phase diagram is then constructed where we characterize the transmittance of each of the surface patterns at varying levels of pre-strain.

4:06PM H40.00009 Elastic theory of origami-based metamaterials, FREDERIC LECHENAULT, Laboratoire de Physique Statistique, ENS, Paris, V. BRUNCK, Lab. de Physique Statistique, Ecole Normale Superieure, UPMC, Univ. Paris 06, Univ. Paris-Diderot, CNRS, Paris, France, A. REID, Lab. de Physique Statistique, Ecole Normale Superieure, UPMC, Univ. Paris 06, Univ. Paris-Diderot, CNRS, Paris, France & NC State Univ, M. ADDA-BEDIA, Lab. de Physique Statistique, Ecole Normale Superieure, UPMC, Univ. Paris 06, Univ. Paris-Diderot, CNRS, Paris, France — Origami offers the possibility for new metamaterials whose overall mechanical properties can be programmed by acting locally on each crease. Starting from a thin plate and having knowledge about the properties of the material and the folding procedure, one would aim to determine the shape taken by the structure at rest and its mechanical response. We introduce a vector deformation field acting on the imprinted network of creases, that allows to express the geometrical constraints imposed upon them by the connecting elements. Whereas networks of featureless nodes connected by central-force springs have been well-studied, many real-world systems such as frictional granular packings, gear assemblies, and flexible beam meshes incorporate torsional degrees of freedom on the nodes, coupled together with transverse shear forces exerted by the connecting elements. We study the consequences of such torsional constraints on the mechanics of periodic isostatic networks as a foundation for mechanical metamaterials. We demonstrate the existence of soft modes of topological origin, that are protected against disorder or small perturbations of the structure analogously to their counterparts in electronic topological insulators. We have built a lattice of gears connected by rigid beams that provides a real-world demonstration of a torsional metamaterial with topological edge modes and mechanical Weyl modes.

4:18PM H40.00010 Self-Folding With Graphene Bimorphs, MARC MISKIN, KYLE DORSEY, PETER ROSE, ITAI COHEN, PAUL MCEUEN, Cornell University — We have developed a new technique that let us program two layer stacks, or bimorphs, made of graphene and ultra-thin films to self-fold via differential stress. Our approach works in the extreme regime of bimorph folding: we construct bimorphs that optimize folding efficiency when one layer is atomically thin. The resulting devices controllably fold to micron sized radii of curvature. By applying this technique in concert with lithographic patterning, we have produced a powerful platform to build three dimensional structures at the nanoscale. We demonstrate that this this approach is intrinsically scalable and facilities the construction of both fixed 3d structures and actuation.

¹This research was supported by the ANR grant 14-CE07-0031 METAMAT
4:30PM H40.00011 The role of geometry in 4-vertex origami mechanics, SCOTT WAITUKAITIS, PETER DIELEMAN, MARTIN VAN HECKE, Leiden University, AMOLF — Origami offers an interesting design platform for materials because it strongly couples mechanics with geometry. Even so, most research carried out so far has been limited to one or two particular patterns. I will discuss the full geometrical space of the most common origami building block, the 4-vertex, and show how exotic geometries can have dramatic effects on the mechanics.

4:42PM H40.00012 Generalized Bistability in Origami Cylinders, AUSTIN REID, North Carolina State University, MOKHTAR ADDA-BEDIA, FREDERIC LECHENAUT, Laboratoire de Physique Statistique de l’ENS — Origami folded cylinders (origami bellows) have found increasing range of applications in spaces flight, medicine, and even experimental nuclear physics. In spite of this interest, a general understanding of the dynamics of an origami folded cylinder has been elusive. By solving the fully constrained behavior of a periodic fundamental origami cell defined by unit vectors, we have found an analytic solution for all possible rigid-face states accessible from a cylindrical Miura-ori pattern. Although an idealized bellows has two rigid-face configurations over a well-defined region, a physical device, limited by nonzero material thickness and forced to balance hinge with plate-bending energy, often cannot stably maintain a stowed configuration. We have identified and measured the parameters which control this emergent bistability, and have demonstrated the ability to fabricate bellows with tunable deployability.

4:54PM H40.00013 Origami Optimization: Role of Symmetry in Accelerating Design, PHILIP BUSKOHL, Air Force Research Laboratory, KAZUKO FUCHI, Wright State Research Institute, GIORGIO BAZZAN, UES, Inc, MICHAEL DURSTOCK, GREGORY REICH, JAMES JOO, RICHARD VAIA, Air Force Research Laboratory — Origami structures morph between 2D and 3D conformational states that can be programmed for the form, function and mobility of the structure. Deterministic optimization tools have recently been developed to predict optimal fold patterns with mechanics-based metrics, such as the minimal energy storage, auxetic response and actuation. Origami actuator design problems possess inherent symmetries associated with the grid, mechanical boundary conditions and the objective function, which are often exploited to reduce the design space and computational cost of optimization. However, enforcing symmetry eliminates the prediction of potentially better performing asymmetric designs, which are more likely to exist given the discrete nature of fold line optimization. To better understand this effect, actuator design problems with different combinations of rotation and reflection symmetries were optimized while varying the number of folds allowed in the final design. In each case, the optimal origami patterns transitioned between symmetric and asymmetric solutions depended on the number of folds available for the design, with fewer symmetries present with more fold lines allowed. This study investigates the interplay of symmetry and discrete vs continuous optimization in origami actuators and provides insight into how the symmetries of the reference grid regulate the performance landscape.

1 This work was supported by the Air Force Office of Scientific Research.

5:06PM H40.00014 How do bendy straws bend? A study of re-configurability of multi-stable corrugated shells, NAKUL BENDE, SARAH SELDEN, Univ of Mass - Amherst, ARTHUR EVANS, University of Wisconsin–Madison, CHRISTIAN SANTANGELO, RYAN HAYWARD, Univ of Mass - Amherst, SHI-MING MCEUEN, Cornell University — Shape-programmable systems have evolved to allow for reconfiguration of structures through a variety of mechanisms including swelling, stress-relaxation, and thermal expansion. Particularly, there has been a recent interest in systems that exhibit bi-stability or multi-stability to achieve transformation between two or more pre-programmed states. Here, we study the ubiquitous architecture of corrugated shells, such as drinking straws or bellows, which has been well known for centuries. Some of these structures exhibit almost continuous stability amongst a wide range of reconfigurable shapes, but the underlying mechanisms are not well understood. To understand multi-stability in ‘bendy-straw’ structures, we study the unit bi-conical segment using experiments and finite element modeling to elucidate the key geometrical and mechanical factors responsible for its multi-stability. The simple transformations of a unit segment – a change in length or angle can impart complex re-configurability of a structure containing many of these units. The fundamental understanding provided of this simple multi-stable building block could yield improvements in shape re-configurability for a wide array of applications such as corrugated medical tubing, robotics, and deployable structures.

2 NSF EFRI ODISSEI-1240441

5:18PM H40.00015 Q: How many folded angels can we fit on the head of a pin? A: 22+/−5 , ITAI COHEN, Cornell University, TOM HULL, Western New England University, ROBERT LANG, Lang Origami, CHRISTIAN SANTANGELO, University of Massachusetts, RYAN HAYWARD, Univ of Mass - Amherst, SHI-MING MCEUEN, Cornell University — For centuries, origami, the Japanese art of paper folding, has been a powerful technique for transforming two dimensional sheets into beautiful three dimensional sculptures. Recently, origami has made its foray into a new realm, that of physics, where it has been revolutionizing our concept of materials design. Arguably the greatest strength of this new paradigm is the fact that origami is intrinsically scalable. Thus sculptures built at one size can be shrunk down smaller and smaller. This begs the question: what is the smallest fold one can make? Or in other words how many folded angels can we fit on the head of a pin? This talk takes a deep dive into how origami has been marching smaller and smaller in size. From folding by hand, to self-folding through shape memory alloys and even folding via polymer layers, I will argue that the ultimate limit for scaling down origami is set by folding an ashet of atomic dimensions. I will conclude by showing this vision realized in the folds of a single sheet of graphene.

Tuesday, March 15, 2016 2:30PM - 5:30PM
Session H43 GSNP GSOFT: Aging in the Jammed State

2:30PM H43.00001 A Time-Temperature Transistor - An Application of Aging Dynamics, GREGORY KENNING, Indiana University of Pennsylvania — Aging dynamics occur as systems far from thermodynamic equilibrium evolve towards equilibrium. We have produced a magnetic nanoparticle system composed of Co nanoparticles, which self-assemble during Co deposition on Sb. At a particular time in the formation of the nanoparticles, they are encased in a layer of Sb producing a system far from equilibrium. Magnetization vs. temperature measurements as well as Magnetic Force Microscopy (MFM) indicates that the nanoparticles initially have a large magnetic moment. We observe, as a function of time, an approximately 80% decay in the sample magnetization and an approximately 50% decay in the DC electrical resistivity. MFM suggests that the magnetization decay proceeds from the magnetic nanoparticles losing their net moments possibly due to spin rearrangement. Evidence also suggests that the initial magnetic moments, drive the Sb layer semiconducting. As the net moments of the magnetic nanoparticles decrease, the Sb reverts back to its semi-metal behavior with the accompanying decrease in the electrical resistivity. The magnetization and resistance decays follow the same Arrhenius type behavior. By varying the Co layer thickness, the Arrhenius parameters can be tuned. We have been able to tune the parameters making these materials excellent candidates for sensors for the accompanying decrease in the electrical resistivity. The magnetization and resistance decays follow the same Arrhenius type behavior. By varying the Co layer thickness, the Arrhenius parameters can be tuned. We have been able to tune the parameters making these materials excellent candidates for sensors for the electrical resistivity.

2:42PM H43.00002 Density variations of plastic carriers in metallic glasses during aging, YUE FAN, Oak Ridge National Lab, TAKUYA IWASHITA, University of Tennessee, TAKESHI EGAMI, University of Tennessee; Oak Ridge National Lab — Thermally induced deformation in metallic glasses was investigated by sampling the potential energy landscape (PEL) and probing the changes in the atomic properties (e.g. energy, displacement, stress). We demonstrate that there exists a universal plastic carrier in amorphous materials, which corresponds to the hopping between local minima on PEL. However very interestingly, the density of plastic carrier is largely affected by the aging history of the glasses. The higher fictive temperature (i.e. fast cooling rate), the larger density of plastic carrier is contained in the system. In particular, we observe a scaling of $ρ \propto \exp(-\alpha/T_{fict})$, which is consistent with the prediction of shear transformation zone theory. The work is supported by U.S. Department of Energy.
2:54PM H43.00003 Aging and memory effects in the spin jam states of densely populated frustrated magnets, ANJANA SAMARAKOON, SEUNG-HUN LEE, University of Virginia, TAKU SATO, Tohoku University, Katahira, Sendai, Japan; HAIDONG ZHOU, RYAN SINCLAIR, University of Tennessee, JUNJIE YANG, TIANRAN CHEN, GIA-WEI CHERN, ISRAEL KLIICH, University of Virginia — Defects and randomness has been largely studied as the key mechanism of glassiness find in a dilute magnetic system. Even though the same argument has also been made to explain the spin glass like properties in dense frustrated magnets, the existence of a glassy state arise intrinsically from a defect free spin system, far from the conventional dilute limit with different mechanisms such as quantum fluctuations and topological features, has been theoretically proposed recently. We have studied field effects on zero-field cooled and field cooled susceptibility bifurcation and memory effects below freezing transition; of three different densely populated frustrated magnets which glassy states we call spin jam, and a conventional dilute spin glass. Our data show common behaviors among the spin jam states, which is distinct from that of the conventional spin glass. We have also performed Monte Carlo simulations to understand the nature of their energy landscapes.

3:06PM H43.00004 Time Dependence of the freezing temperature for thin film spin glasses1, RAYMOND ORBACH, The University of Texas at Austin — There have been many measurements of the dependence of the “freezing temperature”, \( T_f \), on the thickness \( L \) of thin film spin glasses. \( T_f \) decreases with decreasing \( L \), but never vanishes. This contribution suggests that the dependence of \( T_f \) on \( L \) is a time dependent relationship. Because the lower critical dimension of a spin glass, \( d_c \geq 2.5 \), when the spin glass correlation length \( \xi(t,T) \) grows to \( L \), the spin glass dimensionality crosses over to the glassy state. The approach to spin glass order is then determined by the time evolution of the spin glass correlation length. The glass ordering dynamics are then activated, with activation energy equal to a largest barrier \( \Delta_{max}(L) \) and an associated activation time \( \tau \). For measurements at time scales such that \( \xi(t,T) < L \), the effective dimension \( d = 3 \), and the characteristic cup and knee of a spin glass is observed. For experimental time scales greater than \( \tau \), with \( \xi(t,T) \approx L \), the zero-field cooled magnetization has grown to the field-cooled value of the magnetization, leading to the identification of \( T_f \). Quantitative agreement with experiment is exhibited.

1Supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-SC0013599

3:18PM H43.00005 Intermittent Aging Dynamics in a Metallic Glass Studied by X-ray Photon Correlation Spectroscopy, ZACH EVENSON, Technical University Munich / Maier-Leibnitz Zentrum (MLZ), BEATRICE RUTA, ESRF - The European Synchrotron, SIMON HECHLER, MORITZ STOLPE, Saarland University, ELOI PINEDA, Universitat Politècnica de Catalunya-BarcelonaTech, ISABELLA GALLINO, RALF BUSCH, Saarland University — Although physical aging is a universal feature of glasses and other non-equilibrium matter, the atomic-level processes involved are still a puzzling. Here we study the microscopic aging dynamics of a metallic glass using coherent X-rays. Contrary to the common assumption of a steady slowing down of the dynamics usually observed in macroscopic studies, we show that the structural relaxation processes underlying aging in this metallic glass are intermittent and highly heterogeneous at the atomic scale. Moreover, physical aging is triggered by cooperative atomic rearrangements, driven by the relaxation of internal stresses. These results strengthen the similarities between metallic glasses and non-equilibrium soft materials and suggest a common microscopic origin stemming from a complex energy landscape.

3:30PM H43.00006 Record Dynamics and the Parking Lot Model for granular dynamics, PAOLO SIPANI, University of Southern Denmark, STEFAN BOETTCHER, Emory University — Also known for its application to granular compaction (E. Ben-Naim et al., Physica D, 1988), the Parking Lot Model (PLM) describes the random parking of identical cars in a strip with no marked bays. In the thermally activated version considered, cars can be removed at an energy cost and, in thermal equilibrium, their average density increases as temperature decreases. However, equilibration at high density becomes exceedingly slow and the system enters an aging regime induced by a kinematic constraint, the fact that parked cars may not overlap. As parking an extra car reduces the available free space, the next parking event is even harder to achieve. Records in the number of parked cars mark the salient features of the dynamics and are shown to be well described by the log-Poisson statistics known from other glassy systems with record dynamics. Clusters of cars whose positions must be rearranged to make the next insertion possible have a length scale which grows logarithmically with age, while their life-time grows exponentially with size. The implications for a recent cluster model of colloidal dynamics, (S. Boettcher and P. Sibani, J. Phys.: Cond. Matter, 2011 N. Becker et al., J. Phys.: Cond. Matter, 2014) are discussed.

3:42PM H43.00007 Non-equilibrium phenomena in disordered colloidal solids, PETER YUNKER, Georgia Institute of Technology — Colloidal particles are a convenient tool for studying a variety of non-equilibrium phenomena. I will discuss experiments that investigate the aging and non-equilibrium growth of disordered solids. In the first set of experiments, colloidal glasses are rapidly formed to study aging in jammed packings. A colloidal fluid, composed of micron-sized temperature-sensitive pNIPAM particles, is rapidly quenched into a colloidal glass. After the glass is formed, collective rearrangements occur as the glass ages. Particles undergo irreversible rearrangements, which break nearest-neighbor pairings and allow the glass to relax. These irreversible rearrangements are accompanied by large clusters of fast moving particles; the number of particles involved in these clusters increases as the glass ages, leading to the slowing of dynamics that is characteristic of aging. In the second set of experiments, we study the role particle shape, and thus, interparticle interaction, plays in the formation of disordered solids with different structural and mechanical properties. Aqueous suspensions of colloidal particles with different shapes evaporate on glass slides. Convective flows during evaporation carry particles from drop center to drop edge, where they accumulate. The resulting particle deposits grow heterogeneously from the edge on the air-water interface. Three distinct growth processes were discovered in

4:18PM H43.00008 Correlated Clusters in Aging Colloidal Glass1, DOMINIC ROBE, STEFAN BOETTCHER2, Emory University, PETER YUNKER1, Georgia Tech — A numerical model of correlated domains in glassy colloids is recreated, following its development by Becker, et. al.[1] The model is a course grained representation of 2D colloidal systems inspired by record dynamics, and produces emergent dynamic heterogeneity and aging. Results from the original development are reproduced, and compared to the same observables in an experimental system of bidisperse microgel spheres studied by Yunker, et. al.[2] Basic observables such as particle persistence and mean square displacement are measured at different waiting times to observe aging. Four-point correlation lengths are also examined for signs of dynamic heterogeneity. Results from both the numerical and experimental systems are consistent with the predictions of record dynamics, that aging systems evolve on a logarithmic time scale.

1Supported from the Villum Foundation is gratefully acknowledged

2Website: http://www.physics.emory.edu/faculty/boettcher/
3Website: https://www.physics.gatech.edu/user/peter-yunker
4:30PM H43.0009 Universal Scaling in the Aging of the Strong Glass Former SiO2. KATHARINA VOLLMAYR-LEE, Bucknell University; HORACIO CASTILLO, Department of Physics and Astronomy and Nanoscale and Quantum Phenomena Institute; CHRISTOPHER GORMAN, University of California, Santa Barbara — We show that the aging dynamics of a strong glass former displays a strikingly simple scaling behavior. Using molecular dynamics simulations, we quench the system from high temperature to 2500 K, below the glass transition and investigate dynamic heterogeneities as a function of waiting time, the time elapsed since the quench. We find that both the dynamic susceptibility and the probability distribution of the local incoherent intermediate scattering function can be described by simple scaling forms in terms of the global incoherent intermediate scattering function. The scaling forms are the same that have been found to describe the aging of several fragile glass formers. Furthermore, we find that the aging dynamics is controlled by a unique aging clock which is the same for Si and O atoms.

We acknowledge the support via NSF REU Grant PHY-1156964, DFG via SFB 602 and FOR1394, and DOE under grant DE-FG02-06ER46300 and NSF Grant PHY-1062693.

4:42PM H43.00010 Aging near the wall in colloidal glasses, CONG CAO, XINRUI HUANG, ERIC WEEKS, Emory University — In a colloidal glass system, particles move slower as sample ages. In addition, their motions may be affected by their local structure, and this structure will be different near a wall. We examine how the aging process near a wall differs from that in the bulk of the sample. In particular, we use a confocal microscope to observe 3D motion in a bidisperse colloidal glass sample. We find that flat walls induce the particles to organize into layers. The aging process behaves differently near the boundary, especially within the first three layers. Particle motion near the wall is noticeably slower but also changes less dramatically with age. We compare and contrast aging seen in samples with flat and rough walls.

4:54PM H43.00011 Thermal fluctuations and elastic relaxation in the compressed exponential dynamics of colloidal gels, MEHDI BOUZID, JADER COLOMBO, EMANUELA DEL GADO, Georgetown University — Colloidal gels belong to the class of amorphous systems; they are disordered elastic solids that can form at very low volume fraction, via aggregation into a rich variety of networks. They exhibit a slow relaxation process in the aging regime similar to the glassy dynamics. A wide range of experiments on colloidal gels show unusual compressed exponential of the relaxation dynamical properties. We use molecular dynamics simulation to investigate how the dynamic change with the age of the system. Upon breaking and reorganization of the network structure, the system may display stretched or compressed exponential relaxation. We show that the transition between these two regimes is associated to the interplay between thermally activated rearrangements and the elastic relaxation of internal stresses. In particular, ballistic-like displacements emerge from the non local relaxation of internal stresses mediated by a series of “micro-collapses”. When thermal fluctuations dominate, the gel restructurating involves instead more homogeneous displacements across the heterogeneous gel network, leading to a stretched exponential type of relaxation.

5:06PM H43.00012 Power-law creep and residual stresses in carbopol microgels, PIERRE LIDON, SEBASTIEN MANNEVILLE, Physics Laboratory - Ecole Normale Superieure de Lyon - France — We report on the interplay between creep and residual stresses in carbopol microgels. When a constant shear stress \( \sigma \) is applied below the yield stress \( \sigma_y \), the strain is shown to increase as a power law of time, \( \gamma(t) = \gamma_0 + (t/\tau)^\alpha \), with exponent \( \alpha \approx 0.38 \) that is strongly reminiscent of Andrade creep in hard solids. For applied shear stresses lower than some characteristic value of about \( \sigma_y/10 \), the microgels exhibit a more complex creep behavior that we link to the existence of residual stresses and to weak aging of the system after preshear. The influence of the preshear protocol, of boundary conditions and of microgel concentration on residual stresses is investigated.

We discuss our results in light of previous works on colloidal glasses and other soft glassy systems.

5:18PM H43.00013 Creep and aging in jammed granular materials, ISHAN SRIVASTAVA, TIMOTHY FISHER, Purdue University — Granular materials flow (or unjam) when stressed above the Coulomb yield stress, but a slow creep is observed when the applied stresses are low. In this work, using a recently introduced enthalpy-based variable-cell simulation method, we will present results on the creep and slow aging dynamics in granular systems comprised of soft particles of varying shape that are hydrostatically jammed and subjected to an external stress. We observe a two-stage creep with an initial fast exponential evolution followed by a slow logarithmic evolution over long time scales. We correlate the slow creeping dynamics with micromechanical evolution at the grain scale, such as increasing dynamical heterogeneity and force-chain rearrangements. Results will also be presented on the effect of grain shape (faceted vs. spherical) on the creep and aging dynamics. Finally, a continuum granular fluidity model is developed to rationalize these observations.

Tuesday, March 15, 2016 2:30PM - 5:18PM –
Session H51 GPC DFD GSNP: Climate as a Non-equilibrium and Stochastic System
Hilton Baltimore Holiday Ballroom 2 - Juan Restrepo, Oregon State University

2:30PM H51.00001 Fluctuations and Response in Geophysical Fluid Dynamics, VALERIO LUCARINI, University of Hamburg — The climate is a complex, chaotic, non-equilibrium system featuring a limited horizon of predictability, variability on a vast range of temporal and spatial scales, instabilities resulting into energy transformations, and mixing and dissipative processes resulting into entropy production. Despite great progresses, we still do not have a complete theory of climate dynamics able to account for instabilities, equilibration processes, response to changing parameters of the system, and multiscale effects. We will outline some possible applications of the response theory developed by Ruelle for non-equilibrium statistical mechanical systems, showing how it allows for setting on firm ground and on a coherent framework concepts like climate sensitivity, climate response, and climate tipping points, and to construct parametrizations for unresolved processes. We will show results for comprehensive global climate models. The results are promising in terms of suggesting new ways for approaching the problem of climate change prediction and for using more efficiently the enormous amounts of data produced by modeling groups around the world. Ref: V. Lucarini, R. Blender, C. Herbert, F. Ragone, S. Pascale, J. Wouters, Mathematical and Physical Ideas for Climate Science, Reviews of Geophysics 52, 809-859 (2014).

3:06PM H51.00002 Balanced Dynamics in the Madden-Julian Oscillation, SHARON SESSIONS, STIPO SENTIC, New Mexico Tech, ZELJKA FUCHS, University of Split, Croatia, and New Mexico Tech, DAVID RAYMOND, New Mexico Tech — Balanced dynamics describes the response of the tropical thermodynamic environment to changes in the atmospheric vorticity patterns. Observations and numerical simulations have demonstrated that positive mid-tropospheric vorticity anomalies produce a more stable thermodynamic environment with cool anomalies at low levels and warm anomalies aloft. The increase in atmospheric stability creates more bottom-heavy convective profiles which are highly conducive for developing tropical cyclones. Balanced dynamics may also play a role in other varieties of tropical convection, including the most significant source of intraseasonal variability: the Madden-Julian Oscillation (MJO). Using data from DYNAMO—a field program aimed to investigate the dynamics of the MJO—we investigate the role of balanced dynamics in the Madden-Julian Oscillation.

This work supported by the NSF.
3:18PM H51.00003 Stochastic dynamics of melt ponds and sea ice-albedo climate feedback . IVAN SUDAKOV, Department of Physics, University of Dayton — Evolution of melt ponds on the Arctic sea surface is a complicated stochastic process. We suggest a low-order model with ice-albedo feedback which describes stochastic dynamics of melt ponds geometrical characteristics. The model is a stochastic dynamical system model of energy balance in the climate system. We describe the equilibria in this model. We conclude the transition in fractal dimension of melt ponds affects the shape of the sea ice albedo curve.

3:30PM H51.00004 A Novel Method to Unravelling Energy Pathways in the Ocean . HUSSEIN ALUIE, University of Rochester — Large-scale currents and eddies pervade the ocean and play a prime role in the general circulation and climate. The coupling between scales ranging from $\mathcal{O}(10^{-4})$ km down to $\mathcal{O}(1)$ mm presents a major difficulty in understanding, modeling, and predicting oceanic circulation and mixing, where the energy budget is uncertain within a factor possibly as large as ten. Identifying the energy sources and sinks at various scales can reduce such uncertainty and yield insight into new parameterizations. To this end, we refine a novel coarse-graining framework, which accounts for the spherical geometry of the problem, to directly analyze the coupling between scales. We apply these tools to strongly eddying high-resolution simulations using LANL’s Parallel Ocean Program (POP).

4:06PM H51.00005 The impact of the diurnal insolation cycle on the tropical cyclone heat engine . MORGAN E. O’NEILL, Department of Earth and Planetary Sciences, Weizmann Institute of Science, DIAMILET PEREZ-BETANCOURT, Program in Atmospheres, Oceans and Climate, Massachusetts Institute of Technology, ALLISON A. WING, Lamont-Doherty Earth Observatory, Columbia University — A hurricane, or tropical cyclone, is understood as a heat engine that moves heat from the warm sea surface to the cold tropopause. The efficiency of this engine depends in part on the strength and duration of solar heating. Over land, peak rainfall associated with individual thunderstorms occurs in the late afternoon. Over ocean, with its markedly higher surface heat capacity, deep convection responds more to radiational cooling than daytime surface heating. However, the role of daily varying solar forcing on the dynamics of tropical cyclones is poorly understood. Recently, Dunion et al. (2014) reported significant, repeating diurnal behavior propagating outward from tropical cyclone centers, using infrared imagery from nine years of North Atlantic tropical cyclones. We study the impact of the diurnal cycle on tropical cyclones using a high resolution 3D numerical model, the System for Atmospheric Modeling (Khairoutdinov and Randall 2003). Simulations are run with and without variable sunlight. We are able to reproduce the observational finding of Dunion et al. (2014), and further identify a diurnally-varying residual circulation in the tropical cyclone at midlevels. The impact of the diurnal cycle on the equilibrium dynamics of tropical cyclones is also discussed.

4:18PM H51.00006 Towards a General Turbulence Model for Planetary Boundary Layers Based on Direct Statistical Simulation 1, BRAD MARSTON, BAYLOR FOX-KEMPER, JOE SKITKA, Brown University — Sub-grid turbulence models for planetary boundary layers are typically constructed additively, starting with local flow properties and including non-local (KPP) or higher order (Mellor-Yamada) parameters until a desired level of predictive capability is achieved or a manageable threshold of complexity is surpassed. Such approaches are necessarily limited in general circumstances, like global circulation models, by their being optimized for particular flow phenomena. By using direct statistical simulation (DSS) that is based upon expansion in equal-time cumulants we offer the prospect of a turbulence model that is equally applicable to all flow types and able to take advantage of the wealth of nonlocal information in any flow. We investigate the feasibility of a second-order closure (CE2) by performing simulations of the ocean boundary layer in a quasi-linear approximation for which CE2 is exact. As oceanographic examples, wind-driven Langmuir turbulence and thermal convection are studied by comparison of the statistics of quasi-linear and fully nonlinear simulations. We also characterize the computational advantages and physical uncertainties of CE2 defined on a reduced basis determined via proper orthogonal decomposition (POD) of the flow fields.

1Supported in part by NSF DMR-1306806

4:30PM H51.00007 Non-equilibrium Statistical Mechanics and the Sea Ice Thickness Distribution . JOHN WETTLAUFER, SRIKANTH TOPPALADODDI, Yale University — We use concepts from non-equilibrium statistical physics to transform the original evolution equation for the sea ice thickness distribution $g(h)$ due to Thorndike et al., (1975) into a Fokker-Planck like conservation law. The steady solution is $g(h) = \mathcal{A}(q)h^{\epsilon}e^{-h/H}$, where $q$ and $H$ are expressible in terms of moments over the transition probabilities between thickness categories. The solution exhibits the functional form used in observational fits and shows that for $h \ll 1$, $g(h)$ is controlled by both thermodynamics and mechanics, whereas for $h \gg 1$ only mechanics controls $g(h)$. Finally, we derive the underlying Langevin equation governing the dynamics of the ice thickness $h$, from which we predict the observed $g(h)$. This allows us to demonstrate that the ice thickness field is ergodic. The genericity of our approach provides a framework for studying the geophysical scale structure of the ice pack using methods of broad relevance in statistical mechanics.

2Swedish Research Council Grant No. 638-2013-9243, NASA Grant NNH13ZDA001N-CRYO and the National Science Foundation and the Office of Naval Research under OCE-1332775 for support.

4:42PM H51.00008 Large-eddy simulation of the transient and near-equilibrium behavior of precipitating shallow convection . THIJS HEUS, Cleveland State University, AXEL SEIFERT, Deutscher Wetter Dienst, Offenbach, Germany, ROBERT PINCUS, University of Colorado, BJORN STEVENS, Max Planck Institute for Meteorology, Hamburg, Germany — Cloud-aerosol remain one of the largest uncertainties in climate modeling. Many of the postulated cloud-aerosol interactions involve precipitation to limit cloud size and life time, in particular for barely precipitating shallow cumulus clouds. If the precipitation exceeds a certain threshold, it will create feedback on the cloud field through cold pools and mesoscale organization. Such mesoscale responses have mostly been ignored so far in the discussion of aerosol indirect effects. We study the sensitivity of trade wind cumulus clouds to perturbations in cloud droplet number concentrations. Over time, the cloud system approaches a radiative-convective equilibrium state. The transient behavior and the properties of the near-equilibrium cloud field depend on the microphysical state and therefore on the cloud droplet number density. The primary response of the cloud field to changes in the cloud droplet number density is deepening of the cloud layer, and results in a shorter cloud life time. If the atmospheric time scales are long enough compared to the microphysical time scales, the cloud field may reach a near-equilibrium regime. In this regime, the decrease in cloud cover compensates much of the brightening of the clouds, and the overall effect on the albedo is small.

4:54PM H51.00009 Statistical state dynamics of jet/wave coexistence in beta-plane turbulence . NAVID CONSTANTINOU, Scrips Inst. of Oceanography, Univ of California - San Diego, BRIAN FARRELL, Department of Earth and Planetary Sciences, Harvard University, PETROS IOANNOU, Physics Department, National and Kapodistrian University of Athens — Jets are commonly observed to coexist in the turbulence of planetary atmospheres with planetary scale wave fields and embedded vortices. These large-scale coherent structures arise and are maintained in the turbulence on time scales long compared to dissipation or advective time scales. The emergence, equilibrium at finite amplitude, maintenance and stability of these structures pose fundamental theoretical problems. The emergence of jets and vortices from turbulence is not associated with an instability of the mean flow and their equilibration and stability at finite amplitude does not arise solely from the linear or nonlinear dynamics of these structures in isolation from the turbulence surrounding them. Rather the dynamics of these large-scale structures arises essentially from their cooperative interaction with the small-scale turbulence in which they are embedded. It follows that fundamental theoretical understanding of the dynamics of jets and vortices in turbulence requires adopting the perspective of the statistical state dynamics (SSD) of the entire turbulent state. In this work a theory for the jet/wave coexistence regime is developed using the SSD perspective.
Irvine, PNAS (In press).

Controlled distortions of the underlying lattice can induce a topological phase transition that switches the edge mode chirality. This effect allows the direction and are unaffected by disorder. We observe these edge modes in experiment and verify their robustness to disorder and the insertion of obstacles.

Chicago — Topological mechanical meta-materials are artificial structures whose unusual properties are protected very much like their electronic and optical counterparts. I will present an experimental and theoretical study of a new kind of active meta-material comprised of coupled gyroscopes on a lattice that breaks time-reversal symmetry. The vibrational spectrum displays a sonic gap populated by topologically protected edge modes which propagate in only one direction and are unaffected by disorder. We observe these edge modes in experiment and verify their robustness to disorder and the insertion of obstacles. Controlled distortions of the underlying lattice can induce a topological phase transition that switches the edge mode chirality. This effect allows the direction of the edge current to be determined on demand.

Curvature and one-dimensional sources of mean curvature, and our cutting and pasting rules maintain the intrinsic bond lengths on both the lattice and its dual. We find that a small set of rules is allowed providing a framework for exploring and building kirigami - folding, cutting, and pasting the edges of paper. These rules are very general and apply to pattern defects in elastic materials, thus promising improved control over hierarchical bending, buckling or folding processes. Generally, this study suggests that kirigami is a powerful tool for generating new structures.

Spherical, ellipsoidal and toroidal surfaces over a wide range of system sizes. However, both the localization of individual defects and the orientation of defect chains depend strongly on the local Gaussian curvature and its gradients across a surface. Our results imply that curvature and topology can be utilized to tailor the mechanical properties of materials.


We explore and develop a simple set of rules that apply to cutting, pasting, and folding honeycomb lattices. We consider origami-like structures that are extrinsically flat away from zero dimensional sources of Gaussian curvature and one-dimensional sources of mean curvature, and our cutting and pasting rules maintain the intrinsic bond lengths on both the lattice and its dual lattice. We find that a small set of rules is allowed providing a framework for exploring and building kirigami - folding, cutting, and pasting the edges of paper.


We investigate the influence of curvature and topology on crystalline wrinkling patterns in generic elastic bilayers. Our numerical analysis predicts that the total number of defects created by adiabatic compression exhibits universal quadratic scaling for spherical, ellipsoidal and toroidal surfaces over a wide range of system sizes. However, the localization of individual defects and the orientation of defect chains depend strongly on the local Gaussian curvature and its gradients across a surface. Our results imply that curvature and topology can be utilized to tailor the mechanical properties of materials.

Brown University — It has been claimed that graphene, with the elastic modulus of 1TPa and theoretical strength as high as 130 GPa, is the strongest material. However, from an engineering point of view, it is the fracture toughness that determines the actual strength of materials, as crack-like flaws (i.e., cracks, holes, notches, corners, etc.) are inevitable in the design, fabrication, and operation of practical devices and systems. Recently, it has been demonstrated that graphene has very low fracture toughness, in fact close to that of ideally brittle solids. These findings have raised sharp questions and are calling for efforts to explore effective methods to toughen graphene. Recently, we have been exploring the potential use of topological effects to enhance the fracture toughness of graphene. For example, it has been shown that a sinusoidal graphene containing periodically distributed disclination quadrupoles can achieve a mode I fracture toughness nearly twice that of pristine graphene. Here we report working progresses on further studies of topological toughening of graphene and other 2D materials. A phase field crystal method is adopted to generate the atomic coordinates of material with specific topological patterns. We then perform molecular dynamics simulations of fracture in the designed samples, and observe a variety of toughening mechanisms, including crack tip blunting, crack trapping, ligament bridging, crack deflection and daughter crack initiation and coalescence.

Joint work with Norbert Stoop, Romain Lagrange, Jorn Dunkel and Pedro M. Reis
8:00AM K40.00001 Combinatorial Mechanical Metamaterials, MARTIN VAN HECKE, Amolf Amsterdam & Leiden University — The structure of most mechanical metamaterials is periodic so that their design space is that of the unit cell. Here we introduce a combinatorial strategy to create a vast number of distinct mechanical metamaterials, each with a unique spatial texture and response. These are aperiodic stackings of anisotropic building blocks, and their functionality rests on both the block design and their stacking configuration which is governed by a tiling problem. We realize such metamaterials by 3D printing, and show that they act as soft machines, capable of pattern recognition and pattern analysis.

8:12AM K40.00002 Geometry Driven Pathways in Hierarchical Mechanical Metamaterials, CORENTIN COULAI, Leiden University / AMOLF, ALBERICO SABBADINI, Leiden University, MARTIN VAN HECKE, Leiden University / AMOLF — Using exactly positioned vacancies in flexible tessellations of squares, we create novel hierarchical mechanical metamaterials that can exhibit multiple shape changes under mechanical actuation. By designing bending, buckling and self-contact interactions, we unravel the link between geometry and dynamical pathways and engineer 2D transformers, which explore complex sequences of symmetrical shapes.

8:24AM K40.00003 Rigidity loss in disordered network materials, WOUTER G. ELLENBROEK, Eindhoven University of Technology, VARD A F. HAGH, AVISHEK KUMAR, Arizona State University, M.F. THORPE, Arizona State University and University of Oxford, MARTIN VAN HECKE, Leiden University and AMOLF — Weakly jammed sphere packings show a very peculiar elasticity, with a ratio of compression modulus to shear modulus that diverges as the number of contacts approaches the minimum required for rigidity. Creating artificial isotropic network materials with this property is a challenge: so far, the least elaborate way to generate them is to actually simulate weakly compressed repulsive spheres. The next steps in designing such materials hinge upon the combination of the dynamical properties of the sphere-packing derived network are essential for its elasticity. We elucidate the topological aspects of this question by comparing the rigidity transition in these networks to that in other random spring network models, including the common bond-diluted triangular net and a self-stress-free variant of that. We use the pebble game algorithm for identifying rigid clusters in mechanical networks to demonstrate that the marginally rigid state in sphere packings is perfectly isostatic everywhere, and the addition or removal of a single bond creates a globally stressed or globally floppy network, respectively. By contrast, the other classes of random network random networks show a more localized response to addition and removal of bonds, and, correspondingly, a more gradual rigidity transition.

8:36AM K40.00004 Foam-like compression behavior of fibrin networks, XIAOJUN LIANG, University of Pennsylvania, OLEG KIM, University of Notre Dame, RUSTEM LITVINOV, JOHN WEISSEL, University of Pennsylvania, MARK ALBER, University of Notre Dame, PRASHANT PUROHIT, University of Pennsylvania — The rheological properties of fibrin networks have been of long-standing interest, especially shear and tensile responses. Their compressive behavior, however, remains unexplored. We show that the compressive behavior of fibrin networks consists of three regimes: 1) an initial linear regime, in which most fibers are straight, 2) a plateau regime, in which more and more fibers buckle and collapse, and 3) a markedly non-linear regime, in which network densification occurs by bending of buckled fibers and inter-fiber contacts. Importantly, the spatially non-uniform network deformation included formation of a moving phase boundary along the axis of strain, which segregated the fibrin network into two phases with different fiber densities and structure. The Young’s modulus of the linear phase depends quadratically on the fibrin volume fraction while that in the densified phase depends cubically on it. The viscoelastic plateau regime corresponds to a change of volume fraction in mixture of these two phases. We model this regime using a continuum theory of phase transitions and analytically predict the storage and loss moduli. We show they are in good agreement with the experimental data. Our work shows that fibrin networks are a member of a broad class of natural cellular materials.

8:48AM K40.00005 Topological boundary modes in jammed matter, DANIEL SUSSMAN, OLAF STENULL, TOM LUBENSKY, University of Pennsylvania — Granular matter at the jamming transition is poised on the brink of mechanical stability, and hence it is possible that these random systems have topologically protected surface phonons. Studying two model systems for jammed matter, we find states that exhibit distinct mechanical topological classes, protected surface modes, and ubiquitous Weyl points. The detailed statistics of the boundary modes enable tests of a standard understanding of the detailed features of the jamming transition, and show that parts of this argument are invalid.

9:00AM K40.00006 Rigidity Percolation in Mechanical Metamaterials, LUUK LUBBERS, MARTIN VAN HECKE, Leiden University / AMOLF — We explore rigidity percolation of non-generic diluted tilings of rigid squares coupled by hinges. These compose the backbone of a range of mechanical metamaterials, and allow for a single degree of freedom motion even for full filling. We numerically study the onset and nature of additional floppy modes which arises when sufficient square tiles are removed.

9:12AM K40.00007 to be determined by you, JULIA GREER, California Institute of Technology — No abstract available.

9:48AM K40.00008 Multistable Compliant Auxetic Metamaterials Inspired by Geometric Patterns in Islamic Arts, AHMAD RAFSANJANI, DAMIANO PASINI, Mechanical Engineering Department, McGill University, PASINILAB TEAM — Beyond their aesthetic significance, geometric patterns in Islamic arts can offer a rich source of inspiration that can be used to create new mechanical metamaterials. In this work, we follow this route and present a new class of compliant mechanical metamaterials which simultaneously exhibit negative Poisson’s ratio and structural bistability. Designed by finite element simulations, this multifunctional metamaterial is fabricated by perforating a symmetric cut pattern into a sheet of natural rubber. Its building blocks are rotating units with square or triangular shapes connected together with compliant flexure hinges. Under the action of uniaxial extension, the relative rotation between the adjacent members triggers snap-through instability and brings together auxeticity and structural bistability. As a result, this metamaterial can accomplish reversible reconfiguration between two stable arrangements.

10:00AM K40.00009 The topology of gyroscopic metamaterials, LISA M. NASH, University of Chicago, DUSTIN KLECKNER, University of California, Merced, ALISMARY READ, University of Chicago, VINCENZO VITELLI, Institutut-Lorentz, Leiden University, ARI M. TURNER, Johns Hopkins University, WILLIAM T.M. IRVINE, University of Chicago — Mechanical metamaterials can have topological protected states, much like their electronic and optical counterparts. We recently demonstrated this in experiment by building a meta-material composed of coupled gyroscopes on a honeycomb lattice. This system breaks time-reversal symmetry and exhibits topologically protected one-way edge modes. In this talk we will explore the relationship between the topology of the band structure and the geometry of the lattice.
10:12AM K40.00010 Modeling the Mechanical Metamaterials with Confinement Controlled Response. JITIN SINGH, CORENTIN COULAIL, BASTIAAN FLORIJN, MARTIN VAN HECKE, Univ of Leiden / AMOLF. — Much of the physics of two-dimensional mechanical metamaterials can be understood from tilting of rigid-polygons connected by hinges. Here we map recently introduced programmable mechanical metamaterials which are elastic slabs patterned with circular holes of two different sizes to a tilting of hinged rectangles. Torsional springs in the hinges and linear springs at the outside of this mechanism allow us to capture the experimentally observed mechanical response, and we connect the physical design parameters to the shape of the rectangles, and the strength of the torsional springs. We finally show that this soft mechanism provides us with an inverse design tool for metamaterials.

10:24AM K40.00011 Taming the Exceptional Points of Parity-Time Symmetric Acoustics. MARC DUBOIS, CHENGZHI SHI, Univ of California - Berkeley, YUN CHEN, LEI CHENG, Fudan University, HAMIDREZA RAMEZANI, YUAN WANG, XIANG ZHANG, Univ of California - Berkeley — Parity-time (PT) symmetric concept and development lead to a wide range of applications including coherent perfect absorbers, single mode lasers, unidirectional cloaking and sensing, and optical isolators. These new applications and devices emerge from the existence of a phase transition in PT symmetric complex-valued potential obtained by balancing gain and loss materials. However, the systematic extension of such devices is adjourned by the key challenge in the management of the complex scattering process within the structure in order to engineer PT phase and exceptional points. Here, based on active acoustic elements, we experimentally demonstrate the simultaneous control of complex-valued potentials and multiple interference inside the structure at any given frequency. This method broadens the scope of applications for PT symmetric devices in many fields including optics, microwaves, electronics, which are crucial for sensing, imaging, cloaking, lasing, absorbing, and absorbing, etc.

10:36AM K40.00012 Overcoming dissipation with structure: Stable propagation of mechanical signals in soft mechanical metamaterials. KATIA BERTOLDI, JORDAN RANEY, Harvard University, NEEL NADKARNI, California Institute of Technology, CHIARA DARAIO, ETH, DENNIS KOCHMANN, California Institute of Technology, JENNIFER LEWIS, Harvard University — Soft structures with rationally designed architectures capable of large, nonlinear deformation present opportunities for the design of unprecedented, highly-tunable devices and machines. However, the highly-dissipative nature of soft materials has inherently limited the way in which such systems can be used. Here we present an architected soft system comprised of elastomeric, bistable beam elements connected by elastomeric linear springs. The dissipative nature of the polymer readily damps linear waves, preventing propagation of any mechanical signal beyond a short distance, as expected. However, the unique architecture of the system enables propagation of stable, nonlinear solitary transition waves with constant velocity and pulse geometry over arbitrary distances. Since the high damping of the material removes all other linear, small amplitude excitations, the desired pulse propagates with high fidelity and controllability. This phenomenon can be used for control signals as we demonstrate through the design of soft diodes and soft mechanical logic gates.

10:48AM K40.00013 Combinatorial Origami. PETER DIELEMAN, SCOTT WAITUKAITIS, MARTIN VAN HECKE, Leiden University, FOM Institute AMOLF. — To design rigidly foldable quadrilateral meshes one generally needs to solve a complicated set of constraints. Here we present a systematic, combinatorial approach to create rigidly foldable quadrilateral meshes with a limited number of different vertices. The number of discrete, 1 degree-of-freedom folding branches for some of these meshes scales exponentially with the number of vertices on the edge, whilst other meshes generated this way only have two discrete folding branches, regardless of mesh size. We show how these two different behaviours both emerge from the two folding branches present in a single generic 4-vertex. Furthermore, we model generic 4-vertices as a spherical linkage and exploit a previously overlooked symmetry to create non-developable origami patterns using the same combinatorial framework.

Wednesday, March 16, 2016 8:00AM - 10:36AM Session K43 GSNP: Complex Networks and their Applications I 346 - Flaviano Morone, City College of New York

8:00AM K43.00001 Influence maximization in complex networks through optimal percolation. FLAVIANO MORONE, HERNAN MAKSE, City College of New York. CUNY COLLABORATION, CUNY COLLABORATION. — The whole frame of interconnected complex networks hinges on a specific set of structural nodes, much smaller than the total size which, if activated, would cause the spread of information to the whole network, or, if immunized, would prevent the diffusion of a large scale epidemic. Localizing this optimal, that is, minimal, set of structural nodes, called influencers, is one of the most important problems in network science. Here we map the problem onto optimal percolation in random networks to identify the minimal set of influencers, which arises by minimizing the energy of a many-body system, where the form of the interactions is fixed by the non-backtracking matrix of the network. Big data analyses reveal that the set of optimal influencers is much smaller than the one predicted by previous heuristic centralities. Remarkably, a large number of previously neglected weakly connected nodes emerges among the optimal influencers. Reference: F. Morone, H. A. Makse, Nature 524,65-68 (2015)

8:12AM K43.00002 Collective opinion formation on fluctuating networks. VUDTIWAT NGAM-PRUETIKORN, Okinawa Institute of Science and Technology, GREG STEPHENS, Vrije Universiteit Amsterdam & Okinawa Institute of Science and Technology. — Thanks to the advent of online social networks, not only are we more connected than ever but we are also able to design and maintain our own social networks. An insight into this phenomenon will be key to understanding modern societies. To this end, we argue that active network maintenance exposes individuals to selective exposure (preference for agreeing information sources) and we explore how this could affect the structure of social networks and collective opinion formation. More technically, we investigate opinion dynamics on a complex network with fast stochastic rewiring. We show that selective exposure while inducing segregation of agents with different opinions, stabilises consensus state regardless of opinion update rules. We argue further that selective exposure can lead to a shorter time to consensus. The time to consensus has non-trivial dependence on the magnitude of selective exposure. Moreover, we find for some opinion updating rules, selective exposure can increase the lifetime of opinion segregation (polarisation of opinions).

8:24AM K43.00003 Choice Shift in Opinion Network Dynamics. MICHAEL GABBAY, University of Washington. — Choice shift is a phenomenon associated with small group dynamics whereby group discussion causes group members to shift their opinions in a more extreme direction so that the mean post-discussion opinion exceeds the mean pre-discussion opinion. Also known as group polarization, choice shift is a robust experimental phenomenon and has been well-studied within social psychology. In opinion network models, shifts toward extremism are typically produced by the presence of stubborn agents at the extremes of the opinion axis, whose opinions are much more resistant to change than moderate agents. However, we present a model in which choice shift can arise without the assumption of stubborn agents; the model evolves member opinions and uncertainties using coupled nonlinear differential equations. In addition, we briefly describe the results of a recent experiment conducted involving online group discussion concerning the outcome of National Football League games as described. The model predictions concerning the effects of network structure, disagreement level, and team choice (favorite or underdog) are in accord with the experimental results.

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1 This research was funded by the Office of Naval Research and the Defense Threat Reduction Agency.
8:36AM K43.00004 Social Network Influence and Personal Financial Status, SHAOJUN LUO, FLAVIANO MORONE, City College of CUNY, CARLOS SARRAUTE, Grandata, Buenos Aires, Argentina, HERMAN MAKSE, City College of CUNY — Networks of social ties emerging from individual economic needs display a highly structured architecture. In response to socio-economic demands, people reshape their circle of contacts for maximizing their social status, and ipso facto, the pattern of their interconnections is strongly correlates with their personal financial situation. In this work we transform this qualitative and verbal statement into an operative definition, which allows us to quantify the economic wellness of individuals trough a measure of their collective influence. We consider the network of mobile phone calls made by the Mexican population during three months, in order to study the correlation of person’s economic situation with her network location. Notably, we find that rich people tend to be also the most influential nodes, i.e., they self-organize to optimally position themselves in the network. This finding may be also raised at the level of a principle, a fact that would explain the emergence of the phenomenon of collective influence itself as the result of the local optimization of socio-economic interactions. Our method represents a powerful and efficient indicator of socio-economic robustness, which may be applied to maximize the effect of large scale economic intervention and stimulus policies.

8:48AM K43.00005 More Opportunities than Wealth: Inequality and Emergent Social Classes in a Network of Power and Frustration, CRISTIANO NISOLI, Los Alamos National Laboratory, BENOIT MAHAULT, Service de Physique de l’Etat Condense, CNRS UMR 8506, CEA-Saclay, 91191 Gif-sur-Yvette, France, AVADH SAXENA, Los Alamos National Laboratory — We introduce a minimal agent-based model to qualitatively conceptualize the allocation of limited wealth among more abundant opportunities. There the interplay of power, satisfaction and frustration determines the distribution, concentration, and inequality of wealth. Our framework allows us to compare subjective measures of frustration and satisfaction to collective measures of fairness in wealth distribution, such as the Lorenz curve and the Gini index. We find that a completely libertarian, law-of-the-jungle setting, where every agent can acquire wealth from, or lose wealth to, anybody else invariably leads to large inequality. The picture is however dramatically modified when hard constraints are imposed over agents, and they are limited to share wealth with neighbors on a network. We address dynamical societies via an out of equilibrium coevolution of the network, driven by a competition between power and frustration. The ratio between power and frustration controls different dynamical regimes separated by kinetic transitions and characterized by drastically different values of the indices of equality. In particular, it leads to the emergence of three self-organised social classes, lower, middle, and upper class, whose interactions drive a cyclical regime.

9:00AM K43.00006 Dynamic networks community detection via low rank component recovery of adjacency matrices, WEI BAO, GEORGE MICHAILIDIS, University of Michigan, Ann Arbor — Dynamic community detection in networks has been of high interest due to its various applications. In this work, we apply low rank extraction technique on adjacency matrices to approximate the community structures. Not only can the low rank approximation yield nice transition point times where significant changes in the community structures occur, but also can increase the accuracy of the core community structures recovered in the peace time ranges by averaging the low rank components. A systematic methodology has been proposed as how to accomplish the target. Factor model, and stochastic block model (including weighted scenario) have been tested for the robustness of our model. Besides, applications on both Kuramoto model and US Senate Roll Call data are also carried out and interesting results are obtained.

9:12AM K43.00007 Multiway spectral community detection in networks, XIAO ZHANG, MARK NEWMAN, Univ of Michigan - Ann Arbor — Spectral methods are widely used for community detection in networks because of their high efficiency and amenability to formal analysis. However, spectral algorithms have been limited to the division of networks into only two or three communities. Here we present a spectral algorithm that can divide a network into any number of a priori specified communities. We give a formal analysis of the algorithm via a mapping to a vector partitioning problem, which we solve using a fast heuristic. We then apply our algorithm to a variety of real world networks and find it to give superior results. We also give demonstrative applications of the algorithm to real-world networks and find that it produces results in good agreement with expectations for the networks studied.

9:24AM K43.00008 Utilizing Maximal Independent Sets as Dominating Sets in Scale-Free Networks, N. DERZSY, Rensselaer Polytechnic Institute, F. MOLNAR JR., Northwestern University, B. K. SZYMANSKI, G. KORNIS, Rensselaer Polytechnic Institute — Dominating sets provide key solution to various critical problems in networked systems, such as detecting, monitoring, or controlling the behavior of nodes. Motivated by graph theory literature [Erdos, Israel J. Math. 4, 233 (1966)], we studied maximal independent sets (MIS) as dominating sets in scale-free networks. We investigated the scaling behavior of the size of MIS in artificial scale-free networks with respect to multiple topological properties (size, average degree, power-law exponent, assortativity), evaluated its resilience to network damage resulting from random failure or targeted attack [Molnar et al., Sci. Rep. 5, 8321 (2015)], and compared its efficiency to previously proposed dominating set selection strategies. We showed that, despite its small set size, MIS provides very high resilience against network damage. Using extensive numerical analysis on both synthetic and real-world (social, biological, technological) network samples, we demonstrate that our method effectively satisfies four essential requirements of dominating sets for their practical applicability on large-scale real-world systems: 1.) small set size, 2.) minimal network information required for their construction scheme, 3.) fast and easy computational implementation, and 4.) resiliency to network damage.

9:36AM K43.00009 Growing Networks with Positive and Negative Links, CORYNNE DECH, SHADRACK ANTWI, LEAH SHAW, College of William and Mary — Scale-free networks grown via preferential attachment have been used to model real-world networks such as the Internet, citation networks, and social networks. Here we investigate signed scale-free networks where an edge represents a positive or negative connection. We present analytic results and simulation for a growing signed network model. We compare the signed network to an unsigned scale-free network. We discuss several options for preferential attachment in a signed network that could be further adapted to model the accumulation of links over time in real-world signed networks.

9:48AM K43.00010 Robustness of networks of networks with degree-degree correlation, BYUNGJOON MIN, City College of New York, SANTIAGO CANALS, Instituto de Neurociencias, HERNAN MAKSE, City College of New York — Many real-world complex systems ranging from critical infrastructure and transportation networks to living systems including brain and cellular networks are not formed by an isolated network but by a network of networks. Randomly coupled networks with interdependency between different networks may easily result in abrupt collapse. Here, we seek a possible explanation of stable functioning in natural networks of networks including functional brain networks. Specifically, we analyze the robustness of networks of networks focused on one-to-many interconnections between different networks and degree-degree correlation. Implication of the network robustness on functional brain networks of rats is also discussed.

10:00AM K43.00011 Degree distributions of bipartite networks and their projections, DEMIVAL VASQUES FILHO, DION O'NEALE, University of Auckland — Bipartite networks play an important role in the analysis of social and economic systems as they explicitly separate two distinct sets of nodes. The links between individuals or nodes in the bipartite network are of particular interest. Here we consider a general class of bipartite graphs characterized by a degree distribution on one set of nodes. Our results provide an analytic understanding of degree distributions of projections with respect to the degree of nodes in the original bipartite network. We consider random bipartite graphs with arbitrary degree sequences on either side of the projection, and demonstrate that the degree distribution of the projection follows a trend that can be predicted from the degree distribution on the original bipartite network.
10:12AM K43.00003 Effects of Microstructural Geometry for Computing Closure Models in Multiscale Modeling of Shocked Particle Laden Flow, OISHIK SEN, H.S. UDAYKUMAR, Univ of Iowa, GUSTAAF JACOBS, San Diego State University — Interaction of a shock wave with dust particles is a complex physical phenomenon. A computational model for studying this two-phase system is the Particle-Source in Cell (PSIC) approach. In this method, the dust particles are tracked as point particles in a Lagrangian frame of reference immersed in a compressible fluid. Two-way interaction between the carrier and the dispersed phases is ensured by coupling the momentum and energy transfer between the two phases as source terms in the respective governing equations. These source terms (e.g., drag force on particles) may be computed from resolved numerical simulations by treating each macroscopic point particle as an ensemble of cylinders immersed in a compressed fluid. However the drag so computed must be independent of the geometry of the mesoscale. In this work, the effect of the stochasticity of the microstructural geometry in construction of drag laws from resolved mesoscale computations is studied. Several different arrangement of cylinders are considered and the mean drag law as a function of Mach Number and Volume Fraction for each arrangement is computed using the Dynamic Kriging Method. The uncertainty in the drag forces arising because of the arrangement of the cylinders for a given volume fraction is quantified as 90% credible sets and the effect of the uncertainty on PSIC computations is studied.

Wednesday, March 16, 2016 8:00AM - 11:00AM — Session K53 DFD GSOFT GSNP: Granular and Multiphase Flows Hilton Baltimore Holiday Ballroom 4 -

8:00AM K53.00001 Ferrofluid-based Diamagnetic Particle Separation in U-shaped Microchannels, YILONG ZHOU, XIANGCHUN XUAN, Clemson University — We demonstrate in this talk a continuous-flow sheath-free separation method of diamagnetic particles in ferrofluids through U-shaped microchannels. Due to the action of a size-dependent magnetic force, diamagnetic particles are focused into a single stream in the inlet branch of the U-turn and then continuously separated into two streams in its outlet branch. We also develop a 3D numerical model to predict and understand the diamagnetic particle transport during the separation process. The numerical predictions are found to agree well with the experimental observations in a systematic study of multiple parameter effects including ferrofluid flow rate, concentration and magnet-channel separation method of diamagnetic particles in ferrofluids through U-shaped microchannels. Due to the action of a size-dependent magnetic force, diamagnetic particles are focused into a single stream in the inlet branch of the U-turn and then continuously separated into two streams in its outlet branch. We also develop a 3D numerical model to predict and understand the diamagnetic particle transport during the separation process. The numerical predictions are found to agree well with the experimental observations in a systematic study of multiple parameter effects including ferrofluid flow rate, concentration and magnet-channel separation.

1This work was supported by NSF.

10:12AM K43.00012 Spectra of Adjacency Matrices in Networks with Extreme Introverts and Extroverts, KEVIN E. BASSLER, Department of Physics, University of Houston, ROYCE K.P. ZIA, Department of Physics and Astronomy, Iowa State University, and Department of Physics, Virginia Tech — In recent studies of networks with preferred degrees (suitable for describing social networks in which individuals tend to prefer a certain number of contacts), the XIE model of extreme introverts and extroverts was found to display remarkable collective behavior and to raise interesting theoretical issues. Though this system is defined through its dynamics, i.e., introverts/extroverts always cut/add links, the steady state turns out to be a Boltzmann-like distribution. While the intra-group links are static, the cross-links are dynamic and lead to an ensemble of bipartite graphs, with extraordinary long-ranged correlations between elements of the incidence matrix (details in JSTAT P07013, 2015). Here, we report simulation studies of a different perspective of networks, namely, the spectra associated with this ensemble of adjacency matrices. As a baseline, we first consider the spectra associated with (the adjacency matrices of) a simple random (Erdős-Rényi) ensemble of bipartite graphs, where simulation results can be understood analytically.

Work supported by the NSF through grants DMR-1206839 and DMR-1507371.

10:24AM K43.00013 Complex root networks of Chinese characters, PO-HAN LEE, Affiliated Senior High School of National Taiwan Normal University, Taipei, Taiwan, JIA-LING CHEN, Chinese Department, National Taiwan Normal University, Taipei, Taiwan, PO-CHENG WANG, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan, TING-TING CHI, Chinese Department, National Taiwan Normal University, Taipei, Taiwan, ZHI-REN XIAO, ZIH-JIAN JHANG, Physics Department, National Taiwan University, Taipei, Taiwan, YEONG-NAN YEH, Institute of Mathematics, Academia Sinica, Nankang, Taipei, Taiwan, YIH-YIH CHEN, Physics Department, National Taiwan University, Taipei, Taiwan, CHIN-KUN HU, Institute of Physics, Academia Sinica, Taipei, Taiwan — There are several sets of Chinese characters still available today, including Oracle Bone Inscriptions (OBI) in Shang Dynasty, Chu characters (CC) used in Chu of Warring State Period, Small Seal Script in dictionary Shuowen Jiezi (SJ) in Eastern Han Dynasty, and Kangxi Dictionary (KD) in Qing Dynasty. Such as Chinese characters were all constructed via combinations of meaningful patterns, called roots. Our studies for the complex networks of all roots indicate that the roots of the characters in OBI, CC, SJ and KD have characteristics of small world networks and scale-free networks.

1This work was supported by the NSF through grants DMR-1206839 and DMR-1507371.
8:36AM K53.00004 Time dependent behavior of impact angle in turbulent pipe flows experiencing erosion.\textsuperscript{1} ANADOR GUZMAN, Pontificia Universidad Catolica de Chile, DIEGO OYARZUN\textsuperscript{2}, Universidad de Santiago de Chile, MAGDALENA WALCZAK\textsuperscript{1}, JAVIERA AGUIRRE\textsuperscript{1}, Pontificia Universidad Catolica de Chile — Erosion-corrosion in pipe systems transporting slurry turbulent flows is of a great importance in industrial and mining applications, where large volumes of suspended solids are sent up to hundreds of kilometers, to be further processed. The slurry is typically sent over large diameter steel pipes, which not always have an anti-abrasion coating. During the transport, the thickness of the pipe diminishes and eventually leaks and breaks, due to the combined effects of wear and corrosion. The processes of pipe degradation are further enhanced by the content of the slurry electrolytes that might switch from neutral to aggressive. The understanding of these processes in terms of operational parameters is critical for anticipating and mitigating a catastrophic outcome. This paper describes turbulent flow numerical simulations in a slurry transporting steel pipe with an emphasis on the correlation between the time dependent impact angle in the vicinity of the steel pipe and the rate of material loss. Full numerical simulations in a 3D long domain by using an Eulerian–Eulerian two phase flow approach coupled to a n–e–sion turbulent model are performed for different solid particle concentration and flow velocity and compared to existing experimental and numerical results for validation with and without gravity. Time-dependent axisymmetric turbulent flow simulations are performed for determining both the time dependent behavior of the axial and radial velocities near the pipe wall and the impact angle.

\textsuperscript{1}Financial support from Conicyt through the Fondecyt proposal 1141107 is acknowledged

\textsuperscript{2}Assistant Professor of Mechanical Engineering

8:48AM K53.00005 Caustics and the growth of droplets\textsuperscript{1} RAMA GOVINDARAJAN, S RAVICHANDRAN, TIFR Centre for Interdisciplinary Sciences, Hyderabad, India, SAMRIDDHI RAY, International Centre for Theoretical Sciences, TIFR, Bangalore, P DEEPU, TIFR Centre for Interdisciplinary Sciences, Hyderabad, India — Caustics are formed when inertial particles of very different velocities collide in a flow, and are a consequence of the dissipative nature of particle motion in a suspension. Using a model vortex-dominated flow with heavy droplets in a saturated environment, we investigate the dynamics of caustics and the way they form only within a neighborhood around a vortex, the square of whose radius is proportional to the product of circulation and particle inertia. Droplets starting close to this critical radius congregate very close together, resulting in large spikes in (Lagrangian) number density. Allowing for merger when droplets collide, we show that droplets starting out close to the critical radius display a much more rapid growth in size than those starting elsewhere, and a large fraction of the large droplets are those that originate within the caustics-forming region. We test these predictions in a two-dimensional simulation of turbulent flow. We hope that our study will be of interest in long-standing problems of physical interest such as the mechanism of broadening of droplet spectra in a turbulent flow.

\textsuperscript{1}Support from the Ministry of Earth Sciences, Government of India for the project Coupled physical processes in the Bay of Bengal and monsoon air-sea interaction under OMM is gratefully acknowledged

9:00AM K53.00006 Soft Sphere Suspensions: Flow and Relaxation. MARCEL WORKAMP, JOSHUA A. DIJKSMAN, Physical Chemistry and Soft Matter, Wageningen University — We experimentally study the role of particle elasticity on the rheology of soft sphere suspensions. Experiments allow us to probe the role of elastic timescales, relaxation and anisotropy in a custom 3D printed shear cell. We find robust rheological features, such as a flow instability, that are not well captured by existing models for suspension flows. In addition, we find relaxation effects after shear even in the absence of shear or thermal fluctuations. We aim to integrate these findings in the emerging unified framework for structured fluids.

9:12AM K53.00007 Impact cratering on granular beds: From the impact of raindrops to the strike of hailstones\textsuperscript{1} LEONARDO GORDILLO, JUNPING WANG, FRED JAPARDI, WARREN TEDDY, MING GAO, XIANG CHENG, CEMS — University of Minnesota — Impact craters generated by the impacts of a small object onto a granular bed strongly depend on the material properties of impactors. As an example, impact cratering by liquid drops and by solid spheres exhibits qualitatively different power-law scalings for the size of resulting impact craters. While the basic energy conservation and dimensional analysis provide simple guiding rules, the detailed dynamics governing the relation between these power-law scalings is still far from clear. To analyze the transition between liquid-drop and solid-sphere impact cratering, we investigate impact cratering by liquid drops for a wide range of viscosities over 7 decades. Using high-speed photography and laser profilometry, we delineate the liquid-to-solid transition and show the emergence of the two asymptotic behaviors and their respective power laws. We find that granular avalanches triggered by impacts are crucial in understanding the energy partition between impacted surfaces and impactors, which directly determines the observed scaling relations. A simple model is constructed for the initial stage of the impact that explains the energy partition during crater formation.

\textsuperscript{1}We acknowledge the support of NSF CAREER DMR-1452180. LG acknowledges fundings from CONICYT/BECAS CHILE 74160007.

9:24AM K53.00008 Scaling of liquid-drop impact craters in granular media\textsuperscript{1} RUNCHEN ZHAO, QIANYUN ZHANG, HENDRO TJUGITO, MING GAO, XIANG CHENG, University of Minnesota — Granular impact cratering by liquid drops is a ubiquitous phenomenon, directly relevant to many important natural and industrial processes such as soil erosion, drip irrigation, and dispersion of micro-organisms in soil. Here, by combining the high-speed photography with high precision laser profilometry, we investigate the liquid-drop impact dynamics on granular surfaces and monitor the morphology of resulting craters. Our experiments reveal novel scaling relations between the size of granular impact craters and important control parameters including the impact energy, the size of impinging drops and the degree of liquid saturation in a granular bed. Interestingly, we find that the scaling for liquid-drop impact cratering in dry granular media can be quantitatively described by the Schmidt-Holsapple scaling originally proposed for asteroid impact cratering. On the other hand, the scaling for impact craters in wet granular media can be understood by balancing the inertia of impinging drops and the strength of impacted surface. Our study sheds light on the mechanism governing liquid-drop impacts on dry/wet granular surfaces and reveals a remarkable analogy between familiar phenomena of raining and catastrophic asteroid strikes.

\textsuperscript{1}Scaling of liquid-drop impact craters in granular media

9:36AM K53.00009 Scaling of granular convective velocity and timescale of asteroidal resurfacing. TOMOYA YAMADA, KOUSUKE ANDO, TOMOKATSU MOROTA, HIROAKI KATSURAGI, Department of Earth and Environmental Sciences, Nagoya University — Granular convection is one of the well-known phenomena observed in a vertically vibrated granular bed. Recently, the possible relation between granular convection and asteroidal surface processes has been discussed. The granular convection on the surface of small asteroids might be induced by seismic vibration resulting from meteorite impacts. To quantitatively evaluate the timescale of asteroidal resurfacing by granular convection, the granular convective velocity under various conditions must be revealed. As a first step to approach this problem, we experimentally study the velocity scaling of granular convection using a vertically vibrated glass-beads layer. By systematic experiments, a scaling form of granular convective velocity has been obtained. The obtained scaling form implies that the granular convective velocity can be written by a power-law product of two characteristic velocity components: vibrational and gravitational velocities. In addition, the system size dependence is also scaled. According to the scaling form, the granular convective velocity is almost proportional to gravitational acceleration. Using this scaling form, we have estimated the resurfacing timescale on small asteroid surface.
9:48AM K53.00010 The Larger the Viscosity, the Higher the Bounce, MENACHEM STERN, MARTIN KLEIN SCHAARSBERG, IVO PETERS, KEVIN DODGE, WENDY ZHANG, HEINRICH JAEGGER, The Physics Department and the James Franck Institute, The University of Chicago — A low-viscosity liquid drop can bounce upon impact onto a solid. A high-viscosity drop typically just flattens, i.e., it splats. Surprisingly, our experiments with a droplet made of densely packed glass beads in silicone oil display the opposite behavior: the low-viscosity oil suspension drops splats.

The high-viscosity oil suspension bounces. Increasing solvent viscosity increases the rebound energy. To gain insight into the underlying mechanism, we model the suspension as densely packed elastic spheres experiencing viscous lubrication drag between neighbors. The model reproduces the observed trends. Plots of elastic compression and drag experienced by the particles show that rebounds are made possible by (1) a fraction of the impact energy being stored during initial contact via elastic compression, (2) a rapid broadening of local lubrication drag interactions at the initial impact site into a spatially uniform upward force throughout the drop. Including finite wall drag due to the presence of ambient air into the numerical model diminishes and eventually cuts off the rebound.

10:00AM K53.00011 Percolation velocity dependence on local concentration in bidisperse granular flows1, RYAN P. JONES, HONGYI XIAO, ZHEKAI DENG, PAUL B. UMBANHOWAR, RICHARD M. LUEPTOW, Northwestern University —

The percolation velocity, \( u_p \), of granular material in size or density bidisperse mixtures depends on the local concentration, particle size ratio, particle density ratio, and shear rate, \( \gamma \). Discrete element method computational results were obtained for bounded heap flows with size ratios between 1 and 3 and for density ratios between 1 and 4. The results indicate that small particles percolate downward faster when surrounded by large particles than large particles percolate upward when surrounded by small particles, as was recently observed in shear-box experiments. Likewise, heavy particles percolate downward faster when surrounded by light particles than light particles percolate upward when surrounded by heavy particles. The dependence of \( u_p/\gamma \) on local concentration results in larger percolation flux magnitudes at high concentrations of large (or light) particles compared to high concentrations of small (or heavy) particles, while local volumetric flux is conserved. The dependence of \( u_p/\gamma \) on local concentration can be incorporated into a continuum model, but the impact on global segregation patterns is usually minimal.

1Partially funded by Dow Chemical Company and NSF Grant No. CBET-1511450

10:12AM K53.00012 Impact of Overburden on Segregation in Sheared Granular Flow, ALEXANDER M. FRY, PAUL B. UMBANHOWAR, RICHARD M. LUEPTOW, Northwestern University — Dense granular materials tend to segregate into size or density graded regions when subjected to shear. Previous experiments demonstrated that overburden — normal confining pressure on a granular system — can slow the rate of size segregation in an annular shear cell. Here, we explore the effects of overburden on sheared granular material through Discrete Element Method (DEM) simulations in a planar shear cell geometry in which shear is applied by a moving bottom wall, while a massive upper wall provides the overburden. Segregation decreases with increasing overburden, but the picture is complicated by concurrent changes in the streamwise velocity profile. To decouple these effects, we also test an idealized system in which a desired streamwise velocity profile — and therefore shear rate — is imposed by applying additional horizontal forces to each particle. Based on this approach, we link the effect of overburden on segregation to the grain-scale behavior of the system. Partially funded by Procter & Gamble.

10:24AM K53.00013 Impact of a hydrophobic granular stream in water, BRIAN UTTER, Bucknell University, HARRY MANDELES, JACOB PARKHOUSE, James Madison University — We experimentally investigate the flow of a stream of hydrophobic granular particles impacting a water surface from above. The granular sample is composed of a mixture of hydrophobic and hydrophilic grains and the concentration, stream diameter, and drop height are independently controlled. While granular flows are common in nature and industry, effects of surface chemistry on flow behavior have received relatively little attention. The present experiment complements rheological measurements performed in parallel and aims to elucidate prior experiments on hydrophobic samples in a rotating drum. The present experimental geometry allows us to compare the behavior of granular streams to prior work on impacts of solids and fluid streams. Sequential images of the granular stream in water are taken and analyzed. We present data on the size, length, and shape of the aggregate streams with variations in concentration, entering stream diameter, and drop height. We find that increased hydrophobic grain concentration leads to increased aggregation due to an effectively cohesive interaction mediated by entrained air. At lower concentrations, the stream exhibits a lateral instability. Finally, we will make connections to rheology and rotating drum results.

1This work was supported by NSF CBET award 1067598.

10:36AM K53.00014 Numerical Simulation and Performance Optimization of a Magnetophoretic Bio-separation chip, MATIN GOLOZAR, JEFF DARABI, MAJID MOLKI, Southern Illinois University Edwardsville — Separation of micro/nanoparticles is important in biomedicine and biotechnology. This research presents the modeling and optimization of a magnetophoretic bio-separation chip for the isolation of biomaterials, such as circulating tumor cells (CTCs) from the peripheral blood. The chip consists of a continuous flow through microfluidic channels that contains locally engineered magnetic field gradients. The high gradient magnetic field produced by the magnets is spatially non-uniform and gives rise to an attractive force on magnetic particles that move through the flow channel. The computational model takes into account the magnetic and fluidic effects, we also test an idealized system in which a desired streamwise velocity profile — and therefore shear rate — is imposed by applying additional horizontal forces to each particle. Based on this approach, we link the effect of overburden on segregation to the grain-scale behavior of the system. Partially funded by Procter & Gamble.

10:48AM K53.00015 A Statistical investigation of sloshing parameters for multiphase offshore separators, MD MAHMUD, Lamar University, RAFIGUL KHAN, Cameron Corporation, QIANG XU, University of Chicago — A low-viscosity liquid drop can bounce upon impact onto a solid. A high-viscosity drop typically just flattens, i.e., it splats. Surprisingly, our experiments with a droplet made of densely packed glass beads in silicone oil display the opposite behavior: the low-viscosity oil suspension drops splats.

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Lamar University, Beaumont, TX 77710

1Partially funded by Dow Chemical Company and NSF Grant No. CBET-1511450

10:50AM K53.00016 The Larger the Viscosity, the Higher the Bounce, MENACHEM STERN, MARTIN KLEIN SCHAARSBERG, IVO PETERS, KEVIN DODGE, WENDY ZHANG, HEINRICH JAEGGER, The Physics Department and the James Franck Institute, The University of Chicago — A low-viscosity liquid drop can bounce upon impact onto a solid. A high-viscosity drop typically just flattens, i.e., it splats. Surprisingly, our experiments with a droplet made of densely packed glass beads in silicone oil display the opposite behavior: the low-viscosity oil suspension drops splats.

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1Partially funded by Dow Chemical Company and NSF Grant No. CBET-1511450
Wednesday, March 16, 2016 11:15AM - 2:15PM –
Session L3 DCMP GSNP GSOFT: Buckley, Lilienfeld and Onsager Prize Session  Ballroom III -
Sharon Glotzer, University of Michigan

11:15AM L3.00001 Photonic Crystals-Inhibited Spontaneous Emission: Optical Antennas-Enhanced Spontaneous Emission, ELI YABLONOVITCH, UC Berkeley Electrical Engineering and Computer Sciences Dept. — Photonic crystals are also part of everyday technological life in opto-electronic telecommunication devices that provide us with internet, cloud storage, and email. But photonic crystals have also been identified in nature, in the coloration of peacocks, parrots, chameleons, butterflies and many other species.

In spite of its broad applicability, the original motivation of photonic crystals was to create a “bandgap” in which the spontaneous emission of light would be inhibited. Conversely, the opposite is now possible. The “optical antenna” can accelerate spontaneous emission. Over 100 years after the radio antenna, we finally have tiny “optical antennas” which can act on molecules and quantum dots. Employing optical antennas, spontaneous light emission can become faster than stimulated emission.

11:51AM L3.00002 Julius Edgar Lilienfeld Prize: Lilienfeld Prize Lecture: Emergent Behavior in Quantum Matter, DAVID PINES, Physics Dept., U C Davis and UIUC, Santa Fe Institute — We live in an emergent universe in which interactions between the basic building blocks of matter and their environment give rise to unpredicted and unexpected emergent behavior at every scale. As physicists we seek to identify the organizing principles responsible for that behavior, construct soluble models that incorporate these, and explain experiment. In this lecture, I illustrate this approach to understanding emergent behavior in quantum matter through three examples: collective modes in electron, helium, and nuclear liquids; the emergence of superconductivity in conventional and unconventional superconductors, nuclei, and neutron stars; and the emergence of heavy electrons in Kondo lattice materials.

12:27PM L3.00003 Lars Onsager Prize: Phase transitions in massive data acquisition, MARC MEZARD, Ecole normale superieure - PSL Research University — The rapid increase in the amount of data that is presently being generated, acquired and processed opens new perspectives in many branches of science. In order to take full advantage of this data revolution, and to turn it into a major tool for scientific discoveries, new concepts and methods need to be developed, thus allowing us to focus on the extraction of significant information. Referring to the case of compressed sensing, the talk will show how ideas and methods in statistical physics -from spin glass theory to crystal nucleation - can help design faster, less destructive, and more efficient signal acquisition protocols, with possible applications in numerous fields -from magnetic resonance imaging to astronomy, tomography, or gene interaction network reconstruction.

1:03PM L3.00004 Lars Onsager Prize: The mean field solution for Hard Sphere Jamming and a new scenario for the low temperature landscape of glasses, GIORGIO PARISI, University of Rome, “La Sapienza”, Italy — In a hard spheres systems particles cannot overlap. Increasing the density we reach a point where most of the particles are blocked and the density cannot be increased any more: this is the jamming point. The jamming point separates the phase, where all the constraint can be satisfied, from an unsatisfiable phase, where spheres do have to overlap. A scaling theory of the behavior around the jamming critical point has been formulated and a few critical exponents have been introduced. The exponents are apparently super-universal, as far as they do seem to be independent from the space dimensions. The mean field version of the model (i.e. the infinite dimensions limit) has been solved analytically using broken replica symmetry techniques and the computed critical exponents have been found in a remarkable agreement with three-dimensional and two-dimensional numerical results and experiments. The theory predicts in hard spheres (in glasses) a new transition (the Gardener transition) from the replica symmetric phase to the replica broken phase at high density (at low temperature), in agreement with simulations on hard sphere systems. I will briefly discuss the possible consequences of this new picture on the very low temperature behavior of glasses in the quantum regime.

1:39PM L3.00005 Lars Onsager Prize: Optimization and learning algorithms from the theory of disordered systems, RICCARDO ZECCHINA, Politecnico di Torino — The extraction of information from large amounts of data is one of the prominent cross disciplinary challenges in contemporary science. Solving inverse and learning problems over large scale data sets requires the design of efficient optimization algorithms over very large scale networks of constraints. In such a setting, critical phenomena of the type studied in statistical physics of disordered systems often play a crucial role. This observation has lead in the last decade to a cross fertilization between statistical physics, information theory and computer science, with applications in a variety of fields. In particular a deeper geometrical understanding of the ground state structure of random computational problems and novel classes of probabilistic algorithms have emerged. In this talk I will give a brief overview of these conceptual advances and I will discuss the role that subdominant states play in the design of algorithms for large scale optimization problems. I will conclude by showing how these ideas can lead to novel applications in computational neuroscience.

Wednesday, March 16, 2016 11:15AM - 2:15PM –
Session L40 GSNP GSOFT: Geometry and Dynamics of Slender Structures  343 - James Hanna,
Virginia Tech

11:15AM L40.00001 Hamiltonian formulations in the computation of extremely deformed nano-scale hyper-elastic rods, JOHN H. MADDOCKS, EPFL FSB MATHEGEO LCVM — There has been a recent resurgence of interest in models exploiting elastic filaments and ribbons, motivated in large part by nano-scale applications, including DNA. Such models are frequently near-inextensible or nearly unsharable. I will describe how such systems can be modelled as a smooth limit within a hierarchy of perturbed Hamiltonian formulations of the governing equations. Examples include a sequence-dependent double-strand birod model of DNA, where a more familiar rod model can be obtained as a smooth limit in which the intra-strand degrees of freedom are frozen.

11:51AM L40.00002 A conserved quantity in thin body dynamics, JAMES HANNA, HODJAT PENDAR, Virginia Tech — We use an example from textile processing to illustrate the utility of a conserved quantity associated with metric symmetry in a thin body. This quantity, when combined with the usual linear and angular momentum currents, allows us to construct a four-parameter family of curves representing the equilibrium of a rotating, flowing string. To achieve this, we introduce a non-material action of mixed Lagrangian-Eulerian type, applicable to fixed windows of axially-moving systems. We will point out intriguing similarities with Bernoulli’s equation, discuss the effects of axial flow on rotating conservative systems, and make connections with 19th- and 20th-century results on the dynamics of cables.
12:03PM L40.00003 Tearing of thin spherical shells adhered to equally curved rigid substrates.
CONNOR MCMAHAN, ANNA LEE, JOEL MARTHELOT, PEDRO REIS, Massachusetts Institute of Technology — Lasik (Laser-Assisted in Situ Keratomileusis) eye surgery involves the tearing of the corneal epithelium to remodel the corneal stroma for corrections such as myopia, hyperopia and astigmatism. One issue with this procedure is that during the tearing of the corneal epithelium, if the two propagating cracks coalesce, a flap detaches which could cause significant complications in the recovery of the patient. We seek to gain a predictive physical understanding of this process by performing precision desktop experiments on an analogous system. First, thin spherical shells of nearly uniform thickness are fabricated by the coating of hemispherical molds with a polymer solution, which upon curing yields an elastic and brittle structure. We then create two notches near the equator of the shell and tear a flap by pulling tangentially to the spherical substrate, towards its pole. The resulting fracture paths are characterized by high-resolution 3D digital scanning. Our primary focus is on establishing how the positive Gaussian curvature of the system affects the path of the crack tip. Our results are directly contrasted against previous studies on systems with zero Gaussian curvature, where films were torn from planar and cylindrical substrates.

12:15PM L40.00004 Cracks in Sheets Draped on Curved Surfaces, NOAH P. MITCHELL, James Franck Institute, University of Chicago, VINZENZ KONING, VINZENZO VITELLI, Institutu-Lorentz for Theoretical Physics, Universiteit Leiden, WILLIAM T. M. IRVINE, James Franck Institute, University of Chicago — Conforming materials to surfaces with Gaussian curvature has proven a versatile tool to guide the behavior of mechanical defects such as folds, blisters, scars, and pleats. In this talk, we show how curvature can likewise be used to control material failure. In our experiments, thin elastic sheets are confined on curved geometries that stimulate or suppress the growth of cracks, and steer or arrest their propagation. By redistributing stresses in a sheet, curvature provides a geometric tool for protecting certain regions and guiding crack patterns. A simple model captures crack behavior at the onset of propagation, while a 2D phase-field model successfully captures the crack’s full phenomenology.

12:27PM L40.00005 Pick-up, impact, and peeling. , HARMHEET SINGH, JAMES HANNA, Virginia Tech — We consider a class of problems involving a one-dimensional, extensible body with a propagating discontinuity (shock) associated with partial contact with a rigid obstacle providing steric, frictional, or adhesive forces. This class includes the pick-up and impact of an axially flowing string or cable, and the peeling of an adhesive tape. The dynamics are derived by applying an action principle to a non-material volume. The resulting boundary conditions provide momentum and energy jump conditions at the shock. These are combined with kinematic conditions on velocities and accelerations to obtain families of steady-state solutions parameterized by the shock velocity and momentum and energy sources. We find relationships between the jump in stress, injection of momentum, and dissipation of energy, which we apply to specific cases and compare with other results in the literature on chain fountains, falling folded chains, and impulsively loaded cables. Time permitting, we will briefly discuss the possibility of using kinematic conditions and information about accelerating or otherwise unsteady forms of the adjoining bulk solutions to construct an equation of motion of the shock.

12:39PM L40.00006 Effect of boundary conditions on the buckling instabilities of a ribbon under twist. , CASEY TRIMBLE, ARSHAD KUDROLLI, Department of Physics, Clark University — We investigate the buckling instabilities of a thin flat sheet in the shape of a ribbon which is held at its ends and twisted under tension. Recently it was shown that such a system with clamped boundary conditions exhibited a rich variety of buckled shapes with longitudinal and transverse wrinkles as a function of applied twist and tension for a given ribbon aspect ratio and elastic modulus [1], which could be described by a far from threshold analysis of the covariant form of the Foppl-von Karman equations [2]. Here, we focus on the effect of the boundary conditions on the observed buckled patterns by constraining the ends only at the mid-point towards imposing free boundary conditions normal to the ribbon. In particular, we compare and contrast the observed phase diagram and the shape of the longitudinal and transverse buckled modes as a function of applied constraints. [1] J. Chopin and A. Kudrolli, Phys. Rev. Lett. 111, 174302 (2013). [2] J. Chopin, V. Demery, and B. Davidovitch J. Elast. 119, 137 (2015).

12:51PM L40.00007 Multi-stability and bifurcations of a thin band. , TIAN YU, JAMES HANNA, Department of Biomedical Engineering and Mechanics, Virginia Tech — Thin band- or strip-like structures are common motifs in flexible and deployable systems, serving as integrated connectors, hinges, and umbilicals. The morphing systems impose variable constraints on these components, inducing complex responses. We experimentally investigate a simple configuration representing the above type, a thin elastic band with end constraints on position and orientation. These constraints correspond to a combination of compression and shear with respect to a flat rectangular rest configuration. We vary the aspect ratio of the band, and the position and clamping angle at its ends. The buckled structure remains developable up to limiting deformations that approach one of two states, each dominated by two singularities. At intermediate deformations, the structure may adopt many distinct stable states. Transitions between these states can be smooth or violent, and depend strongly on constraints such as the clamping angle. Time permitting, we will relate our results to the behavior of anisotropic rods, and of strips subjected to twisting and extension.

1:03PM L40.00008 Finite and infinite wavelength elastocapillary instabilities with cylindrical geometry, JOHN BIGGINS, CHEN XUAN, Cambridge University — In an elastic cylinder with shear modulus $\mu$, radius $R_0$ and surface tension $\gamma$ we can define an emergent elastocapillary length $l = \gamma/\mu$. When this length becomes comparable to $R_0$, the cylinder undergoes a Rayleigh-Plateaux type instability, but surprisingly, with infinite wavelength $\lambda$ rather than with wavelength $\lambda \sim R_0 \sim l$. Here we take advantage of this infinite wavelength behaviour to construct a simple 1-D model of the elastocapillary instability in a cylindrical gel which permits a high-amplitude fully non-linear treatment. In particular, we show that the instability is sub-critical and entirely dependent on the elastic cylinder being subject to tension. We also discuss elastocapillary instabilities in a range of other cylindrical geometries, such as a cylindrical cavities through a bulk elastic solid, or a solid cylinder embedded in a bulk elastic solid, and show that in these cases instability has finite wavelength. Thus infinite wavelength behaviour is a curiosity of elastic cylinders rather than the generic behaviour or elastocapillary instabilities.

1:15PM L40.00009 Sequential buckling of an elastic wall1, JOSE BICO, HADRIEN BENSE, LUDOVIC KEISER, BENOIT ROMAN, PMMH, ESPCI, Paris, France, FRANCISCO MELO, Universidad de Santiago de Chile, MANOUK ABKARIAN, Centre de Biochimie Structurale, Montpellier, France — A beam under quasistatic compression classically buckles beyond a critical threshold. In the case of a free beam, the lowest buckling mode is selected. We investigate the case of a long wall grounded of a compliant base and compressed in the axial compression. In the case of a wall of slender rectangular cross section, the selected buckling mode adopts a nearly fixed wavelength proportional to the height of the wall. Higher compressive loads only increase the amplitude of the buckle. However if the cross section has a sharp shape (such as an Eiffel tower profile), we observe successive buckling modes of increasing wavelength. We interpret this unusual evolution in terms of scaling arguments. At small scales, this variable periodicity might be used to develop tunable optical devices.

1Supported by NSF DMR - 1508186
1We thank ECOS C12E07, CNRS-CONICYT, and Fondecyt Grant No. N1110922 for partially funding this work.
that is capable of constructing such objects, along with many other non-Euclidean plates. This work is the first to address the unusual mechanical properties of constrained non-Euclidean elastic objects. We also present a novel experimental system of the model allows us to calculate key quantities of interest in closed form. By varying the parameter $\alpha$ the target node with stopping probability node to a randomly chosen node in network B, called the target node. We then assign the neighbors of the source node to the neighborhood of the target node localization of node placement in network B using a single parameter. Starting from an unassigned node in network A, called the source node, we first map this surfaces with different extensions leads to a complete degeneracy of the bulk elastic energy of the minimal spring under elongation. This degeneracy is removed of the minimal spring is hyperbolic, and can be embedded as a minimal surface. We argue that the existence of a continuous set of such isometric minimal preferential curvature can be related to an effective compression, and hence a confining force that can vary spatially. This suggests a simple experimental setup, where we have characterised a variety of wrinkle patterns that can be generated for different mechanical properties and natural curvatures.

In two dimensions this type of problem is typically considered by the model of an Euler-RAN, Max Planck Institute for Dynamics and Self-Organization, ELENI KATIFORI, University of Pennsylvania, LUCAS GOEHRING, Max Planck Institute for Dynamics and Self-Organization — The wrinkling and folding transitions of thin elastic sheets have been extensively studied in the last decade. The exchange of energy from stretching to bending acts as a paradigm for a whole range of elastic instabilities, including the wrinkling of the gut, and the crinkling of leaves. In two dimensions this type of problem is typically considered by the model of an Euler-elastic in compressive confinement. We show that, even without any external forces, an elastic surface supported by a fluid can bend and wrinkle when it acquires a non-zero natural curvature. Locally, we will demonstrate how a preferential curvature can be related to an effective compression, and hence a confining force that can vary spatially. This suggests a simple experimental setup, where we have characterised a variety of wrinkle patterns that can be generated for different mechanical properties and natural curvatures.

Anomalously soft non-Euclidean spring, IDO LEVIN, ERAN SHARON, Hebrew Univ of Jerusalem — In this work we study the mechanical properties of a frustrated elastic ribbon spring - the non-Euclidean minimal spring. This spring belongs to the family of non-Euclidean plates: it has no spontaneous curvature, but its lateral intrinsic geometry is described by a non-Euclidean reference metric. The reference metric of the minimal spring is hyperbolic, and can be embedded as a minimal surface. We argue that the existence of a continuous set of such isometric minimal surfaces with different extensions leads to a complete degeneracy of the bulk elastic energy of the minimal spring under elongation. This degeneracy is removed only by boundary layer effects. As a result, the mechanical properties of the minimal spring are unusual: the spring is ultra-soft with rigidity that depends on the thickness, $t$, as $t^{-1/2}$, and does not explicitly depend on the ribbon’s width. These predictions are confirmed by a numerical study of a constrained spring. This work is the first to address the unusual mechanical properties of constrained non-Euclidean elastic objects. We also present a novel experimental system that is capable of constructing such objects, along with many other non-Euclidean plates.

Wednesday, March 16, 2016 11:15AM - 1:51PM – Session L43 GSNP: Complex Networks and their Applications II 346 - Mason Porter, Oxford University

Flexible embedding of networks, JUAN FERNANDEZ-GRACIA, CAROLINE BUCKEE, JUKKA-PEKKA ONNELA, Harvard T.H. Chan School of Public Health — We introduce a model for embedding one network into another, focusing on the case where network A is much bigger than network B. Nodes from network A are assigned to the nodes in network B using an algorithm where we control the extent of localization of node placement in network B using a single parameter. Starting from an unassigned node in network A, called the source node, we first map this node to a randomly chosen node in network B, called the target node. We then assign the neighbors of the source node to the neighborhood of the target node using a random walk based approach. To assign each neighbor of the source node to one of the nodes in network B, we perform a random walk starting from the target node with stopping probability $\alpha$. We repeat this process until all nodes in network A have been mapped to the nodes of network B. The simplicity of the model allows us to calculate key quantities of interest in closed form. By varying the parameter $\alpha$, we are able to produce embeddings from very local ($\alpha = 1$) to very global ($\alpha \rightarrow 0$). We show how our calculations fit the simulated results, and we apply the model to study how social networks are embedded in geography and how the neurons of C. Elegans are embedded in the surrounding volume.

Exploring many-body physics with deep networks, GIACOMO TORLAI, University of Waterloo, JUAN CARRASQUILLA, Perimeter Institute, DAVID SCHWAB, Northwestern University, ROGER MELKO, University of Waterloo — The introduction of neural networks with deep architecture has led to a revolution, giving rise to a new wave of technologies empowering our modern society. Although data science has been the main focus, the idea of generic algorithms which automatically extract features and representations from raw data is quite general and applicable in multiple scenarios. Motivated by the effectiveness of deep learning algorithms in revealing complex patterns and structures underlying data, we are interested in exploiting such tool in the context of many-body physics. In this talk we will focus on how to extract information about the physics of a many-body system from the generative training of a deep network, and ultimately consider discriminative tasks, such as phase diagrams estimation and critical points detection. We will discuss results for different classical spin systems, including models with quenched disorder.

Random walks on networks, ISAAC DONNELLY, Northeastern — Random walks on lattices are a well used model for diffusion on continuum. They have been modelled as diffusive systems, systems with forcing and reactions as well as a combination of the three. We extend the traditional random walk framework to the network to obtain novel systems. As an example due to the small graph diameter, the early time behaviour of subdiffusive dynamics dominates the observed system which has implications for models of the brain or airline networks.

I would like to thank the Australian American Fulbright Association
11:51AM L43.00004 The Impact of Selectivity on Fitness Evolution in the Multi-Generational Matching Problem

STEPHEN DIPPLE, TAO JIA, GYORGY KORNISS, BOLESLAW SZYMANSKI, Rensselaer Polytechnic Institute — The stochastic matching hypothesis has been found to produce self-similar pairing without explicitly requiring self-similarity in the rules for matching. Here, we introduce an added complexity of selectivity in which the relative probability of being matched are modified. This allows for probing in areas between the currently established matching hypothesis, random matching, and the extreme case of super selectivity, where only the very best fitness matches for nodes are created. A higher selectivity parameter has been found to indirectly increase the number of matches in the system monotonically. A fairly simple model is then implemented to produce offspring who inherit fitness based on the inherited fitness distribution which is a function of the parents’ fitness. While the results show that the specific distribution used may limit the inherited quality factors to a too narrow range to be broadly applicable, the model does expose some interesting patterns in fitness evolution across multiple generations in the context of selectivity and network degree distribution.

1:03PM L43.00005 A matrix product algorithm for stochastic dynamics on locally tree-like graphs

THOMAS BARTHIEL, Duke University, Department of Physics, CATERINA DE BACCO, SILVIO FRANZ, Université Paris-Sud, LPTMS — In this talk, I describe a novel algorithm for the efficient simulation of generic stochastic dynamics of classical degrees of freedom defined on the vertices of locally tree-like graphs. Such models correspond for example to spin-glass systems, Boolean networks, neural networks, or other technological, biological, and social networks. Building upon the cavity method and ideas from quantum many-body theory, the algorithm is based on a matrix product approximation of the so-called edge messages - conditional probabilities of variable vertex trajectories. The matrix product edge messages (MPEM) are constructed recursively. Computation costs and accuracy can be tuned by controlling the matrix dimensions of the MPEM in truncations. In contrast to Monte Carlo simulations, the approach has a better error scaling and works for both, single instances as well as the thermodynamic limit. Due to the absence of cancellation effects, observables with small expectation values can be evaluated accurately, allowing for the study of decay processes and temporal correlations with unprecedented accuracy. The method is demonstrated for the prototypical non-equilibrium Glauber dynamics of an Ising spin system. Reference: arXiv:1508.03295.

12:27PM L43.00007 Properties of the networks of same-spin sites in each Ising Model macrostate

ROBERT HOSKEN, The Aerospace Corporation — An Ising Model macrostate contains all the microstates with the same energy. Each macrostate is labeled in an energy two-space by the two sums in the Hamiltonian, one for the magnetism and the other for the interaction energy. In a single macrostate, a network can be defined for all the up-spin sites and another network for all the down-spin sites. An exact formula has been derived that explicitly provides the total number of connection links (edges) in both of these macrostate networks. This derivation follows from a meticulous analysis of the calculation of the sum of the product of spins in the Hamiltonian. It is applicable to one, two, and three dimension Ising models with periodic boundary conditions. The formula permits calculation of the total number of nearest-neighbor connections for all of the sites, and thus the average number of connections per site. The number of connections can be used to calculate the probability that a nearest neighbor in a particular direction at a spin site has the same spin. This probability can be used to infer the closeness of any macrostate to the ferromagnetic ground states, the paramagnetic region, or the anti-ferromagnetic ground states. Note that these properties of each macrostate do not require knowledge of the number of microstates in the macrostate (the density of states).

12:39PM L43.00008 Upper Bound for the Ordering Transition on an Ising Model on a Graph

TIMOTHY DOWNING, LEONID PRYADKO, Univ of California - Riverside — We present an upper bound for the ordering transition of a ferromagnetic Ising model on a graph. Namely, we show that at any given temperature, the magnetic susceptibility per spin cannot exceed that on an infinite tree, the universal cover of the original graph. Exact solution of the Ising model on the tree can be obtained using Bethe-Peierls expansion (also known as Belief Propagation). The corresponding transition point is given by a solution of an eigenvalue problem.

1:27PM L43.00009 Spectral renormalization group theory on nonspatial networks

ASLI TUNCER, AYSE ERZAN, Istanbul Tech Univ — We recently proposed a "spectral renormalization group" scheme, for non-spatial networks with no metric defined on them. We implemented the spectral renormalization group on two deterministic non-spatial networks without translational invariance, namely the Cayley tree and diamond lattice. The thermodynamic critical exponents for the Gaussian model are only functions of the spectral dimension, \( \tilde{d} \). The Gaussian fixed point is stable up to second order on these lattices with \( \tilde{d} = 2 \), the lower critical dimension for the Ising universality class. This is expected for the Cayley tree, but for the diamond lattice it is an indication that the perturbation expansion up to second order breaks down at \( \tilde{d} = 2 \), as it does for the Wilson scheme on the square lattice. On generalized diamond lattices, with \( 2 < \tilde{d} < 4 \), we find non-Gaussian fixed points with non-trivial exponents. For \( \tilde{d} > 4 \), the critical behavior is once again mean field.

1:03PM L43.00010 Real beards and real networks: a spin-glass model for interacting individuals

DION O'NEALE, University of Auckland — "I want to be different, just like all the other different people" sang the band King Missile. Whether they are the Beatniks of the 1950s, the punks of the 1970s, or the hipsters of today, non-conformists often tend to look the same, seemingly at odds with their goal of non-conformity. The spin-glass model, originally developed to describe the interaction of magnetic spins, and since applied to situations as diverse as the electrical activity of networks of neurons, to trades on a financial market, has recently been used in social science to study populations of interacting individuals comprised of a mix of both conformists and anti-conformists - or hipsters. Including delay effects for the interactions between individuals has been shown to give a system with non-trivial dynamics with a phase transition from stable behaviour to periodic switching between two states (let's call them bushy bearded and clean shaven). Analytic solutions to such a model are possible, but only for particular assumptions about the interaction and delay matrices. In this work we will show what happens when the interactions in the model are based on real-world networks with "small-world" effects and clustering.
1:15PM L43.00011 Condensation and transport in the totally asymmetric inclusion process (TASIP)¹, JOHANNES KNEBEL, MARKUS F WEBER, LMU Munich, TORBEN KRUEGER, IST Austria, ERWIN FREY, LMU Munich — Transport phenomena are often modeled by the hopping of particles on regular lattices or networks. Such models describe, e.g., the exclusive movement of molecular motors along microtubules: no two motors may occupy the same site. In our work, we study inclusion processes that are the bosonic analogues of the fermionic exclusion processes. In inclusion processes, many particles may occupy a single site and hopping rates depend linearly on the occupation of departure and arrival sites. Particles thus attract other particles to their own site. Condensation occurs when particles collectively cluster in one or multiple sites, whereas other sites become depleted. We showed that inclusion processes describe both the selection of strategies in evolutionary zero-sum games and the condensation of non-interacting bosons into multiple quantum states in driven-dissipative systems. The condensation is captured by the antisymmetric Lotka-Volterra equation (ALVE), which constitutes a nonlinearly coupled dynamical system. We derived an algebraic method to analyze the ALVE and to determine the condensates. Our approach allows for the design of networks that result in condensates with oscillating occupations, and yields insight into the interplay between network topology and transport properties.

¹Deutsche Forschungsgemeinschaft (SFB-TR12), German Excellence Initiative (Nanosystems Initiative Munich), Center for NanoScience Munich

1:27PM L43.00012 Multi-frequency and edge localized modes in mechanical and electrical lattices, LARS ENGLISH, Dickinson College, FAUSTINO PALMERO, University of Seville, PANAYOTIS KEVREKIDIS, University of Massachusetts — We present experimental evidence for the existence of a type of dynamical, self-localized mode called a multi-frequency breather in both a mechanical lattice of pendula and an electrical lattice. These modes were excited and stabilized by subharmonic driving. We also experimentally characterize dynamical modes that are localized on the edges of the pendulum chain, as well as in 2D electrical lattices. In the latter system, we briefly discuss the role of lattice topology in the stability of such modes.

1:39PM L43.00013 Stokes Trap: Multiplexed particle trapping and manipulation using fluidics, ANISH SHENOY, CHARLES SCHROEDER, University of Illinois at Urbana-Champaign — We report the development of the Stokes Trap, which is a multiplexed microfluidic trap for control over an arbitrary number of small particles in a microfluidic device. Our work involves the design and implementation of “smart” flow-based devices by coupling feedback control with microfluidics, thereby enabling new routes for the fluidic-directed assembly of particles. Here, we discuss the development of a new method to achieve multiplexed microfluidic trapping of an arbitrary number of particles using the sole action of fluid flow. In particular, we use a Hele-Shaw microfluidic cell to generate hydrodynamic forces on particles in a viscous-dominated flow defined by the microdevice geometry and imposed peripheral flow rates. This platform allows for a high degree of flow control over individual particles and can be used for manufacturing novel particles for fundamental studies, using fluidic-directed assembly. From a broader perspective, our work provides a solid framework for guiding the design of next-generation, automated on-chip assays.

11:30AM - 11:30AM Session M1 DPOLY DBIO GSOFT GSNP DFD: Poster Session II (Wednesday, 11:30 am - 2:30 pm) Exhibit Hall EF -

M1.00001 POLYMER PHYSICS —

M1.00002 Morphology Evolution and Dynamic Viscoelastic Behavior of Ternary Elastomer Blends under Shear¹, XIA DONG, XUANGUI LIU, CHARLES C HAN, DUJIN WANG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry CAS — The influence of nanoparticle geometry, such as size and shape, on the phase morphology of partially miscible binary polymer blends under and after shear has been examined by rheological and rheo-optical techniques. The phase morphologies of the solution-processed styrene-butadiene rubber and low vinyl content polyisoprene (SSBR/LPI) blend systems were affected by the dispersion status of fillers which were determined by filler shapes and shear strength. Under weak shear flow, the domain morphology of the OMMT filled blend was much thinner than that of the SiO₂ filled blend. Under strong shear flow, the string-like phase interface of the OMMT filled blend was much blurred compared with that of the SiO₂ filled blend. After shear cessation, the orientation status of OMMT determined the orientation of newborn domains. Combined morphology observation and rheological analysis showed that the anisotropic structure and the unfavorable bending energy of OMMT sheets played important roles on phase morphology and its evolution process during or after shear.

¹The authors thank the financial support from National Natural Science Foundation of China (No.51173195).

M1.00003 Selective crystallization of regioregularity controlled polythiophene for enhancing mechanical stability and electronic performance, HYEONG JUN KIM, KAIST, HOJEONG YU, POESTECH, JAE-HAN KIM, JIN-SUNG KIM, TAEK SOO KIM, KAIST, JOON HAK OH, POESTECH, BUMJOON KIM, KAIST — Considering the many potential applications of organic electronics in portable electronic devices, it is of great importance to develop an electro-active material that possesses mechanical stability and high electronic performance. Coexistence of both properties, however, is very difficult to achieve because good electronic performance is associated with long conjugation length, and high crystallinity often results in stiffness and brittleness. Herein, we utilize P3HT with two different regioregularities: high RR (98) P3HT has high electronic properties but poor mechanical resilience, and low RR P3HT (68) exhibits high elasticity and ductility but poor electronic performance. Selective crystallization of high RR P3HT induced by solution assembly allows construction of percolated networks of high RR P3HT nanowires (NWs) embedded in low RR P3HT matrix. Only 5 wt high RR P3HT is required to reach a hole mobility comparable to that of high RR P3HT, and high RR NWs embedded in film exhibits 20 times higher elongation at break. Selective self-assembly allows us to overcome the fragile nature of highly crystalline conjugated polymers without losing their electronic properties.
M1.00004 Development of flash nanoprecipitation as a scalable platform for production of hybrid polymer-inorganic Janus particles1, VICTORIA E. LEE, ROBERT K. PRUD'HOMME, RODNEY D. PRIESTLEY, Princeton University — Polymer Janus particles, containing two or more distinct domains, can act as supports for inorganic nanoparticles, stabilizing them against aggregation and templating anisotropic functionalization of the microparticles. This anisotropy can be advantageous for applications such as biofuel upgrading, biosensors, and responsive materials. Here, we introduce flash nanoprecipitation (FNP) as a scalable, fast process to create hybrid polymer-inorganic Janus particles with control of particle size and anisotropy. During FNP, polymer Janus particles form by rapid intermixing of a polymer solution with a poor solvent, inducing polymer precipitation and phase separation. Inorganic nanoparticles are then adsorbed selectively onto one domain of the polymer support by exploiting electrostatic interactions between the charged particles. By tuning polymer concentration and ratio in the feed stream, the particle size and anisotropy can be controlled. We further demonstrate that these hybrid particles can simultaneously stabilize emulsions and selectively catalyze the degradation of dye in one phase.

1With support from the Princeton Imaging Analysis Center

M1.00005 Control of dynamical self-assembly of strongly Brownian nanoparticles through convective forces induced by ultrafast laser, SERIM ILDAY, GURSOY B. AKGUC, ONUR TOKEL, GAITH MAKEY, OZGUN YAVUZ, KORAY YAVUZ, IHOR PAVLOV, F. OMER ILDAY, OGUZ GULSEREN, Bilkent Univ — We report a new dynamical self-assembly mechanism, where judicious use of convective and strong Brownian forces enables effective patterning of colloidal nanoparticles that are almost two orders of magnitude smaller than the laser beam. Optical trapping or tweezing effects are not involved, but the laser is used to create steep thermal gradients through multi-photon absorption, and thereby guide the colloids through convective forces. Convective forces can be thought as a positive feedback mechanism that helps to form and reinforce pattern, while Brownian motion act as a competing negative feedback mechanism to limit the growth of the pattern, as well as to increase the possibilities of bifurcation into different patterns, analogous to the competition observed in reaction-diffusion systems. By steering stochastic processes through these forces, we are able to gain control over the emergent pattern such as to form-deform-reform of a pattern, to change its shape and transport it spatially within seconds. This enables us to dynamically initiate and control large patterns comprised of hundreds of colloids. Further, by not relying on any specific chemical, optical or magnetic interaction, this new method is, in principle, completely independent of the material type being assembled.

M1.00006 Amphiphilic Soft Janus Particles as Interfacial Stabilizers, WENDA WANG, SUNNY NIU, CHRIS SOSA, ROBERT PRUD'HOMME, RODNEY PRIESTLEY, Princeton Univ, PRIESTLEY POLYMER GROUP TEAM, PRUD'HOMME RESEARCH GROUP TEAM — Janus particles, which incorporate two or more “faces” with different chemical functionality, have attracted great attention in scientific research. Amphiphilic Janus particles have two faces with distinctly different hydrophobicity. This can be thought of as colloidal surfactants. Theoretical studies on the stabilization of emulsions using Janus particles have confirmed higher efficiency. Herein we synthesize the narrow distributed amphiphilic polymeric Janus particles via Precipitation-Induced Self-Assembly (PIA). The efficiency of the amphiphilic Janus particles are tested on different oil/water systems. Biocompatible polymers can also be used on this strategy and may potentially have wide application for food emulsion, cosmetics and personal products.

M1.00007 Time-resolved SANS studies on block copolymer micelles with varying core-solvent interactions, TYLER COOKSEY, AVANTIKA SINGH, MARIA MARQUEZ, MEGAN ROBERTSON, University of Houston — The self-assembly of block copolymer micelles occurs through a relaxation process dominated by the exchange of individual polymer chains. The objective of this work is to probe the single chain exchange of block copolymer micelles with varying core-solvent interactions, utilizing time-resolved neutron scattering (TR-SANS). The interactions between the core-forming polymer and the solvent has many implications for the micelle structure, including the aggregation number, micelle size, and interfacial tension. However, few studies have investigated the effect of the core polymer-solvent interactions on the dynamics of micelle formation. We will focus our study on poly(epsilon-caprolactone-block-ethylene oxide) block copolymers forming micelle structures in mixtures of water and tetrahydrofuran (THF). It was observed that changing the THF concentration, which varies the degree of repulsion between the core and solvent, greatly influences the single chain exchange rate in this system.

M1.00008 Spectroscopic Analysis of 10MAG/LDAO Reverse Micelles to Determine Characteristic Properties and Behavioral Extrema, JOSHUA BERG2, CARA MAWSON2, ZACH NORRIS, NATHANIEL NUCCI, Rowan University — Reverse micelles are spontaneously organizing complexes of surfactant that encapsulate a nanoscale pool of water in a bulk non-polar solvent. Reverse micelle (RM) mixtures have a wide range of applications, including biophysical investigation of protein systems. A new RM mixture composed of decyl-1-monoglycerol (10MAG) and lauryldimethylammonium-N-oxide (LDAO) was recently described. This mixture has the potential to prove more widely applicable for use of RMs in applications that involve encapsulation of macromolecules, yet little is known about the phase behavior or size of reverse micelles created by this mixture. Data describing such behaviors for this mixture are presented here. We have used dynamic light scattering (DLS) and fluorescence spectroscopy to investigate the size and partitioning behavior of RMs in varying mixtures of 10MAG, LDAO, water, pentane, and hexanol. These data demonstrate that the 10MAG/LDAO RM mixture exhibits markedly different phase and RM size behavior than that of commonly used RM surfactant mixtures. The implications of these findings for use of the 10MAG/LDAO mix for RM applications will also be addressed.

1Funding provided by Rowan University
2co-presenting author
3co-presenting author

M1.00009 Photolithography and Fluorescence Correlation Spectroscopy used to examine the rates of exchange in reverse micelle systems, JOSHUA BERG, CARA MAWSON, KYRON JOHNSON, SARAH KESSLER, ANNE REBECCA, NATHAN WOLF, MICHAEL LIM, NATHANIEL NUCCI, Rowan University — Reverse micelles are molecular complexes that encapsulate a nanoscale pool of water in a surfactant shell dissolved in non-polar solvent. These complexes have a wide range of applications, and in all cases, the degree to which reverse micelles (RM) exchange their contents is relevant for their use. Despite its importance, this aspect of RM behavior is poorly understood. Photolithography is employed here to create micro and nano scale fluidic systems in which mixing rates can be precisely measured using fluorescence correlation spectroscopy (FCS). Micro-channel patterns are etched using reactive ion etching process into a layer of silicon dioxide on crystalline silicon substrates. Solutions containing mixtures of reverse micelles, proteins, and fluorophores are placed into reservoirs in the patterns, while diffusion and exchange between RMs is monitored using a FCS system built from a modified confocal Raman spectrometer. Using this approach, the diffusion and exchange rates for RM systems are measured as a function of the components of the RM mixture.

1Funding provided by Rowan University
M1.00010 Self-assembly of mixed lipids into bicelles and vesicles: molecular dynamics simulations. HARI SHARMA, ZILU WANG, ELENA DORMIDONTOVA, Department of Physics and Institute of Materials Science, University of Connecticut, Storrs, CT — Formation of complex supramolecular nanostructures, such as micelles, bicelles, vesicles (liposomes) etc. via self-assembly of simple molecules has provided a new pathway for the design and development of effective drug carriers. Solid nanoparticles or functional biopolymers, such as DNA, RNA, peptides can be encapsulated into these carriers for controlled delivery or selective targeting. We performed coarse grained molecular dynamics simulation using the MARTINI force field to study the self-assembly of a binary surfactant mixture composed of long and short phospholipids, DPPC and DHPC, in the ratio 3:1. We found that at low temperature lipids self-assemble into a bicelle (nanodisc) with the longer lipid mainly forming the interior and short lipid the rim of the bicelle. At higher temperature the nanodisc transforms into a vesicle with homogeneously distributed lipids. The structural changes of these nanodiscs and vesicles imposed by gold nanoparticle encapsulation and pegylation will be addressed.

M1.00011 Directed Assembly of Gold Nanoparticles via Polymer Single Crystals, SHAN MEI, HAO QI, TIAN ZOU, CHRISTOPHER LI, None, SOFT MATERIAL LAB TEAM — Gold nanoparticles (AuNPs) have attracted great attention due to their unique properties and potential applications. In recent years, more efforts have been made to the assembly of AuNPs into various ordered structures such as AuNP wires and sheets in order to transfer their properties from nanoscale to macroscale, as well as exploring new properties. In this work we report a method to assemble AuNP into well defined, free standing frame structure using poly(ethylene oxide) (PEO) lamellar single crystal as the template. By controlling the single crystal size and functioning pattern, we are able to tune the width and size of the AuNP frame. We consider this approach to be an efficient and precise way to assemble AuNP and this methodology could be applied to other metal or semiconductor NPs.

M1.00012 Synthesis of Poly(N-isopropylacrylamide) Microcapsules for Drug Delivery Applications via UV Aerosol Photopolymerization. NICOLE ROBERSON, DANIEL DENMARK, SARATH WITANACHCHI, University of South Florida — Hybrid drug delivery systems composed of thermoresponsive polymers and magnetic nanoparticles have been developed using chemical methods to deliver controlled amounts of a therapeutic agent to target tissue. These methods can be expensive, time intensive, and produce impure composites due to the use of surfactants during polymer synthesis. In this study, UV aerosol photopolymerization is used to synthesize N-isopropylacrylamide (NIPAM) monomers, N,N-methylenebisacrylamide (MBA) crosslinker, and irgacure 2959 photoinitiator into the transporting microcapsule for drug delivery. The method of UV aerosol photopolymerization allows for the continuous, cost effective, and time efficient synthesis of a high concentration of pure polymers in a short amount of time; toxic surfactants are not necessary. Optimal NIPAM monomer, MBA crosslinker, and irgacure 2959 photoinitiator concentrations were tested and analyzed to synthesize microcapsules. Characterizations were performed using UV-visible spectroscopy, Atomic Force Microscopy, and light scattering to determine the size of the synthesized polymer microcapsules of about 30 micrometers in size is effective through UV aerosol photopolymerization. Findings will contribute greatly to the field of emergency medicine.

M1.00013 Tertiary phase diagram of cellulose, ionic liquid and organic solvent, XIN ZHANG, DOUG HENDERSON, Department of Materials Science and Engineering, University of Maryland, MADHUSUDAN TYAGI, YIMIN MAO, NCCR, GAITHERSBURG, MD, ROBERT M. BRIBER, HOWARD WANG, Department of Materials Science and Engineering, University of Maryland — Cellulose is the most abundant natural polymer and a key material widely used in a variety of applications. Understanding the phase behavior of molecular solutions of cellulose is key to realize advanced technologies beyond cellulose fibers. It has been reported that certain ionic liquid/organic solvent mixtures dissolve cellulose. In this study, the tertiary phase diagram of microcrystalline cellulose, 1-Ethyl-3-methylimidazolium acetate (EMIMAc), and dimethylformamide (DMF) mixtures has been determined using optical cloud point method and small angle neutron scattering (SANS). Data indicate that a molar ratio of EMIMAc to cellulose repeating unit equal or greater than 3 is necessary but not sufficient in forming one-phase homogeneous solutions. A miscibility gap exists in the dilute regime, where a minimum of 5 mol% of EMIM Ac in DMF is needed to form homogenous solutions. SANS show that cellulose chains adopt Gaussian-like conformation in homogenous solutions. The solutions exhibit the characteristics of upper critical solution temperature. Clustering of cellulose chains occurs at low EMIMAc/DMF or EMIMAc/cellulose ratio, or at low temperatures. The mechanism of cellulose dissolution in tertiary mixture is discussed.

M1.00014 Thin blend films of cellulose and polyacrylonitrile, RUI LU, XIN ZHANG, Department of Materials Science and Engineering, University of Maryland, College Park, MD, YIMIN MAO, NCCR, NIST, GAITHERSBURG, MD, ROBERT BRIBER, HOWARD WANG, Department of Materials Science and Engineering, University of Maryland, College Park, MD — Cellulose is the most abundant renewable, biocompatible and biodegradable natural polymer. Cellulose exhibits excellent chemical and mechanical stability, which makes it useful for applications such as construction, filtration, bio-scaffolding and packaging. To further expand the potential applications of cellulose materials, their alloying with synthetic polymers has been investigated. In this work, thin films of cotton linter cellulose (CLC) and polyacrylonitrile (PAN) blends with various compositions spanning the entire range from neat CLC to neat PAN were spun cast on silicon wafers from common solutions in dimethyl sulfoxide / ionic liquid mixtures. The morphologies of thin films were characterized using optical microscopy, atomic force microscopy, scanning electron microscopy and X-ray reflectivity. Morphologies of as-cast films are highly sensitive to the film preparation conditions; they vary from featureless smooth films to self-organized ordered nano-patterns to hierarchical structures spanning over multiple length scales from nanometers to tens of microns. By selectively removing the PAN-rich phase, the structures of blend films were studied to gain insights in their very high stability in hot water, acid and salt solutions.

M1.00015 Process Dependence of Cellulose Nanofiber Fabrication, DOUG HENDERSON, XIN ZHANG, Department of Materials Science and Engineering, University of Maryland-College Park, MD, YIMIN MAO, NCCR, NIST, GAITHERSBURG, MD, SOO-HWAN JANG, LIANGBING HU, ROBERT BRIBER, HOWARD WANG, Department of Materials Science and Engineering, University of Maryland-College Park, MD — Cellulose nanofibers (CNF) are the most abundant natural nanomaterial on earth with potential applications in renewable energy, polymer nanocomposites and flexible electronics. CNF can be produced through TEMPO oxidation which separates the hierarchical structure of cellulose fibers into smaller micro- and nanofibers by altering their surface chemistry, inducing a repulsive electrostatic charge on the fibers. This work investigated the structural evolution of CNF during production. Samples were prepared by removing and quenching aliquots during the TEMPO reaction. The fibers were washed, filtered and re-dispersed into D2O for small angle neutron scattering (SANS) measurements. The SANS data was analyzed to track the changes in the CNF structure as a function of reaction time.

M1.00016 Multi-scale Characterization of Cellulose TEMPO-Nanofiber Suspension, YIMIN MAO, Dept. of Materials Sci. and Eng., Univ. of Maryland, College Park; NIST Center for Neutron Research, National Institute of Standards and Technology, KAI LIU, BENJAMIN HSIAO, Chemistry Department, Stony Brook University — Cellulose nanofiber (CNF) suspensions were characterized at multiple length scales. CNF suspension was prepared by applying 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) oxidation method to dry wood pulp. TEMPO method was able to produce fine fibers with a cross section dimension being in the order of magnitude of several nanometers, and length being several hundred nanometers. The surface was negatively charged. Charge density was characterized by Zeta-potential measurement. Both small-angle X-ray (SAXS) and small-angle neutron (SANS) methods were employed to examine fiber dimensions in solution. Data fitting indicated that newly-developed ribbon model was able to capture the structural evolution of CNF during production. The characterization was used to gain insights into how cellulose crystals were biologically synthesized and packed in nature. Multi-angle dynamic light scattering (DLS) was used to study CNF’s diffusion properties. A strong scattering-angle dependence of autocorrelation function was observed. The characterization is useful to understanding suspension quality of CNF, and can provide guideline for follow-up research aimed for a variety of applications.
M1.00017 Controlling the structure and rheology of TEMPO-oxidized cellulose in zinc chloride aqueous suspensions for fabricating advanced nanopaper. SHA WANG, XIN ZHANG, LIANGBING HU, ROBERT BRIBER, HOWARD WANG, Dept. Materials Science and Engineering, University of Maryland, College Park, LINXIN ZHONG, State Key Laboratory of Pulp and Paper Engineering, South China University of Technology — Due to its abundance, low-cost, biocompatibility and renewability, cellulose has become an attractive candidate for a functional material for various advanced applications. A key to novel applications is the control of the structure and rheology of suspensions of fibrous cellulose. Among many different approaches of preparing cellulose suspensions, zinc chloride addition to aqueous suspensions is regarded as an effective practice. In this study, effects of ZnCl2 concentration on TEMPO-oxidized cellulose (TOC) nanofiber suspensions have been investigated. Highly-transparent cellulose nanofiber suspensions can be rapidly obtained by dissolving TOC in 60 wt. % zinc chloride aqueous solutions at room temperature, whereas a transparent zinc ion cross-linked TOC gel could be obtained with zinc chloride concentration as low as 10 wt.% The structural and rheological characteristics of TOC/ZnCl2 suspensions have been measured to correlate with the performance of transparent and flexible nanocellulose paper subsequently produced via vacuum filtration or wet-casting processes.

M1.00018 All-or-none folding of a polymer in confinement1, MARK TAYLOR, Hiram College — A flexible homopolymer chain with sufficiently short-range interactions undergoes a discontinuous transition from an expanded coil to a compact crystalline analogue to the all-or-none folding transition exhibited by fast-folding proteins. One anticipates that geometric confinement will reduce the entropy of the unfolded chain, thereby stabilizing the folded state and shifting the transition to higher temperature. In this work we study a flexible square-well N-mer chain (monomer diameter d) located between two hard walls forming a slit-like pore (width W) with the chain end-tethered to one wall. We carry out Monte simulations with Wang-Landau sampling to construct the single-chain density of states and use both microcanonical and canonical analyses to characterize phase transitions. When the slit width is similar to the size of the folded chain we observe a modest stabilization effect. Further reduction of the slit width geometrically prohibits the chain from folding into the free-end ground state. However, a discontinuous all-or-none folding transition still occurs to a flattened crystallite that spans the pore. All-or-none folding persists even to the limit of a very narrow pore (W d) where the ground-state structure is a quasi-two-dimensional crystal.

M1.00019 Exploring the existence of two Tgs in thin, supported polymer films1, ERIC CHEN, ETHAN GLOR, GABRIEL ANGRAND, ZAHRA FAKHRAAI, Univ of Pennsylvania, FAKHRAAI GROUP TEAM — Ellipsometry has commonly been used to characterize the glass transition temperature (Tg) and other properties of nanoscale thin films. In some ultra-thin films the glass transition broadens and even becomes two distinct transitions, as previously observed in free-standing polystyrene, thin films. However, for most polymers, the second, lower Tg is located below the condensation temperature of water, generating large errors in determining the lower Tg, which is associated with the layer close to the free interface. Here we designed a vacuum stage with a base pressure of <1×10⁻⁶ torr, equipped with a Linkam temperature stage with a temperature range of 153 K-873 K to study the properties of thin polymer films, supported on a substrate, in a broad temperature range and explore the existence of two Tgs in these systems. The stage was machined from aluminum and used infra-red quartz windows to allow the transmission of polarized light without distortion. The vacuum allows for accurate ellipsometry measurements of the properties of thin polymer films, such as expansion coefficient and Tg, at temperatures well below room temperature, without artifacts due to water condensation.

M1.00020 Limits of single-molecule super-resolution microscopy in thin polymer films, MUZHO WANG, MARCELO DAVANCO, JAMES M. MARR, J. ALEXANDER LIDDLE, JEFFREY W. GILMAN, National Institute of Standards and Technology — Structural characterization by super-resolution microscopy has become increasingly widespread, particularly in the biological community. The technique is powerful because it can produce real-space images with resolutions of tens of nanometers, while sample preparation is relatively non-invasive. Previous studies have applied these techniques to important scientific problems in the life sciences, but relatively little work has explored the attainable limit of resolution using samples of known structure. In this work, we apply photo-activated localization microscopy (PALM) to polymer films that have been nanopatterned using electron-beam lithography. Trace amounts of rhodamine spinoamide dye are dispersed into nanostructured poly(methyl methacrylate), and UV-induced switching of the fluorophores enables nanoscale resolution of single molecules to generate a final composite super-resolution image. Features as small as 50 nm are clearly resolvable. To determine the ultimate resolution limit, we investigate sources of error in the system, particularly from systematic mislocalizations due to the effect of fluorophore orientation on the single-molecule point-spread function.

M1.00021 Phase separated microstructure and dynamics of polyurethane elastomers under strain, CIPRIAN IACOB, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802 USA, AJAY PADASALGIKAR, Implantable Electronic Systems Division, St. Jude Medical, Rogers, MN, USA, JAMES RUNT, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802 USA, AJAY PADASALGIKAR, Implantable Electronic Systems Division, St. Jude Medical, Rogers, MN, USA, JAMES RUNT, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802 USA — The molecular mobility of polyurethane elastomers is of the utmost importance in establishing physical properties for uses ranging from automotive tires and shoe soles to more sophisticated aerospace and biomedical applications. In many of these applications, chain dynamics as well as mechanical properties under external stresses/strains are critical for determining ultimate performance. In order to develop a more complete understanding of their mechanical response, we explored the effect of uniaxial strain on the phase separated microstructure and molecular dynamics of the elastomers. We utilize X-ray scattering to investigate segment and hard domain orientation, and broadband dielectric spectroscopy for interrogation of the dynamics. Uniaxial deformation is found to significantly perturb the phase-separated microstructure and chain orientation, and results in a considerable slowing down of the dynamics of the elastomers. Attenuated total reflectance Fourier transform infrared spectroscopy measurements of the polyurethanes under uniaxial deformation are also employed and the results are quantitatively correlated with mechanical tensile tests and the degree of phase separation from small-angle X-ray scattering measurements.

M1.00022 Phase behavior of the thermoresponsive polymer Poly(N-isopropyl acrylamide) at variable pressure, ALFONS SCHULTE, Department of Physics and College of Optics and Photonics, University of Central Florida, Orlando, FL 32817-2385, KORA-LEE CLAUDE, SIMON PINZEK, PETER MILLER-BUSCHBAUM, CHRISTINE PAPADAKIS, TU Munchen, Physik-Department, LS FLORIDA 32817-2385, KORA-LEE CLAUDE, SIMON PINZEK, PETER MILLER-BUSCHBAUM, CHRISTINE PAPADAKIS, TU Munchen, Physik-Department, LS M1.00023 Exploring the existence of two Tgs in thin, supported polymer films, ERIC CHEN, ETHAN GLOR, GABRIEL ANGRAND, ZAHRA FAKHRAAI, Univ of Pennsylvania, FAKHRAAI GROUP TEAM — Ellipsometry has commonly been used to characterize the glass transition temperature (Tg) and other properties of nanoscale thin films. In some ultra-thin films the glass transition broadens and even becomes two distinct transitions, as previously observed in free-standing polystyrene, thin films. However, for most polymers, the second, lower Tg is located below the condensation temperature of water, generating large errors in determining the lower Tg, which is associated with the layer close to the free interface. Here we designed a vacuum stage with a base pressure of <1×10⁻⁶ torr, equipped with a Linkam temperature stage with a temperature range of 153 K-873 K to study the properties of thin polymer films, supported on a substrate, in a broad temperature range and explore the existence of two Tgs in these systems. The stage was machined from aluminum and used infra-red quartz windows to allow the transmission of polarized light without distortion. The vacuum allows for accurate ellipsometry measurements of the properties of thin polymer films, such as expansion coefficient and Tg, at temperatures well below room temperature, without artifacts due to water condensation.

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M1.00023 Complex Cure Kinetics of the Hydroxyl-Epoxide Reaction in DGEBA Epoxy Hardened with Diethanolamine. WINDY ANGIPINK, JOHN MCCOY, New Mexico Institute of Mining and Technology. JAMIE KROPKA, MATHIAS CELINA, Sandia National Laboratories. — The curing of a diglycidyl ether of bisphenol-A epoxy over long time periods. The cure was studied at various temperatures. We develop a Monte Carlo simulation to study the structure of adsorbed molecules. 

M1.00024 Relaxation Characteristics of 828 DGEBA Epoxy Over Long Time Periods. JASMIN HOO, RILEY C. REPROGLE, BRIAN WISLER, GABRIEL K. ARECHEVERRA, JOHN D. MCCOY, New Mexico Institute of Mining and Technology. JAMIE M. KROPKA, KEVIN N. LONG, Sandia National Laboratories. — The mechanical relaxation response in uniaxial compression of a diglycidyl ether of bisphenol-A epoxy was studied over long time periods. The curing was performed at various temperatures. The mechanical relaxation response was studied using isothermal modulated differential scanning calorimetry, microcalorimetry, and infrared spectroscopy. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

M1.00025 Effect of Structure on Charge Mobility in Partially Ordered Polymeric Systems. WAYLON LUO, KIRAN KHANAL, JUTTA LUETTMER-STRATMANN, University of Akron. — The performance of thin film organic semiconductor devices depends on the mobility of the charge carriers, which is strongly affected by the structure of the material. Accounting for these effects in device simulations is difficult since the size of the active layer is too large to generate realistic morphologies from molecular simulations of the constituents. In this work, we present Monte Carlo simulations of a coarse-grained lattice model for dense polymeric systems with a semiflexible component that undergoes a transition to (partially) ordered states at low temperatures. To investigate charge transport, the lattice polymer configurations become part of a model device, which consists of a layer of the material between two electrodes at different potentials. We determine the mobility from Monte Carlo simulations of charge carriers. To model the effect of polymer chain connectivity on charge transport we include an energetic barrier to hopping between sites on different chains; energetic disorder is taken into account by averaging over many polymer configurations. We find that ordering in the material leads to strong mobility anisotropies with increased mobility for transport parallel to the ordered domains and reduced mobility for perpendicular transport.

M1.00026 Improved electrospinning processing of PU/PEDOT:PSS for electronic textile applications. ERIN EVKE, Materials Engineering, AARON CLIPPINGER, Biomedical Engineering, CLAYSON SPACKMAN, JOHN SON SAMUEL, Mechanical, Aerospace and Nuclear Engineering, RAHMI OZSIK, Materials Engineering, Rensselaer Polytechnic Institute. — Poly(3,4-ethylenedioxythiophene) poly(4-styrenesulfonate), PEDOT:PSS, is an electrically conductive polymer used in electronic textile (e-textile) applications, such as electrochromic textiles, strain sensors, and resistive heaters. In the current study, PEDOT:PSS is blended with varying concentrations of polyurethane (PU) to investigate the effect on the mechanical properties of PU/PEDOT:PSS fibers. The fibers are produced via modified electrospinning process where the jet is collected close to the tip of the needle, thereby, enabling the collection of straight fibers by a rotating spool. The electrical conductivity and mechanical properties of PU/PEDOT:PSS fibers are characterized to understand the effect of PU concentration and the processing parameters.

M1.00027 Monte-Carlo simulations of a coarse-grained model for α-oligothiophenes. AMANI AL-MUTAIRI, JUTTA LUETTMER-STRATMANN, Department of Physics, University of Akron. — The interface of an organic semiconductor in contact with a metal electrode has important effects on the performance of thin-film devices. However, the structure of this layer is not easy to model. Oligothiophenes are small, π-conjugated molecules with applications in organic electronics that also serve as small-molecule models for polythiophenes. α-heithiophene (6T) is a six-ring molecule, which adsorption on noble metal surfaces has been studied extensively (see, e.g., Ref. [1]). In this work, we develop a coarse-grained model for α-oligothiophenes. We describe the molecules as linear chains of bonded, discotic particles with Gay-Berne potential interactions between non-bonded ellipsoids. We perform Monte Carlo simulations to study the structure of isolated and adsorbed molecules. [1] M. Kiel et al. Phys. Rev. B 75, 195439 (2007).

M1.00028 Conductance Thin Film Model of Flexible Organic Thin Film Device using COMSOL Multiphysics. CAROLYN CARRADORE-SANTIAGO, JOSEE VEDRINE-PAULUS, University of Puerto Rico at Humacao. — We developed a virtual model to analyze the electrical conductivity of multilayered thin films placed above a graphene conducting and flexible polyethylene terephthalate (PET) substrate. The organic layers of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT-PSS) as a hole conducting layer, poly(3-hexylthiophene-2,5-diy) (P3HT), as a p-type, phenyl-C61-butyric acid methyl ester (PCBM) and as n-type, with aluminum as a top conductor. COMSOL Multiphysics software was used to develop the virtual model to analyze potential variations and conductivity through the thin-film layers. COMSOL Multiphysics software allows simulation and modeling of physical phenomena represented by differential equations such as heat transfer, fluid flow, electromagnetism, and structural mechanics. In this work, using the AC/DC, electric currents module we defined the geometry of the model and properties for each of the six layers: PET/graphene/PEDOT-PSS/P3HT/PCBM/aluminum. We analyzed the model with varying thicknesses of graphene and active layers (P3HT/PCBM). This simulation allowed us to analyze the electrical conductivity, and visualize the model with varying voltage potential, or bias across the plates, useful for applications in solar cell devices.
M1.00029 Photopatterned surface relief gratings in azobenzene-amorphous polycarbonate thin films, MORTEN VOLLMANN, Technical University Berlin, PETER GETEK, University of Applied Sciences Berlin, KELLIE OLEAR, CODY COMBS, BENJAMIN CAMPOS, EDMUND WITKOWSKI, The College of New Jersey, ERIN CAIN, Temple University, DAVID MCCGE, The College of New Jersey — Photoinduced orientation of azobenzene chromophores in polymeric host materials has been broadly explored for optical processing applications. Illumination of the chromophore with polarized light rotates the trans isomer perpendicular to the polarization, resulting in spatially modulated birefringence. The photoinduced anisotropy may also drive mass transport, with surface relief patterns being observed in a wide variety of systems. Here we report photoinduced birefringence in a guest-host system of Disperse red 1- amorphous polycarbonate (DRI-APC). Birefringence was induced with a 490 nm laser and probed at 633 nm, with typical values of Δn = 0.01 in 2 micron thick films. Illumination of DRI-APC with intensity and/or polarization gratings also resulted in sinusoidal surface relief patterns with periodicity 1- 3 micron as controlled by the interbeam crossing angle of the 490 nm writing beams; the surface modulation was +/− 20 nm as measured by atomic force microscopy. Photopatterned DRI-APC is advantageous for applications given the ease of thin-film fabrication and the high glass transition temperature of APC, resulting in robust optically-induced surface gratings.

M1.00030 Morphology of conjugated polymer/insulating polymer blends from inkjet printing and its correlation to the function of field-effect transistors, HUIPENG CHEN, GUOCHEN ZHENG, LIQIN HU, HUHIUANG YANG, TAILIANG GUO, Fuzhou University — Printed electronics is a rapidly developing field of research which covers any electronic devices or circuits that can be processed using direct printing techniques. Among those printing techniques, inkjet printing is a technique of increasing interest for organic field-effect transistors (FETs) due to its fully data driven and direct patterning. In this work, the morphology of conjugated polymer/insulating polymer blends from inkjet printing and their FET properties has been investigated. The crystallinity and packing of conjugated polymer has been examined by synchrotron x-ray diffraction. The detailed information about the interface and domains of polymer blends were investigated by small angle neutron scattering. It is found that the domains and polymer interface were crucial to the FET properties. Finally, the relationship between morphology and function has been established for polymer blends FET from inkjet printing.

M1.00031 Solvent-vapor concentration imparts selectivity on the propagation front during polymeric transformation in molecular- semiconductor thin films, GEOFFREY PURDUM, Dept. of Chemical and Biological Engineering, Princeton University, THOMAS GESSNER, R. THOMAS WEITZ, BASF SE, GMV 67056, Germany, YUEH-LIN LOO, Dept. of Chemical and Biological Engineering, Princeton University — Post-deposition processing allows precise control over the structural development of molecular- semiconductor thin films. In particular, solvent-vapor annealing converts thin films of a core-chlorinated naphthalene diimide from its triclinic polymorph to its monoclinic polymorph. By tuning the concentration of solvent vapor, we can simultaneously impact the morphology of the resulting monoclinic thin film. At low solvent-vapor concentrations, transformation in-plane is isotropic; we observe comparable transformation rates along the b- and c-axes, resulting in plate-like domains. At high solvent-vapor concentrations, transformation along the c-axis is instead favored, resulting in the formation of needle-like domains. Extended solvent-vapor annealing at these conditions can lead to isolated needles in the active channels of field-effect transistors; these devices exhibit electron mobilities exceeding 1 cm²/Vs.

M1.00032 Charge conduction in partially fluorinated discotic liquid crystals, MITCHELL POWERS, ZHE LI, ROBERT TWIEG, BRETT ELLMAN, Kent State University — Motivated by the role of electrostatic interactions on stacking of partially fluorinated conjugated compounds, we present mobility measurements of, e.g., 1,4-difluoro-2,3,6,7,10,11-hexakispentaloxytriphenylene (2F-HAT5) in discotic mesophases across a wide range of temperature and applied electric field. Charge conduction in this case is well described by a disorder driven hopping model. 2F-HAT5 exhibits a mobility of approximately 2x10⁻³ cm²/Vs, similar to the parent triphenylene, and has a weak temperature dependence throughout it’s discotic mesophase, which extends below room temperature. We compare results on this and related compounds to various theoretical models.

M1.00033 Gated Seebeck using Polymerized Ionic Liquid Gate Dielectrics, ELAYNE THOMAS, BOHHOSAN POPERE, HAIYU FANG, MICHAEL CHABINYC, RACHEL SEGALMAN, Univ of California - Santa Barbara — Thermoelectric materials have the ability to convert a temperature gradient into usable electric power via the Seebeck effect. This phenomenon is directly related to the material’s Seebeck coefficient and electrical conductivity, which are in turn linked to its electron (or hole) mobility and carrier concentration. Organic semiconductors show promise for thermoelectric applications due to their flexibility and low-temperature manufacturing techniques; however, the role of ionized dopants on charge transport in these materials remains poorly understood. In this work, we use polymerized ionic liquids (PILs) as a gate dielectric in organic field-effect transistors to directly control the concentration of charges in the conducting channel. We report a method to tune the carrier concentration in the transistor channel via electrostatic gate modulation. We observe carrier concentration levels that are comparable to traditional doping methods with the added ability to precisely tune the concentration of charges induced. With this process, we aim to gather new information on the effect of ions on the performance of organic semiconductors in hopes of better understanding charge transport in conducting polymers on a molecular level.

M1.00034 Electrospray Composite Nanofibers of Semiconductive Polymers for Coaxial PN Junctions, WILLIAM SERRANO, SYLVIA THOMAS, University of South Florida at Tampa — The objective of this research is to investigate the conditions under which high-performance organic field-effect transistors (FETs) can be fabricated. Electrosprinning, a low cost, fast and reliable method, with a coaxial syringe arrangement will be used to fabricate these fibers. With the formation of coaxial coaxial arrangements, there will be investigations of dimensionality crossovers e.g., from one-dimensional (1D) to two-dimensional (2D). Coaxial core/shell fibers have been realized as seen in a recent publication on an electrospray nanofiber p-n heterojunction of oxides (BiFeO₃ and TiO₂, respectively) using the electrosprining technique with hydrothermal method. In regards to organic semiconductor coaxial p-n junction nanofibers, no reported studies have been conducted, making this study fundamental and essential for organic semiconducting nano devices for flexioble electronics and multi-dimensional integrated circuits.

M1.00035 A novel Graphene Oxide film: Synthesis and Dielectric properties, BETUL CANIMKURBEY, SAIT EREN SAN, Gebze Technical University, MUHAMMAD YASIN, National University of Science and Technology, MUHAMMET ERKAN KSE, Gebze Technical University — In this work, we used Hummers method to synthesize Graphene Oxide (GO) and its parallel plate impedance spectroscopic technique to investigate dielectric properties. Graphene Oxide films were coated using drop casting method on ITO substrate. To analyze film morphology, atomic force microscopy was used. Dielectric measurements of the samples were performed using impedance analyzer (HP-4194) in frequency range (100 Hz to 10MHz) at different temperatures. It was observed that the films’ AC conductivity σac varied with angular frequency, ω as ω², with S<1. The electrical properties of GO showed changes depending on both frequency and temperature. We observed GO film contains direct current (DC) and Correlated Barrier Hopping (CBH) conductivity mechanisms at low and high frequency ranges, respectively. Using solution processed Graphene Oxide will provide potential for organic electronic applications through its photon absorption and transmittance capability in the visible range and excellent electrical parameters.
M1.00036 Synthesis and Characterization of Plant based Polyythiophene Copolymers for Light Harvesting Applications. UDARI KODITHWAKKU, PRASHANTHA MALAVI ARACHCHI, DILRU RATNAWEERA, University of Sri Jayewardenepura, Sri Lanka — Polyythiophenes became more attractive in diverse applications due to some of their inherent properties including thermal and environmental stability as well as optical and electronic conductive properties. Commonly thiophene monomers are obtained from byproducts of crude oils. The current study discuss for the first time the synthesis and characterization of light harvesting polyythiophenes copolymers from thiophene derivatives extracted from Tagetes species. There were mainly two thiophene derivatives, 5-(3-buten-1-ynyl)-2, 2-bithienyl and 2, 2', 5', 2"-terthienyl (terthiophene), in the roots of the plant. Chemical oxidative radical polymerization was followed during the synthesis of copolymers with various block compositions of plant based terthienophenes and 3-hexyl terthienophenes. Structural characterization of the synthetic products was done using FTIR, NMR, UV-vis, XRD and DSC techniques. Polyythiophene homopolymers obtained from plant based terthienophenes have limited processability of solar cells due to poor solubility in common organic solvents. A significant solubility improvement was observed with copolymers having minor contributions of 3-hexythiophenes.

1Research Grants, University of Sri Jayewardenepura, Sri Lanka

M1.00037 Synthesis and Photoelectrochemistry Characterization of Polymer based on 4,7-Di(thiophen-2-yl)-benzo[c][1,2,5]thiadiazole, (DTBT). LUZ MARIA LAZO JIMENEZ1, Instituto de Ciencias Nucleares, UNAM., BERNARDO ANTONIO FRONTANA-URIBE2, Centro Conjunto de Investigacion en Quimica Sustenable, CCIQS-UNAM-UAEM. — Poly[4,7-di-(thiophen-2-yl)-benzo[c][1,2,5] thiadiazole], P(DTBT), is used in polymer:PCMB blends as active layer on organic photovoltaic devices, (OPV); DTBT-based copolymers show well-reversible oxidation and reduction electrochemical processes. These processes indicate their high electrochemical stability suitable for n- and p-doping. This is a typical feature benzothiadiazole containing molecules. In the present study the synthesis conditions of the monomer, 4,7-di-(thiophen-2-yl)-benzo[c][1,2,5] thiadiazole based on Stille coupling reactions has been investigated and its respectively polymer P(DTBT) was prepared by repetitive potential-sweep anodic oxidation of the corresponding monomer DTBT onto Pt disk or indium tin oxide (ITO) electrodes. Electrochemical cyclic voltammetry (CV) was performed to determine the HOMO and the LUMO energy levels of the conjugated DTBT and P(DTBT), both exhibit amphoteric redox properties, n- and p- doping process. The optical gap estimated from electrochemical measurements of the polymer (P(DTBT)) was found to be 1.77 eV, which is close to the reported band gap (1.1-1.2 eV) determined by optical absorption technique. Photoelectrochemical characterization of P(DTBT) was realized from UV-Vis-NIR spectra recorded at different applied potentials. These results are correlated with the charge-transfer phenomena in the polymers applied as active layer on OPV’s.

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M1.00038 Electrosprinning Nanofiber Based Organic Solar Cell1, ZHENHUA YANG, YING LIU, STONY BROOK UNIVERSITY, MARIA MOFFA, CNR-Istituto Nanoscienze, CHANG-YONG NAM, Brookhaven National lab, DARIO PISIGNANO, CNR-Istituto Nanoscienze, MIRIAM RAFAILOVICH, STONY BROOK UNIVERSITY — Bulk heterojunction (BJH) polymer solar cells are an area of intense interest due to their potential to result in printable, inexpensive solar cells which can be processed onto flexible substrates. The active layer is typically spin coated from the solution of polymer derivatives (donor) and fullerens (acceptor) and interconnected domains are formed because of phase separation. However, the power conversion efficiency (PCE) of BJH solar cell is restricted by the presence of undesirable morphological features, including dead ends or isolated domains. Here we MEH-PPV:PVP:PCBM electrosprinn nanofiber into BJH solar cell for the active layer morphology optimization. Large interfacial area between donor and acceptor is attained with electrosprinng method and the high aspect ratio of the MEH-PPV:PVP:PCBM nanofiber allows them to easily form a continuous pathway. The surface morphology is investigated with atomic force microscopy (AFM) and scanning electron microscopy (SEM). Electrosprinn nanofibers are discussed as a favorable structure for application in bulk-heterojunction organic solar cells.

1Electrosprining Nanofiber Based Bulk Heterojunction Organic Solar Cell

M1.00039 Asymmetrical Zinc Phthalocyaninmes as Dye-Sensitized Solar Cells. GULENAY TUNC, YUNUS YAVUZ, AYSEGUL GUREK, BETUL CANIMKURBEY, ARIF KOSEMEN, SAIT EREN SAN, VEFA AHSEN, Gebze Technical University — Dye-sensitized solar cells (DSSCs) have received increasing attention due to their high incident to photon efficiency, easy fabrication and low production cost. Theoretical research efforts have been devoted to the development of new and efficient sensitizers suitable for practical use. In TiO2-based DSSCs, efficiencies of up to 11.4% under simulated sunlight have been obtained with rutheniumpolypyrrolid complexes. However, the main drawback of ruthenium complexes is the lack of absorption in the red region of the visible light and the high cost. For this reason, dyes with large and stable p-conjugated systems such as porphyrins and phthalocyanines are important classes of potential sensitizers for highly efficient DSSCs. Phthalocyanines (Pcs) have been widely used as sensitizers because of their improved light-harvesting properties in the far red- and near-IR spectral regions and their extraordinary robustness [1]. In this work, a series of asymmertic Zn(II) Pcs bearing a carboxylic acid group and six hexylthia groups either at the peripheral or non-peripheral positions have been designed and synthesized to investigate the influence of the COOH group and the positions of hexylthia groups on the dye-sensitized solar cell (DSCC) performance.

M1.00040 Highly conductive polymer electrolyte membranes modified with polyethylene glycol-bis-carbamate1, GUOPENG FU, Univ of Akron, JANEL DEMPESEY, John Carroll University, THEIN KYU, Univ of Akron — By virtue of its non-flammability and chemical stability, polyethylene glycol (PEG) networks have shown potential application in all solid-state polymer electrolyte membranes (PEM). However, room temperature ionic conductivity of these PEG based PEMs is inherently low. Plasticization of these PEMs is needed to improve the ionic conductivity. It was demonstrated by this group that small-molecule plasticizers such as succinonitrile, ethylene carbonate, or urea-carbamate can boost the ionic conductivity. It was demonstrated by this group that small-molecule plasticizers such as succinonitrile, ethylene carbonate, or urea-carbamate can boost the ionic conductivity of solid-state polymer electrolyte membranes. Polyethylene glycol bis-carbamate (PEGBC) was synthesized via condensation reaction of polyethylene glycol diamine and ethylene carbonate. The PEGBC modified PEM has shown higher ionic conductivity relative to the unmodified PEM. Moreover, PEGBC modified PEM has a better thermal stability relative to ethylene carbonate based liquid electrolyte with enhanced ionic conductivity.

1Supported by NSF-DMR 1161070, 1502543 and REU 1359321

M1.00041 Neutron Vibrational Spectroscopy and modeling of polymer/dopant interactions. ADAM MOULE, THOMAS HARRELSON, University of California, Davis, YONGQIANG CHENG, ANIBAL RAMIREZ-CUESTA, Oak Ridge National Lab, ROLAND FALLER, University of California, Davis, DAVID HUANG, University of Adelaide, Australia — Neutron vibrational spectroscopy (VISION and ORNL) is a powerful technique to determine the configurations of organic species in amorphous samples. We apply this technique to samples of the semiconducting polymer regio-regular P3HT to determine the molecular configurations outside of the crystalline domains, which have never been investigated. Application of density functional theory modeling using crystal field theory and for the single molecule approach yield a variety of configurations of the polymer backbone and side chains. These results demonstrate that only 1% of the volume corresponds to the assumed crystal structure solved using x-ray diffraction. In addition we investigate the configurations of P3HT with the molecular dopant 4TCTNQ and determine that the charging of the polymer backbone leads to increased side chain stiffness. These results have significant implications for design of organic electronic devices based on thiophenes.
Assembly polyvinylidene fluoride (PVDF) and trifluoroethylene (TrFE) copolymers on the characteristic relaxation timescale of the particular material. Subsequently, we use the aligned polymeric films as templates for synthesis of single- and various block-copolymer thin films including PS-b-PMMA, PS-b-PEO, PS-b-P2VP, PS-b-PI and observe different responsiveness to the shearing rate depending on the global alignment of block copolymer domains assessed by GISXAS diffraction studies and real-space SEM imaging. We demonstrate monolithic alignment of induced in block copolymer films by rastering narrowly focused laser line over the light-absorbing substrate. Extremely steep temperature gradients accelerate accelerated self-assembly of block copolymer thin films utilizing laser light, called Laser Zone Annealing (LZA). In our approach, steep temperature transients are displayed a similar trend, with the room temperature spontaneous polarization decreasing by 44% from 13.8 $\mu$C/cm$^2$ to 7.7 $\mu$C/cm$^2$, as a function of TrFE content (0-50%) in the temperature range of 0-400 K. There is a very good agreement between the experimentally obtained and the computed values of the lattice parameters, thermal expansion coefficients, elastic constants, polarization, and pyroelectric coefficients. A continuous decrease in Young’s modulus with increasing TrFE content was observed and attributed to the increased intramolecular and intermolecular repulsive interactions between fluorine atoms. The computed polarization displayed a similar trend, with the room temperature spontaneous polarization decreasing by 44% from 13.8 $\mu$C/cm$^2$ to 7.7 $\mu$C/cm$^2$. Our results show that molecular dynamics can be used as a practical tool to predict the mechanical and polarization-related behavior of ferroelectric poly(vinylidene fluoride-trifluoroethylene). Such an atomistic model can thus serve as a guide for practical applications of this important multifunctional polymer.

M1.00043 Temperature dependent structural, elastic, and polar properties of ferroelectric polyvinylidene fluoride (PVDF) and trifluoroethylene (TrFE) copolymers, FU-CHANG SUN, AVINASH DON-GARE, ALEXANDRU ASANDEI, University of Connecticut, PAMIR ALPAY, University of Connecticut, SERGE NAKHMANSON, University of Connecticut, UNIVERSITY OF CONNECTICUT TEAM — We use molecular dynamics to calculate the structural, elastic, and polar properties of crystalline ferroelectric $\beta$-poly(vinylidene fluoride), PVDF (CH$_2$=CF$_2$)$_n$, and randomized trifluoroethylene TrFE (CHF$_2$-CF$_2$)$_n$, as a function of TrFE content (0-50%) in the temperature range of 0-400 K. There is a very good agreement between the experimentally obtained and the computed values of the lattice parameters, thermal expansion coefficients, elastic constants, polarization, and pyroelectric coefficients. A continuous decrease in Young’s modulus with increasing TrFE content was observed and attributed to the increased intramolecular and intermolecular repulsive interactions between fluorine atoms. The computed polarization displayed a similar trend, with the room temperature spontaneous polarization decreasing by 44% from 13.8 $\mu$C/cm$^2$ to 7.7 $\mu$C/cm$^2$. Our results show that molecular dynamics can be used as a practical tool to predict the mechanical and polarization-related behavior of ferroelectric poly(vinylidene fluoride-trifluoroethylene). Such an atomistic model can thus serve as a guide for practical applications of this important multifunctional polymer.

M1.00044 Understanding Nonlinear Dielectric Properties in a Biaxially Oriented Poly(vinylidene fluoride) Film at Both Low and High Electric Fields, YUE LI, College of Polymer Science and Engineering, Sichuan University, LEI ZHU, Department of Macromolecular Science and Engineering, Case Western Reserve University, CASE WESTERN RESERVE UNIVERSITY TEAM, SICHUAN UNIVERSITY TEAM — Understanding nonlinear dielectric behavior in polymer materials is crucial to their potential application as next generation high energy density and low loss dielectrics. In this work, we studied nonlinear dielectric properties of a biaxially oriented poly(vinylidene fluoride) (PVDF) film under both low and high electric fields. It was observed that the low-field dielectric nonlinearity for the BOPVDF disappeared above 10 Hz at room temperature, suggesting that the low-field dielectric nonlinearity originated from ionic migration of impurity ions rather than dipolar relaxation of the amorphous segments. Above the coercive field (EC ≈ 70 MV/m), bipolar electric displacement-electric field (D-E) loop tests were used to extract the nonlinear behavior for pure PVDF crystals, which had a clear origin of ferroelectric switching of polar crystalline dipoles and domains and nonpolar-to-polar ($\alpha \rightarrow \beta$) phase transformations. Using HVBDS, it was observed that the ferroelectric switching of polar crystalline domains and domains in BOPVDF above the EC always took place between 20 and 500 Hz, regardless of a broad range of temperature from -30 to 100 C. This behavior was drastically different from the amorphous PVDF films, which had a strong dependence on frequency over orders of magnitude.

M1.00045 Correlating Thin-Film Radical Density with Charge Transport in Open-Shell Conducting Macromolecules, MARTHA HAY, ELIZABETH JERGENS, BRYAN BOUDOURIS, Purdue University — Within the class of radical polymers, stable open-shell species serve as the medium for charge transport by undergoing oxidation-reduction (redox) reactions. The kinetics of these reactions are rapid enough that they are not considered rate-limiting in the electronic interactions of these materials. Rather, the proximity of these radical sites is paramount as a synthetic handle. Unfortunately, controlling the density of radicals has proven challenging in radical polymer systems. Often radical functionality is imparted to a polymer, rather than polymerizing a radical-containing monomer unit. This can prove troublesome as longer reaction times, in the interest of higher radical functionality, can lead to the elimination of radicals. Thus, the consequential altering of the radical electronic interactions is not well understood. We have synthesized a series of polynorbornene-based radical monomers at controlled radical loadings such that the radical density was preserved from monomer to polymer synthesis. As such, we attribute any change in the macroscopic transport properties to a change in the spacing between radical sites. These results elucidate the role of radical site distribution on the electronic performance of nitroxide-based radical polymers.

M1.00046 Polyvinylidene fluoride molecules in nanofibers, imaged at atomic scale by aberration corrected electron microscopy, DARRELL RENEKER, JOSEPH GORSE, DINESH LOLLALA, Lawrence Berkeley National Laboratory, JIAYUAN MIAO, PHILLIP TAYLOR, Case Western Reserve University, CHRISTIAN KISIELOWSKI, Lawrence Berkeley National Laboratory, JIAYUAN MIAO, PHILLIP TAYLOR, Case Western Reserve University, George Chase, The University of Akron — Atomic scale features of polyvinylidene fluoride molecules (PVDF) were observed. Electron micrographs of thin, self-supporting PVDF nanofibers showed conformations of the backbone atoms, as well as the conformation of backbone segments. Rows of CF2 groups, at 0.25 nm intervals, marked the paths of segments of the PVDF molecules. The fact that an electron microscope image of a segment of a PVDF molecule depended upon the particular azimuthal alignment, along which the segment was viewed, enabled observation of twist around the molecular axis. The 0.2 nm side-by-side distance between the two fluorine atoms attached to the same carbon atom was clearly resolved. Morphological and chemical changes produced by energetic electrons, ranging from no change to fiber scission, were clearly visible. Relative movements of segments of the PVDF molecules were observed. Synergism between high resolution electron micrographs and images created by molecular dynamic modeling was demonstrated. This paper is at the threshold of growing usefulness of electron microscopy to the science and engineering of polymer and other molecules.

M1.00047 Design of Free-Standing Microstructured Conducting Polymer Films for Enhanced Particle Removal from Non-Uniform Surfaces, JENNIFER LASTER, NICHOLAS DEOM, BRYAN BOUDOURIS, STEPHEN BEAUDOIN, Purdue University — Particle removal from surfaces is important for a wide range of industrial applications (e.g., microelectronics fabrication). One of the main forces of particle adhesion to a surface is the van der Waals attraction force, which will be the focus of this effort. The surface features of interacting bodies can play a controlling role in the adhesion of particles by increasing or decreasing the amount of mass within the range of strong van der Waals forces. In order to control these interactions, specific geometries can be designed in order to manipulate the micro- and nanostructure of a material, which can conform to the features of a corresponding substrate increasing the overall contact area between the two surfaces. In this work, microstructured films of the conducting polymer polypyrrole (PPy) were synthesized through template-assisted electropolymerization techniques. The removal of fluorescently-labeled polystyrene beads from aluminum surfaces of varying roughness was measured and compared for microstructured and flat PPy films. The microstructured films were found to have an overall increase in the amount of particles removed from the aluminum surfaces; this demonstrates the ability to manipulate particle adhesion through advanced nanostructured polymer templating.

1Research carried out in part at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-88CH10886.

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Out-of-plane Block Copolymer Microdomains in High Aspect-Ratio Templates

KARIM GADELRAI, WUBIN BA, ALFREDO ALEXANDER-KATZ, CAROLINE ROSS, Massachusetts Inst of Tech/MIT — Directed self-assembly (DSA) of block copolymers BCP proved to be a power approach for nanoscale fabrication. In addition, BCP with highly incompatible blocks (high Flory-Huggins interaction parameter (χ)) offer improvement in resolution of the BCP patterns. Unfortunately, high-χ BCPs usually exhibit large differences in surface affinity between the two blocks, forming a surface layer of the lower surface energy block and favoring in-plane orientation of lamellae or cylindrical microdomains. Here, we explore the conditions under which a high-χ BCP creates an out-of-plane lamellar structure using high aspect ratio trenches with preferential walls. We employ self-consistent field theory (SCFT) and single mode expansion of Ginzburg-Landau free energy expression to analytically construct a phase diagram of the in- and out-of-plane lamellae as a function of aspect ratio and surface affinity. It is found that achieving an out of plane lamellar structure necessitates a coupling between aspect ratio and surface functionality. In particular, strong side wall attraction results in out-of-plane lamellae when the trench aspect ratio is greater than unity. The results are validated for a polystyrene-block-polydimethylsiloxane (PS-PDMS) system within trenches made using interference lithography.

Vertically Aligned Nanoplate Particles Directed by Block Copolymer Domains for Anisotropic Properties

NADIA KROOK, University of Pennsylvania, JEFFREY METH, DuPont, CHRISTOPHER MURRAY, ROBERT RIGLEMAN, RUSSELL COMPOSTO, University of Pennsylvania — During common processing methods, anisotropic fillers in polymer nanocomposites align in the direction of flow, parallel to the surfaces, thus enhancing properties in the plane of the substrate. This research aims to create thin film nanocomposites with perpendicularly aligned anisotropic particles to improve properties in the out-of-plane direction. The demonstrated work explores vertical orientation of rare-earth fluoride nanoparticles in lamellar-forming (polystyrene-b-methyl methacrylate) to establish a platform that controls the alignment of any planar particle. Currently, gadolinium fluoride (GdF₃) rhombohedral nanoparticles with the longest and shortest diagonal dimensions of ~30 nm and ~25 nm, respectively, have been specially synthesized with the potential to intercalate the block copolymer (BCP) domains. By employing a ternary brush blend layer to neutralize silicon substrates to both BCP domains, vertical lamelae orientation has been enabled with an optimum film thickness of ~110 nm. The GdF₃ surfaces are chemically modified to drive the plates to a specific BCP domain. After surface solution modification, the dispersion of GdF₃ in homopolymer will first be shown followed by morphology results from integrating GdF₃ into the BCP using scanning and transmission electron microscopy.

The role of ultra-fast solvent evaporation on the directed self-assembly of block polymer thin films

GUNNAR NELSON, J. WONG, C. DRAPES, M. GRANT, A. BARUTH, Creighton University — The directed self-assembly of nanostructures in block polymer thin films via solvent vapor annealing is complicated by several factors, including evaporation rate. Solvent vapor annealing exposes a disordered film to solvent(s) in the vapor phase, increasing mobility and tuning surface energy, with the intention of producing an ordered structure. Recent theoretical predictions reveal the solvent evaporation affects the resultant nano-structuring. In a competition between phase separation and kinetic trapping during drying, faster solvent removal can enhance the propagation of a given morphology into the bulk of the thin film down to the substrate. Recent construction of a purpose-built, computer controlled solvent vapor annealing chamber provides control over forced solvent evaporation down to 15 ms. This is accomplished using pneumatically actuated nitrogen flow into and out of the chamber. Furthermore, in situ spectral reflectance, with 10 ms temporal resolution, monitors the swelling and evaporation. Presently, cylinder-forming polystyrene-block-polylactide thin films were swollen with 40% (by volume) tetrahydrofuran, followed by immediate evaporation under a variety of designed conditions. This includes various evaporation times, ranging from 15 ms to several seconds, and four unique rate trajectories, including linear, exponential, and combinations. Atomic force microscopy reveals specific surface, free and substrate, morphologies of the resultant films, dependent on specific evaporation conditions. Funded by the Clare Boothe Luce Foundation and Nebraska EPSCoR.
The morphology of A2B miktoarm polymer in thin film, HYEYOUNG KIM, Univ of Mass - Amherst, BEOM-GOO KANG, University of Tennessee, ZHIWEI SUN, JAEWON CHOI, THOMAS RUSSELL, Univ of Mass - Amherst — The morphologies of A2B mikto-arm polymer consisted of poly(2-vinyl pyridine) and polystyrene ((P2VP)2PS) in thin film were examined. Solvent vapor annealing produces films with lamellae perpendicular to the substrate within a very short time. The change in the morphology for different periods of time, corresponding to different swelling ratios was observed by grazing incidence small angle x-ray scattering and scanning force microscopy. This morphology showed the smaller height difference between PS and P2VP microdomains, when compared to the corresponding diblock copolymer. We also observed the long-range ordering formed on the saw-tooth pattern. Thermal annealing, on the other hand, resulted in the lamellae being oriented parallel to the substrate, where unusual behavior was depending on the film thickness and surface energy of substrate.

Simple, generalizable route to highly aligned block copolymer thin films, ZHE QIANG, KEVIN CAVICCHI, BRYAN VOGT, University of Akron, UNIVERSITY OF AKRON TEAM — Macroscopic alignment of block copolymer domains in thin films is desired for many applications, such as cell responsive surfaces or optical polarizers. Alignment generally requires specialized tools that apply external fields, shear force gradient, or produce topological patterned substrates. This requirement limits the broad academic application of aligned BCPs. Here, we describe a simple modification of commonly utilized solvent vapor annealing (SVA) process for macroscopic alignment of BCPs. Adhering a flat, crosslinked elastomer pad to the BCP film leads to differential swelling between the elastomer pad and BCP to produce a shear force that aligns the ordered BCP domains. The role of elastomer properties, solvent quality, drying rate and degree of segregation of the block copolymer will be discussed to provide generalized rules for alignment with this technique. Cylindrical nanostructures formed in polystyrene-block-polydimethylsiloxane can be transformed into arrays of silica lines and increasing the thickness from a monolayer to bilayer can effectively halve the spacing of the lines. These results illustrate a generalized method for BCP alignment and a potential route for the generation of complex hierarchical assembled structures.

Sulfation effect on levan polysaccharide chains structure with molecular dynamics simulations, BINNAZ COSKUNKAN, Yeditepe University, DENIZ TURGUT, DENIZ RENDE, Rensselaer Polytechnic Institute, SEYDA MALTA, Yeditepe University, NIHAT BAYSAL, RAHMI OZISIK, Rensselaer Polytechnic Institute, EBRA TOKSOY-ONER, Marmara University — Diversity in conformations and structural heterogeneity make polysaccharides the most challenging biopolymer type for experimental and theoretical characterization studies. Levan is a biopolymer chain that consists of fructose rings with β(2→6) linkages. It is a glycan that has great potential as a functional biopolymer in foods, feeds, cosmetics, pharmaceutical and chemical industries. Sulfated polysaccharides are group of macromolecules with sulfated groups in their hydroxyl parts with a range of important biological properties. Sulfate groups and their positions have a major effect on anticoagulant activity. It is reported that sulfate modified levan has anticoagulant activity such as heparin. In the current study, the effect of sulfation on the structure and dynamics of unmodified and sulfate modified levan are investigated via fully atomistic Molecular Dynamics simulations in aqueous media and varying salt concentrations at 310 K.

The Effects of pH and Temperature on the Nanostructure of Chitosan Films, RAMONA LUNA, AHMED TOUHAMI, University of Texas Rio Grande Valley — Developing a matrix that can mimic tissue-like environment for cell cultures and molecular studies can help reduce the loss of some cell functions that occur when investigations are performed in vitro. Of particular interest is chitosan (CS): abundant and renewable biopolymer that is also biodegradable and non-toxic. The present study focuses on synthesizing CS films under various conditions and for multiple applications. We are using several techniques to characterize the physicochemical properties of the synthesized films. The contact angle technique is used to determine the hydrophobicity, hydrophilicity, and the surface free energy. The atomic force microscopy is used to determine the nanostructure, and nanomechanical properties. Here we specifically investigated the effect of the pH and the temperature on the nanostructure of the CS films. AFM images showed remarkable changes in the surface nanostructures that increase the roughness of the films when the pH of the solution increases. However, the surface free energy of these films has not shown any significant changes with the pH. By investigating the properties of these films, the needed biomaterial platform for a specific biological system can be designed and manipulated to increase its performance and lifetime.

Characterization of Nanoparticle Aggregation in Biologically Relevant Fluids, KATHLEEN MCGNIS, JOERG LAHANN, University of Michigan — Nanoparticles (NPs) are often studied as drug delivery vehicles, but little is known about their behavior in blood once injected into animal models. If the NPs aggregate in blood, they will be shunted to the liver or spleen instead of reaching the intended target. The use of animals for these experiments is costly and raises ethical questions. Typically dynamic light scattering (DLS) is used to analyze aggregation behavior, but DLS cannot be used because the components of blood also scatter light. As an alternative, a method of analyzing NPs in biologically relevant fluids such as blood plasma has been developed using nanoparticle tracking analysis (NTA) with fluorescent filters. In this work, NTA was used to analyze the aggregation behavior of fluorescent polystyrene NPs with different surface modifications in blood plasma. It was expected that different surface chemistries on the particles will change the aggregation behavior. The effect of the surface modifications was investigated by quantifying the percentage of NPs in aggregates after addition to blood plasma. The use of this characterization method will allow for better understanding of particle behavior in the body, and potential problems, specifically aggregation, can be addressed before investing in in vivo studies.

Ring Structure of Center of Spacetime, DNA, and Extraterrestrial Being, DAYONG CAO, AEAA — There is a balance of the flat universe between the stellar matter and the dark massenergy (include dark matter and dark energy) which make of dark hole which has the center of the spacetime. The Einstein’s equation has the other formula of the structure of the center of spacetime. There are also balance system between the solar system and its companion dark hole, and between the Milky Way galaxy and its center of the huge dark hole. The model of stellar matter can explain of the structure of molecule by electromagnetic interaction (of the spacetime effect). The ring structure both the nucleic acid and protein is like the structure of the center of the spacetime. It produced by an interaction of double helix between dark massenergy and stellar matter when the companion dark hole of sun seasonal impacted near solar system, and took dark comets and dark massenergy on the earth, and made extinctions while they were producing new DNA of lives, broke the old one to the petroleum, natural gas, and coal. DNA of extraterrestrial being who live on system of the companion dark hole may have special ring structure with the double helix. A new big extinction is coming for human being and extraterrestrial being.
M1.00060 Coacervate Core Micelles for the Dispersion and Stabilization of Organophosphate Hydrolase in Organic Solvents. CAROLYN MILLS, ALLIE OBERMEYER, XUEHUI DONG, BRADLEY D. OLSEN, Massachusetts Institute of Technology — Bulk organophosphate (OP) nerve agents are difficult to decontaminate on site and dangerous to transport. The organophosphate hydrolase (OPH) enzyme is an efficient catalyst for hydrolyzing, and thus decontaminating, these compounds, but suffers from poor stability in the hydrophobic bulk OP environment. Here, we exploit the complex coacervation phase separation phenomenon to form complex coacervate core micelles (C3Ms) that can protect this OPH enzyme under these conditions. Stable C3Ms form when mixing a charged-neutral block copolymer methyl-quaternized poly(4-vinylpyridine)-block-poly(oligo(ethylene glycol) methacrylate) (Qdpvp-b-POEMGA), a homopolymer poly(acrylic acid) (PAA), and OPH under certain conditions. The C3Ms are then transferred into two organic solvents, ethanol and dimethyl methylphosphonate (DMMP), which is a good simulant for the physical properties of the OP compounds. The C3Ms retain their nanostructures in the organic solvents. The activity test of OPH indicates that the C3Ms successfully protect OPH activity in organic solvents.

M1.00061 Fluorescence Recovery after Photobleaching in Confined Polymer Thin Films. LAURA A. G. GRAY, CLIFFORD P. BRANGWYNE, RODNEY D. PRIESTLEY, Princeton Univ, Dept. of Chemical and Biological Engineering — Over the past twenty years many studies have shown a reduction in the glass transition temperature (Tg) of thin polymer films confined on the nanoscale when supported on non-attractive substrates or free-standing. The depth dependence of Tg has been measured using thin layers of fluorescently tagged polymer to localize the dye within a larger polymer film stack, revealing a decrease in local Tg tens of nanometers into the film. These results have been explained by the propagation of enhanced mobility from the free-surface into the polymer film. Fewer direct measurements of molecular mobility have been made in confined polymer films. Here, we present the results of fluorescence recovery after photobleaching (FRAP) experiments investigating the mobility of fluorescently doped and labeled methacrylate-based polymers confined in thin film geometries. Bleaching and recovery was monitored using a laser-scanning confocal microscope that enabled us to bleach arbitrary micron-sized shapes to monitor diffusion in polymer melts.

M1.00062 Using Atomic Molecular Dynamics Simulations to Guide Development of Coarse-Grained Models of Polyethylene glycol (PEG), Elastic-like peptides (ELP) and Collagen-like peptides (CMP) For Biomaterial Design. FRANCESCA STANZIONE, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716. ARTHI JAYARAMAN, Department of Chemical and Biomolecular Engineering, Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716. — Molecular dynamics (MD) is a well established technique to study the structure and dynamics of biomolecular systems. While atomistic simulations maintain chemical details, they are computationally intensive, thus limiting the accessible time, the length scales and the sampling. To overcome these limitations, coarse-grained (CG) models have proven to be successful in reproducing experimentally relevant length and time scales with reasonable computational expense. CG models can be developed to be phenomenological by effectively reproducing experimental results or can be developed by mapping rigorously to structural information provided by atomistic MD simulations. The latter method is recommended for biomolecules and biomaterials since atomistic simulations capture the detailed effect of the medium on interactions that affect the structure, dynamics and functional properties of the biomolecules, and that can be programmed into the CG models. In this poster we highlight three different cases where atomistic MD simulations provide such essential information to guide CG models: Polyethylene glycol, Elastic-like peptides and Collagen-like peptides based biomaterials.

M1.00063 The influence of ionic strength on DNA diffusion in gel networks1. YUANXI FU, AH-YOUNG JEE, HYEONG-JU KIM, STEVE GRANICK, Institute for Basic Science — Cations are known to reduce the rigidity of the DNA molecules by screening the negative charge along the sugar phosphate backbone. This was established by optical tweezer pulling experiment of immobilized DNA strands. However, little is known regarding the influence of ions on the motion of DNA molecules as they thread through network meshes. We imaged in real time the Brownian diffusion of fluorescent labeled lambda-DNA in an agarose gel network in the presence of salt with monovalent or multivalent cations. Each movie was analyzed using home-written program to yield a trajectory of center of the mass and the accompanying history of the shape fluctuations. One preliminary finding is that ionic strength has a profound influence on the slope of the trace of mean square displacement (MSD) versus time.1The influence of ionic strength on DNA diffusion in gel networks

M1.00064 Active microrheology of entangled blends of DNA and Actin link polymer flexibility to induced molecular deformations and stress propagation. ROBERT FITZPATRICK, RAE ROBERTSON-ANDERSON, University of San Diego, ANDERSON RESEARCH TEAM — Actin is a ubiquitous structural protein in the cytoskeleton that gives cells shape and rigidity, and plays important roles in mechanical processes such as cell motility and division. Actins diverse roles stem from its ability to polymerize into semiflexible filaments that are less than one persistence length (\(17 \text{ nm}\)) in length, and form entangled networks that display unique viscoelastic properties. We previously found that entangled actin networks propagate microscale forces over several persistence lengths (\(\lambda_0 \text{ m}\)) and takes minutes to relax. DNA, oppositely, has thousands of persistence lengths (50 nm) per chain, exhibits minimal force propagation, and takes only seconds to re-equilibrate. To directly determine the role of flexibility in mechanical response and force propagation of entangled networks, we use optical tweezers and fluorescence microscopy to investigate blends of actin and DNA. We use optically driven microparticles to perturb the network far from equilibrium and measure the force the network creates in response to the induced force. We simultaneously track partially labeled actin filaments during the perturbation and subsequent relaxation period. We characterize filament deformation and show explicitly how induced microscale forces propagate through the network.

M1.00065 Deep image analysis of entangled ring-shaped DNA. HYEONGJU KIM, AH-YOUNG JEE, STEVE GRANICK, Institute for Basic Science — Ring-shaped DNA entangled in aqueous actin networks and observed by super-resolution microscopy (STED; stimulated emission depletion) offers rich data for comparison with unresolved questions of polymer physics. Using home-written software, we calculated not only the center of mass (CoM) and CoM trajectories of hundreds of molecules, but also analyzed conformation dynamics with statistical analysis including wavelet transformation and a correlation matrix approach. The analysis reveals some surprising aspects unanticipated by classical theories.

M1.00066 Quantifying the effects of cyclic defects on the mechanical properties of polymer gels. RUI WANG, MINGJIANG ZHONG, KEN KAWAMOTO, JEREMIAH JOHNSON, BRADLEY OLSEN, Massachusetts Institute of Technology — Understanding the correlation between the topology and properties of polymer gels is an outstanding challenge in polymer science. Classical theories of gel elasticity assume acyclic tree-like network topology; however, all polymer gels inevitably possess cyclic defects: loops that have profound, yet previously unpredictable, effect on gel properties. Here, we develop a modified phantom network theory that describes the effects of loops on the modulus of polymer gels. We demonstrate that small loops (primary and secondary loops) have vital effect on the modulus; whereas this negative impact decreases rapidly as the loop order increases, especially for networks with higher junction functionalities. Loop effect is non-local, which can propagate to its neighborhood strands. We show that adjacent loops weaken the network cooperatively, resulting in the nonlinear decrease of the dimensionless modulus (\(G/vkT\), where \(v\) is the total density of polymer strands) with the loop fraction. The theory is in good agreement with the experimental data without any fitting parameters.
**M1.00067 Degrafting of polymer brushes from substrates enables insight about the brush structure and facilitates surface patterning.** ROHAN PATIL, North Carolina State Univ, SALOMON TURGAN-COHEN, Kettering University, JIRI SROGL, North Carolina State Univ, DOUGLAS KISEROW, US Army Research Office, JAN GENZER, North Carolina State Univ — Polymers end-grafted to surfaces or interfaces, commonly referred to as polymer brushes, enable tailoring physico-chemical properties of material surfaces. Many applications of polymer brushes require information about the molecular weight (MW) and grafting density (GD) of polymer brushes. For brushes synthesized by surface initiated polymerization (SIP) determining these attributes was always a challenge. We have developed a simple method of measuring MW and GD of these systems by degrafting SIP from silica-based surfaces by using tetrabutyl ammonium fluoride (TBAF), which attacks selectively Si-O bonds and enables complete degrafting of poly(methyl methacrylate) (PMMA) brushes from silica based substrates without damaging the backbone. The rate of PMMA degrafting decreases with reaction time and depends on the concentration of TBAF, temperature, and the initial GD of the system. The molecular weight distribution of the degrafted PMMA was measured using size exclusion chromatography. The GD was calculated from known MW and dry thickness of the PMMA brush. Spatial patterns of degrafted regions on the substrate can be prepared by either localizing the TBAF to certain regions or by gradually immersing homogeneous samples into TBAF solution.

**M1.00068 Driving Organic Molecule Crystallization with Surface Reconstructions.** JESSICA BICKEL, GIANFRANCO TROVATO, Cleveland State University — This work examines how surface reconstructions can drive crystallization of organic molecules via self-assembly. Organic electronic molecules have low conductivities compared to inorganic materials, but crystallizing these polymers increases their conductivity. This project uses surface reconstructions with periodically repeating topographies to drive the crystallization process. The samples are grown by placing a drop of a dilute PEDOT solution on the clean Si(001)-(2x1) or Si(111)-(7x7) surface reconstruction and heating the surface up to both evaporate the solvent and promote diffusion of the polymer to the thermodynamically defined lowest energy position. The resulting samples are characterized by scanning tunneling microscopy (STM) with respect to their crystallinity and electronic properties. Of particular interest is whether there is a preferential location for the PEDOT molecule to adsorb and whether there are any conformational changes upon adsorption that modify the HOMO-LUMO gap. This work is being done in a new pan-style RHK-STM enclosed in a glovebox at Cleveland State University. The glovebox has O₂ and H₂O levels of less than 1ppm. This allows for sample preparation and imaging in a controlled environment that is free from contamination.

**M1.00069 The Study of Intercalation Length between dPS Films and PS-grafted Layers.** HOYEON LEE, SEONGJUN JO, Yonsei University, TOYOAKI HIRATA, Kyusu University, NORIFUMI L. YAMADA, J-PARC, KEIJI TANAKA, Kyusu University, DU YEOL RYU¹, Yonsei University — In polymer thin film system, the type of interfacial interaction is a critical parameter to determining the thermal and physical properties of polymer films. Interestingly, the interfacial energy of grafted substrates with polymer chains is remarkably altered by simply controlling grafting density, which has been referred to as autopolymerization. In this study, we investigated the interpenetrating interfaces between deuterated polystyrene (dPS) and grafted substrates with the same chemical identity. PS-grafted substrates were prepared using a grafting-to approach with hydroxyl end-functionalized polystyrene (PSOH) in a dry brush regime, where the brush thickness and grafting density were determined based on the chain length (or molecular weight, Mᵢ) of PSOHs. The penetration lengths (ξ) at interfaces between dPS and PS-grafted layers were characterized using neutron reflectivity (NR) measurements (performed at the SOFIA beam-line at J-PARC, Japan).

¹academic adviser

**M1.00070 Glass transition dynamics and charge carrier mobility in conjugated polyfluorene thin films.** HUI QIN, DAN LIU, TAO WANG, Wuhan University of Technology — Conjugated polymers are commonly used in organic optoelectronic devices, e.g. organic photovoltaics (OPVs), light-emitting diodes (LEDs) and field effect transistors (FETs). In these devices, the conjugated polymers are prepared as thin films with thicknesses in the range of tens to hundreds of nanometers, and are interfaced with different function layers made from organic or inorganic materials. We have studied the glass transition temperature (Tg) of poly(9,9-diocylfluorene)-co-N-(1,4-butylphenyl)diphenylamine) (TFB) thin films supported on different substrates, as well as their SCLC charge carrier mobility in photodiodes. Both Monotonic and non-monotonic Tg deviations are observed in TFB thin films supported on Si/SiOx and PEDOT-PS, respectively. With low to moderate thermal crosslinking, the thickness dependent Tg deviation still exists, which diminishes in TFB films with a high crosslinking degree. The vertical charge carrier mobility of TFB thin films extracted from the SCLC measurements is found increase with film thickness, a value increases from 1 to 50 x 10⁻⁶ cm² V⁻¹ s⁻¹ in the thickness range from 15 to 180 nm. Crosslinking was found to reduce the mobility of TFB thin films. The Tg deviations are also discussed using the classic layered models in the literature. Our results provide a precise guide for the fabrication and design of high performance optoelectronic devices.

**M1.00071 Bending and Fracture in Thin Polymer Films during Capillary Origami Assembly.** TIMOTHY TIWOGH, ANDREW EROLL, North Dakota State Univ — Capillary origami uses liquid tension to bend thin films into useful shapes and structures. The ability to scale this process to the microscopic range has led to growing interest in capillary origami and many potential applications. Clearly, the creation of three dimensional structures from flat sheets depends deeply on a combination of properties: fluid tensions, film thickness, film modulus and importantly the films fracture properties. Fractures in a film are a critical component of macroscopic origami but macroscopic methods for creating these fractures are not possible at the microscopic scale. We present an experimental investigation of the interplay of capillary forces and material properties in the creation of controlled fractures in thin polymer films. Specifically, we use capillary forces to lift and bend a thin polymer film to the point of fracture using a variety of film thicknesses and material properties and attempt to model the basic underlying physics. We observe the creation of delaminations and fractures at pre-determined sites that can be tailored to specific shapes to be utilized in capillary origami.

**M1.00072 Confinement Effect on the Effective Viscosity of Plasticized Polymer Films.** FEI CHEN, D. PENG, Boston University Physics Department, Y. OGATA, K. TANAKA, Kyusu University Department of Applied Chemistry, Z. YANG, Soochow University Department of Polymer Science and Engineering, Y. FUJII, National Institute for Materials Science (Japan), N. L. YAMADA, Neutron Science Laboratory High Energy Accelerator Research Organization (Japan), C. H. LAM, Hong Kong Polytechnic University Department of Applied Physics, OHPELIA K. C. TSUI, Boston University Physics Department — We have measured the effective viscosity of polystyrene films with a small (4 wt%) added amount of diocyl phthalate (DOP) deposited on silica. A broad range of molecular weights, Mₑ, from 13.7 to 2,100 kg/mol was investigated. Our result shows that for the thin films with Mₑ < ~100 kg/mol, the addition of DOP causes the effective viscosity to decrease by a factor of ~4, independent of Mₑ. But for the higher Mₑ films, the effective viscosity of the DOP added films creeps towards that of the neat films with increasing Mₑ. A model assuming the effective viscosity to be dominated by enhanced surface mobility for the lower Mₑ films, but surface-promoted interfacial slippage for the higher Mₑ films is able to account for the experimental observations.

We are grateful to the support of National Science Foundation through the project DMR-1310536.
M1.00073 Adhesion and Wetting in Soft Polymeric Systems, ANDREY DOBRYNIN, ZHEN CAO, Univ of Akron, MARK STEVENS, Sandia National Laboratories — We have developed a generalized model of particle/surface interactions describing adhesion and wetting phenomena. We show that for an elastic nanoparticle with radius $R_p$ and shear modulus $G_p$ interacting with an elastic substrate having shear modulus $G_s$, the crossover between adhesion and wetting-like behavior is determined by a dimensionless parameter $\beta = \gamma_s (G_s/2G_p)^{1/3} W^{-1/3}$. In the limit of small values of the parameter $\beta < 1$, our model reproduces JKR model for particle adhesion on elastic substrates (adhesion regime). However, in the opposite limit, $\beta > 1$, the capillary forces play a dominant role and determine particle/substrate interactions (wetting regime). We extended our approach to describe the detachment of rigid nanoparticles from elastic surfaces. Simulation results confirm that the detachment force, $f^*$, depends on a dimensionless parameter $\delta = \gamma_s (G_s R_p)^{1/3} W^{1/3}$, which corresponds to the ratio of the surface energy of the neck and the substrate elastic energy. In the case when $\delta < 1$, the critical detachment force takes a critical value calculated in the framework of the JKR model, $f = 1.5 \pi W R_p$ (JKR regime). However, in the opposite limit, the critical detachment force scales as $f^* \propto \gamma_s^{3/2} R_p^{1/2} G_p^{1/2}$ (necking regime). All simulation data can be described by a crossover function $f^* \propto \gamma_s^{3/2} R_p^{1/2} G_p^{1/2} \delta^{-1.89}$.

1 NSF DMR-1409710

M1.00074 Novel adhesion properties of irreversibly adsorbed polymer chains, ZHIZHAO CHEN, MANI SEN, JUSTIN CHEUNG, DEBORAH BARKLEY, NAISHENG JIANG, WENDUO ZENG, MAYA K. ENDOH, TADANORI KOGA, Stony Brook University — The stability of thin polymer films on solids is of vital interest in traditional technologies and in new emerging nanotechnologies. We recently found that nanoscale structures of polymer chains adsorbed onto a silicon (Si) substrate (“adsorbed nanolayers”) play a crucial role in the thermal stability of the film. To understand the adhesion mechanism at the adsorbed polymer-free polymer interface, we mimicked the interface by preparing bilayers where a 200 nm-thick polymer film and an adsorbed nanolayer, both prepared on Si, were pressed together at high temperature. The bilayers were then subjected to an adhesion test by measuring the critical normal force required to separate the two films. Polystyrene was used as a model. The results are intriguing as they show an absence of adhesion between the “flattened” adsorbed chains, which lie flat together at high temperature. The bilayers were then subjected to an adhesion test by simulating the JKR model, $f = 1.5 \pi W R_p$ (JKR regime). However, in the opposite limit, the critical detachment force scales as $f^* \propto \gamma_s^{3/2} R_p^{1/2} G_p^{1/2} \delta^{-1.89}$ (necking regime). All simulation data can be described by a crossover function $f^* \propto \gamma_s^{3/2} R_p^{1/2} G_p^{1/2} \delta^{-1.89}$.

1 We acknowledge the financial support from NSF Grant No. CMMI-1332499.

M1.00075 Entropic Segregation of Short Polymers to the Surface of a Polydisperse Blend, PENDAR MAHMoudI, MARK MATSEn, University of Waterloo — Surface effects become particularly important for micro-sized and even more so for nano-sized objects. Naturally, enthalpic preferences will cause certain components of a multi-component material to segregate to a surface, but in polymeric materials this can also happen as a result of purely entropic reasons. To demonstrate this, we consider the effect of a surface on a binary blend of chemically identical long and short polymers, using self-consistent field theory. Despite the absence of any enthalpic preference, the short polymers are found to segregate to the surface. We investigate how the amount of the surface excess and its decay length depends on the polymeric model, the molecular weights of the two polymers and the blend composition.

1 This work was supported by NSERC of Canada.

M1.00076 Effect of tacticity on the structure and glass transition temperature of polystyrene thin films, YERGOU TATEK, SOLOMON NEGASH, Addis Ababa University, MESFIN TSIige, The University of Akron — Detailed atomistic Molecular Dynamics simulations are performed to explore the effect of tacticity on the glass transition temperature as well as other pertinent structural properties of films of polystyrene (PS) chains adsorbed onto two distinct types of solid substrates. The investigated systems consist of thin films made of isotactic, syndiotactic and atactic PS chains adsorbed on graphite and hydroxylated silica surfaces. The structure of the films is investigated in terms of film density profiles and side chains and backbone orientations. Simulations results reveal a marked dependence of the film structure on substrate type while the absence of a strong correlation between structure and tacticity is observed. Moreover, it is found that the glass transition temperature is substrate dependent and takes larger values for films adsorbed on graphite surface, irrespective of chain tacticity.

M1.00077 Capillary wrinkling of thin bilayer polymeric sheets, JOOYOUNG CHANG, NARAYANAN MENON, THOMAS RUSSELL, Univ of Mass - Amherst — We have investigated capillary force induced wrinkling on a floated polymeric bilayer thin sheet. The origin of the wrinkle pattern is compressional hoop stress caused by the capillary force of a water droplet placed on the floated polymeric thin sheet afore investigated. Herein, we study the effect of the differences of surface energy arising from the hydrophobicity of Polystyrene (PS Mw: 97 K, Contact Angle: 88°) and the hydrophilicity of Poly(methylmethacrylate) (PMMA Mw: 99K, Contact Angle: 68°) on two sides of a bilayer film. We measure the number and the length of the wrinkles by broadly varying the range of thicknesses of top (9 nm to 550 nm) and bottom layer (25 nm to 330 nm). At the same, there is only a small contrast in mechanical properties of the two layers (PS E = 3.4 GPa, and PMMA E = 3 GPa). The number of the wrinkles is not strongly affected by the composition (PS(Top)/PMMA(Bottom) or PMMA(Top)/PS(Bottom)) and the thickness of each and overall bilayer system. However, the length of the wrinkle is governed by the contact angle of the drop on the top layer of bilayer system. We also compare this to the wrinkle pattern obtained in monolayer systems over a wide range of thickness from PS and PMMA (7 nm to 1 μm).

1 W.M. Keck Foundation

M1.00078 Role of monomer sequence and backbone structure in polypeptoid and polypeptide polymers for anti-fouling applications, ANASTASIA PATTerson, GEORGIos RIZIS, UC Santa Barbara, BRANDON WENNING, Cornell University, JOHN FINLAY, Newcastle University, CHRISTOPHER OBER, Cornell University, RACHEL SEGALMAN, UC Santa Barbara — Polymeric coatings rely on a fine balance of surface properties to achieve biofouling resistance. Bioinspired polymers and oligomers provide a modular strategy for the inclusion of multiple functionalities with controlled architecture, sequence and surface properties. In this work, polypeptoid and polypeptide functionalized coatings based on PEO and PDMS block copolymers were compared with respect to surface presentation and fouling by Ulva linza. While polypeptoids and polypeptides are simple isothers of each other, the lack of backbone chirality and hydrogen bonding in polypeptoids leads to surprisingly different surface behavior. Specifically, the polypeptoids surface segregate much more strongly than analogous polypeptide functionalized polymers, which in turn affects the performance of the coating. Indeed, polypeptide functionalized surfaces were significantly better both in terms of anti-fouling and fouling release than the corresponding polypeptide-bearing polymers. The role of specific monomer sequence and backbone chemistry will be further discussed in this poster.
M1.00079 Conformation and hydration of surface grafted and free polyethylene oxide chains in solutions, UDAYA DAHAL, Department Dept. of Physics and Institute of Materials Science, Univ. of Connecticut. ZILU WANG, Dept. of Physics and Institute of Materials Science, Univ. of Connecticut — Due to the wide application of polyethylene oxide (PEO), ranging from biomedicine to fuel cells, it is one of the most studied polymers in the scientific world. In order to elucidate detailed molecular-level insights on the impact of surface grafting on PEO conformation, we performed atomistic molecular dynamics simulations of PEO chains in solution and grafted to a flat gold surface in different solvents. We examined the hydration as well as conformation of the free chain compared to the grafted polymer in pure water and mixed solvents. We find that grafted chains are stiffer and have a stronger tendency to form helical structures in isobutyril acid or mixture of isobutyric acid and water solution than the free chains in corresponding solutions. For grafted chains exposed to pure water the random coil conformation is retained at low grafting density, but becomes stretched and more dehydrated as the grafting density or temperature increases.

M1.00080 Charge transport and structural dynamics in ultra-thin films of polymerized ionic liquids, MAXIMILIAN HERES, TYLER COSBY, Univ of Tennessee, Knoxville, STEFAN BERDZINSKI, VERONICA STREHMEL, Department of Chemistry and Institute for coatings and surface chemistry, Hochschule Niederrhein University of Applied Sciences, ROBERTO BENSON, JOSHUA SANGORO, Univ of Tennessee, Knoxville — Ion conduction and structural dynamics in a series of ultra-thin films of imidazolium based polymerized ionic liquids are investigated using broadband dielectric spectroscopy, atomic force microscopy, and ellipsometry. No alteration in the characteristic charge transport rate is observed between bulk sample and films as thin as 12nm. These results are discussed within the recent approaches proposed to explain the confinement effects on structural dynamics in polymers and low molecular weight ionic liquids.

M1.00081 Molecular dynamics simulations and morphology analysis of TEM imaged PVDF nanofibers, JIAYUAN MIAO, Case Western Reserve University, DARRELL RENEKER, MESFIN TSIGE, University of Akron, PHILIP TAYLOR, Case Western Reserve University — With the goal of elucidating the structure of polyvinylidene fluoride (PVDF) nanofibers, all-atom molecular dynamics simulations were performed, and the results compared with structures observed in high resolution transmission electron microscopy (TEM) at the molecular level. Simulation shows that the stability of the β-phase component in a PVDF nanofiber is influenced by its thickness and processing history. When exposed to irradiation, as in a TEM observation, the structure is then further modified by the effects of chain scission. The transformation from the α phase into a paraelectric phase can explain the spindle formation and serpentine motion of molecular segments observed by Zhong et al. (Polymer, 54, 2013, 3745-3756) in irradiated PVDF nanofibers. From a comparison between simulated and experimental TEM images it was possible to identify numerous features that are useful in unveiling the inherent structure of PVDF nanofibers. The experimental TEM images appear to match well with those predicted by a model based on α-phase PVDF, while also being consistent with an alternative model (Nanoscale 2015, DOI: 10.1039/c5nr01619c).

M1.00082 Processing and characterization of natural fiber reinforced thermoplastic composites using micro-braiding technique. SATOSHI KOBAYASHI, Tokyo Metropolitan Univ, SHINJI OGIHARA, Tokyo University of Science — In the present study, we investigate fatigue properties of green composites. A hemp fiber yarn reinforced poly(lactic acid) composite was selected as a green composite. Unidirectional (UD) and textile (Textile) composites were fabricated using micro-braiding technique. Fatigue tests results indicated that fatigue damages in UD composites was splitting which occurred just before the final fracture, while matrix crack and debonding between matrix and fiber yarn occurred and accumulated stably in Textile composites. These results were consistent with modulus reduction and acoustic emission measurement during fatigue tests.

M1.00083 Deformation Behavior during Processing in Carbon Fiber Reinforced Plastics, SHINJI OGIHARA, Tokyo University of Science, SATOSHI KOBAYASHI, Tokyo Metropolitan University — In this study, we manufacture the device for measuring the friction between the prepreg curing process and subjected to pull-out tests with it. The prepreg used in this study is a unidirectional carbon/epoxy, produced by TORAY designation of T700SC/2592. When creating specimens 4-ply prepgres are prepared and laminated. The 2-ply prepregs in the middle are shifted 50mm. In order to measure the friction between the prepreg during the cure process, we simulate the environment in the autoclave in the device, and we experiment in pull-out test. Test environment simulating temperature and pressure. The speed of displacement should be calculated by coefficient of thermal expansions (CTE). By calculation, 0.05mm/min gives the order of magnitude of displacement speed. In this study, 3 pull-out speeds are used: 0.01, 0.05 and 0.1mm/min. The specimen was heated by a couple of heaters, and we controlled the heaters with a temperature controller along the curing conditions of the prepreg. We put pressure using 4 bolts. Two strain gages were put on the bolt. We can understand the load applied to the specimen from the strain of the bolt. Pressure was adjusted the tightness of the bolt according to curing conditions. By using such a device, the pull-out test performed by tensile testing machine while adding temperature and pressure. During the 5 hours, we perform experiments while recording the load and stroke. The shear stress determined from the load and the stroke, and evaluated.

M1.00084 Localized Memory Effect of Elastomers Filled with Nanoparticles, SHOUBO LI, XIAORONG WANG, Chemical Engineering, Tongji University, Shanghai — When a filler-reinforced elastomer compound is oscillatory sheared or pressed at a small fixed strain (e.g., 2%) for a period of time, it can produce a localized memory perturbation in its dynamic spectrum. Typically, a localized memory appears near the applied strain amplitude in the loss modulus spectrum. Sequential holding the system at two strains can produce one or two holes depending on the deformation history. While this discovery of localized memory effect seems to be significant and compelling, its generality in vulcanized elastomers containing various fillers has not yet been tested extensively. In this work, we intend to expand on our previous work of a colloidal silica-filled model system to carbon black-filled rubber. We also examine the effect of filler volume fraction in rubber compounds on the spectral memory phenomenon.

M1.00085 Mechanical Properties of Cellulose Microfiber Reinforced Polyolefin, SATOSHI KOBAYASHI, HIROYUKI YAMADA, Tokyo Metropolitan Univ — Cellulose microfiber (CeF) has been expected as a reinforcement of polymer because of its high modulus and strength and lower cost. In the present study, mechanical properties of CeF/polyolefin were investigated. Tensile modulus increased with increasing CeF content. On the other hand, tensile strength decreased. Fatigue properties were also investigated with acoustic emission measurement. Stiffness of the composites gradually decreased with loading. Drastic decrease in stiffness was observed just before the final fracture. Based on the Mori-Tanaka’s theory, the method to calculate modulus of CeF were proposed to evaluate dispersion of CeF.
M1.00086 Soft composites with the twisted plywood microstructure, a lesson from nature.

1, YONGJIN KIM, ALFRED CROSBY, Univ of Mass - Amherst, CROSBY RESEARCH GROUP TEAM — The twisted plywood microstructure, consisting of rigid structural units within a continuous matrix, is known to be prevalent in many natural materials, including exoskeletons of crustaceans, scales of fish, and even bones of mammals. Although it is yet to be resolved whether this structure is a product of evolution or an inevitable consequence of chirality of building blocks, nature utilizes the structure extensively to create various components. Previous studies have focused on fabricating and characterizing synthetic composites with similar structures; however, these composites have been based on a rigid matrix, e.g., an epoxy resin, and hard fibers, e.g., carbon fibers. For this combination of materials, it has been difficult to deconvolute the specific roles of each component. For a better understanding of the advantage of the structure, we have developed flexible composites, comprising a soft matrix and hard fiber bundles at two different size scales. Macroscale engineered samples were created by combining elastomer and hard fibers, while sub-micron composites are fabricated from self-assembled nanoparticle ribbons and hydrogel matrices. The advantageous mechanical response of these flexible twisted plywood composites is characterized and presented.

M1.00087 Modeling heterogeneous polymer-grafted nanoparticle networks having biomimetic core-shell structure

1, BADEL M. MBANGA, VICTOR V. YASHIN, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, USA, NIELS HOLTEN-ANDERSEN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, USA — Inspired by the remarkable mechanical properties of such biological structures as mussel adhesive fibers, we use 3D computational modeling to study the behavior of heterogeneous polymer-grafted nanoparticle (PGN) networks under tensile deformation. The building block of a PGN network is a nanoparticle with grafted polymer chains whose free ends' reactive groups can form both permanent and labile bonds with the end chains on the nearby particles. The tunable behavior of cross-linked PGN networks makes them excellent candidates for designing novel materials with enhanced mechanical properties. Here, we consider the PGN networks having the core-shell structures, in which the type and strength of the inter-particle bonds in the outer shell differ from those in the core. Using the computer simulations, we have obtained and compared the ultimate tensile properties (strength, toughness, ductility) and the strain recovery properties for the uniform samples and various core-shell structures. We demonstrate that the core-shell structures could be designed to obtain highly resilient self-healing materials.

M1.00088 Effects of Dimensionality and Flexibility of Conductive Fillers in Nanocomposites on Percolating Network Formation and Electrical Conductivity

SEULKI KWON, HYUN WOO CHO, BONG JUNE SUNG, Department of Chemistry, Sogang University, Seoul 121-742, Republic of Korea — We conduct extensive langevin dynamics (LD) simulation to explore how the dimensionality and flexibility of conductive fillers in polymer nanocomposites influence their percolation network formation and electrical conductivity. The percolation network formation of nanoparticles in polymer matrices is critical to obtaining desired properties of polymer nanocomposites. Some nanofillers such as carbon nanotubes (CNTs) and graphene nanosheets, are so flexible that they become either wavy or crumpled. Such a variability in nanofiller conformation brings a change to the percolation network, but has been often ignored in the theoretical and computational investigation. We consider three kinds of nanofillers of different dimensionality: zero-dimensional (0D) nanospheres, one-dimensional (1D) nanorods, and two-dimensional (2D) nanoplates. We estimate the percolation network concentration ($\phi_c$) and electrical conductivity with careful finite-size scaling. When the sizes of nanofillers are comparable, the dimensionality of nanofillers influences on $\phi_c$ and electrical conductivity of nanocomposites significantly. The effect of flexibility of nanofillers is less significant than that of dimensionality.

M1.00089 Structure, Nanomechanics and Dynamics of Dispersed Surfactant-Free Clay Nanocomposite Films

XIAO ZHANG, JING ZHAO, University of Akron, CHAD SNYDER, National Institute of Standards and Technology, ALAMGIR KARIM, University of Akron, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY COLLABORATION — Natural Montmorillonite particles were dispersed as tactoids in thin films of polycaprolactone (PCL) through a flow coating technique assisted by ultra-sonication. Wide angle X-ray scattering (WAXS), Grazing-incidence wide angle X-ray scattering (GI-WAXS), and transmission electron microscopy (TEM) were used to confirm the level of dispersion. These characterization techniques are in conjunction with its nanomechanical properties via strain-induced buckling instability for modulus measurements (SIEBIMM), a high throughput technique to characterize thin film mechanical properties. The linear strengthening trend of the elastic modulus enhancements was fitted with Halpin-Tsai (HT) model, correlating the nanoparticle geometric effects, and mechanical behaviors based on continuum theories. The overall aspect ratio of dispersed tactoids obtained through HT model fitting is in reasonable agreement with digital electron microscope image analysis. Moreover, glass transition behaviors of the composites were characterized using broadband dielectric relaxation spectroscopy. The segmental relaxation behaviors indicate that the associated mechanical property changes are due to the continuum filler effect rather than the interfacial confinement effect.

M1.00090 Influence of Surface Coating of Magnetic Nanoparticles on Mechanical Properties of Polymer Nanocomposites

1, ECEM YARAR, GIZEM KARAKAS, Yeditepe University, DENIZ RENDE, RAHMI OZISIK, Rensselaer Polytechnic Institute, SEYDA MALTA, Yeditepe University, — Polymer nanocomposites have emerged as promising materials due to improved properties when compared with conventional bulk polymers. Nanofillers are natural or synthetic organic/inorganic particles that are less than 100 nm in at least one dimension. Even the addition of trace amounts of nanofillers to polymers may lead to unique combinations of properties. Among variety of inorganic nanofillers, iron oxide magnetic nanoparticles are of great interest due to their unique physical and chemical properties, such as low toxicity, biocompatibility, large magnetization and conductivity, owing to their extremely small size and large specific surface area. In this study, approximately 8-10 nm magnetic nanoparticles coated with either citric acid or oleic acid are synthesized and blended with poly(methyl methacrylate) (PMMA) or poly(ethylene oxide) (PEO). The hydrophobicity/hydrophilicity of the polymer and the surface coating on the iron oxide nanoparticles are exploited to control the dispersion state of nanoparticles, and the effect of dispersion on mechanical and thermal properties of the nanocomposites are investigated via experimental methods such as dynamic mechanical analysis and differential scanning calorimetry.

M1.00091 Wide Angle X-Ray Scattering Investigations on Irradiated iPP-VGCNF Nanocomposites

1, ARNOLD FONSECA, DORINA CHIPARA, KAREN LOZANO, MIRCEA CHIPARA, The University of Texas Rio Grande Valley — Isotactic Polypropylene (iPP) has been loaded by various amounts of Vapor Grown Carbon Nanofiber (VGCNF), ranging between 0 and 20 % wt., via melt mixing. The as-obtained nanocomposites were gamma irradiated in air, at room temperature, at a dose rate of about 1 kGy/h and various integral doses ranging between 0 and 28 kGy. by using a 60Co source. Wide Angle X-Ray Spectroscopy has been used to quantify the changes in the crystalline structure and the degree of crystallinity of iPP-VGCNFs nanocomposites. The measurements have been carried out by a Bruker Discover 8 spectrometer. Additional measurements have been performed by Raman spectroscopy using a Renishaw InVia microscope system operating at 532 and 785 nm. The experimental spectra of the nanocomposite were fitted by assuming a superposition of extended Breit-Wigner-Fano line shapes. It is concluded that the observed modifications noticed in these nanocomposites are dominated by the radiation-induced degradation of the polymeric matrix. Differential Scanning Calorimetry data provided additional information regarding the effect of the nanofiller on the degree of crystallinity.
M1.00092 Designing a gel–fiber composite to extract nanoparticles from solution. YA LIU, University of Pittsburgh, OLGA KUKSHENOK, Clemson University, ANNA BALAZS, University of Pittsburgh — Using DPD simulations, we proposed the design of a gel–fiber coating where the components of the system act in concert to extract particles from solution and localize these solids in the underlying gel layer. We model an array of flexible fibers that are embedded in a lower critical solution temperature (LCST) thermo-responsive gel, which swells at lower temperatures and collapses at higher temperatures. The system is immersed in a solution containing dispersed nanoparticles and this fluid is driven to flow by an imposed shear. When the gel is heated, it collapses to expose the fibers, and thereby, triggers the “catch” process. Namely, the fibers can act like “arms” that wrap around the nanoparticle and bring it from the outer solvent into the gel layer. Moreover, we show that depending on the flexibility and hydrophobicity of the fibers, as well as the imposed shear, we can position the nanoparticles at the desired height within the gel layer. Our approach can be utilized for the detection and separation of components in fluids and for the controlled insertion of nanoparticles within a hydrogel at a particular distance from the gel interface.

M1.00093 ABSTRACT WITHDRAWN –

M1.00094 Viscoelastic Analysis of Thermally Stiffening Polymer Nanocomposites1, ANDREW EHLERS*, DENIZ RENDE, Rensselaer Polytechnic Institute, ERKAN SENSES, PINAR AKCORA, Stevens Institute of Technology, RAHMI OZISIK, Rensselaer Polytechnic Institute — Poly(ethylene oxide), PEO, filled with silica nanoparticles coated with poly(methyl methacrylate), PMMA, was shown to present thermally stiffening behavior above the glass transition temperature of both PEO and PMMA. In the current study, the viscoelastic behavior of this nanocomposite system is investigated via noninvasive experiments to complement ongoing rheological studies. Results were compared to neat polymers, PEO and PMMA, to understand the effect of coated nanoparticles.

1This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730. *Undergraduate student.

M1.00095 Controlling the Degradation of Bioreosorbable Polymers1, ISTVAN MORITZ, BRIAN CROWLEY*, ELIZABETH BRUNDAGE*, Materials Science and Engineering, Rensselaer Polytechnic Institute, DENIZ RENDE, Center for Materials, Devices and Integrated Systems, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Bioreosorbable polymers play a vital role in the development of implantable materials that are used in surgical procedures, controlled drug delivery systems; and tissue engineering scaffolds. The half-life of common bioreosorbable polymers ranges from 3 to over 12 months and slow bioresorption rates of these polymers restrict their use to a limited set of applications. The use of embedded enzymes is reported as a strategy to accelerate the degradation of bioreosorbable polymers. However, it was shown that controlled degradative behavior is strongly related to the degradation rate of the polymers and the mechanism of the degradation. Recent results indicate that the internal temperature of iron oxide magnetic nanoparticle-doped PEO samples can be increased via an alternating magnetic field, and temperature increase depends strongly on nanoparticle concentration and magnetic field parameters. The temperature achieved is sufficient to relax the PEO matrix and to enable the diffusion of enzymes from PEO to a surrounding PCL matrix. Current studies are directed at measuring the degradation rate of PCL due to the diffused enzyme.

1This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730. *Undergraduate student.

M1.00096 Interfacial slip in nano filled polymer blends, JOHN MIKHAIL, DI XI, JOSEPH ORTIZ, DILIP GERSAPP, Stony Brook University — The ability to control the interfacial slip in polymer blends is key to strengthening the material. Here, we look at how nano fillers can be used to strengthen the interface. By designing nano fillers with the appropriate surface energy we show how nano fillers can localize at the interface between the two polymer blends. We examine that the aspect ratio of the nano filler has on its ability to reduce the interfacial slip, and look to understand the mechanisms by which the slip is reduced. We look for network formation near the interface as a possible strengthening mechanism.

M1.00097 Nanocellulose Composite Materials Synthesizes with Ultrasonic Agitation, TIMOTHY KIDD, ANDREW FOLKEN, BYRON FRITCH, DEREK BRADLEY, University of Northern Iowa — We have extended current techniques in forming nanocellulose composite solids, suspensions and aerogels to enhance the breakdown of cellulose into its molecular components. Using only mechanical processing which includes ball milling, using a simple mortar and pestle, and ultrasonic agitation, we are able to create very low concentration uniform nanocellulose suspensions in water, as well as incorporate other materials such as graphite, carbon nanotubes, and magnetic materials. Of interest is that no chemical processing is necessary, nor is the use of nanoparticles, necessary for composite formation. Using both graphite and carbon nanotubes, we are able to achieve conducting nanocellulose solids and aerogels. Standard magnetic powder can also be incorporated to create magnetic solids. The technique also allows for the creation of an extremely fine nanocellulose suspension in water. Using extremely low concentrations, less than 1% cellulose by mass, along with careful control over processing parameters, we are able to achieve highly diluted, yet homogenous nanocellulose suspensions. When air dried, these suspensions have similar hardness and strength properties to those created with more typical starting cellulose concentrations (2-10%). However, when freeze-dried, these dilute suspensions form aerogels with a new morphology with much higher surface area than those with higher starting concentrations. We are currently examining the effect of this higher surface area on the properties of nanocellulose aerogel composites and how it influences the impact of incorporating nanocellulose into other polymer materials.

M1.00098 Predicting \( \chi \) for polymers with stiffness mismatch from simulations, DANIEL KOZUCH, WENLIN ZHANG, ENRIQUE GÓMEZ, SCOTT MILNER; Department of Chemical Engineering, Penn State University — The Flory-Huggins \( \chi \) parameter describes the excess free energy of mixing and governs phase behavior for polymer blends and block copolymers. For chemically distinct polymers, the value of \( \chi \) is dominated by the mismatch in cohesive energy densities of the monomers. For blends of chemically similar polymers, the entropic portion of \( \chi \) arising from non-ideal local packing, becomes more significant. Using polymer field theory, Fredrickson, Liu, and Bates predict that a difference in backbone stiffness can result in a positive \( \chi \) for chains consisting of chemically identical monomers. To quantitatively investigate this phenomenon, we perform molecular dynamic (MD) simulations for bead-spring chains which differ only in stiffness. From the simulations, we apply a novel thermodynamic integration to extract \( \chi \) as low as \(-3\) per monomer for blends with mild stiffness mismatch. By introducing a standardized effective monomer, we map real polymers to our bead-spring chains and show that the predicted entropic portion of \( \chi \) is consistent with experimental data.

M1.00099 Comparative Study of Silk-Silk Alloy Materials, YE XUE, Rowan University; Nanjing University, DAVE JAO, Rowan University, WENBING HU, Nanjing University, NATHAN WOLF, EVA-MARIE ROCKS, XIAO HU, Rowan University — Silk fibroin materials can be used for various kinds of biomedical applications. We report a comparative study of silk-silk blend materials using thermal analysis and infrared spectroscopy. Four groups of silk-silk blend films: Mori-Tussah, Mori-Muga, Mori-Eri and Mori-Thai, were fabricated from aqueous solutions and blended at different weight ratios, respectively. These silk-silk blend systems exploit the beneficial material properties of both silks. DSC and temperature-modulated DSC were used to measure the transition temperatures and heat capacity of these water-based silk-silk blend films. Fourier transform infrared spectrometer was used to characterize secondary structures of silk-silk blends. This study demonstrates that Mori silk are fully miscible with Tussah, Muga, Eri and Thai silk at different weight ratios without phase separation. Glass transition temperatures, degradation temperatures and the contents of alpha-helix and random coils of those silk-silk blend films can be controlled by changing the contents of different silks in the blend system. The features of Mori silk combined with the attributes of Tussah, Muga, Eri and Thai silk offer a useful suite of materials for a variety of applications in the future.
M1.00100 Compatibility and Impact Resistance of Biodegradable Polymer Blends Using Clays and Natural Nanotubes, YICHEN GUO, XUE YUAN, XIANGHAO ZUO, MIRIAM RAFAILOVICH, Stony Brook University — Montmorillonite clays and Halloysite nanotubes (HNTs) were modified by surface adsorption of resorcinol di (phenyl phosphate) (RDP) oligomers. Biodegradable poly(lactic acid) (PLA) and poly (butylene adipate-co-butylene terephthalate) (PBAT) polymers were blended together with RDP coated clays and tubes. TEM images of thin sections indicated that even though both RDP coated clay nanotubes and platelets located on the interfacial region between two immiscible polymers, only the platelets, having the larger aspect ratio, were able to reduce the PBAT domain sizes. The ability of clay platelets to partially compatibilize the blend was further confirmed by the dynamic mechanical analysis (DMA) which showed that the glass transition temperatures of two polymers tend to shift closer. Izod impact testing demonstrated that the rubbery PBAT phase greatly increased the impact strength of the unfilled blend, but addition of only 5% clay, filler decrease the impact strength by nearly 50% while a small increase was observed with nanotubes at that concentration. A simple model is proposed. The clay platelets are observed to cover the interfacial area. Although they are effective at reducing the interfacial tension, they block the entanglements between two polymer phase and increase the overall brittleness. On the other hand, the HNTs are observed to lie perpendicular to the interface, which makes them less effective in reducing interfacial tension, but far more effective at retarding micro-crack propagation.

M1.00101 Hybrid Simulation Strategy for Simulating Self-Assembled Polymer Morphologies at the Atomic Scale, SUNGYOUL HWANG, YOUNGKEOL KIM, DOKYEONG KWON, KOOKHEON CHAR, Seoul Natl Univ — There have been many studies to investigate the phase behavior of block copolymers (BCPs) in cylindrical confinement. In the nanometer scale 2D confinement, the phase behavior of BCPs is mainly dependent upon commensurability and interfacial interaction. However, most studies have focused only on the effects of commensurability on the microdomains of BCPs. In this study, we expand the scope to homopolymer-BCP binary blends. Given fraction of homopolymers, the phase behavior of blends is dependent on molecular weight (Mw) of homopolymers. Lamella- and cylinder-forming poly(styrene-b-butadiene) (PS-b-PBD) and PS homopolymers (hPS) were drawn into the pores of anodized aluminum oxide (AAO) membranes in the melt by capillary forces. Based on the detailed observation of the morphologies within porous columns, we analyzed the structural transition of BCPs induced by the presence of hPS and confinement. The effect of hPS on the micro-domain of BCPs is greatly accentuated in nanoscale confinement compared to the bulk state due to the entropic loss of polymer chains. Pore diameters of AAO and Mw of the PS-b-PBD are also controlled so as to examine the effects of confinement on the phase transition of PS-b-PBD/hPS blends.

M1.00102 Controlling Miscibility in Polyethylene-Polynorbornene Block Copolymers via Side-Group Chemistry, WILLIAM MULHEARN, RICHARD REGISTER, Princeton University — Block copolymers containing a crystallizable block, such as polyethylene (PE), and an amorphous block with high glass transition temperature (Tg) are an interesting class of materials since the rigid glassy block can improve the mechanical response of the article under strain by reinforcing the crystal fold surface. However, to prepare an easily processable PE-containing block copolymer it is necessary to avoid microphase separation in the melt by selection of amorphous blocks with weak repulsive interactions against PE (low Flory interaction parameter χ or interaction energy density 1/χ). Most such low-χ polymers are chemically similar to PE, such as copolymers of ethylene and a small amount of an α-olefin, and therefore exhibit similarly low glass transition temperatures. This work investigates a series of low- and high-Tg polymers based on substituted norbornene monomers, polymerized via ring-opening metathesis polymerization (ROMP). Hydrogenated polynorbornene derivatives possess a wide range of glass transition temperatures, and miscibility with PE can be readily tuned by the choice of substituents on the monomers (e.g. aromatic vs. aliphatic groups). Two species investigated, hydrogenated poly(cyclohexyl norbornene) and hydrogenated poly(norbornyl norbornene), have high Tg and also remain miscible with polyethylene to high molecular weight. Additionally, the chemical identity and high thermal stability of these BCPs relative to other post-functionalized BCPs makes them attractive for applications.

M1.00103 Influence of Homopolymers on the Microdomain Behavior of Block Copolymers in 2D Confinement, YOUNGKEOL KIM, SUNGYOUL HWANG, GUIDUK YU, KOOKHEON CHAR, Seoul Natl Univ — Constraints imposed by nanometer scale confinement lead to changes in bulk equilibrium behavior of block copolymers (BCPs). Cylindrical pores with diameters corresponding to the length equivalent of several copolymer chains have been employed to investigate the influence of two-dimensional confinement on the behavior of BCPs. In this study, we expand the scope to homopolymer-BCP binary blends. Given fraction of homopolymers, the phase behavior of blends is dependent on molecular weight (Mw) of homopolymers. Lamella- and cylinder-forming poly(styrene-b-butadiene) (PS-b-PBD) and PS homopolymers (hPS) were drawn into the pores of anodized aluminum oxide (AAO) membranes in the melt by capillary forces. Based on the detailed observation of the morphologies within porous columns, we analyzed the structural transition of BCPs induced by the presence of hPS and confinement. The effect of hPS on the micro-domain of BCPs is greatly accentuated in nanoscale confinement compared to the bulk state due to the entropic loss of polymer chains. Pore diameters of AAO and Mw of the PS-b-PBD are also controlled so as to examine the effects of confinement on the phase transition of PS-b-PBD/hPS blends.

M1.00104 Tunable Surface Energy Interlayer Coating to Control the Phase Behavior of Block Copolymers in 2D Confinement, SUNGYOUL HWANG, YOUNGKEOL KIM, DOKYEONG KWON, KOOKHEON CHAR, Seoul Natl Univ — There have been many studies to investigate the phase behavior of block copolymers (BCPs) in cylindrical confinement. In the nanometer scale 2D confinement, the phase behavior of BCPs is mainly dependent upon commensurability and interfacial interaction. However, most studies have focused only on the effects of commensurability on the microdomains of BCP. In this study, we employed organosilicate (OS) which has tunable surface energy upon adjusting curing temperature as interlayer to examine the phase behavior of BCPs as a function of interfacial energy. The OS interlayer was coated in the inner surface of the pores of anodized aluminum oxide (AAO) pores by template-wetting method and cured in a range of temperature to control the surface energy of the interlayer. Lamellae-forming poly(styrene-b-methyl methacrylate) (PS-b-PMMA) (SMA) in the melt was injected into the OS-coated AAO pores by capillary forces. With the detailed analysis, we note that the self-assembly of SMA within 2D confinement is competitively affected by both entropic and enthalpic effects as the contact interfacial energy is varied. Simply by controlling the curing temperature of the OS interlayer, various morphologies arising from both preferential and commensurate interfacial energies are observed. The OS interlayer is shown to be an effective tool for controlling the morphology of BCPs in 2D confinement.

M1.00105 Bottlebrush Copolymer Morphology Transition: Influence of Side Chain Length and Block Volume Fraction1, YUE GAI, DONG-PO SONG, JAMES WATKINS, Univ of Mass - Amherst — Brush block copolymers synthesized via living ring-opening metathesis polymerization (ROMP) offer unique advantages as template for functional hybrid materials. In addition to only 5% of the block copolymer, the bottlebrush polymer phase transition not only depends on volume fractions of the two blocks but also on side chain length. Here we report the morphology transitions of PS-b-PET copolymer brush copolymer (BBCP) as a function of PET side chain length and block volume fraction. For the BBCP with similar side chain lengths, highly ordered lamellar morphologies were observed with PET volume fractions in a wide range from 32 vol% to 72 vol%, which is significantly different from that of traditional linear block copolymers. This study will lay the groundwork for nanostructure fabrications using the BBCPs and provides new insights into the phase behavior of the new type of materials.

1This work was supported by NSF center for Hierarchical Manufacturing at the University of Massachusetts, Amherst.
M1.00106 Microwave Irradiation on Graphene Dispersed Within Polymeric Matrices. JORGE CISNEROS, BRIAN YUST, MARCIA CHIPARA, Univ of Texas Rio Grande Valley — Graphene is a two dimensional nanomaterial with high thermal and electric conductivity and Young modulus. These features make graphene an ideal reinforcement for polymeric matrices. However, the mechanical features of polymer-carbon nanocomposites are limited by the dispersion of the filler and by the delamination or microcracks initiated at the interface between the polymeric matrix and nanofiller. This last weakness can be addressed by improving the interface via chemical and physical methods. Microwave heating of graphite is a very efficient approach if the polymeric matrix does not also have a strong absorption. During the irradiation, the nanofiller is preferentially heated; the local melting of the polymer at the interface improves the interface by filling the microcracks and delaminations. Nanocomposites of polystyrene-poly(ethylene-ran-butylene)-polystyrene loaded by various amounts of graphene ranging from 0 % to 20 % wt. have been prepared by solution mixing using chloroform as solvent. The as obtained nanocomposites have been subjected to microwave irradiation in an Anton Paar Monowave 300 system operating at 75 W, for various irradiation times 5, 10, 15, 30, 45, and 60 minutes. The effect of microwave irradiation has been studied by Raman spectroscopy.

M1.00107 Acoustic and Ultrasonic Spectral Evolution in Pre- and Post-Damage Self-Healing Poly (Ethylene Co-Methacrylic Acid) Ionomer Samples; JONATHAN BUCKLEY, KENNETH PESTKKA II, Longwood University, STEPHEN KALISTA, Department of Biomedical Engineering, Rensselaer Polytechnic Institute — We measured the pre- and post-damage resonant spectra of several self-healing ionomer samples composed of poly (ethylene co-methacrylic acid) (EMAA). The post-damage results indicate significant time-dependent variation in the acoustic and ultrasonic resonant spectral waveforms of these self-healing samples. These results are consistent with other recent experiments that demonstrate time evolution of resonant frequencies and associated quality factors within samples of post-damage EMAA ionomers. However, in our experiments it was found that, in some circumstances, the quality factors and associated resonant frequencies can exhibit time-dependent variation both before and after external damage. By quantifying time-dependent variations in the spectra of undamaged samples, including quality factor, resonant frequency and spectral waveform, we demonstrate a method to isolate changes in the resonant spectra that are present solely due to the post-damage healing behavior of these EMAA ionomers.

M1.00108 Effect of charge density in chain extension reactions involving complexes of 4, 4'-diaminodiphenylmethane and various alkali metal salts. SUBRAJEET DESHMUKH, KATHERINE CARRASQUILLO, FANG CHANG 'TSAI, LIN A WU, SHAW LING HSU, University of Massachusetts Amherst, UNIVERSITY OF MASSACHUSETTS AMHERST TEAM — Controlling the reaction of methylene diphenyl disiocyanate (MDI)-terminated polyester prepolymer and 4, 4'-diaminodiphenylmethane (MDA) is extremely important in many large scale applications. The ion-diamine complex has the advantage of blocking the instantaneous reaction between the diamine and isocyanate from taking place until it is released at elevated temperatures. We synthesized complexes of MDA with various alkali metal salts. These complexes create a barrier between the diamine and isocyanate thus preventing the premature reaction. We compared the complexes in terms of their dissociation and the subsequent curing with the prepolymer. Charge density had a tremendous effect. DSC showed that Na complexes dissociated at a lower temperature and needed less energy to dissociate than the Li complexes. The effect of change in cation on complex dissociation was more pronounced compared to the change in anion. Also, the ionic liquid introduced greatly altered the dissociation behavior. Temperature and time resolved IR spectroscopy was used to monitor the urea and NH band. By DSC and IR, we showed that NaCl complex is best suited for the curing of prepolymer with regards to curing temperature and energy.

M1.00109 Structural dynamics in polystyrene-b-polyisoprene block copolymers with varying molecular architectures. THOMAS KINSEY, MAXIMILIAN HERES, JIMMY MAYS, ROBERTO BENSON, JOSHUA SANGORO, Univ of Tennessee, Knoxville — A series of polystyrene-polyisoprene block copolymers with different molecular architectures are investigated by broadband dielectric spectroscopy and temperature modulated differential scanning calorimetry. The influence of copolymer composition on segmental and normal mode relaxation dynamics is analyzed. These results are discussed with respect to the current understanding of copolymer dynamics and interactions.

M1.00110 How to Improve Ion Transport in Polymer Nanocomposites? Insights from Atomistic Simulations. SATNOSH MOGURAMPALLY, VENKAT GANESAN, Univ of Texas, Austin — We present different strategies to enhance ion conducting properties of polymer nanocomposite electrolytes and their implications by varying the surface chemistries of the nanoparticles and interactions between nanoparticle and components of polymer-salt mixture. Our molecular dynamics simulations suggest that the ionic mobilities and conductivities correlate with the combined effects of the changes in polymer segmental dynamics and the modifications in the local environment of ionic species arising from the introduction of nanoparticles. In the presence of α, β and γ-Al2O3 nanoparticles, we observe a monotonic decrease of ionic conductivities and mobilities with the nanoparticle loading due to the corresponding slowing of polymer dynamics. However, with the introduction of the repulsive interactions between nanoparticle and components of polymer-salt mixture, we find an increase in the mobility and conductivity of the polymer nanocomposites. However, the repulsive interactions seem to decrease the elastic moduli in contrast to the moduli enhancing effects by attractive interactions.

M1.00111 STRUCTURE OF ANION-CONDUCTING POLYMERS FROM WAXS AND MD SIMULATIONS. BARBARA FRISKEN, SEPEHR TAHAMSEBI, ERIC SCHIBLI, STEVEN HOLDCROFT, Simon Fraser University — The structure of novel polymers for anion exchange membranes (AEMs) is investigated using wide angle X-ray scattering (WAXS) combined with molecular dynamics (MD) simulations using a united-atom force field model based on the Dreiding force field. The polymers being studied are poly(benzimidazole) (PBI) derivatives including poly(dimethylbenzimidazole) (PDDBMI), mesitylene poly(benzimidazole) (mes-PBI), and mesitylene poly(dimethylbenzimidazole) (mes-PDDBMI). WAXS reveals an amorphous structure with two main length scales. By comparing simulation results to WAXS data, we attribute features observed in the scattering data to side-to-side spacing between polymer chains and to the parallel-ring stacking of the benzimidazole rings. Overall, we are able to validate the interpretation of scattering data by combining MD simulations and scattering experiments.

M1.00112 Charge Transport and Dynamics in Confined Phosphonium-based Ionic Liquids1. TYLER COSBY, University of Tennessee, Knoxville, KATSUHIKO TSUNASHIMA, National Institute of Technology, Wakayama College, JOSHUA SANGORO, University of Tennessee, Knoxville — Charge transport and structural dynamics in a homologous series of phosphonium-based ionic liquids confined in silica nanochannels are investigated by broadband dielectric spectroscopy and Fourier transform infrared spectroscopy. The impact of alkyl chain length and hydrophobic aggregation on the physicochemical properties as well as the interplay between confinement effects and pore-wall interactions through silica surface silanization are investigated. The results are discussed within the framework of current understanding of confinement effects in ionic liquid systems, especially in comparison to imidazolium-based ionic liquids.

M1.00113 Charge Transport and Dynamics in Confined Ammonium and Phosphonium-based Ionic Liquids, MATTHEW HARRIS, TYLER COSBY, Univ of Tennessee, Knoxville, KATSUHIKO TSUNASHIMA, National Institute of Technology, Wakayama College, JOSHUA SANGORO, Univ of Tennessee, Knoxville — Charge transport and structural dynamics in a homologous series of ammonium and phosphonium ionic liquids confined in silica nanochannels is investigated by broadband dielectric spectroscopy and Fourier transform infrared spectroscopy. The impact of the central atom of the cation on the physicochemical properties as well as the interplay between confinement effects and pore-wall interactions through silica surface silanization are investigated. The results are discussed within the framework of current understanding of confinement effects in ionic liquid systems, especially in comparison to imidazolium-based ionic liquids.

1 NSF DMR Polymers Program
M1.00114 Amphiphilic Zwitterionic Coatings for Marine Anti-Biofouling Applications.
EDWIN WALKER JR, C. K. PANDIYARAJAN, KIRILL EFIMENKO, JAN GENZER, North Carolina State Univ — Marine biofouling is a problem plaguing the surfaces of cargo ships, military ships and submarines. Previous approaches have relied primarily on the use of Cu-based coatings, which have deleterious effects on aquatic life. Recently, the vast majority of research efforts have focused on the use of polymer brushes synthesized by controlled radical polymerization to create either, the commonly used PEG/PEO materials, amphiphilic alternatives or promising zwitterionic-based moieties. Our approach is based on copolymerizing N, N'-2-dimethylaminoethyl methacrylate (DMAEMA) and propargyl methacrylate (PgMA) in different molar ratios (typically, 1:1 and 3:1) using AIBN-based free radical initiator. The copolymers are then beta-amidized with 1, 3- propane sultone to obtain zwitterionic macromolecules. We create substrate-anchored hydrogels by casting the copolymers as films onto polyurethane-based substrates and crosslink them using a photo-active reagent benzophenone. We investigate the cross-linking reaction with IR, the thickness and swelling as a function of ionic strength and electrolyte using spectrosopic ellipsometry and the wettabily using water contact angle. We study the resistance of the coatings towards non-specific protein adsorption using fibrinogen and BSA.

M1.00115 How does the molecular network structure influence PDMS elastomer wettability?
MATTHEW MELILLO, JAN GENZER, North Carolina State University — Poly(dimethylsiloxane) (PDMS) is one of the most common elastomers, with applications ranging from medical devices to absorbents for water treatment. Fundamental understanding of how liquids spread on the surface of and absorb into PDMS networks is of critical importance for the design and use of another application - microfluidic devices. We have systematically studied the effects of polymer molecular weight, loading of tetra-functional crosslinker, end-group chemical functionality, and the extent of dilution of the curing mixture on the mechanical and surface properties of end-linked PDMS networks. The gel and sol fractions, storage and loss moduli, liquid swelling ratios, and water contact angles have all been shown to vary greatly based on the aforementioned variables. Similar trends were observed for the commercial PDMS material, Sylgard-184. Our results have confirmed theories predicting the relationships between modulus and swelling. Furthermore, we have provided new evidence for the strong influence that substrate modulus and molecular network structure have on the wettability of PDMS elastomers. These findings will aid in the design and implementation of efficient microfluidics and other PDMS-based materials that involve the transport of liquids.

M1.00116 The effects of elastocapillary length on the surface creasing instability of hydrogels
TEETSU OUCHI, Univ of Mass - Amherst, QIHAN LIU, ZHIGANG SUO, Harvard University, RYAN HAYWARD, Univ of Mass - Amherst — Creasing is a mode of surface instability induced by compressing elastomers or gels. Formation of creases is known to proceed by a nucleation and growth process, and the critical nuclei size is thought to be determined by the elastocapillary length (defined by the ratio of surface tension to elastic modulus). Here, we vary the elastocapillary length over the range of 0.008 to 0.4 mm by preparing a series of soft hydrogels with different compositions and contacting them with humidified air. By rapidly applying compression, we are able to achieve strains that exceed the Maxwell strain (where creases become favorable compared to a flat surface) by more than 10%, and which approach Biot’s prediction for linear instability of a compressed half-space. Regardless of the conditions, however, we observe formation of creases only by nucleation and growth, although the density of nucleation sites is found to be sensitive to elastocapillary length. Interestingly, fast propagation of creases (at velocities similar to the speed of sound in the material) are found at strains approaching Biot’s point.

M1.00117 Computer Simulations of Bottlebrush Melts and Soft Networks1
ZHENG CAO, Univ of Akron, JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory, SERGEI SHEIKO, Univ of NC - Chapel Hill, ANDREY DOBRYNIN, Univ of Akron — We have studied dense bottlebrush systems in a melt and network state using a combination of the molecular dynamics simulations and analytical calculations. Our simulations show that the bottlebrush macromolecules in a melt behave as ideal chains with the effective Kuhn length \( K_b \). The bottlebrush induced bending rigidity is due to redistribution of the side chains upon backbone bending. Kuhn length of the bottlebrushes increases with increasing the side-chain degree of polymerization \( n_{sc} \), as \( K_b \propto n_{sc}^{1.4} \). This model of bottlebrush macromolecules is extended to describe mechanical properties of bottlebrush networks in linear and nonlinear deformation regimes. In the linear deformation regime, the network shear modulus scales with the degree of polymerization of the side chains as \( G_0 \propto (n_{sc} + 1)^{-1} \), as long as the ratio of the Kuhn length to the size of the fully extended bottlebrush backbone between crosslinks, \( R_{max} \), is smaller than \( K_b/R_{max} \). Bottlebrush networks with \( K_b/R_{max} \) of 0.5 exhibit behavior similar to that of networks of semiflexible chains with \( G_0 \propto n_{sc}^{1.8} \). In the nonlinear deformation regime, the deformation dependent shear modulus is a universal function of the first strain invariant \( I_2 \) and bottlebrush backbone deformation ratio \( \beta \) describing stretching ability of the bottlebrush backbone between crosslinks.

1 NSF DMR-1409710 DMR-1436201

M1.00118 Modeling polymer gel that strengthen under tension
SANTIDAN BISWAS, VICTOR J. YASHIN, ANNA C. BALAZS, Univ of Pittsburgh — We develop a constitutive model of a responsive polymer gel, which can reversibly form additional crosslinks when under tension. We assume that the polymer chains incorporate the fold domains encompassing the reactive functional groups (cryptic sites). Under extension of the network, the domains unfold and expose the cryptic sites, which can then form stable bonds with the linker chains grafted to the network. Once the deformation is removed, the links detach from the cryptic sites, and unfolded domains go back to the folded configuration thus hiding the cryptic sites. The gel behavior under applied force is described by the equations of elasticity of the polymer network coupled to the kinetic equations for the folding and binding transitions. The developed model could be used for designing new polymer gel-based materials that exhibit self-strengthening in response to a mechanical action.

M1.00119 Modeling thermal-mechanical behavior of networks with reconfigurable crosslinks1
JEH-CHANG YANG, YUAN MENG, MITCHELL ANTHAMATTEN, University of Rochester — Actively moving polymers nearly always involve the storage or release of mechanical energy using external stimuli. Thermomechanical experiments were conducted on well-defined chemical networks bearing both permanent and nonlinear deformation regimes. In the linear deformation regime, the network shear modulus scales with the degree of polymerization of the side chains \( G_0 \propto n_{sc}^{1.8} \). In the nonlinear deformation regime, the deformation dependent shear modulus is a universal function of the first strain invariant \( I_2 \) and bottlebrush backbone deformation ratio \( \beta \).

1 NSF ECCS-1530540

M1.00120 Imparting large macroscopic changes with small changes in polypeptide composition
MICHELLE SING, GARETH MCKINLEY, BRADLEY OLSEN, Massachusetts Institute of Technology — Block copolymers composed of polypeptides provide an excellent platform for exploring the underlying physics surrounding macroscopic associative network behavior. Previous work in our group has elucidated a difference in the mechanical properties of two nearly identical elasin-like polypeptide (ELP) endblocks. In poly[ELP]s, this substitution is known to result in tighter beta turns. These beta turns exhibit slower responses to changes in temperature within the material. Under shear, the modulus for the alanine-containing ELP trilobal is almost three times higher than the glycine-containing ELP. Additionally, preliminary tensile tests show higher stress and strain at break for the alanine ELP trilobal. We are able to explain the reasons for this behavior using a variety of spectroscopic and analytical techniques. Small angle neutron and x-ray scattering indicate differences in ordering between the alanine and glycine containing ELP materials both in shear and in stagnant flow.
M1.00121 Effect of Temperature and Strain on a Self–assembled Gel . SATISH MISHRA, SANTANU KUNDU, Mississippi State University — Gels are widely used in food industry and biomedical field. For physically associating gels, mechanical properties depend on the nature of association between the polymer and the solvent. A thermoreversible, physically associating gel is considered here, which consists of 10% (v/v) poly (methyl methacrylate) - poly (n-butyl acrylate) - poly (methyl methacrylate) in butanol, a midblock selective solvent. Below gelation temperature, the end blocks collapse and form aggregates, and the mid-blocks act as bridges between those aggregates. Rheo-SANS experiments were conducted on these samples where small angle neutron scattering (SANS) and shear-rheology experiments are combined. SANS data were collected over a wide temperature range, from 65C to -10C with and without strain. Near the gelation temperature, SANS data can be fitted with hard sphere model. However, with decrease of temperature, structural changes, due to clustering of aggregates, are observed. The SANS and rheological results in combination provide insight in structural changes of the gel with strain and temperature, respectively.

M1.00122 Rubber Elasticity for percolation network consisting of Gaussian Chains . KENGO NISHI, Georg-August-Universitt Gttingen, MITSUHIRO SHIBAYAMA, TAKAMASA SAKAI, The University of Tokyo — A theory describing the elastic modulus for percolation networks of Gaussian chains on general lattices such as square and cubic lattices is proposed and its validity is examined with simulation and mechanical experiments on well-defined polymer networks. The theory was developed by generalizing the effective medium approximation for Hookean spring network (EMA) to Gaussian chain networks. From EMA theory, we found that the ratio of the elastic modulus at p/C to that at p = 1/C0, must be equal to G0/G0 = (p−2/2−2)f if the position of sites can be determined so as to meet the force balance, where f is the degree of cross-linking reaction. However, the EMA prediction cannot be applicable near its percolation threshold because EMA is a mean field theory. Thus, we combine real-space renormalization and EMA, and propose a theory called real-space renormalized EMA, i.e., REMA. The elastic modulus predicted by REMA is in excellent agreement with the results of simulations and experiments of near-ideal diamond lattice gels.

Please set this talk on Mon, Tue, or Wed (March 14-16) just after its accompanying talk, MAR16-2015-000773.

M1.00123 Nonlinear Stress Relaxation of “Quasi-monodisperse” Polyisoprene and Poly(ptert-butylstyrene) . HIROSHI WATANABE, YUMI MAEDA, Viscoelastic relaxation was examined for entangled miscible blends of cis-polyisoprene (PI) and poly(ptert-butylstyrene) (PtBS) within TPI and TPtBS, changed with the composition wPI and the molecular weights Mw, Mf, and MwPI values were chosen adequately. For example, in a blend with 10 wPI, TPI/TPtBS = 1 and Mw/Mf = 55 and 8.3 for PI and PtBS. Under small strains, this blend exhibited a type-A damping for entangled monodisperse homopolymers. Nevertheless, PI had Mw/Mf = 1 and large M/Mf ratio exhibit very strong type-C damping. Thus, as compared to homopolymers, the nonlinear stress relaxation is enhanced. This suppression is discussed in relation to the slow Rouse retraction of the coexisting PI.

M1.00124 Bidirectional Control of Flow in Thin Polymer Films by Photochemically Manipulating Surface Tension . CHAE BIN KIM, DUSTIN JANES, SUNSHINE ZHOU, AUSTIN DULANEY, CHRISTOPHER ELLISON, The University of Texas at Austin — The Marangoni effect causes transport of liquids in response to surface tension gradients. In a thin polymer film, such flow results in formation of topographic features that could be exploited as a practically useful route to manufacture patterned surfaces. An especially versatile material for this application should be able to be spatially programmed to possess regions of higher or lower relative surface tension so that the direction of flow into or out of those regions can be directed with precision. To this end, we describe here a photopolymer whose melt-state surface tension can be selectively raised or lowered in light exposed regions depending on the wavelength and dose of applied light. The direction of Marangoni flow into or out of irradiated regions agrees with expected surface tension changes associated with each photochemical transformation. We believe this patterning methodology will be potentially useful for high throughput fabrication environments such as roll-to-roll processing that can exploit contact-free and solvent-free topography development.

M1.00125 Dynamics of associating polymers and the sticky Rouse model: a study by combined dielectric and dynamic mechanical techniques . YANGYANG WANG, Oak Ridge National Laboratory, TYLER COSBY, JOSHUA SANGORO, University of Tennessee, Knoxville — Reversible association through non-covalent bonding is ubiquitous in the soft matter world. Despite decades of studies, the dynamics of associating polymers have not been well understood. Here we examine the dynamics of butadiene- and isoprene-based model polymeric systems with pairwise association through hydrogen bonding. Compared to ionomers, where reversible crosslinks are typically not well defined, these hydrogen bonding polymers are associated through strictly binary contacts and thus provide a better opportunity to test theoretical ideas. By combining dielectric spectroscopy and dynamic mechanical measurement, we are able to identify both chain and junction dynamics and analyze their motional coupling mechanism. The results are discussed in the context of the sticky Rouse model.

M1.00126 Evolution of Yield Stress during Structural Relaxation for the Epoxy 828DEA1 . GABRIEL ARECHEDERRA, JOHN MCCOY, New Mexico Tech, JAMIE KROPKA, Sandia National Laboratories — The evolution of yield stress from structural relaxation of diethanolamine cured diglycidyl ether of bisphenol-A, 828DEA, was tracked using uniaxial compression experiments. Samples were aged isothermally for up to 3 months at 5 temperatures ranging from deep in the glass to above Tg. Since 828DEA has remaining reactive potential, it is anticipated that the Tg will continue to evolve throughout the course of the study as new chemical crosslinks are formed. Consequently, it is important to track the evolution of Tg as well as the progression of the fictive temperature in order to interpret the evolution of yield stress.

1 Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE

M1.00127 Can Stress Relaxation Experiments be Used to Assess Deformation Induced Mobility in Glassy Polymers? . JAMIE KROPKA, KEVIN LONG, Sandia National Laboratories — The observance of an increase in glassy polymer relaxation rates under a mechanical deformation is often referred to as deformation induced mobility (DIM). It has been argued that stress relaxation experiments can provide indirect evidence of this phenomenon. Recently, stress relaxation experiments have been interpreted as demonstrating a mobility decrease with increased deformation when very slow strain rates, 1.2 x 10−5 s−1, are used to apply the deformation. This would suggest against generality of DIM and would have significant implications to constitutive models founded on this principle. Here, a mathematical exercise is performed to evaluate the implications of DIM on stress relaxation response. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
M1.00128 Chain networking revealed by molecular dynamics simulation, YEXIN ZHENG, MESFIN TSIGE, SHI-QING WANG, Department of Polymer Science, University of Akron — Based on Kremer-Grest model for entangled polymer melts, we demonstrate how the response of a polymer glass depends critically on the chain length. After quenching two melts of very different chain lengths (350 beads per chain and 30 beads per chain) into deeply glassy states, we subject them to uniaxial extension. Our MD simulations show that the glass of long chains undergoes stable necking after yielding whereas the system of short chains is unable to neck and breaks up after strain localization. During ductile extension the polymer glass made of long chain significant chain tension builds up in the load-bearing strands (LBSs). Further analysis is expected to reveal evidence of activation of the primary structure during post-yield extension. These results tend support to the recent molecular model and are the simulations to demonstrate the role of chain networking. This work is supported, in part, by a NSF grant (DMR-EAGER-1444859).


M1.00129 How plasticizer makes a ductile polymer glass brittle?1, YUE ZHAO, XIAOXIAO LI, SHI-QING WANG, Univ of Akron — During uniaxial extension, a polymer glass of high molecular weight is ductile at high temperatures (still below Tg) and turns brittle when the temperature is sufficiently lowered. Incorporation of small-molecular additives to polymer glasses can speed up segmental relaxation considerably. The effect of such plasticization should be to make the polymers more ductile. We examined the effect of blending a few weight percent of either triphenyl phosphate (TPP) or a mineral oil to a commercial-grade PS and PMMA. Our Instron tests show that the plasticized PS is less ductile. Specifically, at 70 °C, the original PS is ductile at an extensional rate of 0.02 s⁻¹ [1] whereas the PS with 4 wt. % TPP turns brittle. Mechanical spectroscopic measurements show that the alpha relaxation time is shortened by more than two orders of magnitude with 4 wt. % TPP. On the other hand, such anomalous behavior did not occur in PMMA. We need to go beyond the conventional description to rationalize these results. [1] Li, X.; Wang, S. Q. ACS Macro Letters 2015, 1110-1113.

1This work is supported, in part, by a NSF grant (DMR-EAGER-1444859).

M1.00130 Surface diffusion of molecular glasses: Material dependence and impact on physical stability1, SHIANG RUAN, WEI ZHANG, LIAN YU, University of Wisconsin-Madison — Surface diffusion coefficients have been measured for molecular glasses tris-naphthylbenzene (TNB) and PMMA oligomers by surface grating decay. Surface diffusion on TNB is vastly faster than bulk diffusion, by a factor of 10⁸ at Tg, while the process is very slow on PMMA. Along with the previous results on o-terphenyl, nifedipine, indomethacin, and polystyrene oligomers, we find that surface diffusion slows down with increasing molecular size and intermolecular forces, whereas bulk diffusion has a weaker material dependence. The molecular glasses studied show fast crystal growth on the free surface. A general correlation is observed between the coefficient of surface diffusion and the velocity of surface crystal growth, indicating surface crystallization is supported by surface mobility. (Zhu, L., et al. Phys. Rev. Lett. 106 (2011): 256103; Zhang, W., et al. J. Phys. Chem. B 119 (2015): 5071-5078).

1NSF

M1.00131 Liquid Crystalline Phases of Polymer Brushes1, KIANA AMINI, NASSER ABUKHDEIR, MARK MATSEN, University of Waterloo — The phase behavior of liquid-crystal polymeric brushes in solvent are investigated using self-consistent field theory. The polymers are modeled as freely-jointed chain consisting of N rigid segments. The isotropic interactions between the polymer and the solvent are treated using the standard Flory-Huggins theory, while the anisotropic liquid-crystalline (LC) interactions between rigid segments are taken into account using the Mayer-Saupe theory. For weak LC interactions, the brush exhibits the conventional parabolic-like profile, while for strong LC interactions, the polymers crystallize into a dense brush with a step-like profile. At intermediate interaction strengths, we find the microphase-segregated phase observed previously for lattice-model calculations. In this phase, the brush exhibits a crystalline layer next to the grafting surface with an external layer similar to the conventional brush.

1This work was supported by NSERC of Canada.


M1.00132 Thermal Characterization of Thermotropic Nematic Liquid-Crystalline Elastomers, DAVID THOMAS, MATT CARDARELLI, Tufts University, ANTONI SANCHEZ-FERRER, ETH Zurich, BADEL L. MBANGA, TIMOTHY J. ATHERTON, PEGGY CEBE, Tufts University — Nematic Liquid-Crystalline Elastomers (LCEs) are weakly crosslinked polymeric networks that exhibit rubber elasticity and liquid-crystalline orientational order due to the presence of mesogenic groups. Three end-on side-chain nematic LCEs were investigated using real-time synchrotron wide-angle X-ray scattering (WAXS), differential scanning calorimetry (DSC), and thermogravimetry (TG) to correlate thermal behavior with structural and chemical differences among them. The elastomers differed in crystallization density and mesogen composition. Thermally reversible glass transition temperature, Tg, and nematic-to-isotropic transition temperature, Tni, were observed upon heating and cooling for all samples. By varying the heating rate, Tg and Tni were determined at zero heating rate. The temperature dependence of the orientational order parameter was determined from the anisotropic azimuthal angular distribution of the equatorial reflection seen during real-time WAXS experiments. Our results show that the choice of crosslinking unit, its shape, density, as well as the structure of co-monomers, all influence the temperature range over which the thermal transitions take place.

M1.00133 Crystal Growth Theory for Random Copolymers of Crystallizable and Non-crystallizable Units, HERVE MARAND, HADI MOHAMMADI, Virginia Tech, Department of Chemistry — While the presence of randomly distributed non-crystallizable units (e.g. short branches in metallocene linear low density polyethylene) has been carefully considered in the thermodynamics of copolymers crystallization, it has been mostly ignored in the analysis of crystal growth rate data. In this work, we present an extension of the Lauritzen-Hoffman (LH) secondary nucleation theory that considers crystal growth processes for random copolymers of crystallizable and non-crystallizable units. Concentrating on the distribution of crystallizable unit sequence lengths rather than the whole polymer chain, rate equations in the LH theory are modified to account for the population of crystallizable sequences able to form a specific number of folds. We then calculate the flux over the nucleation barrier for each lamellar thickness, the secondary nucleation rate, i, the substrate completion rate, g, and derive the crystal growth rate, G, as a function of crystallization temperature. The model also allows prediction of the lamellar thickness distribution as a function of crystallization temperature. In qualitative agreement with literature data, our model predicts lower crystal growth rates and higher average lamellar thicknesses for m-LLDPE than for linear polyethylene at the same undercooling.
M1.00134 Flow-induced Crystallization of Long Chain Aliphatic Polyamides under a Complex Flow Field1, XIANG DONG, YUNYUN GAO, LILI WANG, DUJIN WANG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry CAS — The present work dealt with the flow-induced multiple orientations and crystallization structure of polymer melts under a complex flow field. This complex flow field is characteristic of the consistent coupling of extensional pulse and closely followed shear flow in a narrow channel. Utilizing an ingenious combination of an advanced micro-injection device and long chain aliphatic polyamides, the flow-induced crystallization morphology was well preserved for ex-situ synchrotron micro-focused wide angle X-ray scattering as well as small angle X-ray scattering. The experimental results clearly indicate that the effect of extensional pulse on the polymer melt is restrained and further diminished due to either the transverse tumble of fountain flow or the rapid retraction of stretched high molecular weight tails. However, the residual shish-kebab structures in the core layer of the far-end of channel suggest that the effect of extensional pulse should be considered in the small-scaled geometries or under the high strain rate condition.  

1The authors thank the financial support from MOST (2013BAE02B02, 2014CB643600) and NSFC(21574140).  

M1.00135 Effects of mechanical strain and heat on the strain-induced crystalline \( \beta \) to \( \alpha \) structural transition of syndiotactic polystyrene. \( \cdot \) FUUYAKI ENDO, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — The polymorphic behavior of syndiotactic polystyrene (sPS) during the \( \beta \) to \( \alpha \) form transition was investigated. sPS presents complex polymorphism with five crystalline forms. Quite a few crystalline structural transitions have also been reported, including our recent discovery of the structural transition from \( \beta \) to \( \alpha \) forms induced by tensile deformation at around 200°C. In this study, we analyzed the individual effects of mechanical strain and heat on the \( \beta \) to \( \alpha \) crystalline structural transformation caused by the mechanical deformation. sPS film samples containing \( \beta \) form crystals were prepared and stretched at 130°C (near the glass transition temperature of sPS), followed by the annealing process of the samples below the melting temperature. X-ray analyses revealed that the stretched sample possessed mesomorphic \( \alpha \) forms, indicating that the mechanical strain could invoke the destruction of \( \beta \) form crystals by producing mesomorphic \( \alpha \) forms. Interestingly, the annealed samples exhibited sharp X-ray reflections typical of \( \alpha \) forms, which became even sharper by the increase in the annealing temperature. It was therefore concluded that the heat could induce the structural transitions from mesomorphic \( \alpha \) forms to perfect \( \alpha \) forms.  

M1.00136 Tracing Poly(ethylene-oxide) Crystallization using Atomic Force Microscopy1, XAVIER CAPALDI, SAMUEL AMANUEL, None — The early stages of nucleation and crystallization of Poly(ethylene-oxide) have been studied using Atomic Force Microscopy equipped with a heating and cooling stage. Effects of molecular weight and sample preparation techniques were studied using amplitude and frequency modulation mapping the viscoelastic behavior at different temperatures and has enabled the development of a relatively new technique for following the evolution of crystallization and melting of a semi-crystalline polymer.  

1Tracing Poly(ethylene-oxide) Crystallization using Atomic Force Microscopy  

M1.00137 Viscoelastic Properties of Fluorinated Ethylene-Propylene (FEP) Random Copolymers1, MEGAN CURTIN*, BENJAMIN WRIGHT*, Chemical and Biological Engineering, RAHMIZI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Fluorinated ethylene-propylene (FEP) random copolymers contain tetrafluoroethylene (TFE) and hexafluoropropylene (HFP) repeat units. FEP is an excellent alternative to poly(tetrafluoroethylene), PTFE, which cannot be melt processed due to its high molecular weight and extensive crystallinity. On the other hand, FEP is a melt processible polymer and offers similar if not the same properties as PTFE. Many studies have been performed on FEP over the years, however, the properties of these polymers strongly depend on the HFP concentration and molecular weight (distribution). Just like PTFE, FEP cannot be dissolved in many solvents, therefore, obtaining molecular weight distribution of these polymers is not possible with commonly used methods. In the current study, we perform rheological analysis of various FEPS and obtain their molecular weight distributions by employing the Tuminelio method.  

1This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730. *Undergraduate students.  

M1.00138 Thermal Properties of Trogamid by Conventional and Fast Scanning Calorimetry1, PEGGY CEBE, JOHN MERFELD, BIN MAO, Tufts University, ANDREAS WURM, EVGENY ZHUARLEV, CHRISTOPHER SCHICK, University of Rostock — We use conventional slow scan rate differential scanning calorimetry, and fast scanning chip-based calorimetry (FSC), to investigate the crystallization and melting behavior of Trogamid, a chemical relative of nylon. Fundamental thermal properties of Trogamid were studied, including the melt crystallization kinetics, heat of fusion, and the solid and liquid state heat capacities. Using slow scan DSC (at 5 K/min), Trogamid displays a glass transition relaxation process at ~133°C, melting endotherm peak at 250°C, and is stable upon repeated heating to 310°C. When using slow scan DSC, the isothermal melt crystallization temperatures were restricted to 225°C or above. Trogamid crystallizes rapidly from the melt and conventional calorimetry is unable to cool sufficiently fast to prevent nucleation and crystal growth prior to stabilization at lower crystallization temperatures. Using FSC we were able to cool nano-gram sizes samples at 2000 K/s to investigate a much lower range of melt crystallization temperatures, from 205-225°C. The experimental protocol for performing FSC on semicrystalline polymers to obtain liquid state heat capacity data will be presented.  

1National Science Foundation, Polymers Program DMR-1206010; DAAAD; Tufts Faculty Supported Leave  

M1.00139 Polymer crystallization in thin films: morphology and physical properties, GIOVANNI KELLY, JULIE ALBERT, Tulane University — Polymer crystallization has been studied both computationally and experimentally for decades, elucidating many of the mysteries surrounding crystallization kinetics and thermodynamics. However, many unanswered questions remain pertaining to the relationships between crystallization phenomena and material properties needed for specific applications that range from drug delivery and tissue engineering to optical devices and mechanically robust membranes. One of the especially interesting facets of polymer crystallization is the behavior observed when these long chain molecules are spatially confined in thin and ultrathin films. Confined geometry leads to chain configurations, and therefore thermal, mechanical, and optical properties, sometimes far removed from reported bulk values. This project aims to study the phenomena exhibited by linear semi-crystalline polymers in thin films as well as this way in which blending with homopolymers, block copolymers, and novel polymer chain architectures affect morphology, biodegradation, optical, thermal, and mechanical properties.  

M1.00140 Morphological Evolution During Tensile Deformation in Semi-Crystalline Precise Functional Copolymers via Fitting of In Situ X-ray Scattering, EDWARD B. TRIGG, L. ROBERT MIDDLETON, University of Pennsylvania, BRIAN S. AIKEN, University of Florida, JASON AZOULAY, DUSTIN MURTAGH, Sandia National Laboratories, KENNETH B. WAGENER, University of Florida, JOSEPH CORDARO, Sandia National Laboratories, KAREN I. WINEY, University of Pennsylvania — Morphological evolution during tensile deformation of semi-crystalline polymers is often described qualitatively. The layered crystal structures of precise copolymers, in which functional groups are bonded at precise intervals along the polymer backbone, allow for quantitative fitting of oriented X-ray scattering peaks to provide additional information. The crystallites in precise poly(ethylene-co-acrylic acid) align with the acid group layers' normal vector perpendicular to the tensile direction, while those in precise poly(ethylene-co-imidazolium bromide) align with the layers' normal vector parallel to the tensile direction. We present fits of in situ X-ray scattering during tensile deformation of semi-crystalline precise copolymers, to quantify the size, shape, and degree of orientation of the crystallites during the deformation process. Mathematical descriptions of the X-ray scattering in these two cases is explored, and a physical explanation for the difference in alignment direction is proposed.
M1.00141 Probing polyethylene crystallization via simultaneous Raman scattering, rheology and microscopy . KALMAN MIGLER, ANTHONY KOTULA, ANGELA HIGHT WALKER, NIST — The structure and rheology of polyolefins during crystallization is of critical importance to the polymer processing industry. Here we present simultaneous Raman scattering, rheological and optical microscopy measurements of crystallizing high density polyethylene during quiescent and slow flow conditions. Raman scattering measurements during quiescent crystallization allow us to quantify three different mass fractions of chain conformers: an amorphous fraction, an orthorhombic crystalline fraction, and a fraction of chains that contain many consecutive trans bonds but are not part of the orthorhombic crystal. These non-crystalline consecutive trans (NCCT) conformers are generated as a precursor to crystallinity. Slow steady shear rates (1 s⁻¹) applied during isothermal crystallization experiments dramatically increase the crystallization rate as well as the amount of NCCT conformers produced. Optical measurements of sheared samples during crystallization reveal the formation of fiber structures that compositionally contain more NCCT conformers than the surrounding melt. The increase in the complex shear modulus commonly measured for crystallizing polyolefines correlates with the growth of chain conformers and the appearance of spherulites within the melt.

M1.00142 Molecular simulations of the formation of semi-crystalline structure from super-cooled polyethylene melt . PENG YI, Johns Hopkins Univ — Formation of semi-crystalline structure is important for industrial processing, but it is scientifically poorly understood due to the strong anisotropy and the conformational flexibility of polymer chains. In this work we report the results of molecular dynamics simulations of homogeneous crystallization from polyethylene melts. A realistic united atom model was used. At room temperature (~30% supercooling), the crystal nucleation and growth lead to a stable semi-crystalline structure, with crystal lamellae separated by amorphous regions. Entanglement in the amorphous region prevents further crystal growth. The crystal-amorphous interface migrates with changing annealing temperature. Chain segments in the amorphous region adopt loop, bridge and tail conformations. Their populations and lengths were calculated and analyzed.

M1.00143 Engineering Multi-scale Electrospin Structure for Integration into Architected 3-D Nanofibers for Cimex Annihilation: Fabrication and Mechanism Study . SHAN HE, LINXI ZHANG, Stony brook university, YING LIU, Advanced Energy Research and Technology Center, MIRIAM RAFAILOVICH, Stony Brook University, GARCIA CENTER FOR POLYMERS AT ENGINEERED INTERFACES TEAM — In this study, engineered electrospin scaffolds with fibers oriented with designed curvature in three dimensions (3D) including the looped structure were developed based on the principle of electrostatic repulsion. Here we illustrate that 3D electrospin polystyrene fibers could closely mimic the unique architectures of multi-direction and multi-layer nano-spiderweb. In contrast to virgin PS, the recycled PS (Dart Styrofoam) are known to contain zinc stearate which acts as a surfactant resulting in higher electrical charge and larger fiber curvature, hence, lower modulus. The surfactant, which is known to decrease the surface tension, may have also been effective at decreasing the confinement of the PS, where chain stretching was shown to occur, in response to the high surface tension at the air interface. Three dimensional flexible architecture with complex structures are shown to be necessary in order to block the motion of Cimex lectularius. Here we show how an engineered electrospin network of surfactant modified polymer fibers with calculated dimensions can be used to immobilize the insects. The mechanical response of the fibers has to be specifically tailored so that it is elastically deformed, without fracturing or flowing. Carefully controlling and tailoring the electrospinning parameters we can now utilize architected 3D nanofiber to create an environmental-friendly Cimex immobilization device which can lead to annihilation solution for all the other harmful insects.

M1.00144 From Non-equilibrium to Equilibrium: Micellar Kinetics seen by Time-resolved Small-angle Scattering . SHAN HE, LINXI ZHANG, Stony brook university, ROBERT BUBECK, Michigan State University, STEVEN KEINATH, Michigan Molecular Institute - Retired — Characterization and molecular simulation of the molecular structure and microstructure of poly(p-phenylene/m-phenylene) copolymers were carried out. Tensile modulus, yield stress, and entanglement molecular weight were modeled as amorphous polymers as a function of m-phenylene content. Significant biphasic character, however, was observed for two copolymers in the melt near 300°C using variable temperature synchrotron-based WAXS. The biphasic nature of the melt may be a contributor to difficulty in melt processing. Precise experimental determinations of entanglement molecular weights were frustrated by the occurrence of significant amounts of nematic mesophase order in the rubbery and melt regimes of two commercial poly(p-phenylene/m-phenylene) examples. Nonetheless, entanglement molecular weights obtained by molecular modeling can be useful for experimental guidance because the level of order in the glassy phase near ambient temperature was found to be low (5 %) regardless of melt processing history. Based on both the modeling and WAXS measurements, it is believed that increasing m-phenylene content reduces modulus, and improves toughness and processibility.


M1.00145 Characterization and Molecular Simulation of Poly(p-phenylene/m-phenylene) Copolymers.1 . ROBERT BUBECK, Michigan State University, STEVEN KEINATH, Michigan Molecular Institute - Retired — Characterization and molecular simulation of the molecular structure and microstructure of poly(p-phenylene/m-phenylene) copolymers were carried out. Tensile modulus, yield stress, and entanglement molecular weight were modeled as amorphous polymers as a function of m-phenylene content. Significant biphasic character, however, was observed for two copolymers in the melt near 300°C using variable temperature synchrotron-based WAXS. The biphasic nature of the melt may be a contributor to difficulty in melt processing. Precise experimental determinations of entanglement molecular weights were frustrated by the occurrence of significant amounts of nematic mesophase order in the rubbery and melt regimes of two commercial poly(p-phenylene/m-phenylene) examples. Nonetheless, entanglement molecular weights obtained by molecular modeling can be useful for experimental guidance because the level of order in the glassy phase near ambient temperature was found to be low (5 %) regardless of melt processing history. Based on both the modeling and WAXS measurements, it is believed that increasing m-phenylene content reduces modulus, and improves toughness and processibility.

1 Beamtime at the Cornell High Energy Synchrotron Source is gratefully acknowledged.
M1.00146 Thermal Conductivity behavior of MWCNT based PMMA and PC composites. GRIJA DUBEY, York College-CUNY, NY11451, PRASHANT JINDAL, University Institute of Engineering & Technology, Panjab University,160014, India, RAJIV BHANDARI, NEHA DHIMAN, CHETAN BAJAJ, VIJAY JINDAL, Department of Physics, Panjab University, Chandigarh 160014, India — Poly methyl methacrylate (PMMA) and Polycarbonate (PC) are low cost polymer materials which can be easily transformed into desired shapes for various applications. However they have poor mechanical, thermal and electrical properties which are required to be enhanced to widen their scope of applications specifically where along with high strength, rapid heat transfer is essential. Multi Walled Carbon nanotubes (MWCNTs) are excellent new materials having extraordinary mechanical and transport properties. We will report results of fabricating composites of varying compositions of MWCNTs with PMMA and PC and their thermal conductivity behaviour using simple transient heat flow methods. The samples in disk shapes of around 2 cm diameters and 0.2 cm thickness with MWCNT compositions varying up to 10 wt% were fabricated. We found that both PMMA and PC measured high thermal conductivity with increase in the composition of CNTs. The thermal conductivity of 10wt% MWCNT/PMMA composite increased by nearly two times in comparison to pure PMMA.

M1.00147 Rheological Properties of a Polybutadiene/Clay Nano-Composite Crosslinked via Thiol-ene Click Chemistry. VIJESH TANNA, H. HENNING WINTER, Univ of Mass - Amherst — We have created an industrially feasible processing method to create a novel polybutadiene/clay nanocomposite. The fabrication step was designed such that the final composite would be chemically crosslinked with exfoliated clay sheets dispersed randomly throughout the polymer matrix. Due to the polybutadiene’s high functionality, the composite’s storage modulus was shown to increase by several orders of magnitude due to crosslinking. In addition, the effect of reinforcements due to clay was shown to double the storage modulus of the composite due to the high elasticity of individual clay sheets. Surprisingly, we observed a critical crossover frequency, below which the mechanical properties, complex modulus, of the neat crosslinked polymer slightly exceed that of the composite. This transition may be due to the large lateral dimensions of the individual clay sheets, hundreds of microns, preventing a small number of crosslinks from forming. We have shown that reinforcement from both chemical crosslinks and clay significantly improves the mechanical properties of the polybutadiene/clay composite and have quantified this reinforcement over a wide range of temperatures and frequencies.

M1.00148 Quantum Molecular Dynamics Validation of Nanocarbon Synthesis by High-Temperature Oxidation of Nanoparticles1, CHUNYANG SHENG, KENICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, Collaboratory for Advanced Computing and Simulations, KOHEI SHIMAMURA, FUYUKI SHIMOJO, Department of Physics, Kumamoto University, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, DEPARTMENT OF PHYSICS, KUMAMOTO UNIVERSITY COLLABORATION, CACS USC COLLABORATION — High temperature oxidation of silicon-carbide nanoparticles (SiC) undergoes a wide range of technologies from high-power electronic switches for efficient electric grid, thermal protection of space vehicles, to self-healing ceramic nanocomposites. Here, multimillion-atom reactive molecular dynamics simulations validated by ab initio quantum molecular dynamics simulations predict unexpected condensation of large graphene flakes during high-temperature oxidation of SiC. In the validation process Small SiC in oxygen environment is chosen to perform QMD simulation, then the QMD results provide the number of Si-O and C-O bonds as a function of time and high temperature. Same QMD simulation is simultaneously performed. We compare the time evolution of different bonds, and observe the condensation of large number of C-cluster nuclei into larger carbon clusters. We further provide the QMD simulation results as an input to a genetic algorithm, which trains the RMD force field parameters, the output force field produce results that are closer to the ground truth QMD simulation results.

1 This research was supported by the Department of Energy (DOE)

M1.00149 Role of Entropic Barriers in Controlling Polymer Diffusion in Polystyrene Nanocomposites, PHILIP GRIFFIN, WEI-SHAO TUNG, University of Pennsylvania, JEFFREY METH, Dupont, NIGEL CLARKE, University of Sheffield, RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania — Polymer diffusion in polymer nanocomposites (PNCs) is significantly modified relative to the neat state. While it is suspected that nanoparticle-induced confinement plays a key role in the diffusion process, a detailed understanding of this process remains nonetheless elusive. We present recent studies of the temperature dependent polymer center-of-mass tracer diffusion coefficient in an athermal PNC comprising polystyrene and phenyl-capped, spherical silica NPs using elastic recoil detection. We find that the polymer tracer diffusion coefficient in the PNC relative to the bulk decreases with increasing nanoparticle concentration and is unexpectedly more strongly reduced at higher temperatures. This unusual temperature dependence of polymer diffusion in PNCs cannot be explained by the reptation model or a modified version incorporating an effective tube diameter, but instead it is the direct result of entropic free energy barriers imposed on polymer chains under confinement.

M1.00150 Morphology and Transport Properties of Novel Polymer Nanocomposites Resulted from Melt Processing of Polyvinylacetaete Substrates Coated with Layer-by-Layer Assemblies, IMAN SOLTANI, RICHARD J. SPONTAK, North Carolina State Univ — Novel polymer nanocomposites (PNCs) were processed through layer-by-layer (LBL) deposition of clay and polyethylene terephthalate ionomer layers on polyvinylacetaete (PVAc) substrates, followed by repetitive melt pressing of coated samples to induce LBL assemblies into the polymer matrix. The increase in the clay content in resulted PNCs prepared through similar LBL coatings, relative to previously studied hydrophobic polystyrene-based nanocomposites, postulated superior clarity of PVAc, with relatively higher hydrophobicity, to interact with LBL assemblies. Also, these PNCs showed relatively good barrier improvement against transport of oxygen and carbon dioxide gases, proposing the scavenging effect of LBL assemblies crushed portions as highly porous structures with high aspect ratios, comprising edge-edge flocculated exfoliated clay platelets, observed through transmission electron micrographs. However, combinative morphological investigations through optical microscopy, x-ray diffractionmetry, and transmission electron microscopy proposed low global dispersion of clay throughout polymeric matrix, conjecturing insufficient intensity of stress applied through cyclic melt pressing, and/or slight thermal degradation of samples via extended times of processing at high temperatures.

M1.00151 Polymer Dynamics by Dielectric Spectroscopy, JENNIFER ZEHNER, KARIN BICHLER, GERALD SCHNEIDER, Louisiana State University Chemistry Department — Theoretical modeling of polymer dynamics is fundamentally important to describe experimental results and to develop new materials. There are many different processes in polymers covering a very broad time range. Dielectric spectroscopy is able to cover a broad frequency range, around 10 decades. Thus many different processes can be studied and it provides a unique means to explore the processes and the time-scales. In our presentation, we emphasize why the line-shape permits to derive information on certain mechanisms. We use entangled melts and demonstrate the influence of entanglements, contour length-fluctuations and constraint release on the spectra and describe it by a theory. Furthermore, we compare it to rheology experiment and demonstrate those parts which are complimentary. We use this knowledge to achieve an advanced understanding of polymer dynamics in nanocomposites.

M1.00152 Polymer Dynamics in Blends, KARIN BICHLER, JENNIFER ZEHNER, GERALD SCHNEIDER, Louisiana State University Chemistry Department — Depending on their miscibility mixtures of polymers or polymers and nanoparticles tend to phase separate. Such systems are of fundamental interest. For example, in case of a blend of two polymer melts a dynamic asymmetry may be generated. It could slow down the chains in one phase or accelerate the chains in the other phase. Due to their heterogeneity these systems are of fundamental interest. Using a certain technique it is very challenging to access all of the information necessary to understand the materials and the interplay between different phases. In order to enhance our understanding, we apply dielectric spectroscopy, scattering experiments and atomic force microscopy to reveal both structure and dynamics and to unravel the fascinating processes.
M1.00153 Nonadiabatic Dynamical Studies of Lead Chalcogenide Quantum Dots (Pb_{16}X_{16}; X = S, Se, Te) Passivated with thin Cadmium Chalcogenide Shells. PATRICK TAMUKONG, SVELTANA KILINA, North Dakota State University — DFT and TDDFT studies of Pb_{16}X_{16}/Cd_{2}S_{2}, Y_{2} (X = S, Se, Te) Core/Shell quantum dots (QDs) have been performed to assess their ground (i.e., the optimized geometries, density of states, projected density of states, and optical absorption spectra), and excited state properties. Most of the heterostructures were analyzed for the first time (e.g., Pb_{16}S_{16}/Cd_{2}S_{2} and Pb_{16}Te_{16}/Cd_{2}Se_{2}). The thin shell core/shell QDs proved to be largely borderline type II with much similarly between QDs containing Cd_{2}S_{2} and Cd_{2}Se_{2} shells, whereas core/shell QDs with a Cd_{2}Te_{2} shell appeared to be borderline type-I. Nonadiabatic DFT-based dynamics, coupled with the surface hopping method, have been done to investigate fates of excited electrons or holes in these systems.

M1.00154 Emergent Magnetism in Mesoporous Materials. SHER ALAM, KEK Accelerator Lab, AJAYAN VINU, University of Queensland — We discuss the emergence of magnetism in Mesoporous Materials. We have obtained experimental results showing a variety of magnetic behaviors arising, by using different types of mesoporous or nanoporous templates. Since the templates allow different magnetic properties to arise naturally we have dubbed this dynamic templating method. Our procedure and results incidentally demonstrates the idea of Nanomorphocomics proposed by Aono, as a MANA concept. Which, simply means to allow different Nano-blocks to interact to obtain a certain desired structure and properties.

M1.00155 Using Self-Similarity to Simulate Meniscus Evolution Around TMV Due to Surface Diffusion. RICHARD POTTER, YUE ZHANG, ZAHRA FAKHRAAI, Univ of Pennsylvania — It has been hypothesized that enhanced surface diffusion allows the formation of stable molecular glasses during physical vapor deposition. The improved properties of these glasses, such as increased density and kinetic stability can help improve material properties in pioneering fields of technology such as organic electronics and pharmaceutical drug delivery. While surface diffusion has been measured previously on the surfaces of organic glasses, direct measurements on the surface of vapor-deposited stable glasses has proven more challenging. This research focuses on a straightforward method for measuring the surface diffusion coefficients of molecular glasses through the use of tobacco mosaic virus (TMV) nanorods as probe particles. In conjunction, mathematical models based on the thin film equation were used to simulate fast meniscus formation around the nanorods on the glassy surface. The evolution of the meniscus is self-similar, which allows quick quantification of the diffusion coefficient, by solving the time evolution for a single experiment. Experimental data were compared and fit to these simulations to derive a quantity for the surface diffusion coefficient, D_s.

M1.00156 Interfacial damping properties of polymeric composites: Effect of interfacial strength. YAPING HUANG, Nanyang Institute of Technology — Experimental studies on interfacial properties of polymeric composites, such as glass transition temperature, showed that the interfacial strength was critical. Numerical studies could also predict interfacial properties based on interfacial strength. In this study, interfacial damping properties and interfacial strength of fiber based polymeric composites were measured by dynamic mechanical tests and micro-indentation technique, showed that the interfacial strength was critical. Numerical studies could also predict interfacial properties based on interfacial strength.

M1.00157 Equilibrium flattening process of irreversibly adsorbed polymer chains on a solid. MANI SEN, Materials Science and Engineering (MSE), Stony Brook University (SBU), NY, NAISHENG JIANG, MAYA ENDOH, TADANORI KOGA, MSE, SBU, DAISUKE KAWAGUCHI, KEJI TANAKA, Kyushu University, Japan — We here report the equilibrium process of adsorbed polymer chains on a solid by sum frequency generation (SFG) spectroscopy. Polystyrene (PS, M_w = 290 kDa) thin films prepared onto quartz prisms (a weakly attractive system) were used as a model system. Spin-cast PS 50 nm films on quartz surface (QS) were annealed at 150 °C for up to 100 h and subsequently rinsed with chloroform to derive the "flattened chains" that lie flat onto the substrate surface. The SFG results for the "matured" flattened chains after annealing for 96 h revealed the strong interfacial orientation of the backbone chains and weak orientation of PS phenyl rings at the QS which is in contrast to a PS spin-cast film annealed at 150 °C for 1 h: the phenyl rings were strongly directed toward the QS, while the backbone chains were weakly orientated at the QS. We postulate that the increase in the number of solid/segment contacts of the backbone chains is the driving force for this equilibrium flattening process. We will also discuss the generality of this flattening process by using solvent-cast PS thin films where the chains are randomly oriented near the QS.

M1.00158 Phase Transitions of 2-Decanol in Nano Pores. SAMUEL AMANUEL, JASON TURNER, CALEB NOVINS, ALEXANDER CLAIN, Dept. of Phys & Astro., Union College — We studied the melting of 2-decanol confined in nano pores, 10-100 nm, using a power-compensated Differential Scanning Calorimeter (DSC). The melting temperature of the nano confined 2-decanol decreases as pore size decreases and a linear relationship is observed between the melting temperature and the inverse of the pore size. This is in agreement with the Gibbs-Thomson prediction. In addition, the apparent heat of fusion of the 2-decanol confined in the nano pores appears to decrease as the size of the pores decreases. However, the apparent heat of fusion of the 2-decanol may not necessarily be true heat of fusion. Annealing, for instance, increases the apparent heat of fusion by as much as 26%. A correction or alternate procedure should be employed to extract the true heat of fusion from DSC measurements, especially when the physical size of the sample is in nano scale or the sample possesses a large surface area to volume ratio.

M1.00159 Heat of fusion of primary alcohol confined in Nano pores. HARRISON GRIFFIN, SAMUEL AMANUEL, Dept. of Phys. & Astro., Union College — Melting behavior of physically confined 1-decanol in nano porous silica was probed using a Differential Scanning Calorimeter (DSC). In agreement with the Gibbs-Thompson prediction, we observe that the melting temperature of the confined 1-decanol scales inversely with the physical size of the pores. Contrary to the assumption used in developing the Gibbs-Thompson equation, however, the apparent heat of fusion decreases as the pore size decreases. Previously, several models have been proposed where the interfacial layer/s of molecules do not participate in the phase transition and thereby would not contribute to the heat of fusion. While these could reconcile the seeming contradiction, annealing the nano confined materials enables some of the interfacial layers to be incorporated into an existing crystal. This leads to an increase in the apparent heat of fusion and a systematic relationship exists between the annealing temperature and the increase in the apparent heat of fusion.

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This work was partially supported by NSF-DMR: 1229142.
M1.00160 Structure and Dynamics of Polymers in Cylindrical Nanoconfinement: A Molecular Dynamics Study. JAMES PRESSLY, ROBERT RIGGLEMAN, KAREN WINEY. Univ of Pennsylvania — The structure and dynamics of polymers under nanoconfinement is critical for understanding how polymers behave in applications from hydraulic fracking to fabricating integrated circuits. We previously used simulations to explore the effect of the diameter of cylindrical pores (d = 10-40σ, where σ is the unit length in reduced units) on polymer end-to-end distance (Rₑₑ,perp, Rₑₑ,par), entanglement density, melt diffusion coefficient (D), and local relaxation time (τₑₑ,perp, τₑₑ,par) at fixed polymer chain length (N = 350). These studies found D, Rₑₑ,perp, and τₑₑ,par increased with increasing confinement while entanglement density, Rₑₑ,perp, and τₑₑ,par decreased. Experiments also found that D increased but to a lesser extent. Here, we examine the molecular weight dependence of these properties using N = 25, 50, 100, 200, 350, and 500 confined to pores of diameter 14σ to examine a range of confinements. Our preliminary results show that as N increases D and Rₑₑ,perp, increase as well, relative to the unconfined state, while entanglement density and Rₑₑ,perp decrease, consistent with our previous work. Interestingly, τₑₑ is shown to be independent of chain length indicating the impact of confinement imposed by reducing pore diameter is distinct from that imposed by increasing chain length.

M1.00161 Man-made Earthquakes & Multifractals in Neutral Fluid Turbulence/Injection1, WH-MAKSOED, Prodi of Physics UI, Depok 16424- INDONESIA — Man-made earthquakes coincide with induced seismicity—typically minor earthquakes & tremors that are caused by human activity that alter the stresses & Strains on the earth crust [Wikipedia—“induced seismicity”]. For these, RD Andrews wrote: “Based on observed seismicity rate & geographical trends following major oil & gas plays with large amounts of produced water, the rates & trends in seismicity are very unlikely to represent a naturally occurring process.” The Philadelphia, Oklahoma, earthquake sequence of 2011, along the Wilzetta faults zone, included the significant foreshock, a main shock of magnetic 5.7, it has been suggested that this sequence represent earthquakes triggered by fluid injection/natural fluid turbulence shows multifractal characteristics, [405J-325-7966 of Dr. G. Randy Keller to UI tuitions of @ Rp. 29, 405, 000.00.

1Acknowledgements to HE. Mr. H. TUK SETYOHADI, Jl. Srigiyaya Raya 3, South-Jakarta, INDONESIA
2of Rabi & Heisenberg hamiltonian oughts to relates to Chris King:“Neurofractal dynamics”

M1.00162 FLUIDS —

M1.00163 Chemically generated convective transport in microfluidic system, OLEG SHKLYAEV, Department of Chemical Engineering, The University of Pittsburgh, SAMBEEATA DAS, ALICIA ALTEMOSE, Department of Chemical Engineering, The University of Pittsburgh, AYUSMAN SEN, Department of Chemistry, The Pennsylvania State University — High precision manipulation of small volumes of fluid, containing suspended micron sized objects like cells, viruses, and large molecules, is one of the main goals in designing modern lab-on-a-chip devices which can find a variety of chemical and biological applications. To transport the cargo toward sensing elements, typical microfluidic devices often use pressure driven flows. Here, we propose to use enzymatic chemical reactions which decompose reagent into less dense products and generate flows that can transport particles. Density variations that lead to flow in the assigned direction are created between the place where reagent is fed into the solution and the location where it is decomposed by enzymes attached to the surface of the microchannel. When the reagent is depleted, the fluid motion stops and particles sediment to the bottom. We demonstrate how the choice of chemicals, leading to specific reaction rates, can affect the transport properties. In particular, we show that the intensity of the fluid flow, the final location of cargo, and the time for cargo delivery are controlled by the amount and type of reagent in the system.

M1.00164 Flow reversal in enzymatic microfluidic pumps, HENRY SHUM, University of Pittsburgh, ISAMAR ORTIZ-RIVERA, ARJUN AGRAWAL, AYUSMAN SEN, Pennsylvania State University, ANNA BALAZS, University of Pittsburgh — A chemical reaction occurring at an enzyme-covered patch in a closed fluid chamber generates local solute concentration gradients and, hence, fluid density gradients. This has recently been shown to drive fluid flows with speeds of the order of microns per second. We develop and analyze a model that accounts for fluid density changes due to consumption of the reaction substrate and accumulation of products for such a fluid pump based on the enzyme urease. Hydrolysis of urea by urease produces ammonium bicarbonate, which leads to a net increase in solution density. Higher density fluid is expected to sink and spread horizontally away from the pump. Modeling reveals, however, that the local fluid density is not necessarily greatest near the pump and fluid flow can even reverse in direction after some time. The qualitative behavior depends on two dimensionless parameters, the ratio of solutal expansion coefficients and the ratio of diffusion coefficients for the reaction substrate and product. The predicted reversal of pumping direction is experimentally verified and we show that the direction of pumping also depends on the amount of enzyme present on the patch. A better understanding of these pumps will aid in the design of responsive, chemically powered microfluidic flow control.

M1.00165 Phase transitions analogy for cavity flows, PETRU FODOR, MIRON KAUFMAN, Physics, Cleveland State University — The fluid flow in cavity type systems, in which one of the walls is moving while the others are stationary, is analyzed using computational modeling, under the assumption of no-slip boundary conditions. By iteratively adapting the mesh used, we are able to map with high spatial resolution the complex flow structures that form at the two types of corners of the cavity, i.e. (i) corners defined by stationary walls, and (ii) corners defined by a stationary and the moving wall, respectively. For the structures that form in the vicinity of the fixed points defined by the corners, we observe that the flow magnitudes and spatial distributions follow scaling laws similar with critical phenomena. In particular, the behavior at the first type of corner is analogous to a to a first-order transition (discontinuity) point, while the behavior at the second one is analogous to a thermodynamic critical point (second-order transition). These results provide a unique insight into the solution to Navier-Stokes equations for cavity flows.

M1.00166 A Statistical investigation of sloshing parameters for multiphase offshore separators, MD MAHMOUD, Lamar University, RAQIFUL KHAN, Cameron Corp, QIANG XU, Lamar University — Liquid sloshing in multiphase offshore separators has been the subject of intense investigations for last several decades both by experiments and simulations. Large number scientists have worked to minimize sloshing impacts and others have developed new methods to describe the sloshing patterns. In addition, complex mathematical models are developed to characterize sloshing phenomenon. However, a comprehensive statistical study of the input parameters and output results is yet to be done. In this study, statistical approaches will be considered to determine the significant parameters for liquid sloshing. The factor analysis and principal component analysis techniques are considered to identify the significant parameters for liquid sloshing. Numerical experiments are carried out through Computation Fluid Dynamics (CFD) technique using ANSYS Fluent software. The input parameters considered here are liquid depth/length ratio, acceleration, wave frequencies, amplitudes in various sea state conditions. The measured variables include hydrodynamic force, pressure, moments, turbulent kinetic energy, height of interfaces. Mathematical correlations may be developed from the data analysis.

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2ETCL Principal Engineer Cameron Corp, 4901 W Sam Houston Pkway, Houston, TX
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M1.00167 Efficient Combustion Simulation via the Adaptive Wavelet Collocation Method, KEVIN LUNG, BRIAN BROWN-DYMOKOSKI, VICTOR GUERRERO, ERIC DORAN, KEN MUSETH, JO BALME, BOB URBERGER, ANDRE KESSLER, STEPHEN JONES, BILLY MOSES, ANTHONY CROGNALE, Space Exploration Tech (SpaX) — Rocket engine development continues to be driven by the intuition and experience of designers, progressing through extensive trial-and-error test campaigns. Extreme temperatures and pressures frustrate direct observation, while high-fidelity simulation can be impractically expensive owing to the inherent multi-scale, multi-physics nature of the problem. To address this cost, an adaptive multi-resolution 3D modeling has been designed which targets the high performance, many-core architecture of GPUs. The adaptive wavelet collocation method is used to maintain a sparse-data representation of the high resolution simulation, greatly reducing the memory footprint while tightly controlling physical fidelity. The tensorial, stencil topology of wavelet-based grids lends itself to highly vectorized algorithms which are necessary to exploit the performance of GPUs. This approach permits efficient implementation of direct finite-rate kinetics, and improved resolution of steep thermodynamic gradients and the smaller mixing scales that drive combustion dynamics. Resolving these scales is crucial for accurate chemical kinetics, which are typically degraded or lost in statistical modeling approaches.

M1.00168 Dual-Mode Measurement and Theoretical Analysis of Evaporation Kinetics of Binary Mixtures, HANYU SONG, Mechanical Engineering, University of Connecticut, CHI-RUEI HE, Chemical Engineering, National Chung Hsing University, CARL BASDEO, QI-QIN LI, ZE-ZHUANG YE, Mechanical Engineering, University of Connecticut, DEVENDRA KALONIA, School of Pharmacy, University of Connecticut, SI-YU LI, Chemical Engineering, National Chung Hsing University, TAI-HSI FAN, Mechanical Engineering, University of Connecticut — Theoretical and experimental investigations are presented for the precision measurement of evaporation kinetics of binary mixtures using a quartz crystal resonator. A thin layer of light alcohol mixture including a volatile (methanol) and a much less volatile (1-butanol) components is deployed on top of the resonator. The normal or acoustic mode is to detect the moving liquid-vapor interface due to evaporation with a great spatial precision on the order of microns, and simultaneously the shear mode is used for in-situ detection of point viscosity or concentration of the mixture near the resonator. A one-dimensional theoretical model is developed to describe the underlying mass transfer and interfacial transport phenomena. Along with the modeling results, the transient evaporation kinetics, moving interface, and the stratification of viscosity of the liquid mixture during evaporation are simultaneously measured by the impedance response of the shear and longitudinal waves emitted from the resonator. The system can be used to characterize complicated evaporation kinetics involving multi-component fuels.

M1.00169 SOFT CONDENSED MATTER

M1.00170 Spin-resolved conductance of Dirac electrons through multibarrier arrays, DIPENDRA DAHAL, Graduate Center and Hunter College of City University of New York, 695 Park Avenue, New York, NY 10065, USA, GODFREY GUMBS, Hunter College of City University of New York, 695 Park Avenue, New York, NY 10065, USA, ANDRII IUROV, Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87106, USA — We use a transfer matrix method to calculate the transmission coefficient of Dirac electrons through an arbitrary number of square potential barrier in gapped monolayer graphene(MLG) and bilayer graphene (BLG). The widths of barriers may not be chosen equal. The shift in the angle of incidence and the width of the barrier required for resonance are investigated numerically for both MLG and BLG. We compare the effects due to energy gap on these two transmission coefficient for each of these two structures (MLG and BLG). We present our results as functions of barrier width, height as well as incoming electron energy as well as band gap and examine the conditions for which perfect reflection or transmission occurs. Our transmission data are further used to calculate conductivity.

M1.00171 Dielectric Screening Response of a Plasmonic "Sandwich", N.J.M. HORING, Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, NJ 07030, GODFREY GUMBS, DIPENDRA DAHAL, Department of Physics and Astronomy, Hunter College, CUNY, New York, NY 10065, ANDRII IUROV, Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87106. — We have formulated the RPA integral equation for a system composed of two identical semi-infinite metallic plasmas with planar bounding surfaces at \( z = \pm d/2 \). The gap between the two metallic bulk plasmas contains a two-dimensional semiconductor plasma at \( z = 0 \). This equation for the inverse dielectric function is solved analytically in position representation for a narrow gap, yielding an explicit formula for the inverse dielectric screening function in terms of the nonlocal 2D semiconductor polarizability and the bulk metallic polarizability, the latter well approximated in the local limit. Based on this solution, we have evaluated the nonlocal plasmon dispersion relation computationally, taking Graphene as the 2D semiconductor plasma. The associated nonlocal Graphene plasmon spectrum coupled to the sandwich system is exhibited in 3D plots, which show a linear mode and another displaced from the bulk plasma frequency.

M1.00172 EM Wave Transmission through a Nano-hole in a Plasmonic Layer, DESIRE MIESSEIN, NORMAN J. MORGENSTERN HORING, HARRY LENZING, Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, NJ 07030, GODFREY GUMBS, Department of Physics and Astronomy, Hunter College, CUNY, New York, NY 10065. — We examine the role of the angle of incidence of an incoming EM wave in its transmission through a subwavelength nano-hole in a thin semiconductor plasmonic layer. Fully detailed calculations and results are exhibited for p- and s-polarizations of the incident wave for a variety of incident angles in the near, middle and far zones of the transmitted radiation. Our dyadic Greens function formulation includes both (1) the electromagnetic field transmitted directly through the 2D plasmonic layer and (2) the radiation emanating from the nano-hole. Interference fringes due to this superposition are explicitly exhibited. Based on an integral equation formulation, this dyadic Greens function approach does not involve any appeal to metallic boundary conditions. It incorporates the role of the 2D plasmon of the semiconductor layer, which is smeared due to its lateral wave number dependence. We find that the interference fringes, which are clustered near the nano-hole, flatten to a uniform level of transmission directly through the sheet alone at large distances from the nano-hole.

M1.00173 Modeling heterogeneous polymer-grafted nanoparticle networks, TAO ZHANG, BADEL MBANGA, VICTOR YASHIN, ANNA BALAZS, Chemical Engineering Department, University of Pittsburgh, Pennsylvania 15261, USA — Via a dynamic 3D computational approach, we simulate the heterogeneous polymer-grafted networks. The nanoparticles rigid cores are decorated with a corona of grafted polymers, which contain reactive functional groups at the chain ends. With the overlap of grafted polymers, these reactive groups can form weak labile bonds, which can reform after breakage, or stronger bonds, which rupture irreversibly and thus, the nanoparticles are interconnected by dual cross-links. Previous work has been done on homogeneous networks, while we introduce the heterogeneity by considering two types of particles having different reactive functional groups, so that the labile bond energy varies depending on types of the two end reactive groups. We study the effect of tensile and rotational deformations on the network morphology, and observe, in particular, the phase separation of the two types of particles. Our results will provide guidelines for designing transformable material that can controllably change structure under mechanical action.
Employ this technique to study star-linear homopolymer mixtures, focusing on the limit of very long homopolymers. Interaction between a star polymer and a linear homopolymer, comparing the results obtained from coarse graining and monomer resolved simulations. We approach is based on the calculation of the effective interaction between a star polymer and a single monomer, which can be used to coarse-grain the interaction of arrested gels. Directed percolation, which is quantitatively associated with the mean number of bonded neighbours. Directed percolation is a universality class of transitions out of equilibrium arrested gel states.

M1.00174 Adhesion of Particulate Materials to Mesostructured Polypyrrole . DARBY HOSS, Purdue University, ROBERT KNEEPER, PETER HOTCHKISS, ALEXANDER TAPPAN, Sandia National Laboratories, BRYAN BOUDOURIS, STEPHEN BEAUDOUIN, Purdue University — Interactions based on van der Waals (vdW) forces will influence the performance and reliability of mesostructured polypyrrole swabs used for the collection and detection of trace particles. The vdW adhesion force between materials is described by the Hamaker constant, and these constants are measured via optical and dielectric properties (i.e., according to Lifshitz theory), inverse gas chromatography (IGC), and contact angle measurements. Here, contact angle measurements were performed on films of several common materials and used to estimate Hamaker constants. This, in turn, will allow for the tuning of the design properties associated with the polypyrrole swabs. A comparison of these results to Hamaker constants estimated using Lifshitz Theory and IGC reveals the fundamental behavior of the materials. The Hamaker constants were then used in a new computational vdW adhesion model. The idealized model describes particle adhesion to an array of mesostructures. This model elucidates the importance of where the particle makes contact with the mesostructure and the independence of vdW forces generated by each mesostructure. These results will facilitate the rational design of polypyrrole swabs optimized for harvesting microscale particles of trace materials.

M1.00175 Droplet Dynamics of a Flowing Emulsion System. OLIVIA CYPULL, KLEBERT FEITOSA, James Madison University — The inner workings of glassy systems have long been a topic of interest for soft material scientists. Similarities between the jamming behavior of emulsions and the glass transition of glassy systems have prompted the conjecture that they might share the same underlying mechanism. Here we study a dense oil-in-water emulsion system forced to flow through a narrow microchannel. By matching the index of refraction of the two phases, we image the internal dynamics of the droplets in a confocal microscope. At low velocity speeds, we find that the velocity along the edge of the microchannel was not significantly different than then the average droplet velocity in the bulk suggesting a near plug flow. By contrast the droplets near the edge experienced more movement perpendicular to the flow indicating the fluidizing effect of the confining walls.

M1.00176 Self-assembly in Dipolar Fluids. MICHELARONTI, SOFIA KANTOROVICH, Univ of Vienna — We are studying low temperature structural transitions in dipolar hard spheres (DHS), combining grand-canonical Monte Carlo simulations and direct analytical theoretical calculations. DHS is characterized by long-range anisotropic interactions: it consists of a point dipole at the center of a hard sphere. We are interested in low temperature and low density phase behaviour of DHS systems. From a theoretical point of view the process of self-assembly is not responsible for a phase transition; this belief was completely overturned by theoretical studies showing that the process of self-assembly is alone capable to induce phase transition. On the other hand in the last year it was found that no sign of critical behaviour is observed, implementing efficient and tailored Monte Carlo algorithms. Moreover a theoretical approach based on Density Functional Theory was developed: a series of structural transitions were discovered providing evidence of a hierarchy in the structures on cooling. We are performing free-energy calculations in order to draw the phase diagram of DHS model. Comparing the numerical results with the theoretical ones shed light on the scenario of temperature induced structural transitions in magnetic nanocollodons.

M1.00177 Deconvolution of the role of metal and pH in metal coordinating polymers. SEETHCAZZELL, NIELS HOLTEN-ANDERSEN, Massachusetts Inst of Tech-MIT — Nature uses metal binding amino acids to engineer both mechanical properties and structural functionality. Some examples of this metal binding behavior can be found in both mussel foot protein and DNA binding protein. The mussel byssal thread contains reversible intermolecular protein-metal bonds, allowing it to withstand harsh intertidal environments. Zinc fingers form intramolecular protein-metal bonds to stabilize the tertiary structure of DNA binding proteins, allowing specific structural functionality. Inspired by both these metal-binding materials, we present mechanical and spectroscopic characterization of a model polymer system, designed to mimic this bonding. Through these studies, we are able to answer fundamental polymer physics questions, such as the role of pH and metal to ligand ratio, illuminating both the macroscopic and microscopic material behavior. These understandings further bio-inspired engineering techniques that are used to design viscoelastic soft materials.

M1.00178 Optically induced thermal response of Chlorophyll for biomedical applications. CHIAWEI TU, SADAT MD EHSAN, YUAN ZHAO, DONGLU SHI, DAVID MAST, Univ of Cincinnati — The heating behavior of Chlorophyll was investigated for possible use in hyperthermia cancer treatments. One measure of hyperthermia effectiveness is the Specific Absorption Rate (SAR) defined as the initial slope of the sample heating behavior, however, for nanoparticle (NP) loaded samples, this initial heating rate is often limited by heat transfer mechanisms from the NPs to the surrounding material and not the initial NP heating. This is especially true for water-based, NP loaded tissue surrogates. Organic solvent dispersed NP loaded samples face the additional problem of heating rate variations due to solvent evaporation effects. We report on measurements of the initial optical heating rates of Chlorophyll and deposited directly on small, Pt thin film resistance temperature detectors (RTDs). Solid state lasers (638 nm and 655 nm) were used to illuminate these samples at different intensities and at specific wavelengths associated with peaks (662 nm) in Chlorophyll's UV-VIS optical absorption spectra while recording the RTD resistance at 0.1 second intervals. This technique significantly reduce evaporation errors we had experienced and has the potential to directly measure the heating behavior of Chlorophyll based NP materials.

M1.00179 Directed percolation identified as equilibrium pre-transition towards non-equilibrium arrested gel states . MARCO LAURATI, RONJA CAPELLMANN, MATTHIAS KOHL, STEFAN EGELHAAF, MICHAEL SCHMIEDEBERG, University of Düsseldorf — The macroscopic properties of gels arise from their slow dynamics and load bearing network structure, which are exploited by nature and in numerous industrial products. However, a link between these structural and dynamical properties has remained elusive. Here we present confocal microscopy experiments and simulations of gel-forming colloid-polymer mixtures with competing interactions. They reveal that gel formation is preceded by continuous and directed percolation. Both transitions lead to system spanning networks, but only directed percolation results in extremely slow dynamics, ageing and a shrinking of the gel that resembles syneresis. Therefore, dynamical arrest in gels is found to be linked to a structural transition, namely directed percolation, which is quantitatively associated with the mean number of bonded neighbours. Directed percolation is a universality class of transitions out of equilibrium, our study hence connects gel formation to a well-developed theoretical framework which now can be exploited to achieve a detailed understanding of arrested gels.

M1.00180 Novel coarse-graining approach for Star polymer and linear Homopolymer mixtures . EMANUELE LOCATELLI, CHRISTOS LIKOS, University of Vienna — We present a novel coarse-graining approach, suitable for star polymer mixtures. The approach is based on the calculation of the effective interaction between a star polymer and a single monomer, which can be used to coarse-grain the interaction between a star and a complex object. The effective interaction has been calculated numerically for star polymers of different functionalities $f$ and for different degrees of polymerization $N$. We find that these potentials can be scaled following the star polymer scaling laws. We test our approach, calculating the effective interaction between a star polymer and a linear homopolymer, comparing the results obtained from coarse graining and monomer resolved simulations. We employ this technique to study star - linear homopolymer mixtures, focusing on the limit of very long homopolymers.
M1.00181 A simple depth-averaged model for dry granular flow. CHI-YAO HUNG, National Taiwan University, COLIN P. STARK. Lamont-Doherty Earth Observatory, Columbia University, HERVE CÁPART, National Taiwan University — Granular flow over an erodible bed is an important phenomenon in both industrial and geophysical settings. Here we develop a depth-averaged theory for dry erosive flows using balance equations for mass, momentum and (crucially) kinetic energy. We assume a linearized GDR-Midi rheology for granular deformation and Coulomb friction along the sidewalls. The theory predicts the kinematic behavior of channelized flows under a variety of conditions, which we test in two sets of experiments: (1) a linear chute, where abrupt changes in tilt drive unsteady uniform flows; (2) a rotating drum, to explore steady non-uniform flow. The theoretical predictions match the experimental results well in all cases, without the need to tune parameters or invoke an ad hoc equation for entrainment at the base of the flow. Here we focus on the drum problem. A dimensionless rotation rate (related to Froude number) characterizes flow geometry and accounts not just for spin rate, drum radius and gravity, but also for grain size, wall friction and channel width. By incorporating Coriolis force the theory can treat behavior under centrifuge-induced enhanced gravity. We identify asymptotic flow regimes at low and high and dimensionless rotation rates that exhibit distinct power-law scaling behaviors.

M1.00182 A Computational Study of the Growth of Hexagonal Ice. , MAXWELL FULFORD, King’s College London, UK, MATTEO SALVALAGLIO, UCL, UK, MICHELE PARRINELLO, ETH Zurich; USI Lugano, CARLA MOLTENI, King’s College London, UK — Hexagonal ice (Ih) has two distinct crystallographic surfaces; a basal and prism surface. At low vapour pressures, Ih forms thin plates and elongated prisms, depending on the temperature and the growth conditions. The base radius on the basal surface is close to the capillary length. In this work, we investigate hexagonal ice Ih growth via molecular dynamics and Metadynamics to study how the interfacial structure at the ice/quasi-liquid and quasi-liquid/vapour interfaces influence the adsorption potential, surface transport properties and growth shape.

M1.00183 The mystery of Coulomb friction in sediment transport1, THOMAS PHTZ, Ocean College, Zhejiang University, ORENCIO DURAN, MARUM-Center for Marine Environmental Sciences, University of Bremen — Nearly all analytical models of sediment transport in Newtonian fluid (e.g., air or water) are based on Bagnold’s assumption of a constant Coulomb friction coefficient (particle-shear-pressure-ratio, µ) at the interface (z0) between sediment bed and transport layer. In fact, this assumption is the main reason why these models predict the sediment load (and subsequently the sediment transport rate) to be proportional to the excess shear stress (τ − τc), a scaling which has been confirmed in many wind-tunnel and flume experiments. Attempts to explain why µ(z0) is constant have usually been based on the sliding-friction analogy or rheology arguments. However, we analytically derive µ(z0) ≈ √3 − 1, where z0 is the location at which the production rate of particle fluctuation energy is maximal. Our derivation is based on the assumption that the rate of collisional transfer of horizontal into vertical kinetic energy is typically much larger than the rate of energy dissipation. Using state-of-the-art numerical simulations of sediment transport in Newtonian fluid, we validate all assumptions and approximation involved in our derivation. Interestingly, the location z0 can significantly deviate from z0 depending on the simulated conditions.

1We acknowledge support from grants National Natural Science Foundation of China (Nos. 1151101041 and 41376095) and Natural Science Foundation of Zhejiang Province (No. LR16E090001).

M1.00184 Core formation by porous flow allowed by hysteresis in melt network topology . SOHEIL GHANBARZADEH, MARC HESSE, MASJA PRODANOVIC, The University of Texas at Austin — The formation of the core via percolation is an attractive process to form planetary cores early in the planets evolution. There is currently a debate whether the ratio of interfacial forces between solid-solid and solid-liquid interfaces, imposing the dihedral angle between the solid grains and the pore fluid, in an olivine-melt matrix allows the formation of a percolating network. We present first computations of equilibrium melt distributions in realistic irregular grains and show that the percolation threshold at dihedral angles above 60 degrees is significantly larger than those previously reported for simple geometries. However, given typical compositions of the terrestrial planets initial porosities after the onset of melting of iron are large, 20-40thousand to form a connected melt network. As the porosity decreases due to melt segregation the network remains connected and allows core formation by porous flow. Only as the porosities approach 1% the iron becoming isolated in pockets along triple junctions. This residual iron may provide an explanation for the formation of dense layers near the core mantle boundary such as.

M1.00185 Spontaneous Pattern Formation of Surface Nanodroplets from Competitive Growth , DETLEF LOHSE, University of Twente, SHUHUA PENG, XUEHUA ZHANG, RMIT, Melbourne — Nanoscale droplets on a substrate are of great interest because of their relevance for droplet-based technologies for light manipulation, lab-on-chip devices, miniaturised reactors, encapsulation and many others. In this work, we focus on the drum problem. A dimensionless rotation rate (related to Froude number) characterizes flow geometry and accounts not just for spin rate, drum radius and gravity, but also for grain size, wall friction and channel width. By incorporating Coriolis force the theory can treat behavior under centrifuge-induced enhanced gravity. We identify asymptotic flow regimes at low and high and dimensionless rotation rates that exhibit distinct power-law scaling behaviors.

M1.00186 Decoupling between Diffusivity and Effective Viscosity in Poly(isobutyl methacrylate) Films with a Thickness-Independent Glass Transition1, KUN GENG, Boston University Physics Department, REIKA KATSUMATA, University of Texas at Austin, McKetta Department of Chemical Engineering, XUANJI YU, Boston University Division of Materials Science and Engineering, HEONJOO HA, AUSTIN R. DULANEY, CHRISTOPHER J. ELLISON, University of Texas at Austin, McKetta Department of Chemical Engineering, OPHÉLIA K.C. TSUI, Boston University Physics Department, Division of Materials Science and Engineering — We report measurements of self-diffusion (D) and effective viscosity (ηeff) on silica-supported poly(isobutyl methacrylate) (PBiMA) thin films, miniaturised reactors, encapsulation and many others. In this work, we establish a basic principle for the symmetrical arrangement of surface nanodroplets during their growth under simple flow conditions. In our model system, nanodroplets nucleate at the rim of spherical cap microstructures on a substrate, due to a pulse of oversaturation is supplied by a solvent exchange process. We find that, while growing at the rim of the microcap, the nanodroplets self-organise into highly symmetric arrangements, with respect to position, size and mutual distance. At low vapour pressures, Ih forms thin plates and elongated prisms, depending on the temperature and the growth conditions.

1We are grateful to the support of NSF through the project DMR-1310536 and DMR-1053293.

M1.00187 Interfacial Bubble Deformations1, BRIAN SEYMOUR, James Madison University, PARVIS SHABANE, Virginia Tech, OLIVIA CYPULL, James Madison University, SHENGFENG CHENG, Virginia Tech, KLEBERT FEITOS, James Madison University — Soap bubbles floating at an air-water experience deformations as a result of surface tension and hydrostatic forces. In this experiment, we investigate the nature of such deformations by taking cross-sectional images of bubbles of different volumes. The results show that as their volume increases, bubbles transition from spherical to hemispherical shape. The deformation of the interface also changes with bubble volume with the capillary rise converging to the capillary length as volume increases. The profile of the top and bottom of the bubble and the capillary rise are completely determined by the volume and pressure differences.

1 James Madison University Department of Physics and Astronomy, 4VA Consortium, Research Corporation for Advancement of Science.
M1.00188 Temperature-dependent neutron diffraction measurements from D₂O hydrating single-supported lipid bilayers of DMPC¹, Z. N. BUCK, J. TORRES, A. MAZZA, H. KAISER, H. TAUB, Univ. of Missouri - Columbia, F. Y. HANSEN, Technical University of Denmark, A. MISKOWIEC, Oak Ridge National Lab, M. TYAGI, NIST Center for Neutron Research. The freezing point depression of water associated with biological membranes, studied principally by NMR, has been of interest for decades. Here we have used neutron diffraction measurements at the University of Missouri Research Reactor (MURR) to investigate the freezing behavior of water associated with single-supported zwitterionic lipid bilayers composed of DMPC. Diffraction patterns obtained as a function of temperature reveal that water freezes abruptly into its hexagonal phase at 270 K with no evidence of amorphous ice. Following the initial crystallization of the membrane-associated water there is a region of continuous hexagonal crystal growth, which is believed to occur in the interfacial water closest to the membrane. The temperature-dependent intensity of the observed Bragg peaks have been compared with that of incoherently elastically-scattered neutrons collected on the High-Flux Backscattering Spectrometer at NIST from an identical sample hydrated with H₂O [2]. We find excellent agreement between the two data sets, suggesting the absence of amorphous solid water and that all the water hydrating a DMPC membrane eventually freezes into the hexagonal crystalline phase. ²M. Bai et al., Europhys. Lett. 98, 48006 (2012).

M1.00189 Elasticity and Extensibility Determine Printability and Spinnability of Polymer Solutions. JELENA DINIC, LEIDY JIMENEZ, VIVEK SHARMA, Univ of Illinois - Chicago — Many advanced manufacturing technologies like inkjet and 3D printing, nano-fiber spinning involve complex free-surface flows, and the formation of columnar necks that undergo spontaneous capillary-driven thinning and pinch-off. The progressive self-thinning of neck is often characterized by self-similar profiles and scaling laws that depend on the relative magnitude of capillary, inertial and viscous stresses for simple (Newtonian and inelastic) fluids. Stream-wise velocity gradients that arise within the thinning columnar neck create an extensional flow field that can orient and stretch macromolecules, contributing extra elastic stresses and extensional viscosity that change thinning and pinch-off dynamics for polymeric complex fluids. Characterizing the filament thinning and break-up kinetics in jetting, dripping and stretching liquid bridge provides invaluable insight into the interplay of elastic, viscous, capillary and inertial stresses relevant for these applications. We elucidate how polymer composition, flexibility and molecular weight determine the thinning and pinch-off kinetics in our experiments. Both effective relaxation time and transient extensional viscosity are found to be strongly concentration dependent even for dilute solutions.

M1.00190 Patterns, Instabilities, Colors, and Flows in Vertical Foam Films. SUBINUER YILXIATI, YIRAN ZHANG, EWELENA WOJCICK, VIVEK SHARMA, Univ of Illinois - Chicago — Understanding and controlling the drainage kinetics of thin films is an important problem that underlies the stability, lifetime and rheology of foams and emulsions. We follow the drainage kinetics of vertical foam films using imaging and color science. Interference between light reflected from two surfactant-laden surfaces that are 100 nm - 10 micron apart leads to thickness-dependent indiscernible colors in the visible region. Below 50 nm the thin films appear as black. In this study, we utilize the thin film interference colors as markers for identifying patterns, instabilities and flows within vertical foam films. We study the emergence of thickness fluctuations near the borders (i.e. marginal regeneration) and within thinning films. Finally, we elucidate how buoyancy, capillarity, convection and gravity-driven instabilities and flows, are affected by the choice and concentration of constituents. We find fascinating examples of two-dimensional hydrodynamics and unexplained, if not unprecedented, drainage kinetics.

M1.00191 Effects of aspect ratio on the phase diagram of spheroidal particles. SONGUL KUTLU, JASON HAAGA, JEFFREY RICKMAN, JAMES GUNTON, Lehigh University — Ellipsoidal particles occur in both colloidal and protein science. Models of protein phase transitions based on interacting spheroidal particles can often be more realistic than those based on spherical molecules. One of the interesting questions is how the aspect ratio of spheroidal particles affects the phase diagram. Some results have been obtained in an earlier study by Odriozola (J. Chem. Phys. 136:134505 (2012)). In this poster we present results for the phase diagram of hard spheroids interacting via a quasi-square-well potential, for different aspect ratios. These results are obtained from Monte Carlo simulations using the replica exchange method. We find that the phase diagram, including the crystal phase transition, is sensitive to the choice of aspect ratio.

M1.00192 Coarse-grained simulation of dynamin-mediated fission. MARCUS MULLER, GUOJIE ZHANG, MARC FUHRMANS, Georg-August University, Goettingen, Germany — Fission is a process in which a region of a lipid bilayer is deformed and separated from its host membrane, so that an additional, topologically independent compartment surrounded by a continuous lipid bilayer is formed. It is a fundamental process in the compartmentalization of living organisms and carefully regulated by a number of membrane-shaping proteins. An important group within these is the dynamin family of proteins that are involved in the final severance of the hourglass-shaped neck, via which the growing compartment remains connected to the main volume until the completion of fission. We present computer simulations testing different hypotheses of how dynamin proteins facilitate fission by constriction and curvature. Our results on constraint-induced fission of cylindrical membrane tubes emphasize the importance of the local creation of positive curvature and reveal a complex picture of fission, in which the topological transformation can become arrested in an intermediate stage if the proteins constituting the fission machinery are not adaptive.

M1.00193 Coarse grained modeling of transport properties in monoclonal antibody solution. JAMES SWAN, GANG WANG, Massachusetts Inst of Tech-MIT — Monoclonal antibodies and their derivatives represent the fastest growing segment of the bio pharmaceutical industry. For many applications such as novel cancer therapies, high concentration, sub-cutaneous injections of these protein solutions are desired. However, depending on the peptide sequence within the antibody, such high concentration formulations can be too viscous to inject via human derived force alone. Understanding how heterogenous charge distribution and hydrophobicity within the monoclonal antibodies is crucial to their application. In this talk, we explore a coarse grained computational model of therapeutically relevant monoclonal antibodies that accounts for electrostatic, dispersion and hydrodynamic interactions between suspended antibodies to predict assembly and transport properties in concentrated antibody solutions. We explain the high viscosities observed in many experimental studies of the same biologics.

M1.00194 Hierarchical Cluster Formation in Concentrated Monoclonal Antibody Formulations. P. DOUGLAS GODFRIN, University of Delaware, JONATHAN ZARZAR, ISIDRO (DAN) ZARRAGA, Genentech, Inc., LIONEL PORCAR, PETER FALUS, Institute Laue-Langevin, NORMAN WAGNER, University of Delaware, YUN LIU, NIST Center for Neutron Research, University of Delaware — Reversible cluster formation has been identified as an underlying cause of large solution viscosities observed in some concentrated monoclonal antibody (mAb) formulations. As high solution viscosity prevents the use of subcutaneous injection as a delivery method for some mAbs, a fundamental understanding of the interactions responsible for high viscosities in concentrated mAb solutions is of significant relevance to mAb applications in human health care as well as of intellectual interest. Here, we present a detailed investigation of a well-studied IgG1 based mAb to relate the short time dynamics and microstructure to significant viscosity changes over a range of pharmaceutically relevant physiochemical conditions. Using a combination of experimental techniques, it is found that upon adding Na₂SO₄, these antibodies dimerize in solution. Proteins form strongly bounded reversible dimers at dilute concentrations that, when concentrated, interact with each other to form loosely bounded, large, transient clusters. The combined effect of forming strongly bounded dimers and a large transient network is a significant increase in the solution viscosity. Strongly bounded, reversible dimers may exist in many IgG1 based mAb systems such that these results contribute to a more comprehensive understanding of the physical mechanisms producing high viscosities in concentrated protein solutions.
M1.00195 Probing matrix and tumor mechanics with in situ calibrated optical trap based active microrheology , JACK RORY STAUNTON, WILFRED VIEIRA, KANDICE TANNER, NIH, TISSUE MORPHODYNAMICS UNIT TEAM — Aberrant extracellular matrix deposition and vascularization, concomitant with proliferation and phenotypic changes undergone by cancer cells, alter mechanical properties in the tumor microenvironment during cancer progression. Tumor mechanics conversely influence progression, and the identification of physical biomarkers promise improved diagnostic and prognostic power. Optical trap based active microrheology enables measurement of forces up to 0.5 mm within a sample, allowing interrogation of in vitro biomaterials, ex vivo tissue sections, and small organisms in vivo. We fabricated collagen I hydrogels exhibiting distinct structural properties by tuning polymerization temperature $T_p$, and measured their shear storage and loss moduli at frequencies 1-15 kHz at multiple amplitudes. Lower $T_p$ gels, with larger pore size but thicker, longer fibers, were stiffer than higher $T_p$ gels; decreasing strain increased loss moduli and decreased storage moduli at low frequencies. We subcutaneously injected probes with metastatic murine melanoma cells into mice. The excised tumors displayed storage and loss moduli 40 Pa and 10 Pa at 1 Hz, increasing to 500 Pa and 1 kPa at 15 kHz, respectively.

M1.00196 Dynamics of Micropipette Vibration During Piezo-assisted Microinjection , MEHDI KARZAR-JEDDI, NEJAT OLGAC, TAI-HSI FAN, Department of Mechanical Engineering, University of Connecticut, Storrs, Connecticut 06269-3139, USA — Microinjection is a well-accepted method to introduce materials such as sperm, DNA materials, or nucleus into a living cell for biomedical applications. The conventional microinjection procedure consists of immobilizing the cell by applying suction through a holding pipette, and then an injecting micropipette penetrates through the cell membrane and introduces the materials into the cell. To assist the penetration process a piezo-generated pulse train is applied to the injecting pipette, which causes an undesirable lateral vibration at the injecting pipette tip. In this research we provide an analytical model to study the response of micropipette to the piezo-pulse train using the Duhamel integral method. Our results show that filling the micropipette tip with mercury causes a larger amplitude stroke vibration in micropipette than that of empty micropipette when it is submerged in the viscous medium surrounding the cell. The mercury introduced larger stroke vibration can cause a larger shear force and assist the penetration of micropipette through the cell membrane.

M1.00197 Characterizing the mechanical behavior of the zebrafish germ layers, DAVID KEALHOFER, FRIEDHELM SERWANE, ALESSANDRO MONGERA, PAYAM ROWGHANIAN, ADAM LUCIO. OTGER CAMPÁS, University of California, Santa Barbara — Organ morphogenesis and the development of the animal body plan involve complex spatial and temporal control of tissue- and cell-level mechanics. A prime example is the generation of stresses by individual cells to reorganize the tissue. These processes have remained poorly understood due to a lack of techniques to characterize the local constitutive law of the material, which relates local cellular forces to the resulting tissue flows. We have developed a method for quantitative, local in vivo study of material properties in living tissue using magnetic droplet probes. We use this technique to study the material properties of the different zebrafish germ layers using aggregates of zebrafish mesodermal and ectodermal cells as a model system. These aggregates are ideal for controlled studies of the mechanics of individual germ layers because of the homogeneity of the cell type and the simple spherical geometry. Furthermore, the numerous molecular tools and transgenic lines already developed for this model organism can be applied to these aggregates, allowing us to characterize the contributions of cell cortex tension and cell adhesion to the mechanical properties of the zebrafish germ layers.

M1.00198 A finite element study of the stability of spontaneous curling of thin shells, XIAOMIN HAN, Thayer School of Engineering, Dartmouth College, QIAOHANG GUO, College of Material Science and Engineering, Fuzhou University, KEVIN CHU, Serendipity Research, IAN TRASE, NAN HU, ZI CHEN, Thayer School of Engineering, Dartmouth College — Thin shells are of great interest in engineering due to their ubiquity in nature. The mechanical instabilities of thin shells are a key factor in understanding many real world phenomena, such as the closure of a Venus flytrap or the curling of a dried leaf. Given the analytical theory that quantitatively described the stability of thin shells subject to surface stress, we are able to identify a dimensionless parameter that controls the stability of thin shells. Finite element analyses are employed to numerically examine the predictions. Bi-layer plates are fabricated where one layer is pre-stretched and has much smaller Young’s modulus than the other layer to examine mechanical instability. By measuring the two principle curvatures on the plate, the onset of bifurcation can be determined. Different initial conditions and material properties are taken into account in the FEA, including initial curvature, Poisson’s ratio, and the magnitude of surface stress. The numerical experiments agree well with the theory.

M1.00199 Diffusion of micrometer-sized soft particles in confinement , BENJAMIN JORDAN, KEVIN APTOWICZ, West Chester University — We investigate the diffusion of micrometer sized poly(N-isopropylacrylamide) (PNIPAM) gel particles in confinement. The influence of confinement on the transport of small particles is becoming increasingly important for microfluidics and bio-fluidics. Analytical solutions to this problem are limited to very unique geometries or gross approximations. Computational methods have provided more insight into the problem as well as experimental investigations. However, most research has focused on the hard-sphere problem. In this work, we will explore the diffusion of soft particles in confinement. The dynamics of the particles confined between two parallel walls is captured with video-microscopy. In addition, we use a recently developed technique to measurement confinement of particles in-situ with a precision of 1%. This poster will present some preliminary results of how confinement affects the diffusion of these soft particles.

M1.00200 Electric Double Layer electrostatics of spherical polyelectrolyte brushes with pH-dependent charge density , HAO LI, GUANG CHEN, SHAYANDEV SINHA, SIDDHARTHASI DAS, Univ of Maryland-College Park, SOFT MATTER, INTERFACES, AND ENERGY LABORATORY (SMIEL) TEAM — Understanding the electric double layer (EDL) electrostatics of spherical polyelectrolyte (PE) brushes, which are spherical particles grafted with PE layers, is essential for appropriate use of PE-grafed micro-nanoparticles for targeted drug delivery, oil recovery, water harvesting, emulsion stabilization, emulsion breaking, etc. Here we elucidate the EDL electrostatics of spherical PE brushes for the case where the PE exhibits pH-dependent charge density. This pH-dependence necessitates the consideration of explicit hydrogen ion concentration, which in turn dictates the distribution of monomers along the length of the grafted PE. This monomer distribution is shown to be a function of the nature of the sphere (metallic or a charged or uncharged dielectric or a liquid-filled sphere). All the calculations are performed for the case where the PE electrostatics can be decoupled from the PE elastic and excluded volume effects. Initial predictions are also provided for the case where such decoupling is not possible.
M1.00201 Unraveling the Nanostructure and Chain Conformation of Peptide-polymer Conjugates in Solution using Small-angle X-ray Scattering. REIDAR LUND, Department of chemistry, University of Oslo, TING XU, UC-Berkeley, HE DONG, Clarkson University — For therapeutics, polymer functionalization, often by poly(ethylene glycol), PEG (“PEGylation”), is an effective method to improve the solubility, increase the life time and protect the proteins from the immune system[1]. However it is essential that the proteins maintain their structural integrity in solution- thus the role of the polymer and their interactions with proteins needs to be understood. In this work we show how small-angle X-ray scattering (SAXS) can be used as a powerful technique to characterize the structural components of peptide-polymer conjugates in solution [2,3]. We specifically show that by applying detailed modeling very detailed structural features can be revealed, including the PEG chain conformation. In the presentation we will provide an overview of the methodology, specifically addressing peptides that form either alpha-helical bundles [2,3] or beta-sheet structures [4,5] and relate their structure in solution to their crystal structure.


M1.00202 Geometric Frustration Selects Morphology in Chiral Filament Bundles1, DOUGLAS HALL, ISAAC BRUSS, UMass Amherst, JUSTIN BARONE, Virginia Tech, GREGORY GRASON, UMass Amherst — Assemblies of twisted filaments appear in a range of biological contexts, from extracellular filament bundles to amyloid fibrils. Owing to numerous distinctions in molecular structures and interactions underlying these diverse assemblies, a framework to predict and classify the basic mechanisms of structure formation in twisted filament assemblies is still lacking. In this study, we model how the size and shape of self-assembled fibers are controlled by competition between the elastic costs of inter-filament frustration, bending deformation of filaments and bundle surface energy. Exploiting a geometric mapping between inter-filament packing in twisted bundles and packing on positively-curved 2D surfaces, we show that the anisotropy of the bundle cross-section is determined by a single parameter describing the competition between elastic and bending costs. We compare the continuum model’s predictions for stability of cylindrical and tape-like twisted morphologies to numerical simulations of cohesive filament bundles and observations of micron-scale amyloid fibers assembled from hydrolyzed protein fragments.

1 NSF (CAREER) DMR-0955760

M1.00203 Controlling the Size and Shape of the Elastin-Like Polypeptide based Micelles, KIRIL STRELETZKY, HANNAH SHUMAN, ADAM MARASCHKY, NOLAN HOLLAND, Cleveland State University — Elastin-like polypeptide (ELP) trimer constructs make reliable environmentally responsive micellar systems because they exhibit a controllable transition from being water-soluble at low temperatures to aggregating at high temperatures. It has been shown that depending on the specific details of the ELP design (length of the ELP chain, pH and salt concentration) micelles can vary in size and shape between spherical micelles with diameter 30-100 nm to elongated particles with an aspect ratio of about 10. This makes ELP trimers a convenient platform for developing potential drug delivery and bio-sensing applications as well as for understanding micelle formation in ELP systems. Since at a given salt concentration, the headgroup area for each foldon should be constant, the size of the micelles is expected to be proportional to the volume of the linear ELP available per foldon headgroup. Therefore, adding linear ELPs to a system of ELP-foldon should result in changes of the micelle volume allowing to control micelle size and possibly shape. The effects of addition of linear ELPs on size, shape, and molecular weight of micelles at different salt concentrations were studied by a combination of Dynamic Light Scattering and Static Light Scattering. The initial results on 50 M ELP-foldon samples (at low salt) show that Rh of mixed micelles increases more than 5-fold as the amount of linear ELP raised from 0 to 50 M. It was also found that a given mixture of linear and trimer constructs has two temperature-based transitions and therefore displays three predominant size regimes.

M1.00204 Directed Assembly of Hierarchically Ordered Clusters from Anisotropic Microparticles1, KOOHEE HAN, BHUVNESH BHARTI, North Carolina State Univ, C. WYATT SHIELDS IV, GABRIEL P. LOPEZ, Duke University, ORLIN D. VELEV, North Carolina State Univ — The directed assembly of colloidal particles with specific connectivity, symmetry, and directional response requires controlled interactions and means of programmable binding force. We will show how patchy microparticles can be hierarchically assembled into ordered clusters, resulting from directional interactions between metal-coated facets. First, we introduce lipid mediated capillary bridging as a new class of binding force for directed assembly of metallo-dielectric patchy microparticles. Iron oxide surface patches on latex microspheres were selectively wetted with liquid lipids, guiding the particle assembly into well-defined 2D and 3D clusters. The temperature driven fluid-to-gel phase transition of the fatty acids acts as a thermal switch for cluster assembly and disassembly. Secondly, we used external fields to bind patchy microspheres based on their polarization configuration and interparticle interaction. We present assembled clusters of cobalt-coated patchy microspheres that can be dynamically reconfigured using external magnetic field. The residual polarization of ferromagnetic cobalt plates allows for preserving the assembled sequence even in the absence of the field and drives dynamic reconfiguration of assembled clusters.

1 NSF Grant DMR-1121107

M1.00205 Aging and nonlinear rheology of thermoreversible colloidal gels, NORMAN WAGNER, MELISSA GORDON, CHRISTOPHER KLOXIN, University of Delaware — Colloidal dispersions are found in a wide variety of consumer products such as paint, food and pharmaceuticals. We investigate gel formation and aging in a thermoreversible gel consisting of octadecyl-coated silica nanoparticles suspended in n-tetradecane. In this system, the octadecyl brush can undergo a phase change allowing the attractions between particles to be tuned by temperature (1.2). By probing the system with steady shear and large amplitude oscillatory shear, we have studied the effect of thermal history and shear history on gel formation and gel mechanical properties during aging. Gels were formed by approaching a common temperature from above and below to determine a reference state from which creep tests were conducted. Creep ringing was observed as expected for the viscoelastic gel. The rheological aging is interpreted in terms of the gel microstructure formed with differing thermal and shear histories to determine how processing affects structure. Recently proposed scaling laws for the rheology and structure under flow are explored within the context of gel aging (3). Through rheological and microstructural measurements, we will further the understanding of gel formation and aging in this model system which may be applied to processing conditions in an industrial setting. 1. Eberle, A.P.R., Wagner, N. J., Akgun, B. & Satija, S. K. Langmuir 26, 3003–3007 (2010). 2. Eberle, A.P.R., Castañeda-Priego, R., Kim, J. M. & Wagner, N. J. Langmuir 28, 1866–1876 (2012). 3. Eberle, A.P.R., et al., Physical Review E, 89, 050302 (2014).
M1.00206 Dissolution of a Colloidal Particle in an Oscillatory Fluid Medium, DEZHUANG YE, JI-QIN LI, Mechanical Engineering, University of Connecticut, ROBIN BOGNER, Pharmaceutical Sciences, University of Connecticut, TAI-HSI FAN, Mechanical Engineering, University of Connecticut — Understanding dissolution kinetics of a colloid particle in an aqueous solution is of great importance in many pharmaceutical and biochemical applications. We present theoretical analysis of low Reynolds number transient dynamics and mass transfer of a dissolving spherical particle in a unidirectional oscillatory flow. The coupling of fluid flow and passive motion of the particle are resolved analytically, and the transient mass transfer associated with the oscillation of the particle is numerically computed. The flow patterns, diffusive and convective transport phenomena, and the dissolution kinetics under various saturation concentrations and flow conditions are characterized by the frequency parameter, Schmidt number, and Peclet number. The result serves as a basic case in determining the efficiency of drug dissolution or reconstitution that depends on various shaking methods.

M1.00207 Effective temperatures and the breakdown of the Stokes-Einstein relation for particle suspensions1, CARLOS MENDOZA, Materials Research Institute UNAM, IVAN SANTAMARA-HOLEK, UMDI-J Facultad de Ciencias UNAM, AGUSTN PREZ-MADRID, Departament de Fisica Fonamental, Universitat de Barcelona — The short- and long-time breakdown of the classical Stokes-Einstein relation for colloidal suspensions at arbitrary volume fractions is explained here by examining the role that confinement and attractive interactions play in the intra- and inter-cage dynamics executed by the colloidal particles. We show that the short-time diffusion coefficient is larger than the one predicted by the classical Stokes-Einstein relation due to a non-equilibrated energy transfer between kinetic and configuration degrees of freedom. This transfer can be incorporated in an effective temperature that replaces the bath temperature in a Generalized Stokes-Einstein relation (GSER). This relation then allows to obtain the diffusion coefficient once the viscosity is known. On the other hand, the temporary cluster formation induced by confinement and attractive interactions of hydrodynamic nature, makes the long-time diffusion coefficient to be smaller than the corresponding one obtained from the classical Stokes-Einstein relation. Additionally, we provide a simple expression based on a differential effective medium theory (DEMT) that allows to calculate the diffusion coefficient at short and long times. Comparison of our results with experiments and simulations for suspensions of hard and porous spheres shows an excellent agreement in all cases.

M1.00208 Hydrodynamic interactions in colloidal systems confined to linear geometries with a singular corner, BINHUA LIN, RYAN ZARCONE, STUART A. RICE, University of Chicago — Here we investigate the question of whether or not the requirement that particles diffuse around a corner affects their hydrodynamic coupling. We report the results of studies of the collective diffusion coefficients of particles in quasi-one-dimensional linear channels of widths 3 and 5um, each with a singular central corner of angle: 60-, 90-, 120-, and 180-degrees. We find that for large angles, the channels are so close in their geometry to 180-degrees that the corner has very little to no effect on the hydrodynamic coupling of particles on opposite sides of the apex. For small angles, the corner’s effect is to increase the particle separation at which the maximum hydrodynamic coupling occurs.

M1.00209 Effect of Salts on Drainage of Foam, SOUMYADIP SETT, University of Illinois at Chicago, STOYAN KARAKASHEV, University of Sofia, Bulgaria, STOYAN SMOUKOV, University of Cambridge, UK, ALEXANDER YARIN, University of Illinois at Chicago — Gravitational drainage from thin planar vertical sodium dodecyl sulfate (SDS) films in the presence of inorganic salts was experimentally studied. Strong ion-specific effects of the counter-ions were found to affect the stability and the rate of drainage of the planar foam films as a function of concentration of the inorganic salts. The counter-ions can either stabilize (below the critical concentration) or destabilize the foam films. We found that the strongest foam stabilizer salt became the strongest foam destabilizer beyond its critical concentration.

M1.00210 The role of the anchoring conditions in the electro rheological behavior of a nematic constrained by two coaxial cylinders and submitted by a pressure drop, DANIEL MARTINEZ SNchez, Universidad Autnoma de la Ciudad de Mxico, JUAN ADRI N REYES CERVANTES, Universidad Nacional Autnoma de Mxico — We study a nematic liquid crystal (LC) filling the region between two coaxial cylinders subjected to the simultaneous action of both a pressure gradient applied parallel to the axis of the cylinders and a radial low frequency electric field. For the LC 4-n-pentyl-4-cyanobiphenyl (SCB), we consider soft anchoring boundary conditions to obtain the configuration of the director and the velocity profile and the pressure gradient for nonslip boundary conditions. Finally, we calculate the effective viscosity, the first normal stress difference, and the dragging forces on the cylinders.

M1.00211 Colloidal particles embedded in liquid crystal droplets, DREW MELCHERT, MONIROSADAT SADATI, YE ZHOU, JUAN J. DE PABLO1, Institute for Molecular Engineering, University of Chicago — In this work, we encapsulate polystyrene and silica particles in nematic liquid crystal (LC) droplets dispersed in water using microfluidic glass capillary devices. While polystyrene particles induce planar anchoring on the surface, silica particles, treated with DMOAP, create homeotropic anchoring of the LC molecules at their surface. Sodium dodecyl sulfate (SDS) is added to the aqueous phase to stabilize LC droplets and promote a radial configuration with point defect in the center of LC droplet. Our experimental and computational studies show that, when trapped inside the LC droplets, particles with both anchoring types become mostly localized at the defect point (at the center) and interact with the radial configuration. Interestingly, a twisting structure is observed for polystyrene particle with strong planar anchoring. Although localization of the particles at the droplet center is the most stable state and with the lowest free energy, off-center positions also emerge, displacing the defect point from the center to near the surface of a radial droplet.

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M1.00212 Coarse-Grained Molecular Monte Carlo Simulations of Liquid Crystal-Nanoparticle Mixtures1, RYAN NEUFELD, GRIGORIY KIMAEV, FRED FU, NASSER M. ABUKHDEIR, University of Waterloo — Coarse-grained intermolecular potentials have proven capable of capturing essential details of interactions between complex molecules, while substantially reducing the number of degrees of freedom of the system under study. In the domain of liquid crystals, the Gay-Berne (GB) potential has been successfully used to model the behavior of rod-like and disk-like mesogens. However, only ellipsoid-like interaction potentials can be described with GB, making it a poor fit for many real-world mesogens. In this work, the results of Monte Carlo simulations of liquid crystal domains using the Zewdie-Corner (ZC) potential are presented. The ZC potential is constructed from an orthogonal series of basis functions, allowing for potentials of essentially arbitrary shapes to be modeled. We also present simulations of mixtures of liquid crystalline mesogens with nanoparticles. Experimentally these mixtures have been observed to exhibit microphase separation and formation of long-range networks under some conditions. This highlights the need for a coarse-grained approach which can capture salient details on the molecular scale while simulating sufficiently large domains to observe these phenomena. We compare the phase behavior of our simulations with that of a recently presented continuum theory.

1This work was made possible by the Natural Sciences and Engineering Research Council of Canada and Compute Ontario.

M1.00213 ABSTRACT WITHDRAWN
M1.00214 Magnetic domains and defects in ferromagnetic liquid crystal colloids realized with optical patterning, ANDREW HESS, QINGKUN LIU, IVAN SMALYUKH, University of Colorado Boulder — A promising approach in designing composite materials with unusual physical behavior combines solid nanostructures and orientationally ordered soft matter at the mesoscale. Such composites not only inherit properties of their constituents but also can exhibit emergent behavior, such as ferromagnetic ordering of colloidal metal nanoparticles forming mesoscopic magnetization domains when dispersed in a nematic liquid crystal. Here we demonstrate the optical patterning of domain structures and topological defects in such ferromagnetic liquid crystal colloids which allows for altering their response to magnetic fields. Our findings reveal the nature of the defects in this soft matter system which is different as compared to non-polar nematic and ferromagnetic systems alike.

1This research was supported by the NSF grant DMR-1420736.

M1.00215 Conformation of charged vesicles: the Debye Huckel and the low curvature limit, KUMARI PRITI SINHA, PROF. ROCHISH M. THAKOAR, Indian Inst of Tech-Bombay — The shape as well as tension and pressure inside an uncharged vesicle are determined by the reduced volume. These parameters are important for a vesicle or a biological cell, since it can affect bio-physical processes such as osmosis and permeation, interaction with external agents such as bio- macromolecules and thermal fluctuations of the bilayer membrane of a vesicle. Charged membranes are ubiquitous in nature, most biological cell bio-membranes are charged, and therefore the knowledge of shape, tension and pressure of charged vesicles is critical. Additionally, the distribution of charges in the inner and outer leaflets is also important as it can affect the spatial interaction of a bilayer membrane with proteins. This work addresses these issues in the low charge and curvature limit. Our analysis indicates that despite a very strong two-way coupling between the charge and the curvature, the shapes of charged vesicles remain similar to that of uncharged vesicles at comparable reduced volumes, even for reasonable values of total charge. However, the tension and pressure values are higher, and are accurately estimated. Similarly the charge distribution on the inner and outer leaflet is strongly affected by the curvature. The value of spontaneous curvature due to charge redistribution is estimated. The insensitivity of the shape to charges persists even when only the outer leaflet is charged instead of charged inner and outer leaflets.

M1.00216 Emergence of DNA-encapsulating liposomes from a DNA-lipid blend film, SHUN-SUKE SHIMOYABASHI, Department of Physics, Kyoto University, MAFUMI HISHIDA, Department of Chemistry, Tashkuba University, TOMO KURIMURA, MASATOSHI ICHIKAWA, Department of Physics, Kyoto University — A Micro-scale giant unilamellar vesicle (GUV) densely encapsulating molecular systems is one of the simplest life-mimicking model systems. The dehydration-rehydration process proposed by Deamer et al. more than 30 years ago generates vesicles to satisfy the constraints of micro-scale size, unilamellarity and densely polymer-encapsulation. Nevertheless, the physico-chemical mechanism of a set of dehydration-rehydration process has been poorly understood. The present study reveals crucial factors on the process through fluorescent microscopic observation and small angle x-ray scattering. From the results, we propose a plausible physical mechanism for the process, making it possible to optimize the encapsulation of any agent. [1] D. W. Deamer, G. L. Barchfeld, J. Mol. Evol, 18, 203-208 (1982). [2] S. F. Shimobyashy and M. Ichikawa, J. Phys. Chem. B 118, 10688-10694 (2014).

1This work was supported by Grant-in-Aid for JSPS Fellows Grant (No. 25-1270) and by KAKENHI (Nos. 26707020, 25103012, and 26115709).

M1.00217 Lipid transfer energetics between free-standing and solid supported membranes: reconciling discrepancies, BENNY WAH, JOSEPH ADAMS, JEFFREY BREIDIGAN, LI GE, PIOTR HorBAl, UnIV. of ILLiNOIS -- ChiCAGO, LIONEL PORCAR, University of Delaware, SUMIT GARG, URSULA PEREZ-SALAS, UnIV. OF ILLiNOIS -- ChiCAGO — The membranes of animal cells have significant variation in the lipid and protein composition. If we weren’t for the active work of proteins that maintain most of these variations, membranes would ultimately homogenize throughout by mixing. It has been long been recognized that the study of the passive movement of lipids between and within membranes can provide insight into this energetic toll. Using small angle neutron scattering, a non-invasive in situ technique, we recently demonstrated that tags or small structure changes in the lipids can have a huge effect on their transport characteristics. In the present study we compare lipid transfer and energetics between supported free standing membranes. We find that exchange and flipping process are comparable while the presence of the surface slightly increases inter and intra-membrane transport rates. The activation energies for exchange appear to be nearly unaffected by the presence of the surface while for flip-flop it slightly increases. The increase in the rates due to the presence of the surface may possibly explain the apparent contradicting behavior previously reported on supported flat membrane systems and in free-standing membranes.

M1.00218 Photo-Regeneration of Severed Gel Using Photo-Controlled Radical Polymerization, AWANEESH SINGH, UnIV. of PITTSBURGH, OLGA KUKSENOK, cement University, JEREMIAH A. JOHNSON, Massachusetts Institute of Technology, ANNA C. BALAZS, UnIV. OF PITTSBURGH — Using the framework of dissipative particle dynamics (DPD) simulation, we developed a novel computational model that enables photo-regeneration of the gel matrix when a significant portion of the material is severed. We considered photo-controlled radical polymerization (photo-CRP) within polymer networks with embedded initiators (initiators for the photo-CRP reaction). These initiators turn on the polymerization process in the presence of light with monomers and cross-linkers in the solution. This “photo-growth” allows us to effectively regenerate severed gels under the application of light. The growth process can be turned off once the polymerization is near completion, which forms a new cross-linked gel that resembles the uncut material. The polymerization rate can be modulated by altering the light intensity.

M1.00219 Frictional Properties of UV illuminated ZnO Thin Films Grown by Pulsed Laser Deposition, HSIANG-CHIH CHIU, HUAN-PU CHANG, FANG-YU LO, YU-TING YEH, Department of Physics, National Taiwan Normal University, DEPARTMENT OF PHYSICS, NATIONAL TAIWAN NORMAL UNIVERSITY COLLABORATION — Zinc Oxide (ZnO) nanostructures have potential applications in nano-electro-mechanical systems (NEMS) due to their unique physical properties. ZnO is also an excellent lubricant and hence a promising candidate for protective coatings in NEMS. By means of atomic force microscopy (AFM), we have investigated the frictional properties of ZnO thin films prepared by pulsed laser deposition technique. In addition, UV illumination is used to convert the surface wettability of ZnO thin films from being more hydrophobic to superhydrophilic via the photo-catalyst effect. We found that the frictional properties of the UV illuminated, superhydrophilic ZnO surface are strongly dependent on the environment humidity. While for hydrophobic ZnO, no such dependence is found. The observed frictional behaviors can be explained by the interplay between the surface roughness, environmental humidity and the presence of nanoscale capillary condensation forming between surface asperities at the tip-ZnO contact. Our results might find applications in future ZnO related NEMS.

M1.00220 Fracture of molecular glasses under tension and fracture-induced crystallization, YINSHAN CHEN, TRAVIS POWELL, LIAN YU, University of Wisconsin-Madison — Molecular glasses are formed and fractured by cooling a liquid on a less thermally expansive substrate. In-plane tension is created by the mismatch of thermal expansion coefficients and accumulates to cause catastrophic network fracture. This simple experiment allowed the measurement of fracture toughness and the heat of fracture of molecular glasses for the first time. For the systems studied (as-terpenyl, indomethacin, and sucrose benzoate), the fracture condition is well described by recent theories and a material-specific energy release rate (fracture toughness) approximately 1 J/m². The heat of fracture was found to be anomalously high relative to the value expected for the energy release rate and the surface area created. The large release of heat is caused by the reduction of heat capacity for a glass film constrained on a rigid substrate. Rapid crystal growth was observed along fracture surfaces. (Ref.: Powell, C. T.; Chen, Y.; Yu, L. J. Non-Crystalline Solids 2015, 429, 122-128)
M1.00221 Supramolecular Hydrogels from Self-Assembly of di-Fmoc-L-lysine. SEYED MEYSAM HASHEMNEJAD, KINSEY NAA, SANTANU KUNDU, Mississippi State University — Mechanical properties and nanostructure of a supramolecular hydrogel formed by self-assembly of di-fluoromethyleneoxycarbonyl-lysine (di-Fmoc-L-lysine) are reported here. Hydrogels were prepared by solvent switch technique in which water was added to a solution of di-Fmoc-L-lysine in dimethyl sulfoxide (DMSO). Mechanical properties of the gels were investigated using shear and cavitation rheology. The gels display strain-softening behavior at moderate strain values. Morphological investigations of the samples were conducted using FTIR and CD spectroscopy, electron microscopy, and atomic force microscopy (AFM). Self-assembled fibers with lateral dimensions ranging from 10 to 50 nm were captured in microscopy studies. FTIR results indicate β-sheet-like conformation of the peptides in the hydrogel.

M1.00222 Predicting out-of-Equilibrium Phase Behavior in the Dynamic Self-Assembly of Colloidal Crystals. JAMES SWAN, ZACHARY SHERMAN, Massachusetts Inst of Tech-MIT — Crystals self-assembled from colloidal particles are useful in an array of well demonstrated applications. During fabrication however, gelation and classification often leave these materials arrested in defective or disordered metastable states. We show how time-dependent, pulsed interparticle interactions can avoid kinetic barriers and yield well-ordered crystalline domains for a suspension of hard, spherical colloidal particles interacting through short-range attractions. This dynamic self-assembly process is analogous to the flashing Brownian ratchet. Although this is an inherently unsteady, out-of-equilibrium process, we can predict its outcome using appropriate time averages of equilibrium equations of state. The predicted phase behavior is tested and validated by examining the fluid/crystal coexistence of such dynamically self-assembling dispersions in Brownian dynamics simulations of sedimentation equilibrium and homogeneous nucleation. We also show that our dynamic self-assembly scheme offers control and tunability over the crystal growth kinetics and can even stabilize nonequilibrium structures.

M1.00223 Achieving synchronization with active hybrid materials: Coupling self-oscillating gels and piezoelectric films. VICTOR V. YASHIN, Department of Chemical Engineering, University of Pittsburgh, STEVEN P. LEVITAN, Department of Electrical and Computer Engineering, University of Pittsburgh, ANNA C. BALAZS, Department of Chemical Engineering, University of Pittsburgh — Our goal is to develop materials that compute by using non-linear oscillating chemical reactions to perform spatio-temporal recognition tasks. The material of choice is a polymer gel undergoing the oscillatory Belousov-Zhabotinsky reaction. The novelty of our approach is in employing hybrid gel-piezoelectric micro-electro-mechanical systems (MEMS) to couple local chemo-mechanical oscillations over long distances by electrical connection. Our modeling revealed that (1) interaction between the MEMS units is sufficiently strong for synchronization; (2) the mode of synchronization depends on the number of units, type of circuit connection (serial of parallel), and polarity of the units; (3) each mode has a distinctive pattern in phase of oscillations and generated voltage. The results indicate feasibility of using the hybrid gel-piezoelectric MEMS for oscillator based unconventional computing.

M1.00224 Rheological Characterization of Bioinspired Mineralization in Hydrogels. ABIGAIL REGITSKY, NIELS HOLTEN-ANDERSEN, Massachusetts Institute of Technology — With increasing amounts of CO$_2$ in the atmosphere linked to potentially catastrophic climate change, it is critical that we find methods to permanently sequester and store CO$_2$. Inspired by the natural biominalization of calcium carbonate (CaCO$_3$), one future goal of this project is to understand the mechanisms of CaCO$_3$ mineralization in order to ultimately optimize a bioinspired hydrogel system, which produces high value industrial powders that consume CO$_2$ as a feedstock. Along the way, we are developing a rheological technique to study mineral nucleation and growth events by measuring the modulations in mechanical properties of a hydrogel system during mineralization. Our initial system consists of a gelatin hydrogel matrix, which is preloaded with calcium ions, and an aqueous solution of carbonate ions, which are allowed to diffuse through the gel to initiate the mineralization process. In order to monitor how the growth of minerals affects the mechanical properties of the gel network, we measure the storage (G') and loss (G'') moduli of the system in situ. Future work will focus on modifying the properties of the minerals formed by changing the polymer used in the hydrogel network and adding other organic molecules into the system.

M1.00225 Hardening and yielding in colloidal gels. EMANUELA DEL GADO, JADER COLOMBO, MEHDI BOUZID, Georgetown University — Attractive colloidal gel networks are disordered elastic solids that can form even in extremely dilute particle suspensions. With interaction strengths comparable to the thermal energy, their stress-bearing network can locally restructure via breaking and reforming inter-particle bonds. We use molecular dynamics simulations of a model system to investigate the strain hardening and the yielding process. During shear start up protocol, the system exhibits strong localization of tensile stresses that may be released through the breaking and formation of new bonds. In this regime, the small amplitude oscillatory shear analysis shows that the storage and the loss modulus follow a power law behavior that are closely reminiscent of experimental observations. At large accumulated strains, the strain-induced reorganization of the gel may trigger flow heterogeneities and eventually lead to the yielding of the gel via a quasi brittle damage of its structure.

M1.00226 Agglomerate Breakdown in Shear Thickening Fluids by Large Amplitude Oscillatory Shear (LAOS). RAN TAO, KIRK D. RICE, GALE A. HOLMES, NIST — Natl Inst of Stds & Tech — Amorphous fumed silica and polypyrrole glycyl (PPG) suspensions were investigated using both steady shear and oscillatory shear rheology. As-mixed and sonicated silica/PPG suspensions show different shear thickening behavior with different critical shear rates as analyzed by the MITLAOS framework as well as the Fourier Transform approach. The as-mixed suspensions show a pronounced decrease in viscosity or modulus over the course of measurement, which is ascribed to an irreversible breakdown of silica-PPG agglomerates induced by shear. We also extend research to study colloidal silica/PPG dispersions under the same LAOS framework. In particular, we seek to understand the impact of the nanoparticle’s structure, i.e., fractal vs. non-fractal, on the oscillatory STF response.

M1.00227 STATISTICAL AND NONLINEAR PHYSICS —

M1.00228 Three Dimensional Observations of Quantum Vortex Dynamics in Superfluid Helium. PETER MEGSON, DANIEL LATHROP, University of Maryland, College Park — Liquid helium, when cooled below 2.17 K, becomes a superfluid with exotic physical properties such as flow without friction. Superfluid flow is irrotational except about line-like topological phase defects with quantized circulation, known as quantum vortices. The dynamics of these vortices include events such as reconnection, wherein vortices meet and exchange tails, and Kelvin wave propagation, a possible mechanism for energy dissipation. We observe the dynamics of fluorescent nanoparticles trapped on the vortices using a newly developed 3D stereographic system. This talk will present new observations of reconnection events and analysis comparing vortex reconnection behavior in three dimensions to previous work that observed such events in two-dimensional projection. In particular, we discuss the power law scaling of vortex separation as a function of time and the effect of the initial angle of separation between the vortex filaments.
M1.00231 Harnessing geometric and magnetic nonlinearities in phononic meta-plates, OSAMA BILAL, ANDRE FOEHR, CHIARA DARAÏO, Department of Mechanical and Process Engineering, ETH-Zurich — Owing to their physical realization, locally resonant metamaterials retain narrow subwavelength band gaps. Moreover, the fixed geometry and dimensions of the unit cell set a hardbound on the central frequency of the operational bandwidth. Real-time tunable metamaterials extend the range of applications and further enable the realization of new sensors, filters, and switches. Our work harnesses the interaction between geometric nonlinearity and nonlinear magnetic potentials to engineer frequency-agile subwavelength band gaps. The concept is general and applicable to various metamaterial systems. Both numerical simulations and experimental realization of the proposed concept will be presented.

M1.00232 Propagation of mechanical waves through a stochastic medium with spherical symmetry, CARLOS AVENDANO, Universidad Autonoma de la Ciudad de Mexico, ADRIAN REYES, Universidad Nacional Autonoma de Mexico — We analyze the propagation of mechanical waves through an anisotropic and inhomogeneous medium with spherical symmetry. We assume that both its elastic and density properties, are random functions of spatial coordinates with specific statistical properties, which allow us to represent media whose properties are not completely determined. We compute the expected value of this system.

M1.00233 A network model of human aging: Limits, errors, and information, SPENCER FARRELL, ARNOLD MITNITSKI, KENNETH ROCKWOOD, ANDREW RUTENBERG, Dalhousie University — The Frailty Index (FI) quantifies human aging using the fraction of accumulated age-related deficits. The FI correlates strongly with mortality and accumulates non-linearly and stochastically with age. Clinical data shows a near-linear relationship of FI ≤ 0.7. We computationally model an aging population using a network model of interacting deficits. Deficits damage and repair at rates that depend upon the average damage of connected nodes. The model is parametrized to fit clinical data. We find that attribution errors, especially false negative, allow the model to recover the frailty limit. Mutual information allows us to assess how well the FI can predict mortality. Mutual information provides a non-parametric measure of how the FI predicts mortality. We find that attribution errors have a small effect on the mutual information when many deficits are included in the model. The mutual information of our model and of the clinical data are comparable.

M1.00234 Changes in the Distribution of Avalanches on a Conical Bead Pile with Cohesion1, JUSTINE WALKER, SUSAN LEHMAN, College of Wooster, KARIN DAHMEN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, JONATHAN UHL, Retired — The probability distributions for avalanches of varying size are experimentally determined for a slowly driven, conical bead pile. The pile is composed of roughly 20,000 steel spheres, 3 mm in diameter, atop a circular base; it is driven by adding one bead at a time to the apex of the pile. We investigate the dynamic response of the pile by recording avalanches off the pile over the course of tens of thousands of bead drops. The avalanching behavior is studied at different drop heights and different amounts of cohesion between the beads. The level of cohesion is tuned through use of an applied uniform magnetic field. Smaller, local avalanches are distinguished from larger, non-local avalanches and the moments of the avalanche distribution are calculated separately for these different populations. The resulting moments scale with cohesion differently, and the results are compared to the scaling predictions from an analytic mean-field model and corresponding simulation of slip avalanches in a shear system [Dahmen, Nat Phys 7, 554 (2011)].

1Research supported by NSF CBET 1336116 and 1336634.

M1.00235 Improving detection of avalanches on a conical bead pile1, AVI VAJPEYI, SUSAN LEHMAN, College of Wooster, KARIN DAHMEN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, JONATHAN UHL, Retired — A conical bead pile subject to slow driving and an external magnetic field is used as a simple system to investigate the variations in the avalanche size probability distribution function. Steel beads are dropped onto the pile from different heights and at different strengths of applied magnetic field. Avalanches are recorded by the change in mass as beads fall off the pile. Experimentally we observe an increasing deviation from power law behavior as the field and thus cohesion between the beads increases. We compare our experimental results for the probability distribution function to the results of an analytic theory from a mean-field model of slip avalanches [Dahmen, Nat Phys 7, 554 (2011)]. The model also makes predictions for avalanche duration, which is not measurable with the existing system. To more fully characterize the avalanching behavior of the pile over time, a high-speed camera has been added to the system to record the largest avalanches and allow more detailed analysis. The conical pile geometry presents a challenge for observation and particle tracking over the full pile. Our implementation scheme and preliminary results from the video analysis are presented.

1Research supported by NSF CBET 1336116 and 1336634.
M1.00236 Effects of sudden density changes in disordered superconductors and semiconductors 1. HIBA ASSO, SHARHWAHAN CHATURVEED, MICHEL PLEXIMILLING, UWE TÄUBER, Department of Physics, Virginia Tech — Vortices in type-II superconductors in the presence of extended, linear defects display the strongly pinned Bose glass phase at low temperatures. This disorder-dominated thermodynamic state is characterized by suppressed lateral flux line fluctuations and very slow structural relaxation kinetics: The vortices migrate between different columnar pinning centers to minimize the mutual repulsive interactions and eventually optimize the system’s pinning configuration. To monitor the flux lines’ late-time structural relaxations, we employ a mapping between an effectively two-dimensional Bose glass system and a modified Coulomb glass model, originally developed to describe disordered semiconductors at low temperatures. By means of Monte Carlo simulations, we investigate the effects of the introduction of random bare site energies and sudden changes in the vortex or charge carrier density on the soft Coulomb gap that appears in the density of states due to the emerging spatial anticorrelations. The non-equilibrium relaxation properties of the Bose and Coulomb glass states and the ensuing aging kinetics are studied through the two-time density autocorrelation function and its various scaling forms.

1 Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

M1.00237 Autonomous Brownian motors driven by nonadiabatic variation of internal parameters, ALEX PLYUKHIN, Saint Anselm College — We study a family of autonomous motors based on a Brownian particle driven from thermal equilibrium by periodic in time variation of the internal potential through which the particle interacts with molecules of the surrounding thermal bath. We demonstrate for such motors the absence of a linear response regime: The average driving force and drift velocity are shown to be quadratic in both the frequency and amplitude of the variation. The adiabatic approximation (of an infinitely slow variation) and the leading correction to it (linear in the variation’s frequency) lead to zero drift and are insufficient to describe the motor’s operation.

M1.00238 Modeling the Earth: Climate on an Icosphere, STEPHANIE FOUTS, Washington and Lee University, L. JONATHAN COOK, Roanoke College — The totally asymmetric simple exclusion process with Langmuir kinetics is a one-dimensional transport model used to study the motion of particles through a lattice. Its applications include systems in the fields of biology, climatology, mathematics, civil engineering, and physics. In our research, we examine the temporal dynamics through the power spectra, as well as the time-averaged particle distribution on the lattice via Monte Carlo simulations. We have applied our particle transport model to an icosahedron in an attempt to model Earth’s changing climate. In our research, we examine the temporal dynamics of the particle distribution on the lattice, as they correspond to seasonal heat fluctuations in the polar and equatorial regions of the globe. Using Monte Carlo simulations, we alter the input parameters of the system to explore the resultant actions of the Earth-system model. Our findings include seasonal oscillations consistent with those seen in reality. We also built a mathematical framework for our model which, when solved numerically, matches the oscillations seen in our physical system.

M1.00239 Directed Nanopatterning with Nonlinear Laser Lithography, ONUR TOKEL, OZGUN YAVUZ, EMRE ERECEK, IHOR PALEV, GRAHID MAKEY, FATIH OMER ILDAY, Bilken University — In spite of the successes of maskless optical nanopatterning methods, it remains extremely challenging to create any isotropic, periodic nanopattern. Further, available optical techniques lack the long-range coverage and high periodicity demanded by photonics and photovoltaics applications. Here, we provide a novel solution with Nonlinear Laser Lithography (NLL) approach. Notably, we demonstrate that self-organized nanopatterns can be produced in all possible Bawais lattice types. Further, we show that carefully chosen defects or structured noise can direct NLL symmetries. Exploitation of directed self-organization to select or guide to predetermined symmetries is a new capability. Predictive capabilities for such far-from-equilibrium, dissipative systems is very limited due to a lack of experimental systems with predictive models. Here we also present a completely predictive model, and experimentally confirm that the emergence of motifs can be regulated by engineering defects, while the polarization of the ultrafast laser prescribes lattice symmetry, which in turn reinforces translational invariance. Thus, NLL enables a novel, maskless nanofabrication approach, where laser-induced nanopatterns can be rapidly created in any lattice symmetry. [1] Nature Photonics, 7, 897 (2013)

M1.00240 purohit@seas.upenn.edu, XIAOJUN LIANG, PRASHANT PUROHIT, University of Pennsylvania — The thermal fluctuations of lipid bilayer membranes are key to their interaction with cellular components as well as the measurement of their mechanical properties. Typically, membrane fluctuations are analyzed by decomposing into normal modes or by molecular simulations. Here we propose a new approach to calculate the projection function of a membrane. We view the membrane as a fluctuating von Karman plate and discretize it into triangular elements. We express its energy as a function of nodal displacements, and then compute the partition function and covariance matrix using Gaussian integrals. We recover well-known results for membrane fluctuations are analyzed by decomposing into normal modes or by molecular simulations. Here we propose a new approach to calculate the partition function of a membrane. We view the membrane as a fluctuating von Karman plate and discretize it into triangular elements. We express its energy as a function of nodal displacements, and then compute the partition function and covariance matrix using Gaussian integrals. We recover well-known results for

M1.00241 Back-and-forth micromotion of aqueous droplets in a dc electric field, TOMO KURIMURA, MASATOSHI CHIKAWA, Kyoto University, MASAFURO TAKINOURA, Tokyo Institute of Technology, KENICHI YOSHIIKAWA, Doshisha University — Recently, it was reported that an aqueous droplet in an oil phase exhibited rhythmic back-and-forth motion under stationary dc voltage on the order of 100 V. Here, we demonstrate that the threshold voltage for such oscillation is successfully decreased to the order of 10 V through downsizing of the experimental system. Notably, the threshold electric field tends to decrease with a nonlinear scaling relationship accompanied by the downsizing. We derive a simple theoretical model to interpret the system size dependence of the threshold voltage. This model equation suggests the unique effect of additional noise, which is qualitatively characterized as a coherent resonance by an actual experiment as a kind of coherent resonance. Our result would provide insight into the construction of micrometer-sized self-commutating motors and actuators in microfluidic and micromechanical devices. [1] TK, MI, MT and KY, Phys.Rev.E 88, 042918 (2013).

M1.00242 Phase Transitions in a Model of Y-Molecules Abstract, DANIELLE HOLZ, DONOVAN RUTH, Lehigh University, RAUL TORAL, Institute for Cross-Disciplinary Physics and Complex Systems, JAMES GUNTON, Lehigh University — Immunglobulin is a Y-shaped molecule that functions as an antibody to neutralize pathogens. In special cases where there is a high concentration of immunoglobulin molecules, self-aggregation can occur and the molecules undergo phase transitions. This prevents the molecules from completing their function. We used a simplified model of 2-Dimensional Y-molecules with three identical arms on a triangular lattice with 2-dimensional Grand Canonical Ensemble. The molecules were permitted to be placed, removed, rotated or moved on the lattice. Once phase coexistence was found, we used histogram reweighting and multicanonical sampling to calculate our phase diagram.

M1.00243 ABSTRACT WITHDRAWN —
M1.00244 Social Network Influence and Personal Financial Status. SHAQIJUN LUO, FLAVIANO MORONE, City College of CUNY, CARLOS SARRAUTE, Grandata, Buenos Aires, Argentina, HERNAN MAKSE, City College of CUNY — Networks of social ties emerging from individual economic needs display a highly structured architecture. In response to socio-economic demands, people reshape their circle of contacts for maximizing their social status, and ipso facto, the pattern of their interconnections is strongly correlates with their personal financial situation. In this work we transform this substance of a topological-statistical point of view into a qualitative definition, which allows for quantifying the economic situation of individuals through a measure of their collective influence. We consider the network of mobile phone calls made by the Mexican population during three months, in order to study the correlation of person’s economic situation with her network location. Notably, we find that rich people tend to be also the most influential nodes, i.e., they self-organize to optimally position themselves in the network. This finding may be also raised at the level of a principle, a fact that would explain the emergence of the phenomenon of collective influence itself as the result of the local optimization of socio-economic interactions. Our method represents a powerful and efficient indicator of socio-economic robustness, which may be applied to maximize the effect of large scale economic intervention and stimulus policies.

M1.00245 Statistical Mechanics of Japanese Labor Markets. HE CHEN¹, Hokkaido University — We introduce a probabilistic model to analyze job-matching processes of recent Japanese labor markets, in particular, for university graduates by means of statistical physics. To make a model of the market efficiently, we take into account several hypotheses. Namely, each company fixes the (business year independent) number of opening positions for newcomers. The ability of gathering newcomers depends on the result of job matching process in past business years. This fact means that the ability of the company is weakening if the company did not make their quota or the company gathered applicants too much over the quota. All university graduates who are looking for their jobs can access the public information about the ranking of companies. By assuming the above essential key points, we construct the local energy function of each company and describe the probability that an arbitrary company gets students at each business year by a Boltzmann-Gibbs distribution. We evaluate the relevant physical quantities such as the employment rate and Gini index. We discuss social inequalities in labor markets, and provide some ways to improve these situations, such as the informal job offer rate, the job-worker mismatch between students and companies.

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M1.00246 Agitated granular rod monolayers: Tetratic or uniaxial nematic?, THOMAS MUELLER, Experimentalphysik V, University of Bayreuth, DANIEL DE LAS HERAS, Theoretischphysik II, University of Bayreuth, INGO REHBERG, KAI HUANG, Experimentalphysik V, University of Bayreuth — The ordering of granular rod monolayers under vertical agitation against gravity is investigated experimentally and compared quantitatively with equilibrium Monte Carlo simulations and density functional theory. At sufficiently high number density, short rods form a tetratic state and long rods form a uniaxial nematic state. The ordering transitions are found to be independent of the agitation frequency and strength, suggesting that the detailed nature of energy injection into such a nonequilibrium system does not play a crucial role. Interestingly, the length-to-width ratio at which the order changes from tetratic to uniaxial is around 7.3 in both experiments and simulations. This quantitative agreement indicates that, despite of driven far from thermodynamic equilibrium, agitated granular systems may share similar features with corresponding equilibrium systems. Finally, we summarize the universal and non-universal aspects between nonequilibrium granular rod and equilibrium liquid crystal systems in a state diagram.

M1.00247 Buckling of Patterned Top Films. DOKYEONG KWON, Seoul Natl Univ, HYO SEON SUH, University of Chicago, KOOKHEON CHAR, Seoul Natl Univ — Buckling of thin films on elastomeric substrates such as polydimethylsiloxane (PDMS) is the well-known phenomenon in buckling instability originating from the moduli mismatch between a substrate and a thin film placed on the top. Recently, many studies on the microstructure created by the buckling with flat top films have been reported and physics behind them has almost been well received. However, only a few work has been done for the buckling structure with micro- or nano-patterned top films and buckling mechanics for patterned top film-PDMS bilayers has not yet been established in detail. Here, we present the buckling of various patterned top films placed on top of elastomeric PDMS substrates. Geometrical patterns were prepared by unconventional lithography techniques such as thermal imprinting of polystyrene (PS) films. Buckling instability was induced by applying mechanical stress to the patterned top surface-PDMS bilayers. Resulting buckled structures showed different mechanical structures as shape and structural parameters of the top thin films were varied. The structural changes were analyzed by introducing a beam theory or a plate theory for the simple modeling of the top surfaces, giving insights on the buckling mechanics of top films with complicated patterns placed on PDMS substrates.

M1.00248 Triggered Snap-Through of Bistable Shells¹, YIJIE CAI, Wuhan University of Technology, SHICHENG HUANG, JAN TRASE, NAN HU, ZI CHEN, Dartmouth College — Elastic bistable shells are common structures in nature and engineering, such as the lobes of the Venus flytrap or the surfaces of a toy jumping poppers. Despite their ubiquity, the parameters that control the bistability of such structures are not well understood. In this study, we explore how the geometrical features of radially symmetric elastic shells affect the shape and potential energy of a shell’s stable states, and how to tune certain parameters in order to generate a snap-through transition from a convex semi-stable state to concave stable state. We fabricated a series of elastic shells with varying geometric parameters out of silicone rubber and measured the resulting potential energy in the semi-stable state. Finite element simulations were also conducted in order to determine the deformation and stress in the shells during snap-through. It was found that the energy of the semi-stable state is controlled by only two geometric parameters and a dimensionless ratio. We also noted two distinct transitions during snap-through, one between monostability shells with varying geometric parameters out of silicone rubber and measured the resulting potential energy in the semi-stable state. Finite element simulations were also conducted to compare the experimental results with the theoretical predictions. In both experiments and simulations, this quantitative agreement indicates that, despite of driven far from thermodynamic equilibrium, agitated granular systems may share similar features with corresponding equilibrium systems.

¹Z.C. acknowledge support from Society in Science-Branco Weiss Fellowship, administered by ETH Zurich.

M1.00250 Thermodynamics and Phase Transitions of Ising Model on Inhomogeneous Stochastic Recursive Lattice 1, RAN HUANG, Shanghai Jiao Tong Univ — As one of the few exactly solvable thermodynamic models, the Ising model on recursive lattice is featured by its impressive advantages and successful applications in various thermodynamic and statistical researches. However this model was considered that, since the recursive calculation demands homogenous structure, it can only describe the bulk and even systems with narrow utilization. In this work we figured out a practical methodology to extend the conventional homogenous structure of single-unit Husimi lattice to be random inhomogeneous lattices with variable units and structures, while keeping the feature of exact calculation. Three designs of inhomogeneous recursive lattices: the random-angel tessellation system, the Husimi lattice of variable units, and the random lattice, to describe the complex systems that can only be solved by approximations or simulations on regular lattices. Our work may enhance the application of the exact calculation on recursive lattices in various fields of materials science and applied physics, especially it may serve as a powerful tool to explore the cross-dimensional thermodynamics and phase transitions. 1 National Natural Science Foundation of China (Grant No. 11505110)

M1.00251 Nonlinear dynamics of Bohmian trajectories in a double-well potential, O. F. DE ALCAI-
TARA BONFIM, Univ of Portland, JOAO FLORENCIO, Universidade Federal Fluminense, RJ-Brazil — We investigate the dynamics of a quantum particle in a one-dimensional double-well potential within the framework of Bohm’s quantum mechanics. We find that the wavefunction of the trajectories is linked to the depth of complexity of the initial wave packet. By increasing the complexity of the wave packet we observe trajectories that are either periodic, quasiperiodic, or chaoticlike.

M1.00252 Nematic-columnar phase transition in oriented hard rectangles, TRISHA NATH, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India, DEEPAK DHAR, Department of Theoretical Physics, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai 400005, India, R. RAJESH, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India — We consider an assembly of monodisperse hard rectangles of size $2 \times d$ on a square lattice with only hard core interactions amongst them. The long axes of the rectangles can be oriented along the horizontal or vertical directions. For large enough aspect ratio, it is known that this system undergoes three phase transitions as the density ($\rho$) of rectangles is increased: first an isotropic-nematic transition (at $\rho_1^*$), second a nematic-columnar transition (at $\rho_2^*$), and third a columnar-sublattice transition (at $\rho_3^*$). In the nematic phase, only the orientational symmetry is broken. The columnar and sublattice phases correspond to additional broken translational symmetries (i.e., perpendicular to the nematic orientation) and both directions respectively. Interestingly, the critical exact value $\rho_2^*$ remains finite, approximately 0.73, even as $d \to \infty$. We develop a systematic high density expansion for the surface tension between two differently-ordered columnar phases. Keeping only the first order perturbative correction term and setting this surface tension to zero, we get an estimate of $\rho_2^*$ in excellent agreement with estimates from Monte Carlo simulations, for all $d \geq 2$.

M1.00253 BIOLOGICAL PHYSICS —

M1.00254 Single-molecule studies of collagen mechanics, NANCY FORDE, NAGHMEH REZAEI, Department of Physics, Simon Fraser University, MICHAEL KIRKNESS, Department of Molecular Biology and Biochemistry, Simon Fraser University — Collagen is the fundamental structural protein in vertebrates. Its triple helical structure at the molecular level is believed to be strongly related to its mechanical role in connective tissues. However, the mechanics of collagen at the single-molecule level remain contentious. Estimates of its persistence length span an order of magnitude, from 15-180 nm for this biopolymer of 300 nm contour length. How collagen responds to applied force is also controversial, with different single-molecule studies suggesting one of three different responses: extending entropically, overwinding, or unwinding, all at forces below 10 pN. Using atomic force microscopy to image collagens deposited from solution, we find that their flexibility depends strongly on ionic strength and pH. To study force-dependent structural changes, we are performing highly parallelized enzymatic cleavage assays of triple helical collagen in our new compact centrifuge force microscope. Because proteolytic cleavage requires a locally unwound triple helix, these experiments are revealing how local collagen structure changes in response to applied force. Our results can help to resolve long-standing debates about collagen mechanics and structure at the molecular level.

M1.00255 Population Dynamics of Viral Inactivation 1, KRISTA FREEMAN, DONG LI, Carnegie Mellon University, MANJA BEHRENS, Lund University, KIRIL STRELETZKY, Cleveland State University, ULF OLSSON, Lund University, ALEX EVILEVITCH, Carnegie Mellon University — We have investigated the population dynamics of viral infection in vitro using time-resolved cryo electron microscopy combined with light and X-ray scattering techniques. Using bacteriophage $\lambda$ as a model system for pressurized double-stranded DNA viruses, we found that virions incubated with their cell receptor eject their genome in a stochastic triggering process. The triggering of DNA ejection occurs in a non-synchronized manner after the receptor addition, resulting in an exponential decay of the number of genome-filled viruses with time. We have explored the characteristic time constant of this triggering process at different temperatures, salt conditions, and packaged genome lengths. Furthermore, using the temperature dependence we determined an activation energy for DNA ejections. The dependences of the time constant and activation energy on internal DNA pressure, affected by salt conditions and encapsidated genome length, suggest that the triggering process is directly dependent on the conformational state of the encapsidated DNA. The results of this work provide insight into how the in vivo kinetics of the spread of viral infection are influenced by intra- and extra cellular environmental conditions. 1 This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1252522.

M1.00256 Theory of sequence-dependent scaling and confinement of viral RNA molecules 1, JOSHUA KELLY, Univ of California - Los Angeles — We present a general theory for the fractal dimensions of the genomic viral RNA molecules of small RNA viruses and apply the theory as well to RNA encapsidation competition experiments. 1 Work supported by NSF

M1.00257 Convex Lens-induced Confinement to Visualize Biopolymers and Interaction Parameters, FRANK STABLE, DANIEL BERARD, GIL HENKIN, MARJAN SHAYEGAN, FRANCOIS MICHAUD, SABRINA LESLIE, McGill University — In this poster, we present a versatile CLIC (Convex Lens-induced Confinement) microscopy system to access a broad range of biopolymer visualization and interaction parameters. In the CLIC technique, the curved surface of a convex lens is used to deform a flexible coverslip above a glass substrate, creating a nanoscale gap that can be tuned during an experiment to load and confine molecules into nanoscale features, both linear and circular, embedded in the bottom substrate. We characterize and model massively parallel DNA nanochannel-based stretching, building on prior work. Further, we demonstrate controlled insertion of reagent molecules within the CLIC imaging chamber. We visualize real-time reaction dynamics of nanocaged species, including dye/DNA intercalation and DNA/DNA ligation reactions, demonstrating the versatility of this nanoscale microscopy platform.
M1.00258 Slow Domain Motions of an Oligomeric Protein from Deep-Sea Hyperthermophile probed by Neutron Spin Echo. DERSINDHU BHOWMIK, UTSAB SHRESTHA, GURPREET DHINDSA, Wayne State University, MELISSA SHARP, European Spallation Source, LAURA R. STINGACIU, Oak Ridge National Laboratory, XIANG-QIANG CHU, Wayne State University, XIANG-QIANG CHU TEAM — Deep sea microorganisms have the ability to survive under extreme conditions, such as high pressure and high temperature[1]. In this work, we used the combination of the neutron spin-echo (NSE) and the small angle neutron scattering (SANS) techniques to study the inter-domain motions of the inorganic pyrophosphate (IPPase) enzyme derived from thermostable microorganisms Thermococcus thioreducens. The IPPase has hexameric quaternary structure with molecular mass of approx. 120kDa (each subunit of 20kDa), which is a large oligomeric structure. The understanding of its slow inter-domain motions can be the key to explain how they are able to perform catalytic activity at higher temperature compared to mesophilic enzymes, thus leading to adapt to extreme environment present at the seabed [1]. The NSE can probe these slow motions directly in the time domain up to several tens of nanoseconds at sub-nanometers length scales, while the corresponding structural change can be explored by the SANS [2]. Our results provide a better picture of the local flexibility and conformational substates unique to these types of proteins, which will help us better understand the relation between protein dynamics and their biological activities. [1] U. R. Shrestha, et. al, PNAS (2015); X.-Q. Chu, et. al, JPCB 116, 9917 (2012). [2] R. Biehl, et. al. Soft Matt. 7, 1299 (2011)

M1.00259 Replica-exchange Wang-Landau simulations of the H0P lattice protein model. GUANGJIE SHI, Center for Simulational Physics, The University of Georgia, THOMAS WÜST, ID Scientific IT Services, ETH Zürich, Switzerland, YING WAI LI, National Center for Computational Sciences, Oak Ridge National Laboratory, DAVID P. LANDAU, Center for Simulational Physics, The University of Georgia — The hydrophobic-polar (HP) lattice protein model has been the subject of intensive investigation in an effort to aid our understanding of protein folding. However, the high ground state degeneracies caused by its simplification stands in contrast to the generally unique native states of natural proteins. Here we proposed a simple modification, by introducing a new type of “neutral” monomer, 0, i.e. neither hydrophobic nor polar, thus rendering the model more realistic without increasing the difficulties of sampling significantly. With the replica exchange Wang–Landau (REWL) scheme, we investigated several widely studied HP proteins and their H0P counterparts. Dramatic differences in both ground state and thermodynamic properties have been found. For example, the H0P version of Crambin shows more clear two-step folding and 3 order of magnitudes less ground state degeneracy than its HP counterpart.

M1.00260 Identifying paths of allosteric communication in the protein BirA through simulations. GREGORY CUSTER, DOROTHY BECKETT, SILVINA MATYSIAK, University of Maryland — Biotin ligase/repressor (BirA) is a bifunctional enzyme which adenylates biotin and transfers the product, biotinyl-5-AMP (bio-5-AMP) to biotin carboxyl carrier protein (BCCP). In the absence of BCCP, bio-5-AMP promotes the dimerization of BirA. In dimer form, the BirAbio-5-AMP complex is able to bind to the biotin operator and prevents further synthesis of biotin. The BirA bio-5-AMP binds away from the dimer interface, so it is acting as an allosteric activator. We perform all-atom molecular dynamics simulations with BirA to look at fluctuations within the protein at equilibrium. We simulate apoBirA, liganded BirA, as well as two mutants, M211A and V219A. In agreement with experimental observations, several loops of the protein become stabilized for the liganded BirA when compared to the apo protein. In addition, changes in the dimer interface are observed for the M211A and V219A mutations, which are located in the ligand binding region. Using inter-residue correlation coefficients and pair energies a communication network through the protein is constructed. With this network we have identified paths which have the potential to be important in allosteric activation of BirA. These paths and the methods we use to identify them will be presented.

M1.00261 Modeling Hand-Over-Hand and Inchworm Steps in Myosin VI, AMANDA JACK, Denison University, IAN LOWE, University of Pennsylvania, RIINA TEHVER, Denison University — Myosin VI is a molecular motor protein that moves along actin filaments to transport cargo within a cell. There is much experimental evidence that the myosin VI dimer moves “hand-over-hand” along actin; however, recent experiments suggest that the protein can also move via an “inchworm” mechanism. We created a mechanochemical kinetic model to predict myosin VI’s behavior under different ATP, ADP, and force conditions, taking these alternative mechanisms into account. Our model’s calculations agree well with experimental results and can also be used to predict myosin VI’s behavior outside experimentally tested regimes, such as under forward force. We also predict an optimized motor function for the protein around physiological (-2 pN) load and anchoring under -3 pN load. By using our model to predict myosin VI’s response to environmental change, we can gain insight into the behavior of a protein that can be difficult to observe experimentally.

M1.00262 Synchrotron radiation circular dichroism spectroscopy study of recombinant T4β folding. YUNG-CHIN HUANG, HSUEH-LIANG CHU, PENG-JEN CHEN, CHIA-CHING CHANG, Natl Chiao Tung Univ — Thymosin beta 4 (T4β) is a 43-aminoc acid small peptide, has been demonstrated that it can promote cardiac repair, wound repair, tissue protection, and involve in the proliferation of blood cell precursor stem cells of bone marrow. Moreover, T4β has been identified as a multifunction intrinsically disordered protein, which is lacking the stable tertiary structure. Owing to the small size and disordered character, the T4β protein degrades rapidly and the storage condition is critical. Therefore, it is not easy to reveal its unfolding mechanism of native T4β. However, recombinant T4β protein (rT4β), which fused with a 5-kDa peptide in its amino-terminal, is stable and possesses identical function of T4β. Therefore, rT4β can be used to study its folding mechanism. By using over-critical folding process, stable folding intermediates of rT4β can be obtained. Structure analysis of folding intermediates by synchrotron radiation circular dichroism (SRCD) and fluorescence spectroscopies indicate that rT4β is a random coli major protein and its hydrophobic region becomes compact gradually. Moreover, the rT4β folding is a two state transition. Thermal denaturation analysis indicates that rT4β lacks stable tertiary structure. These results indicated that rT4β, similar to T4β, is an intrinsically disordered protein.

M1.00263 Structural Properties of Human CaMKII Ca2+/Calmodulin-Dependent Protein Kinase II using X-ray Crystallography. YUNMENG MELODY CAO, Smith College, ETHAN MCSPADDEN, JOHN KURIYAN, U.C. Berkeley, DEPARTMENT OF MOLECULAR AND CELL BIOLOGY AND DEPARTMENT OF CHEMISTRY TEAM — To this day, human memory storage remains a mystery as we can at most describe the process vaguely on a cellular level. Switch-like properties of Calcium/Calmodulin-Dependent Protein Kinase II make it a leading candidate in understanding the molecular basis of human memory. The protein crystal was placed in the beam of a synchrotron source and the x-ray crystallography data was collected as reflections on a diffraction pattern that undergo Fourier transform to obtain the electron density. We observed two drastic differences from our solved structure at 2.75Å to a similar construct of the mouse CaMKII association domain. Firstly, our structure is a 6-fold symmetric dodecamer, whereas the previously published construct was a 7-fold symmetric tetradecamer. This suggests the association domain of human CaMKII is a dynamic structure that is triggered subunit exchange process. Secondly, in our structure the N-terminal tag is docked as an additional beta-strand on an uncapped beta-sheet present in each association domain protomer. This is concrete evidence of the involvement of the polypeptide docking site in the molecular mechanism underlying subunit exchange. In the future, we would like to selectively inhibit the exchange process while not disrupting the other functionalities of CaMKII.
M1.00264 Nanomechanics of Protein Unfolding outside Protease Nanopores. BINQUAN LUAN, RUHONG ZHOU, IBM T J Watson Res Ctr — Protein folding and unfolding have been the subject of active research for decades. Most of previous studies in protein unfolding were focused on temperature, chemical and/or force (such as in AFM) induced denaturations. Recent studies on the functional roles of proteasomes (such as ClpXP) revealed a novel unfolding process in cell, during which a target protein is mechanically unfolded and pulled into a confined, pore-like geometry for degradation. While the proteasome nanomachine has been extensively studied, the mechanism for unfolding proteins with the proteasome pore is still poorly understood. Here, we investigate the mechanical unfolding process of ubiquitin (with or without) an idealized proteasome pore, and compare such process with that in the AFM pulling experiment. Unexpectedly, the required force by a proteosome can be much smaller than that by the AFM. Simulation results also unveiled different nanomechanics, tearing fracture vs. shearing friction, in these two distinct types of mechanical unfoldings.

M1.00265 Coarse Graining to Investigate Membrane Induced Peptide Folding of Anticancer Peptides. SAI GANESAN, HONGCHEONG XU, SILVINA MATSUYAMA, Univ of Maryland-College Park — Information about membrane induced peptide folding mechanisms using all-atom molecular dynamics simulations is a challenge due to time and length scale issues. We recently developed a low resolution Water Explicit Polarizable PROtein coarse-grained Model by adding oppositely charged dummy particles inside protein backbone beads. These two dummy particles represent a fluctuating dipole, thus introducing structural polarization into the coarse-grained model. With this model, we were able to achieve significant (α-) secondary structure content de novo, without any added bias. We extended the model to zwitterionic and anionic lipids, by adding oppositely charged dummy particles inside polar beads, to capture the ability of the head group region to form hydrogen bonds. We use zwitterionic POPC and anionic POPS as our model lipids, and a cationic anticancer peptide, SV51 as our model peptide. We have characterized the driving forces for SV51 folding on lipid bilayers with varying anionic and zwitterionic lipid compositions. Based on our results, dipolar interactions between peptide backbone and lipid head groups contribute to stabilize folded conformations. Cooperativity in folding is induced by both intra peptide and membrane-peptide interaction.

M1.00266 Group transfer theory of single molecule imaging experiments in the F-ATPase biomolecular motor1, SANDOR VOLKAN-KACSO, RUDOLPH MARCUS, California Institute of Technology — I describe a chemo-mechanical theory to treat single molecule imaging and “stalling” experiments on the F-ATPase enzyme. This enzyme is an effective stepping biomolecular rotary motor with a rotor shaft and a stator ring. Using group transfer theoretical approach the proposed structure-based theory couples the binding transition of nucleotides in the stator subunits and the physics of torsional elasticity in the rotor. The twisting of the elastic rotor domain acts as a perturbation upon the driving potential, the Gibbs free energy. In the theory, without the use of adjustable parameters, we predict the rate and equilibrium constant dependence of steps such as ATP binding and phosphate release as a function of manipulated rotor angle. Then we compare these predictions to available data from stalling experiments. Besides treating experiments, the theory can provide guides for atomistic simulations, which could calculate the reorganization parameter and the torsional spring constant. The framework is generic and I discuss its application to other single molecule experiments, such as controlled rotation and other biomolecular motors, including motor-DNA complexes and linear motors. [PNAS, Early Edition, Oct. 19, 2015, doi: 10.1073/pnas.1518489112]

1 The authors would like to acknowledge support from the Office of the Naval Research, the Army Research Office, and the James W. Glanville Foundation.

M1.00267 Molecular Dynamics Simulation and Statistics Analysis Reveals the Defense Response Mechanism in Plants. ZHICHAO LIU, YUNJIE ZHAO, CHEN ZENG, Department of Physics, The George Washington University, COMPUTATIONAL BIOPHYSICS LAB TEAM — As the main protein of the bacterial flagella, flagellin plays an important role in perception and defense response. The newly discovered locus, FLS2, is ubiquitously expressed. FLS2 encodes a putative receptor kinase and shares many homologies with some plant resistance genes and even with some components of immune system of mammals and insects. In Arabidopsis, FLS2 perception is achieved by the recognition of epitope flg22, which induces FLS2 heteromerization with BAK1 and finally the plant immunity. Here we use both analytical methods such as Direct Coupling Analysis (DCA) and Molecular Dynamics (MD) Simulations to get a better understanding of the defense mechanism of FLS2. This may facilitate a redesign of flg22 or de-novo design for desired specificity and potency to extend the immune properties of FLS2 to other important crops and vegetables.

M1.00268 Multiscale modeling of three-dimensional genome. BING ZHANG, PETER WOLYNES, Rice University — The genome, the blueprint of life, contains nearly all the information needed to build and maintain an entire organism. A comprehensive understanding of the genome is of paramount interest to human health and will advance progress in many areas, including life sciences, medicine, and biotechnology. The overarching goal of my research is to understand the structure-function-relationship of the human genome. In this talk, I will be presenting our efforts in moving towards that goal, with a particular emphasis on studying the three-dimensional organization, the structure of the genome with multi-scale approaches. Specifically, I will discuss our recent reconstruction of genome structures at both interphase and metaphase by making use of data from chromosome conformation capture experiments. Computationally modeling of chromatin fiber at atomic level from first principles will also be presented as our effort for studying the genome structure from bottom up.

M1.00269 Quantifying the DNA binding characteristics of ruthenium based threading intercalator Λ-Δ-Λρ with optical tweezers. NICHOLAS BRYDEN, Bridgewater State University, MA. MICAH MCCAULEY, Northeastern University, MA, FREDRIK WESTERLUND, PER LINCOLN, Chalmers University of Technology, Sweden, IOULIA ROUZINA, Ohio State University, OH, MARK WILLIAMS, Northeastern University, MA, THAYAPARAN PARAMANATHAN, Bridgewater State University, MA — Utilizing optical tweezers, biophysics researchers have been able to study drug-DNA interactions on the single molecule level. Binuclear ruthenium complexes are a particular type of drug molecule that have been found to have potential cancer-fighting qualities, due to their high binding affinity and low dissociation rates. These complexes are threading intercalators, meaning that they must thread their bulky side chains through DNA base pairs to allow the central planar moiety to intercalate between the bases. In this study, we explored the binding properties of the binuclear ruthenium complex, Λ-Δ-Λρ (Λβ-[bidpz(phen)Ru2]4+). A single DNA molecule is held at a constant force and the Λ-Δσ solution introduced to the system in varying concentrations until equilibrium is reached. DNA extension data at various concentrations of Λ-Δσ recorded as a function of time provide the DNA binding kinetics and equilibrium binding affinity. Preliminary data analysis suggests that Λ-Δσ exhibits fast binding kinetics compared to the very similar Δ-Δσ. These complexes have the same chemical structure and only differ in their chirality, which suggests that the left handed (Λσ) threading moieties require less DNA structural distortion for threading compared with the right handed (Δσ) threading moieties.

M1.00270 Temperature Dependent Rotational Correlation in Lipids. CHRISTINA OTHON, NEDA DADASHVAND, EDUARDO VEGA LOZADA, Wesleyan University — The lateral heterogeneity of lipid dynamics is explored in free standing lipid monolayers. As the temperature is lowered the lipids exhibit increasingly broad and heterogeneous rotational correlation. This increase in heterogeneity appears to exhibit a critical onset similar to the observed for glass forming fluids. We explore this heterogeneous relaxation by measuring the membrane diffusion of a fluorescent probe (NBD-PC) using wide-field time-resolved fluorescence anisotropy microscopy, in single constituent lipid monolayer of DMPC. The observed relaxation exhibits a narrow, liquid-like distribution at high temperatures (τ > 2.4 ns), consistent with previous experimental measurements by different methods. However, as the temperature is quenched, the distribution broadens, and we observe the appearance of a long relaxation population (16.5 ns). This demonstrates that the nanoscale diffusion and reorganization in lipid structures can be significantly complex, even in the simplest unstructured architectures. This result can have a significant impact on the organization, permeability and energetics of natural membrane structures.
M1.00271 A study of the eigenvectors of low frequency vibrational modes in crystalline cytidine via high pressure infrared absorption and molecular dynamics simulations. CARL STARKEY, University of Toleda, KRISTINA WOODS, Carnegie-Mellon University, SCOTT LEE, University of Toledo — High-pressure infrared absorption experiments and molecular dynamics simulations have been used to study the eigenvectors and eigenvalues of the vibrational modes of crystalline cytidine at 295 K by evaluating the logarithmic derivative of the vibrational frequency with respect to pressure: $\frac{d\omega}{dP}$. Crystalline samples of molecular materials such as cytidine have vibrational modes that are localized within a molecular unit (“internal” modes) as well as modes in which the molecular units vibrate against each other (“external” modes). The value of the logarithmic derivative is a diagnostic probe of the nature of the eigenvector of the vibrational modes, making high pressure experiments a very useful probe for such studies. Internal stretching modes have low logarithmic derivatives while external as well as internal torsional and bending modes have higher logarithmic derivatives. Modes at about 503, 775, 795, 3093 and 3351 cm$^{-1}$ are found to have negative logarithmic pressure derivatives, indicating a weakening of the effective force constants associated with those modes. The two modes above 3000 cm$^{-1}$ are hydrogen-bond-stretching modes. The identity of all of these modes will be determined via molecular dynamical simulations.

M1.00272 Computational Study of Single-molecule fluorescence studies of transition paths in DNA hairpin folding. ERIN FEENEY, COURTNEY CLARK, M1.00276 Single molecule fluorescence studies of transition paths in DNA hairpin folding, M1.00277 Electrical Heart Defibrillation with Ion Channel Blockers, ERIN FEENEY, COURTNEY CLARK, M1.00273 Quantum Computational Calculations of the Ionization Energies of Acidic and Basic Amino Acids: Aspartate, Glutamate, Arginine, Lysine, and Histidine,1, C. P. DE GUZMAN, M. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA, 94508 — An extensive knowledge of the ionization energies of amino acids can provide vital information on protein sequencing, structure, and function. Acidic and basic amino acids are unique because they have three ionizable groups: the C-terminus, the N-terminus, and the side chain. The effects of multiple ionizable groups can be seen in how Aspartate’s ionizable side chain heavily influences its preferred conformation (J Phys Chem A. 2011 April 7; 115(13): 2900–2912). Theoretical and experimental data on the ionization energies of many of these molecules is sparse. Considering each atom of the amino acid as a potential departing site for the electron gives insight on how the three ionizable groups affect the ionization process of the molecule and the dynamic coupling between the vibrational modes. In the following study, we optimized the structure of each acidic and basic amino acid then extracted the three dimensional coordinates of the amino acids. We used ORCA to calculate point energies for a region near the optimized coordinates and systematically went through the x, y, and z coordinates of each atom in the neutral and ionized forms of the amino acid. With the calculations, we were able to graph energy potential curves to better understand the quantum dynamic properties of the amino acids.

M1.00273 Quantum Computational Calculations of the Ionization Energies of Acidic and Basic Amino Acids: Aspartate, Glutamate, Arginine, Lysine, and Histidine.1, C. P. DE GUZMAN, M. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA, 94508 — An extensive knowledge of the ionization energies of amino acids can provide vital information on protein sequencing, structure, and function. Acidic and basic amino acids are unique because they have three ionizable groups: the C-terminus, the N-terminus, and the side chain. The effects of multiple ionizable groups can be seen in how Aspartate's ionizable side chain heavily influences its preferred conformation (J Phys Chem A. 2011 April 7; 115(13): 2900–2912). Theoretical and experimental data on the ionization energies of many of these molecules is sparse. Considering each atom of the amino acid as a potential departing site for the electron gives insight on how the three ionizable groups affect the ionization process of the molecule and the dynamic coupling between the vibrational modes. In the following study, we optimized the structure of each acidic and basic amino acid then extracted the three dimensional coordinates of the amino acids. We used ORCA to calculate point energies for a region near the optimized coordinates and systematically went through the x, y, and z coordinates of each atom in the neutral and ionized forms of the amino acid. With the calculations, we were able to graph energy potential curves to better understand the quantum dynamic properties of the amino acids.

The authors thank Pacific Union College Student Association for providing funds.

M1.00274 Aggregation propensity of critical regions of the protein Tau. MICAIAH MUTHEE, AZKA AHMED, LUCA LARINI, Rutgers University-Camden — The Alzheimer’s disease is an irreversible, progressive brain disorder that slowly destroys memory and thinking skills, which eventually leads to the ability not to carry out the simplest tasks. The Alzheimer’s disease is characterized by the formation of protein aggregates both within and outside of the brain’s cells, the neurons. Within the neurons, the aggregation of the protein tau leads to the destruction of the microtubules in the axon of the neuron. Tau belongs to a group of proteins referred to as Microtubule-Associated Proteins. It is extremely flexible and is classified as an intrinsically unstructured protein due to its low propensity to form secondary structure. Tau promotes tubulin assembly into microtubules thereby stabilizing the cytoskeleton of the axon of the neuron. The microtubular binding region of tau consists of 4 pseudo-phosphorylations. In this study, we will focus on the aggregation propensity of two fragments. In this study we will consider the mutant P301L.

M1.00275 A Novel Approach for Computing Cross-Sections in Ion-Mobility Measurements. LUCA LARINI, OSCAR MARIN, Rutgers University - Camden — Mass spectrometry allows the identification of molecules based on their mass to charge ratio. One of the advantages of this technique is that it is able to distinguish molecules that differ for a small value of the mass. In addition, once the molecule of interest has been selected by the mass spectrometer, it can be further analyzed in an ion mobility tube that can characterize the conformations adopted by the molecule. This is extremely useful when dealing with unstructured proteins that populate multiple conformations. However, ion mobility distinguishes structures based on their cross-section. In order to associate a well-defined tridimensional structure to a specific cross-section, molecular dynamics simulations must be performed first, and then the theoretical cross-section compared to the experimental one. Computing a cross-section starting from molecular dynamics data is extremely computationally expensive. For this reason, we have developed a software that takes advantage of the multicore and multiprocessor architecture of modern computer clusters.

M1.00276 Single molecule fluorescence studies of transition paths in DNA hairpin folding. KATHERINE TRUEX, HOI SUNG CHUNG, JOHN LOUIS, WILLIAM EATON, National Institutes of Health — DNA hairpins are the simplest structures for investigating fundamental aspects of nucleic acid folding mechanisms. For two-state hairpins, all of the mechanistic information on how the hairpin folds is contained in the transition path (TP), the rare event in single molecule trajectories when the free energy barrier between folded and unfolded states is actually crossed. The only previous experimental study of TPs in nucleic acids used optical tweezer measurements and Szabo’s analytical theory for diffusive barrier crossing to recalculate the free energy surface for an indirect determination of average TP times (Neupane et al. PRL 2012). We used confocal single molecule FRET and maximum likelihood analysis of photon trajectories to determine an upper bound of 2.5 μs for the average TP time of a DNA hairpin (Truex et al., PRL 2015), compared to the value of 4 μs predicted by Neupane et al., providing an important test of energy landscape theory. Current experiments are aimed at eventually characterizing structural changes during TPs, which will provide a very demanding test of mechanisms predicted by both theoretical models and simulations.

M1.00277 Electrical Heart Defibrillation with Ion Channel Blockers. ERIN FEENEY, COURTNEY CLARK, STEFFAN PUWAL, Oakland University — Heart disease is the leading cause of mortality in the United States. Rotary electrical waves within heart muscle underlie electrical disorders of the heart termed fibrillation; their propagation and breakup leads to a complex distribution of electrical activation of the tissue (and of the ensuing mechanical contraction that comes from electrical activation). Successful heart defibrillation has, thus far, been limited to delivering large electrical shocks to activate the entire heart and reset its electrical activity. In theory, defibrillation of a system this nonlinear should be possible with small electrical perturbations (stimulations). A successful approach for such a low-energy defibrillator continues to elude researchers. We propose to examine in silica whether low-energy electrical stimulations can be combined with antiarrhythmic, ion channel-blocking drugs to achieve a higher rate of defibrillation and whether the antiarrhythmic drugs should be delivered before or after electrical stimulation has commenced. Progress toward a more successful, low-energy defibrillator will greatly minimize the adverse effects noted in defibrillation and will assist in the development of pediatric defibrillators.
M1.00278 Dynamics of driven transitions between minima of a complex energy landscapes. SAJ TEJA PUSULURI, Department of physics. Ohio University, ALEX H LANG, Computational Neurobiology Laboratory, Salk Institute, PANKAJ MEHTA, Department of physics. Boston University, HORACIO E CASTILLO, Department of physics. Ohio University — We recently modeled cellular interconnection dynamics[1] by using an epigenetic landscape model[2] inspired by neural network models. Given an arbitrary set of patterns, the model can be used to construct an energy landscape in which those patterns are the global minima. Here we study the transitions between stable states of the landscapes thus constructed, under the effect of an external driving force. We consider three different cases: i) choosing the patterns to be random and independently distributed ii) choosing a set of patterns directly derived from the experimental cellular transcription factor expression data for a representative set of cell types in an organism and iii) choosing randomly generated trees of hierarchically correlated patterns, inspired by biology. For each of the three cases, we study the stability of the global minima against thermal fluctuations and external driving forces, and the dynamics of the driven transitions away from global minima. We compare the results obtained in the three cases defined above, and in particular we explore to what degree the correlations between patterns affect the transition dynamics.

References

M1.00279 Anomalous motor mediated cargo transport in microtubule networks. STEVEN VANDAL, Worcester Polytechnic Institute, Dept of Physics, DANIEL MACVEIGH-FIERRO, ZHIYUAN SHEN, Worcester Polytechnic Institute, Dept of Biology and Biotechnology, KYLE LEMOI, Worcester Polytechnic Institute, Dept of Physics, LUIS VIDALI, Worcester Polytechnic Institute, Dept of Biology and Biotechnology, JENNIFER ROSS, University of Massachusetts Amherst, Dept of Physics, EKKA TUTUEL, Worcester Polytechnic Institute, Dept of Physics — Cargo transport is an important biological mechanism by which cells locomote, self-organize, and actively transport organelles. This transport is mediated by the cytoskeletal network and molecular motors; however, it is not known how network self-organization and dynamics affect these transport processes. In order to develop a mechanistic understanding of cargo transport, we use a coarse-grained Brownian dynamics model that incorporates the dynamics of these networks, as well as experimentally determined motor properties. We will test these models with two experimental systems: (1) in vitro microtubule networks with kinesin-1 motors, and quantum dot cargos on recreated microtubule networks, and (2) an excellent model organism, the moss Physcomitrella patens, in which chloroplasts are transported via the microtubule network by means of kinesin-like proteins. Phenomenological network characteristics are made, both in vivo and in vitro, and cargo motility is characterized using Mean Squared Displacement (MSD) measurements. Our simulations shed light on the role of network density and motor properties on the observed transport behavior, and improve our understanding of cargo transport in cells.

M1.00280 Water - Based TiO$_2$ Suspensions: A Raman Study. ROBERTO RANGE, DORINA CHIPARA, BRIAN YUST, DESIRE PADILLA, MICREA CHIPARA, The University of Texas Rio Grande Valley — The antibacterial features of TiO$_2$ are under scrutiny due to the UV radiation, which contributes to the generation of reactive oxygen species, mainly in water environments. A study of TiO$_2$ suspensions in water and broth is reported. TiO$_2$ has a low solubility in water. TiO$_2$ (anatase), with average diameter of 15 nm from Nanostructured & Amorphous Materials, Inc. has been added to the fluid (water, broth) and the mixture was stirred for 1-10 h, followed by a 10-60 minutes sonication. The suspension was left to sediment for 1 day before measurements. Quasistable suspensions of TiO$_2$ in water and broth were investigated by Raman spectroscopy using a Renishaw InVia spectrometer operating at 532 and 785 nm. The spectra of the nanoparticles were simulated by a collection of Breit-Wigner line shapes and the effect of the preparation conditions (stirring and sonication time) on the parameters of Raman lines are reported. The differences are explained by observing that the sonication destroys the agglomerates of anatase resulting in a better dispersion of nanoparticles and consequently a longer sedimentation time. Sample preparation/storage have been done both under dark and UV light conditions.

M1.00281 The broadcasting mechanism of master regulator NFkB switches. DAVIT POTOYAN, Rice University — The transcription factor NFkB is involved in many cellular responses. Therefore there is a large number of sites in the genome to which NFkB binds thereby activating myriad of genes as a response to various environmental stimuli. Kinetics becomes an important feature to reckon with in eukaryotic regulatory networks with many targets like the NFkB system. In particular models based on the classical picture of genetic switches predict slow down regulation of NFkB which can lead to wasteful over-expression of genes. A way to resolve this difficulty is to evolve faster ways of deactivating NFkB. There is evidence from experiments and our simulations that this is done by an InB induced process of stripping NFkB off directly from its genetic sites instead of waiting for an autonomous downregulation. The broadcasting mechanism proposed in this work solves the time scale problem inherent in the classical picture. Using combination of stochastic and deterministic models we show how such a mechanism results in efficient regulation of NFkB network.

M1.00282 Processing oscillatory signals by incoherent feedforward loops. CAROLYN ZHANG, FEILUN WU, RYAN TSOI, IGOR SHATS, LINGCHONG YOU, Duke University — From the timing of amoeba development to the maintenance of stem cell pluripotency, many biological signaling pathways exhibit the ability to differentiate between pulsatile and sustained signals in the regulation of downstream gene expression. While networks underlying this signal decoding are diverse, many are built around a common motif, the incoherent feedforward loop (IFFL), where an input simultaneously activates an output and an inhibitor of the output. With appropriate parameters, this motif can generate temporal adaptation, where the system is desensitized to a sustained input. This property serves as the foundation for distinguishing signals with varying temporal profiles. Here, we use quantitative modeling to examine another property of IFFLs, the ability to process oscillatory signals. Our results indicate that the system’s ability to translate pulsatile dynamics is limited by two constraints. The kinetics of IFFL components dictate the input range for which the network can decode pulsatile dynamics. In addition, a match between the network parameters and signal characteristics is required for optimal “counting”. We elucidate one potential mechanism by which information processing occurs in natural networks with implications in the design of synthetic gene circuits for this purpose.

This work was partially supported by the National Science Foundation Graduate Research Fellowship (CZ).

M1.00283 Shock wave irradiations avoiding fluid flow evoke intracellular Ca2+ signaling. TORU TAKAHASHI, AKIRA TSUKAMOTO, SHIGERU TADA, National Defense Academy of Japan — Shock wave irradiation accelerates therapeutic effects including angiogenesis. One mechanism underlying those effects is cellular responses evoked by shock wave irradiation. Fluid flow is one of major physical phenomena induced by shock wave irradiation. Cellular responses evoked by fluid flow are similar to those evoked by shock wave irradiation. Thus, fluid flow could be responsible for cellular responses evoked by shock wave irradiation. However, it is obscure whether fluid flow is required for the cellular responses evoked by shock wave irradiation. Cellular responses evoked by fluid flow are similar to those evoked by shock wave irradiation. In our study, intracellular Ca2+ signaling was observed in cells seeded in down-sized chambers. In the down-sized chambers, fluid flow was supposed to be suppressed because size of chambers (6 mm in diameter, 1 mm in thickness) was analogous to size of shock wave focus region (3mm in diameter). Dynamics of polystyrene microbeads suspended in the chambers were visualized with a CCD camera and analyzed with a particle image velocimetry (PIV) method to quantify fluid flow in the chamber. As a result, shock wave irradiation evoked intracellular Ca2+ signaling. However, fluid flow was not observed in the chamber due to shock wave irradiation. Thus, it was suggested that physical mechanics, not fluid flow, are further required for evoking intracellular Ca2+ signaling following to shock wave irradiation.
M1.00284 Dynamics of phenotypic reversibility of bacterial cells with oscillating hydrostatic pressure. SUDIP NEPAL, Univ of Arkansas-Fayetteville. PRADEEP KUMAR, Department of Physics, Univ of Arkansas-Fayetteville — Bacterial cells encounter and respond to physiochemical fluctuations. The response depends on the extent and type of the stresses applied. The response of bacterial cells to the fluctuating stress is relatively unknown. Here, we have studied the response of wild type Escherichia coli (E. coli) under fluctuating hydrostatic pressures ranging from 1 atm to 500 atm. High pressure acts as a stress to E. coli since these bacteria are adapted to grow optimally at atmospheric pressure. Cell division of E. coli is inhibited at high pressures resulting in increase in the length of the cells. Cell-length is reversible in nature and bacterial cells revert back to normal size on a time scale that is proportional to the strength and time of continuous pressure applied upon relaxing the high pressure condition. We have studied the dynamics of cellular reversibility of E. coli under the conditions in which continuous pressure is applied and subsequently relaxed over different time scales. We have quantified the dynamics of cellular reversibility with different relaxation times. Furthermore, we propose a model to describe the reversibility of the bacterial cell with the relaxation time. Our theoretical model fits well to the experimental data. We further

M1.00285 Chiral pattern formation in compact microbial colonies. KIRILL KOROLEV, ASHISH BINO GEORGE. Boston University — Chirality is ubiquitous in biology from single molecules to entire populations. Yet, we are still lacking a detailed understanding of how chiral patterns emerge from cell competition and growth, even in simple microbial colonies. Although many microbes grow as dense colonies with no apparent chirality, recent experiments with Escherichia coli have demonstrated that internal dynamics in such populations can be in fact chiral. We show that there is a unique way to extend the commonly-used reaction-diffusion models of colony growth to account for the emergent chirality. This new model connects microscopic and macroscopic chirality and explains the origin of logarithmic spirals separating different sub-populations in a colony. We also show that chirality is substantially enhanced by the cooperativity of the stable cells, which the designed molecules composed of strains with different chiralities and growth rates, our model predicts a very rich set of possible dynamics. For example, different chiralities can result in either sharp boundaries between the strains or promote their intermixing depending on the preferred twisting directions of the strains.

M1.00286 Adhesion of Mycobacterium smegmatis to Charged Surfaces and Diagnostics Implications. DIANE GORSE, ALI DHINOJWALA, Univ of Akron, FRANCISCO MOORE, Univ of Akron, NSF — Pulmonary tuberculosis (PTB) causes more than 1 million deaths annually. Smear microscopy is a primary rapid detection tool in areas where 95 % of PTB cases occur. This technique, in which the sputum of a symptomatic patient is stained and examined using a light microscope for Mycobacterium tuberculosis (MTB) shows sensitivity between 20 and 60 %. Insufficient bacterial isolation during sample preparation may be a reason for low sensitivity. We are optimizing a system to capture bacteria on the basis of electrostatic interactions to more thoroughly isolate bacteria from suspension and facilitate more accurate detection. Silica supports coated with positively-charged polyelectrolyte, poly(diallyldimethylammonium chloride), captured approximately 4.1 times more Mycobacterium smegmatis, a model organism for MTB, than was captured on negatively-charged silica substrates. Future experimentation will employ branched polymer systems and seek to justify the use of colloidal stability theories to describe initial capture.

M1.00287 Cell motility and antibiotic tolerance of bacterial swarms. WENLONG ZUO1, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — Many bacteria species can move across moist surfaces in a coordinated manner known as swarming. It is reported that swarm cells show higher tolerance to a wide variety of antibiotics than planktonic cells. We used the model bacterium E. coli to study how motility affects the antibiotic tolerance of swarm cells. Our results provide new insights for the control of pathogenic invasion via regulating cell motility.

M1.00288 The Effect of Graphene Oxide/Reduced Graphene Oxide Functionalized with Metal Nanoparticles on Dermal, Bacterial, and Cancerous/Non-Cancerous Epithelial Cells1, ARTHUR CHEN, MIRIAM RAFAILOVICH, MARCIA SIMON, State Univ of NY- Stony Brook, JAE HEE CHO, Boston University, JOHN JEROME, Suffolk University — Graphene and metal nanoparticles are permeating health care products but their effects and combined on human skin are uncertain. This project studied the effect of graphene oxide (GO) and reduced graphene oxide (rGO) functionalized with Ag or Pt nanoparticles (Ag/PtNPs) on bacterial, dermal (DFBC’s), and cancerous (SCC13’s) and non-cancerous (DO33’s) epidermal cells. GO was functionalized with AgNPs or PtNPs, forming metallized-GO; then reduced with NaBH4. FTIR and SEM confirmed the synthesis and composition. Confocal and SEM showed that Ag-rGO, depending on nanoparticle size, killed either S. Aureus or K. Pneumoniae, while Pt-rGO and rGO had no effect. Rhodamine staining revealed that Ag-rGO was very toxic to SCC13’s, but only slightly toxic to DO33’s. Pt-rGO and rGO had little effect on SCC13’s and DO33’s. At high concentrations all GO solutions inhibited cell growth but were not cytotoxic. Optical microscopy displayed that every GO/rGO solution adhered to DFBC’s and influenced their direction of growth, making GO/rGO potentially applicable for wound healing.

M1.00289 The functional consequences of non-genetic diversity in cellular navigation1. THIERRY EMONET, ADAM J WAITE, NICHOLAS W FRANKEL, YANN DUFOUR, JESSICA F JOHNSTON, Yale University — Substantial non-genetic diversity in complex behaviors, such as chemotaxis in E. coli, has been observed for decades, but the relevance of this diversity for the population is not well understood. Here, we use microfluidics to show that non-genetic diversity leads to significant structuring of the population in space and time, which confirms predictions made by our theoretical model of chemotaxis. We then use genetic tools to show that altering the expression level of a single chemotaxis protein is sufficient to alter the distribution of swimming behaviors, which directly determines the performance of a population in a gradient of attractant, a result also predicted by our model.

M1.00290 Allosteric Small-Molecule Inhibitors of the AKT Kinase. D. S. DALAFAVE, The College of New Jersey — This research addresses computational design of small druglike molecules for possible anticancer applications. AKT and SGK are kinases that control important cellular functions. They are highly homologous, having similar activators and targets. Cancers with increased SGK activity may develop resistance to AKT-specific inhibitors. Our goal was to design new molecules that would bind both AKT and SGK, thus preventing the development of drug resistance. Most kinase inhibitors target the kinase ATP-binding site. However, the high similarity in this site among kinases makes it difficult to target specifically. Furthermore, mutations in this site can cause resistance to ATP-competitive kinase inhibitors. We used existing AKT inhibitors as initial templates to design molecules that could potentially bind the allosteric sites of both AKT and SGK. Molecules with no implicit toxicities and optimal drug-like properties were used for docking studies. Binding interactions were measured by molecular models of AKT. Design molecules formed with AKT and SGK were calculated. Possible applications of the designed putative inhibitors against cancers with overexpressed AKT/SGK is discussed.
M1.00291 Effects of Chemotherapy-Induced Alterations in Cell Mechanical Properties on Cancer Metastasis, SRUTI PRATHIVADHI, ANDREW EKPENYONG, MICHAEL NICHOLS, CAROLYN TAYLOR, JIANHAO NING, Creighton University — Biological cells can modulate their mechanical properties to suit their functions and in response to changes in their environment. Thus, mechanical phenotyping of cells has been employed for tracking stem cell differentiation, bacterial infection, cell death, etc. Malignant transformation of cells also involves changes in mechanical properties. However, the extent to which mechanical properties of cancer cells contribute to metastasis is not well understood. Yet, more than 90% of all cancer deaths are directly related to metastasis. Transit of cells through the microcirculation is one of the key features of metastasis. We hypothesize that cancer treatment regimens do inadvertently alter cell mechanical properties in ways that might promote cancer metastasis. We use a microfluidic microrotation mimicetic (MMM) platform which mimics the capillary constrictions of the pulmonary and peripheral microcirculation to determine if in-vivo-like mechanical stimuli can evoke different responses from cells subjected to various cancer drugs. In particular, we show that cancer cells treated with chemotherapeutic drugs such as daunorubicin, become more deformable at short timescales (0.1 s) and transit faster through the device. Our results are first steps in evaluating the pro- or anti-metastatic effects of chemotherapeutic drugs based on their induced alterations in cell mechanical properties.

M1.00292 Collective motion in Proteus mirabilis swarms, XU HAORAN, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — Proteus mirabilis is a Gram-negative, rod-shaped bacterium. It is widely distributed in soil and water, and it is well known for exhibiting swarming motility on nutrient agar surfaces. In our study, we focused on the collective motility of P. mirabilis and uncovered a range of interesting phenomena. Here we will present our efforts to understand these phenomena through experiments and simulation.

M1.00293 Swimming and transport of bacteria in time-periodic flows, REBECCA WINTER, ALISON PATTESON, DAVID GAGNON, PAULO ARRATIA, Univ of Pennsylvania — The transport of bacteria can be highly influenced by external flows in oceans, rivers, and intestinal tracts. This has implications in biological systems for the performance of major biological processes, such as biofilm formation. In this study, we experimentally investigate the aggregation and transport of swimming Vibrio cholerae bacteria in time-periodic flows. Bacteria are placed in a well-characterized flow, and bacterial concentrations are recorded for a range of Reynolds numbers (Re) that spans two orders of magnitude, from 0.1 to 10. It is generally found that bacteria deplete from regions of high deformation rate and accumulate near vortices. This phenomenon seems to be dictated by a combination of bacterial activity and background flow vorticity.

M1.00294 Emergence of collective motion in bacterial suspensions, SONG LIU, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — It is well known that bacterial suspensions will exhibit collective motion at high concentrations, in which both steric and hydrodynamic interactions play important roles. We aim to investigate whether steric and hydrodynamic interactions are of equal importance to the emergence of collective motion. Here we will present our efforts to experimentally tune the relative strength of these interactions in bacterial suspensions. Our preliminary results suggest that the transition to collective motion may depend on the interplay between steric and hydrodynamic interactions.

M1.00295 Effect of microemulsions on cell viability of human dermal fibroblasts, JUYI LI, TATSIANA MIRONAVA, MARCIA SIMON, MIRIAM RAFAILOVICH, NISSIM GARTI, State Univ of NY— Stony Brook — Microemulsions are optically clear, thermostable and isotropic mixture consisting of water, oil and surfactants. Their advantages of ease preparation, spontaneous formation, long-term stability and enhanced solubility of bioactive materials make them great potential vehicles for research and pharmaceutical applications. In this study, comparative in vitro cytotoxicity tests were performed to select a best formulation of microemulsion with the least toxicity for human dermal fibroblasts. Three different kinds of oils and six different kinds of surfactants were used to form microemulsions by different ratios. The effect of oil type and surfactant type as well as their proportions on cell proliferation and viability were tested.

M1.00296 Experimental evolution of E. coli, MENGSHI ZHANG, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — The evolution from unicellular to multicellular behavior is an essential step in the history of life. Our aim is to investigate the emergence of collective behavior in the model organism Escherichia coli (E. coli) and its selection advantages, such as better utilization of public goods. Our preliminary results suggest that the evolution of collective behavior may be a natural response to stressed conditions.

M1.00297 Centrosome Positioning in 1D Cell Migration, KATRINA ADLERZ, HELIM ARANDA-ESPINOZA, Univ of Maryland-College Park — During cell migration, the positioning of the centrosome and nucleus define a cell's polarity. For a cell migrating on a two-dimensional substrate the centrosome is positioned in front of the nucleus. Under one-dimensional confinement, however, the centrosome is positioned behind the nucleus in 60% of cells. It is known that the centrosome is positioned by CDC42 and dynein for cells moving on a 2D substrate in a wound-healing assay. It is currently unknown, however, if this is also true for cells moving under 1D confinement, where the centrosome position is often reversed. Therefore, centrosome positioning was studied in cells migrating under 1D confinement, which mimics cells migrating through 3D matrices. 3 to 5 µm fibronectin lines were stamped onto a glass substrate and cells with fluorescently labeled nuclei and centrosomes migrated on the lines. Our results show that when a cell changes directions the centrosome position is maintained. That is, when the centrosome is between the nucleus and the cell's trailing edge and the cell changes direction, the centrosome will be translocated across the nucleus to the back of the cell again. A dynein inhibitor did have an influence on centrosome positioning in 1D migration and change of directions.
M1.00298 Active microtubule sliding in C. elegans. WILLIAM WEIGAND, Univ of San Diego, ASHLEY MESSMORE, University of California, San Diego, RAE ANDERSON, Univ of San Diego — The sea anenid, *Chaetopterus variopedatus*, secretes a bioluminescent mucus that also exhibits complex viscoelastic properties. The constituents of the mucus are relatively unknown but it does play an important role in the development of the worms’ parchment-like housing tubes. In order to determine how and why this mucus can exhibit material properties ranging from fluidity to rigidity we perform microtubule experiments. We determine the microscale viscoelastic properties by using optical tweezers to produce small oscillations in the mucus which allow us to determine both the linear storage and loss moduli (G’, G”) along with the viscosity of the fluid. By varying the size of the microspheres (2-10 m) and oscillation amplitude (5-10 m) we are able to determine the dominant intrinsic length scales of the molecular mesh comprising the mucus. By varying the oscillation frequency (1-15Hz) we determine the crossover frequency at which G’ surpasses G”, to quantify the longest relaxation time of the mesh network. Initial results show a strong dependence on bead size which indicate that the dominant entanglement length scale of the mucus mesh is ~5 µm. Microspheres of this size exhibit a wide variety of stress responses in different regions of the mucus demonstrating the substantial microscale heterogeneity of the mucus. We carry out measurements on a population of worms of varying size and age to determine mucus variability between worms.

M1.00299 Regulation of muscle contraction by Drebrin-like protein 1 probed by atomic force microscopy. RENATA GARCES, EUGENIA BUTKEVICH, MITJA PLATEN, CHRISTOPH F. SCHMIDT, Third Institute of Physics - Biophysics, Georg August University, Göttingen, BIOPHYSICS TEAM — Sarcomeres are the fundamental contractile units of striated muscle cells. They are composed of a variety of structural and regulatory proteins functioning in a precisely orchestrated fashion to enable coordinated force generation in striated muscles. Recently, we have identified a C. elegans drebrin-like protein 1 (DBN-1) as a novel sarcomere component, which stabilizes actin filaments during muscle contraction. To further characterize the function of DBN-1 in muscle cells, we generated a new dbn-1 loss-of-function allele. Absence of DBN-1 resulted in a unique worm movement phenotype, characterized by hyper-bending. It is not clear yet if DBN-1 acts to enhance or reduce the capacity for contraction. We present here an experimental mechanical study on C. elegans muscle mechanics. We measured the stiffness of the worm by indenting C. elegans with a micron-sized sphere adhered to the cantilever of an atomic force microscope (AFM). Modeling the worm as a pressurized elastic shell allows us to monitor the axial tension in the muscle through the measured stiffness. We compared responses of wild-type and mutant C. elegans in which DBN-1 is not expressed.

M1.00300 Measuring shear force transmission across a biomimetic glycocalyx. ISABEL BRAY, DYLAN YOUNG, JAN SCRIMGEOUR, Department of Physics, Clarkson University, Potsdam NY 13699 — Human blood vessels are lined with a low-density polymer brush known as the glycocalyx. This brush plays an active role in defining the mechanical and biochemical environment of the endothelial cell in the blood vessel wall. In addition, it is involved in the detection of mechanical stimuli, such as the shear stress from blood flowing in the vessel. In this work, we construct a biomimetic version of the glycocalyx on top of a soft deformable substrate in order to measure its ability to modulate the effects of shear stress at the endothelial cell surface. The soft substrate is stamped on to a glass substrate and then enclosed inside a microfluidic device that generates a controlled flow over the substrate. The hydrogel chemistry has been optimized so that it reliably stamps into a defined shape and has consistent mechanical properties. Fluorescent microbeads embedded in the gel allow measurement of the surface deformation, and subsequently, calculation of the shear force at the surface of the soft substrate. We investigate the effect of the major structural elements of the glycocalyx, hyaluronic acid and charged proteoglycans, on the magnitude of the shear force transmitted to the surface of the hydrogel.

M1.00301 Measuring shear force transmission across a biomimetic glycocalyx. ISABEL BRAY, DYLAN YOUNG, JAN SCRIMGEOUR, Department of Physics, Clarkson University, Potsdam NY 13699 — Human blood vessels are lined with a low-density polymer brush known as the glycocalyx. This brush plays an active role in defining the mechanical and biochemical environment of the endothelial cell in the blood vessel wall. In addition, it is involved in the detection of mechanical stimuli, such as the shear stress from blood flowing in the vessel. In this work, we construct a biomimetic version of the glycocalyx on top of a soft deformable substrate in order to measure its ability to modulate the effects of shear stress at the endothelial cell surface. The soft substrate is stamped on to a glass substrate and then enclosed inside a microfluidic device that generates a controlled flow over the substrate. The hydrogel chemistry has been optimized so that it reliably stamps into a defined shape and has consistent mechanical properties. Fluorescent microbeads embedded in the gel allow measurement of the surface deformation, and subsequently, calculation of the shear force at the surface of the soft substrate. We investigate the effect of the major structural elements of the glycocalyx, hyaluronic acid and charged proteoglycans, on the magnitude of the shear force transmitted to the surface of the hydrogel.

M1.00302 Micro-mechanical model for the tension-stabilized enzymatic degradation of collagen tissues. THAO NGUYEN, Mechanical Engineering, Johns Hopkins University, JEFFERY RUBERTI, Department of Bioengineering, Northeastern University — We present a study of how the collagen fiber structure influences the enzymatic degradation of collagen tissues. Experiments of collagen fibrils and tissues show that mechanical tension can slow and halt enzymatic degradation. Tissue-level experiments also show that degredation rate is minimum at a stretch level coincident with the onset of strain-stiffening in the stress response. To understand these phenomena, we developed a micro-mechanical model of a fibrous collagen tissue undergoing enzymatic degradation. Collagen fibers are described as sinusoidal elastic beams, and the tissue is described as a distribution of fibers. We assumed that the degradation reaction is inhibited by the axial strain energy of the crimped collagen fibers. The degradation rate law was calibrated to experiments on isolated single fibrils from bovine sclera. The fiber crimp and properties were fit to uniaxial tension tests of tissue strips. The fibril-level kinetic and tissue-level structural parameters were used to predict tissue-level degradation-induced creep rate under a constant applied force. We showed that we could accurately predict the degradation-induced creep rate of the pericardium and cornea once we accounted for differences in the fiber crimp structure and properties.

M1.00303 Mechanical model of kinesin moving on microtubule. KIWING TO, Institute of Physics, Academia Sinica, YA-CHANG CHOU, Yi-FENG HSIAO, KUAN-HUA CHEN, Department of Physics, National Tsing Hua University — Kinesins are biomolecules that serve as intercellular motors for carrying cellular cargos along microtubules. Although the mechanism of converting the chemical energy of ATP to mechanical work is not fully understood, the motion of a kinesin on a microtubule has been measured and two different mechanisms, namely the hand-over-hand and inchworm, has been proposed. The particular shape of kinesin and microtubules suggest a possible mechanism for force generation similar to Brownian ratchet. Work is not fully understood, the motion of a kinesin on a microtubule has been measured and two different mechanisms, namely the hand-over-hand and inchworm, has been proposed. The particular shape of kinesin and microtubules suggest a possible mechanism for force generation similar to Brownian ratchet. Although the mechanism of converting the chemical energy of ATP to mechanical work is not fully understood, the motion of a kinesin on a microtubule has been measured and two different mechanisms, namely the hand-over-hand and inchworm, has been proposed. The particular shape of kinesin and microtubules suggest a possible mechanism for force generation similar to Brownian ratchet.

M1.00304 Food category consumption and obesity prevalence across countries: an application of Machine Learning method to big data analysis. JOCELYN DUNSTAN, Johns Hopkins Bloomberg Public Health School, SAEIDEH FALLAH-FINI, Cal Poly Pomona, CLAUDIA NÄU, THOMAS GLASS, Johns Hopkins Bloomberg Public Health School, GLOBAL OBESITY PREVENTION CENTER TEAM — The applications of sophisticated mathematical and numerical tools in public health has been demonstrated to be useful in predicting the outcome of public intervention as well as to study, for example, the main causes of obesity without doing experiments with the population. In this project we aim to understand which kind of food consumed in different countries over time best defines the rate of obesity in those countries. The use of Machine Learning is particularly useful because we do not need to create a hypothesis and test it with the data, but instead we learn from the data to find the groups of food that best describe the prevalence of obesity.
M1.00305 An analytically tractable model for community ecology with many species1, BENJAMIN DICKENS, Department of Physics, Boston University . CHARLES FISHER, Bayesian Inference Group, Pfizer, Cambridge, MA, PANKAJ MEHTA, Department of Physics, Boston University . PANKAJ MEHTA BIOPHYSICS THEORY GROUP TEAM — A fundamental problem in community ecology is to understand how ecological processes such as selection, drift, and immigration yield observed patterns in species composition and diversity. Here, we present an analytically tractable, presence-absence (PA) model for community assembly and use it to ask how ecological traits such as the strength of competition, diversity in competition, and stochasticity affect species composition in a community. species can immigrate into the community from a regional species pool and can go extinct due to competition and stochasticity. Despite its simplicity, the PA model reproduces the qualitative features of more complicated models of community assembly. In agreement with recent work on large, competitive Lotka-Volterra systems, the PA model exhibits distinct ecological behaviors organized around a special ("critical") point corresponding to Hubbell's neutral theory of biodiversity. Our results suggest that the concepts of "phases" and phase diagrams can provide a powerful framework for thinking about community ecology and that the PA model captures the essential ecological dynamics of community assembly.

1PM was supported by a Simons Investigator in the Mathematical Modeling of Living Systems and a Sloan Research Fellowship

M1.00306 Speeding up evolution , WOUTER HOFF, Oklahoma State University — Proteins and cells offer great opportunities for green chemistry and renewable energy. However, few of these possible applications have been put into practice because of details that turn out to be major barriers to cost-efficient implementation and that prove difficult to solve by genetic engineering. A better understanding of molecular evolution promises a novel approach to addressing these important challenges. While major advances have been made, major gaps remain in understanding the evolution of proteins. Different approaches to accelerating molecular evolution into targeted directions will be discussed, including recent progress on evolution in non-homogeneous environments.

M1.00307 Population heterogeneity promotes a preference for blind cooperation1, ALFONSO PEREZ-ESCUEDERO, JONATHAN FRIEDMAN, JEFF GORE, Massachusetts Institute of Technology — Game theory—and common sense—recommend to carefully weigh costs and benefits before deciding on a course of action. Yet we often disapprove of people who do so, even when their actual decision benefits us. For example, we prefer people who directly agree to do us a favor over those who agree only after securing enough information to ensure that the favor will not be too costly. Why should we care about how people make their decisions, rather than just focus on the decisions themselves? Hoffman et al. (2015) have shown that such aversion to information gathering may be beneficial when it is strong enough to increase the level of cooperation. Here we show that the same type of aversion arises in heterogeneous populations, but for a different reason: individuals who seek additional information may reveal themselves to be undesirable partners, since they are less likely to cooperate in the future when conditions change. Aversion to information gathering thus facilitates preferential interactions with blind cooperators, who are more favorable partners. Due to this new mechanism the prevalence of such aversion rapidly increases with population diversity, because partner discrimination is more useful in populations which harbor partners of a more varied quality.

1We gratefully acknowledge funding from the Paul G. Allen Family Foundation, EMBO and Human Frontier Science Program

M1.00308 Complex sound stimuli representation by small neural groups in subcortical auditory structure . DOMINIKA LYZWA, Institute of Neuroscience, Newcastle University & Institute for Nonlinear Dynamics, University of Goettingen — The neural representation of complex natural sound stimuli in higher auditory structures is not yet well understood. Based on neurophysiological recordings from the mammalian auditory midbrain, neural responses to complex (natural and also artificial) sounds are investigated and mapped with respect to temporal and spectral neural tuning in the subcortical structure. The mapping includes spiking activity of single neurons and small neural clusters and local field potential activity. A neural model is presented which captures the mapping and also the similarity of responses across the auditory structure, and is used to predict responses to novel sound.

1Financial support by Bernstein Focus Neural Technology Goettingen, grant number 01GQ0811

M1.00309 A phylogenetic study of the section moduli of the humerus in bipedal theropod dinosaurs , SCOTT LEE, ZACHARY RICHARDS, University of Toledo — The section modulus of a bone is a measure of its ability to resist bending torques. Carnivorous dinosaurs including Tyrannosaurus and Allosaurus had strong humeri, presumably to hold struggling prey during hunting. The herbivorous dinosaurs of Ornithomimosauria had weak arm bones. This is believed to reflect the fact that their arms were never subjected to large bending torques. Carnivorous dinosaurs including Therizinosaurus had arms as strong as found in the carnivorous dinosaurs. This is consistent with the hypothesis that their manus suggests a digging lifestyle. Other groups including Oviraptorosauria, Troodontidae, Dromaeosauridae and Compsognathidae are also examined.

M1.00310 Physics of the Brain: Interaction of the Optical-Fiber-Guided Multi-Ultraviolet-Photon Beams with the Epilepsy Topion, (the Seizure Onset Area)1, V. ALEXANDER STEFAN, Institute for Advanced Physics Studies, Stefan University, La Jolla, California 92037 — A novel method for the possible prevention of epileptic seizures is proposed, based on the multi-ultraviolet-photon beam interaction with the epilepsy topion, (nonlinear coupling of an ultra high frequency mode to the brain beta phonons). It is hypothesized that epilepsy is a chaotic-dynamics phenomenon: small electrical changes in the epilepsy-topion lead, (within the 10s of milliseconds), to the onset of chaos, (seizure—excessive electrical discharge), and subsequent cascading into adjacent areas. The ultraviolet photons may control the imbalance of sodium and potassium ions and, consequently, may prove to be efficient in the prevention of epileptic seizures.

1Supported by Nikola Tesla Labs, Stefan University.


3 H.P. Zaveri et al., Localization-related epilepsy exhibits significant connectivity away from the seizure-onset area, Neuroreport, 20(9), 891-5, Jun17, 2009.
M1.00311 Asynchronous electrical activity in epileptic seizures. KATHERINE HOLMAN, Towson University, EUGENE LIM, Ohio Wesleyan University, STEPHEN GLISKE, WILLIAM STACEY, University of Michigan, CHRISTIAN FINK, Ohio Wesleyan University — High-frequency oscillations (HFOs) have been postulated to be potential biomarkers for focal epileptic seizures, with fast ripples (>250 Hz) as the most interesting candidate. The mechanisms underlying the generation of fast ripples, however, are not well understood. In this study, we draw upon results from previous computational studies on HFOs to develop a new mathematical model from first principles describing the generation of HFOs through asynchronous neuronal firing. Asynchrony in the model is obtained with the introduction of two parameters of heterogeneity: variability in the inter-spike interval (ISI) and jitter. The model predicts the generation of harmonic narrow-band oscillations if the heterogeneity-governing parameters do not differ from the predefined ISI by more than 20%. Comparisons against results from a separately constructed computational model verify the accuracy of the model in study. These results provide us with a rigorous framework in which we may investigate the mechanisms driving the generation of abnormal HFOs, and may serve as groundwork for future research in epileptogenesis.

1 NSF Grant 1003992, Ohio Wesleyan University SSRP

M1.00312 Columnar organization of orientation domains in V1. JOSCHA LIEDTKE, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — In the primary visual cortex (V1) of primates and carnivores, the functional architecture of basic stimulus selectivities appears similar across cortical layers (HUBEL & WIESEL, 1962) justifying the use of two-dimensional cortical models and disregarding organization in the third dimension. Here we show theoretically that already small deviations from an exact columnar organization lead to non-trivial three-dimensional functional structures. We extend two-dimensional random field models (Schnabel et al., 2007) to a three-dimensional cortex by keeping a typical scale in each layer and introducing a correlation length in the third, columnar dimension. We examine in detail the three-dimensional functional architecture for different cortical geometries with different columnar correlation lengths. We find that (i) topological defect lines are generally curved and (ii) for large cortical curvatures closed loops and reconnecting topological defect lines appear. This theory extends the class of random field models by introducing a columnar dimension and provides a systematic statistical assessment of the three-dimensional functional architecture of V1 (see also [Tanaka et al., 2011]).

M1.00313 A Topological Perspective of Neural Network Structure. ANN SIZEMORE, CHAD GIUSTI, University of Pennsylvania, MATTHEW CIESLAK, SCOTT GRAFTON, University of California Santa Barbara, DANIELLE BASSETT, University of Pennsylvania — The wiring patterns of white matter tracts between brain regions inform functional capabilities of the neural network. Indeed, densely connected and cyclically arranged cognitive systems may communicate and thus perform distinctly. However, previously employed graph theoretical statistics are local in nature and thus insensitive to such global structure. Here we present an investigation of the structural neural network in eight healthy individuals using persistent homology. An extension of homology to weighted networks, persistent homology records both circuits and cliques (all-to-all connected subgraphs) through a repetitive thresholding process, thus perceiving structural motifs. We report structural features found across patients and discuss brain regions responsible for these patterns, finally considering the implications of such motifs in relation to cognitive function.

M1.00314 Automated Region of Interest Detection of Fluorescent Neurons for Optogenetic Stimulation. JONATHAN MISHLER, DIETMAR PLENZ, Natl Inst of Mental Health - NIMH — With the emergence of optogenetics, light has been used to simultaneously stimulate and image neural clusters in vivo for the purpose of understanding neural dynamics. Spatial light modulators (SLMs) have become the choice method for the targeted stimulation of neural clusters, offering unprecedented spatio-temporal resolution. By first imaging, and subsequently selecting the desired neurons for stimulation, SLMs can reliably stimulate those regions of interest (ROIs). However, as the cluster size grows, manually selecting the neurons becomes cumbersome and inefficient. Automated ROI detectors for this purpose have been developed, but rely on neural fluorescent spiking for detection, requiring thousands of image frames. To overcome this limitation, we present an automated ROI detection algorithm utilizing neural geometry and stationary information from a few hundred imaging frames that can be adjusted for sensitivity.

M1.00315 An in vivo analysis of facial muscle change treated with botulinum toxin type A using digital image speckle correlation. YAN XU, SAMANTHA PALMACCIO PALMACCIO, DUC BUI, ALEXANDER DAGUM, MIRIAM RAFAILOVICH, State Univ of NY- Stony Brook — Been famous for clinical use from early 1980s, the neuromuscular blocking agent Botulinum toxin type A (BTX-A), has been used to reduce wrinkles for a long time. Only little research has been done to quantify the change of muscle contraction before and after injection and most research paper depend on subjective evaluation from both patients and surgeons. In our research, Digital Image Speckle Correlation (DISC) was employed to study the mechanical properties of skin, contraction mode of muscles (injected) and reaction of neighbor muscle group (un-injected). At the same time, displacement patterns (vector maps) generated by DISC can predict injection locus for surgeons who normally handle it depending only on visual observation.

M1.00316 Learning physical biology via modeling and simulation: A new course and textbook for science and engineering undergraduates. PHILIP NELSON, Univ Pennsylvania — To a large extent, undergraduate physical-science curricula remain firmly rooted in descriptive approaches, despite the fact that much current research involves quantitative modeling. Not only does our pedagogy not reflect current reality; it also creates a spurious barrier between the fields, reinforcing the narrow silos that prevent students from connecting them. I’ll describe an intermediate-level course on “Physical Models of Living Systems.” The prerequisite is first-year university physics and calculus. The course is a response to rapidly growing interest among undergraduates in a broad range of science and engineering majors. Students acquire several research skills that are often not addressed in traditional undergraduate courses: • Basic modeling skills; • Probabilistic modeling skills; • Data analysis methods; • Computer programming using a general-purpose platform like MATLAB or Python; • Pulling datasets from the Web for analysis; • Data visualization; • Dynamical systems, particularly feedback control.

1 Partially supported by the NSF under Grants EF-0928048 and DMR-0832802.

M1.00317 Light, Imaging, Vision: An interdisciplinary undergraduate course. PHILIP NELSON, Univ Pennsylvania — The vertebrate eye is fantastically sensitive instrument, capable of registering the absorption of a single photon, and yet generating very low noise. Using eyes as a common thread helps motivate undergraduates to learn a lot of physics, both fundamental and applied to scientific imaging and neuroscience. I’ll describe an undergraduate course, for students in several science and engineering majors, that takes students from the rudiments of probability theory to the quantum character of light, including modern experimental methods like fluorescence imaging and Frustr resonance energy transfer. After a digression into color vision, we then see how the Feynman principle explains the apparently wavelike phenomena associated to light, including applications like diffraction, subdiffraction imaging, total internal reflection and TIRF microscopy. Then we see how scientists documented the single-quantum sensitivity of the eye seven decades earlier than ‘ought’ to have been possible, and finally close with the remarkable signaling cascade that delivers such outstanding performance. Course materials are available upon request.

1 Partially supported by the NSF under Grants EF-0928048 and DMR-0832802.

2 A second oral abstract is allowed if it’s to Biophysics Education.
M1.00318 A Comparative Study Environmental and Radiological Causes Of Cancer In River Nile State, Sudan. EYAD HAMID, International University of Africa. HATIM KHAIR, King Mohamed Ibn Saud University — The causes of cancer in River Nile State are differ between environmental and radiological, this paper tried to make comparison between the two causes, to determine the real cause behind the large rising of cancer cases in this state, considering the daily habits for the patients and the possible contamination in the natural resources around them. The noticeable thing that most of cancer cases are might be due to the high concentration of nitrate pollutant detected in natural resources such as drinking water; also by looking to the radioactive elements we see there’s high concentration of some radioactive elements specially the K-40 which found in Portuclaca Oleraceae.

M1.00319 Dissociative Electron Attachment, ESMERALDA ARREOLA, None, ESMERALDA ARREOLA COLLABORATION, LEIGH HARGREAVES COLLABORATION — Since the pioneering work of Boudiaf et al. [1], it has been understood that electrons, even with energies near or below the ionization threshold, are capable of initiating strand-breaks in human DNA. This discovery raised important questions for cancer treatments, since sub-ionizing electrons are known to be the most copiously produced secondary product of radiation therapy. But even to date these factors are largely excluded from dosimetry calculations. This lack of inclusion is, at least in part, certainly due to the dearth of fundamental data describing low-energy electron interactions with a nucleating process, yet a firm basis of DNA. Under the organic perovskite structure and electronic properties is missing. Particularly, explaining certain physical phenomena, specifically a low recombination rate and high mobility of charge carriers still remain controversial. We theoretically investigate possible formation of hole polarons adopting methodology used for oxide perovskites. The perovskite studied here is the ABX$_3$: Structure, A being an organic cation, B lead and C a halogen; the combinations studied allow for possible formation of hole polarons adopting methodology used for oxide perovskites. It is shown that a localized state is realized with the Hubbard correction in systems with an electron removed, residing in the band gap.

M1.00320 ENERGY RESEARCH AND APPLICATIONS —

M1.00321 Photocurrent Enhancement in the ICG Dye Sensitized ZnO Nanowire Device¹, GEN LONG, MICHAEL BEATTIE, HUIZHONG XU, MOSTAFA SADOQI, Department of Physics, St John’s University — In this presentation, we report a systematic study of photocurrent in ICG dye sensitized ZnO nanowire/FTO devices. ZnO nanowire is grown by hydrothermal method, with length of ~200nm to 1 µm and diameter of ~30 to 60nm. ICG dye is incorporated by immersing ZnO grown FTO substrate. Different concentrations, solvents of ICG dye, sizes of ZnO nanowires and annealing temperatures and atmosphere after immersion were studied. The synthesized nanostructures and devices were characterized by XRD, UV-VIS absorption, SEM, AFM, solar simulator, etc. And an enhancement in the photocurrent due to ICG is observed.

¹The authors thank Center for Functional Nanomaterials of DOE for providing facilities access.

M1.00322 DFT+U Modeling of Hole Polarons in Organic Lead Halide Perovskites, ERIC WELCH, Texas State Univ-San Marcos, PAUL ERHART, Chalmers Institute of Technology, LUISA ŠCOLFARO, ALEX ZAKHIDOV, Texas State Univ-San Marcos — Due to the ever present drive towards improved efficiencies in solar cell technology, new and improved materials are emerging rapidly. Organic halide perovskites are a promising material for solar cells, and a fundamental understanding of the organic perovskite structure and electronic properties is missing. Particularly, explaining certain physical phenomena, specifically a low recombination rate and high mobility of charge carriers still remain controversial. We theoretically investigate possible formation of hole polarons adopting methodology used for oxide perovskites. The perovskite studied here is the ABX$_3$: Structure, A being an organic cation, B lead and C a halogen; the combinations studied allow for possible formation of hole polarons adopting methodology used for oxide perovskites. It is shown that a localized state is realized with the Hubbard correction in systems with an electron removed, residing in the band gap of each different structure. Thus, hole polarons are expected to be seen in these perovskites.

M1.00323 Photovoltaic enhancement via hot electron induced thermionic emission from quantum dots, ANDREI SERGEEV, KIMBERLY SABLON, U.S. Army Research Laboratory, Adelphi, MD 20783, USA — Quantum dot (QD) nanomaterials provide numerous possibilities for nanoscale engineering of photoelectron processes for specific applications, such as lighting, sensing, and energy conversion. It has been found that QDs may increase the photovoltaic conversion efficiency due to enhanced coupling with electromagnetic radiation, multiple exciton generation, and two-step light absorption. The hot electron induced thermionic emission from QDs is a novel mechanism, which may be significantly enhanced due to optimization of QD parameters. In this two-step process the photoelectrons excited from the valence band to localized quantum dot states are extracted from QDs via thermionic emission, which may be initiated by thermal phonons, hot phonons, and hot electrons. Strong interaction between the localized quantum dot electrons and hot photoelectrons excited by high energy photons substantially increases the conversion efficiency due to use of energy of sub-bandgap photons and energy of hot photoelectrons, which otherwise would be lost in relaxation processes. Here we present the theoretical model of the conversion via thermionic emission from quantum dots, results of optimization of photoelectron processes, and experimental data, which evidence in favor of this mechanism.

M1.00324 Strain-induced tuning of surface energetics, electron conductivity and reduction drive in spinel LiMn$_2$O$_4$ cathodes², IVAN SCIVETTI, GILBERTO TEOBALDI, University of Liverpool — LiMn$_2$O$_4$ (LMO) implementing in cathodes of rechargeable Li-ion batteries (LIBs) is hampered by the limited lifetime of the material and the stability of its interfaces, starting from the Solid Electrolyte Interphase [1,2]. Recent experiments [2] and Density Functional Theory (DFT) simulations [3] indicate that the formation and effectiveness of the SEI on LMO is related to the surface orientation. In this context, we analyse the role of geometrical strain for the relative energy, magnetic ordering and the reduction drive of several LMO surfaces. DFT simulations reveal LMO surfaces to be markedly sensitive to geometrical strain. Strain lower than 10% can lead to insulator-metal and ferromagnetic-antiferromagnetic transitions, alter the relative energy of LMO surfaces, and induce changes as large as 1.0 eV in the surface chemical potential, thence the reduction drive. Prompted by advances in the synthesis of metal-oxide core-shell nanostructures [4], the use of strained LMO coating to enhance SEI-formation is put forward as a potential nano-engineered strategy for longer lived SEI on LMO substrates.

1. JCPC 2012, 116, 9682-9661
4. ACS Nano 2012, 6, 5531

²EU FP7 project SIRBATT (Ref. 608502, end date: August 2016)
M1.00325 Defect physics vis-à-vis electrochemical performance in layered mixed-metal oxide cathode materials1,2 . KHANG HOANG, North Dakota State University, MICHELLE JOHANNES, Naval Research Laboratory — Layered mixed-metal oxides with different compositions of (Ni,Co,Mn) [NCM] or (Ni,Co,Al) [NCA] have been used in commercial lithium-ion batteries. Yet their defect physics and chemistry is still not well understood, despite having important implications for the electrochemical performance. In this presentation, we report a hybrid density functional study of intrinsic point defects in the compositions LiNi1/3Co1/3Mn1/3O2 (NCM1/1) and LiNi1/3Co1/3Al1/3O2 (NCA1/1) which can also be regarded as model compounds for NCM and NCA. We will discuss defect landscapes in NCM1/1 and NCA1/3 under relevant synthesis conditions with a focus on the formation of metal antisite defects and its implications on the electrochemical properties and ultimately the design of NCM and NCA cathode materials.

M1.00326 Modified Graphene Oxide for Long Cycle Sodium-Ion Batteries1 . MUHAMED SHAREEF, Kansas State University, HARRISON GUNN, Syracuse University, VICTORIA VOIGT, GURPREET SINGH, Kansas State University — Hummer’s process was modified to produce gram levels of 2-dimensional nanosheets of graphene oxide (GO) with varying degree of exfoliation and chemical functionalization. This was achieved by varying the weight ratios and reaction times of oxidizing agents used in the process. Based on Raman and Fourier transform infra red spectroscopy we show that potassium permanganate (KMnO4) is the key oxidizing agent while sodium nitrate (NaNO3) and sulfuric acid (H2SO4) play minor role during the exfoliation of graphite. Tested as working electrode in sodium-ion half-cell, the GO nanosheets produced using this optimized approach showed high rate capability and exceptionally high energy density of ~500 mAh/g for up to at least 100 cycles, which is among the highest reported for sodium/graphite electrodes. The average Coulombic efficiency was approximately 99 %.

1 Funded by KY EPSCoR, project number T1 2014-2019

M1.00327 Use of TiO2 nano particles in Sulfur electrodes to enhance cyclability of Li-S batteries1 . RUCHIRA DHARMASENA, GAMINI SUMANASEKERA, Department of Physics- University of Louisville, JACEK JASINSKI, ARJUN THAPA, MAHENDRA SUNKARA, Conn center-University of Louisville — Herein we investigate a novel and facile technique to fabricate Sulfur cathode for Li-S batteries with better cyclability and higher stable gravimetric capacity of around 750 mAh/g over 50 cycles. In this study we have experimented the use of TiO2 nano particles to prevent polysulfide dissolution into the electrolyte. Absorption and adsorption properties of TiO2 nano particles are used to trap Lithium Polysulfides. Excellent electrical conductivity property of carbonized polycrylonitrile (PAN) carbon fibers is effectively used in this technique to establish better electrical connection to Sulfur in the bulk electrode. The thermal annealing technique we use in this work introduces a facile way to load Sulfur into the electrode. Mechanical properties of the Sulfur electrode is improved using a relatively easy way to sustain expansion and contraction at stable coulombic capacity with almost 100 % efficiency. The mechanism of the said Sulfur electrode is discussed in detail using cyclic voltammetry and Impedance spectrum analysis.

1 NSF Grant No. 1454151

M1.00328 Incorporation of Platinum and Gold Partially Reduced Graphene Oxide in Polymer Electrolyte Membrane Fuel Cells for Increased Carbon Monoxide Tolerance1,2 . LEE BLACKBURN, REBECCA ISSEROFF, MIRIAM RAFAILOVICH, State Univ of NY- Stony Brook, JAYMO KANG, University of California, Berkeley . HONGFEI LI, MOLLY GENTLEMAN, State Univ of NY- Stony Brook, QIAO QIAO, Brookhaven National Laboratory — Polymer Electrolyte Membrane Fuel Cells (PEMFCs) can potentially provide “green” energy but the platinum catalyst’s susceptibility to carbon monoxide (CO) poisoning reduces output power. This project hypothesized that gold and platinum-partially reduced graphene oxide (Au/Pt-prGO) catalysts, incorporated into the electrodes and Nafion membrane of a PEMFC, will increase CO tolerance. Aliquots of graphene oxide (GO) were functionalized with platinum and/or gold nanoparticles. Partial reduction with NaBH4 prevented precipitation. Raman Spectroscopy and HRTEM verified the chemical identity, structure, and presence of the materials. Setups were tested in a PEM fuel cell with a gas feed containing 1000 ppm of CO, and averaged an output power >200% over the control, with the most effective sample, Pt-prGO Electrode + Membrane, yielding an output power >250% greater than the control. Additionally, each setup’s poisoned output power (PPr) was compared to its highest possible output power (P0). AuPt-prGO Electrode + Membrane produced 100% of its highest possible output power when poisoned, displaying 100% resistance to all CO poisoning at the resistances tested.

1 Funded by KY EPSCoR, project number T1 2014-2019

M1.00329 Harvesting Energy from the Flow-Induced Flutter of a ‘Piezoleaf’. ANDRE RUAS, SANTIAGO ORREGO, KYLE DORAN, AARON RIPS, KOUROSH SHOELE, SUNG HOON KANG, RAJAT MITTAL, Johns Hopkins University — The objective of our research is to examine energy harvesting from the flow-induced flutter of a small piezoelectric membrane, which we call a ‘Piezoleaf’. Piezoleaves are small, low-cost, low-maintenance devices capable of powering small portable electronics or wireless sensors in remote areas. It is well known that piezoelectric membranes subjected to time-varying strains generate electrical energy that can be harvested. In the current project, we have designed and constructed a new, low-speed wind-tunnel (1’x1’, cross-section) to analyze the flow-induced flutter and energy harvesting performance of a small (approximately 1”x2”) piezoleaf. One of the novel features of this research is that the membrane is fixed at its trailing-edge (i.e. an inverted flag) since this is expected to generate more energy than a regular flag configuration. Guided by numerical simulation, we are conducting tests of this configuration in our wind tunnel for various wind speeds (maximum speeds of about 10 m/s) to examine the effect of wind-speed on the flutter and energy harvesting. High-speed videography is also being used to examine the dynamics of the flag and results from this project will be presented.

M1.00330 High Temperature Concentrated Solar Power Using Liquid Metal , ASEGUH HENRY, Georgia Institute of Technology — One of the most attractive ways to try and reduce the cost of concentrated solar power (CSP) is to increase the system efficiency and the biggest loss in the system occurs in the conversion of heat to electricity via heat engine. Heat engines that utilize turbomachinery currently operate near their thermodynamic limitations and thus one of the only ways to improve heat engine efficiency is to increase the turbine inlet temperature. Significant effort is being devoted to the development of supercritical CO2 heat engines, but the most efficient heat engines are combined cycles, which reach efficiencies as high as 60%. However, such heat engines require turbine inlet temperatures ~1300-1500C, which is far beyond what is currently feasible with the state of the art molten salt infrastructure. In working towards the development of a system that can operate in the 1300-1500C temperature range, the most significant challenges lie in the materials and forming functional and reliable components out of new materials. One of the most attractive options from a cost and heat transfer perspective is to use liquid metals, such as tin and aluminum-silicon alloys along with a ceramic based infrastructure. This talk will overview ongoing efforts in the Atomistic Simulation and Energy (ASE) research group at Georgia Tech to develop prototype components such as an efficient high temperature cavity receiver, pumps and valves that can make a liquid metal based CSP infrastructure realizable.
about thermoelectric property of SnSe

Eutectic SnSe solar cell is one of the most promising thin film solar cells and its highest efficiency has reached 21%. To keep improving the efficiency of CdTe solar cells, a few issues need to be addressed, one of which is the back contact. The back contact of CdTe solar cells are mostly Cu-based, and the problem with Cu-based back contact is that Cu diffuses into the grain boundary and into the CdS/CdTe junction, causing degradation problem at high temperature and under illumination. To continue improving the efficiency of CdTe/CdS solar cells, a good ohmic back contact with high work function and long term stability is needed. In this work, we report our studies on the potential of conducting polymer being used as the back contact of CdTe/CdS solar cells. Conducting polymers are good candidates because they have high work functions and high conductivities, are easy to process, and cost less, meeting all the requirements of a good ohmic back contact for CdTe. In our studies, we used poly(3,4-ethylenedioxythiophene) (PEDOT:PSS) with different conductivities and compared them with traditional Cu-based back contact. It was observed that the CdTe solar cell performance improves as the conductivity of the PEDOT:PSS increase, and the efficiency (9.1%) is approaching those with traditional Cu/Au back contact (12.5%).

1Cdium Telluride Solar Cells with PEDOT:PSS Back Contact

M1.00331 Interface Conductance Modal Analysis , ASEGUN HENRY, Georgia Institute of Technology — A formalism termed the interface conductance modal analysis (ICMA) method will be presented, which allows for calculations of the modal contributions to thermal interface conductance within the context of molecular dynamics (MD) calculations, which inherently include anharmonicity to full order. The eight modes of vibration are calculated from harmonic lattice dynamics (LD) calculations, however the generality of ICMA formalism also allows for incorporation of anharmonic LD results into the calculations. The formalism is based on a modal decomposition of the heat flow across an interface, which is then substituted into expressions for the conductance either based on equilibrium or nonequilibrium MD. Several example cases will be covered and the interesting insights that emerge from the ICMA analyses will be discussed in detail. The ICMA method enables more in-depth study of various effects such as temperature, anharmonicity, interdiffusion, roughness, imperfections, dislocations, stress, changes in crystal structure through a single unified model, as it can essentially treat any material or object where the atoms vibrate around equilibrium sites (e.g, ordered or disordered solids and molecules).

M1.00333 Transport and thermoelectric properties of hot-pressed SnSe3, NGUYEN VAN QUANG1, NGUYEN THI MINH HAI, DUONG ANH TUAN, DUONG VAN THIET, CHO SUNGLAE2. University of Ulsan, SONG JAE YONG, PARK HYUNMIN, Korea Research Institute of Standards and Science, JAE YONG SONG COLLABORATION, HYUN-MIN PARK COLLABORATION — Recently, SnSe has been reported as ultralow thermal conductivity material which make it become a very high thermoelectric fingure of merit ZT material, up to 2.6 at 923 K. But, it is hard to use SnSe for applications in high temperature range because SnSe decomposes at 700 K. Therefore, searching for crystalline materials with high ZT value at lower temperature is still an attracted field of research. SnSe is also 2D material which is expected to have low lattice thermal conductivity. However, less is known about thermoelectric property of SnSe. Eutectic SnSe thin films, has been reported as promoting low-temperature thermoelectric material with ZT =0.56 at 593 K. Here, we prepared the polycrystalline SnSe3 using hot pressure method. At temperature range up to 573 K, it exhibited an anisotropic n-type charge carrier. Ultra low thermal conductivity is achieved along parallel direction, however, ZT value is still very low whose maximum was 0.045 at 573 K due to

M1.00334 Correlation between dimensional crossover and thermoelectric performance in conducting polymer , JUNHYEON JO, IN-SEON OH, MI-JIN JIN, JUNG-WOO YOO, Ulsan National Institute of Science and Technology (UNIST) — Conjugated polymers are emerging as attractive thermoelectric materials, resulting from low thermal conductivity, easy process and variable potentials for change. Recently, there are significant improvements of the Seebeck coefficient (S) and electric conductivity (σ) in the conjugated polymers by adding chemical additives to reform its ordinary disordered structure system. However, the relation between thermoelectricity and charge transport in the system is not well understood, which gives us a new challenge to improve thermoelectricity in the organic system. Here, we studied thermoelectric performance of dimethyl sulfoxide (DMSO) doped poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) with adding variable amounts of fluorosurfactant Zonyl. The charge transport in this disordered system was analyzed within variable range hopping (VRH), which showed the change of hopping dimensionality with further molecular dopants. The morphological change and its effect on charge transport and thermoelectric performance were further investigated through AFM, XPS, etc. As a result, we found the optimal condition for increasing both the Seebeck coefficient and electric conductivity, resulting in a significant improvement for the power factor ($S^2\sigma$).

M1.00335 ABSTRACT WITHDRAWN —

M1.00336 Structural And Magnetic Properties In Off-Stoichiometric MnNiGe Based Thin Film And Bulk Compounds , ANIL ARYAL, ABDIEL QUETZ, SUDIP PANDEY, SIUC, USA, IGOR RODIONOV, VALERII PRUDNIKOV, Moscow State Univ,Russia, TAPAS SAMANTA, LS, USA, ALEXANDER GRANOVSKY, Moscow State Univ,Russia, ANDREI SOKOLOV, UML, USA, IGOR DUBENKO, SIUC, USA, SHANE STADLER, LS, USA, NAUSHAD ALI, SIUC,USA — The crystal structure, magnetic properties and magnetic-to-electrical effect in NiMnGe based thin film and bulk compounds are studied by room temperature XRD and magnetization measurements.The bulk compounds Ni0.95Cr0.05Mn1.07Ge1.05 and Ni0.95Cr0.05Mn1.07Ge1.03 were prepared by arc melting process. Thin film was obtained from Ni0.95Cr0.05Mn1.05Ge1.05 target using Pulsed Laser Deposition technique on MgO substrate. Both bulk and thin film crystalizes into hexagonal structure. For bulk Ni0.95Cr0.05Mn1.05Ge1.05, a first order magnetostructural transition from antiferromagnetic orthorhombic to ferromagnetic hexagonal structure was observed near transition temperature 134 K followed by the second order transition (SOT) from ferromagnetic to paramagnetic near Curie temperature $T_c = 204$ K. In case of thin film only the presence of SOT was observed near $T_c$. For Ni0.95Cr0.07Mn1.07Ge1.05, $\Delta T = 0.65K$ near $T_c = 209 K$ for $\Delta H = 1.8 T$ was observed. This work was supported by the U.S. DOE Award No. DE-FG02-06ER46291 & DE-FG02-13ER46946. Authors at Moscow State Univ. acknowledge Russian Foundation for Basic Research (Grant No. 15-02-01976). A. Sokolov acknowledges support from NSF DMR-1310542 grant.

M1.00337 Efficiency, Power and Period of a model quantum heat engine working in a finite time1, MULUGETA BEKELE, Associate Professor of Physics, AAU, TOLASA A DIMA, Graduate student, MEKUANNENT ALEYME, Lecturer: Debre Tabor University, WARGA CHEGENO, Lecturer: Wolkite University — We take a spin-half quantum particle undergoing Carnot type cyclic process in a finite time assisted by two heat reservoirs and an external magnetic field. We find that the power of the heat engine is maximum at a particular period of the cyclic process and efficiency at the maximum power is at least half of the Carnot efficiency. We further apply the Omega-criterion for a figure of merit representing a compromise between useful power and lost power determining the corresponding efficiency for the optimization criterion to be at least three fourth of the Carnot efficiency.

1The authors are thankful to the International Science programme, IPS, Uppsala, Sweden for their support to our research lab.
M1.00338 Enhancing photovoltaic efficiency through radiative cooling of solar cells below ambient temperature.  
Taqiyah Safi, Jeremy Munday, University of Maryland, College Park — Sunlight heats up solar cells and the resulting elevated solar cell temperature adversely affects the photovoltaic efficiency and the reliability of the cell. Currently, a variety of active and passive cooling strategies are used to lower the operating temperature of the solar cell. Passive radiative cooling requires no energy input, and is ideal for solar cells; however, previously demonstrated devices still operate above the ambient, leading to a lower efficiency as compared to the ideal Shockley-Queisser limit, which is defined for a cell in contact with an ideal heat sink at ambient temperature (300 K). In this talk, we will describe the use of radiative cooling techniques to lower the cell temperature below the ambient temperature. We show that by combining specifically designed radiative cooling structures with solar cells, efficiencies higher than the limiting efficiency achievable at 300 K can be obtained for solar cells in both terrestrial and extraterrestrial environments. We show that these structures yield an efficiency 0.87% higher than a typical PV module at operating temperatures in a terrestrial application. We also demonstrate an efficiency advantage of 0.4-2.6% for cells in an extraterrestrial environment in near-earth orbit.  

M1.00339 Li-air, rechargeable, solid-state batteries using graphene and boron nitride aerogel matrices.  
Onur Ergen, Thang Thoan Pham, Sally Demais-Turner, Alex Zettl, University of California at Berkeley — The recent explosion of research on Li-air batteries has provided new insights into developing more efficient air cathodes. Graphene and boron nitride aerogel matrix is anticipated to be an ideal candidate to produce a high throughput air-breathing system. We developed a Li-Air battery model that accounts for efficient O2 throughput. These unique aerogel matrices exhibit the ability to orient the O2 passing through and keep out H2O, CO2, and N2. Thus, the solid-state cells demonstrate a long cycle life, thermal stability, and high rechargeable characteristics. These cells also show an explicit discharge capacity with a constant discharge current density of 0.1mA/cm2.  

M1.00340 Experimental characterization of a small custom-built double-acting gamma-type stirling engine.  
Peter Intsiful, Prairie View A & M University; Prairie View, TX, Francis Mensah, Virginia Union University, Richmond, VA, Arthur Thorpe, Howard University, Washington, DC — This paper investigates characterization of a small custom-built double-acting gamma-type stirling engine. Stirling-cycle engine is a reciprocating energy conversion machine with working spaces operating under conditions of oscillating pressure and flow. These conditions may be due to compressibility as well as pressure and temperature fluctuations. In standard literature, research indicates that there is lack of basic physics to account for the transport phenomena that manifest themselves in the working spaces of reciprocating engines. Previous techniques involve governing equations: mass, momentum and energy. Some authors use engineering thermodynamics. None of these approaches addresses this particular engine. A technique for observing and analyzing the behavior of this engine via parametric spectral profiles has been developed, using laser beams. These profiles enabled the generation of pv-curves and other trajectories for investigating the thermos-physical and thermos-hydrodynamic phenomena that manifest in the exchangers. The engine’s performance was examined. The results indicate that with current load of 35.78A, electric power of 0.505 kW was generated at a speed of 240 rpm and 29.50 percent efficiency was obtained.  

M1.00341 Effects of pH on the characteristics of ZnS thin films grown by using the CBD method  
Heejin Ahn, Dongchan Lee, Su Jung Park, Youngho Um, Univ of Ulsan — In CIGS-based thin film solar cells, a chemically deposited ZnS buffer layer with high resistivity is generally used between the absorber layer and transparent conducting oxide layer. In this work, we report a chemical process to prepare ZnS films by the CBD technique based on the typical bath deposition. The influences of ammonia (NH4OH) and Na2EDTA (Na2C16H10N2O8) as complexing agents on structural, morphological, and optical properties of ZnS thin films are investigated ranging pH concentration from 5 to 10. To investigate effects of pH on the characteristics of ZnS thin films, by using UV-visible transmittance, atomic force microscopy, and optical absorption were investigated. With changing the pH range, the ZnS thin films demonstrate high transmittance of 75-80% in the visible region, indicating the films are potentially useful in photovoltaic applications. The results will be presented in detail.  

M1.00342 Silicon and phosphorus dual doped graphene as the promising metal-free catalysts for oxygen reduction reaction  
Zhansheng Lu, Shuo Li, Zongxian Yang, Henan Normal University, Ruqian Wu, University of California Irvine — The pathways of oxygen reduction reaction (ORR) on the metal-free silicon and phosphorus dual doped graphene (Si-P-G) catalyst are systematically investigated based on the dispersion-corrected density functional theory (DFT-D) method. It is found that the Si-P-G can be stable at high temperature from the first-principles molecular dynamics simulation and the local region of dopants displays an important role in adsorption and reduction of oxygen. Both of the four-electron O2 direct dissociation and the two-electron OOH dissociation pathways are probable for ORR on the Si-P-G, while the latter pathway is mainly followed by the pathway of the OH hydrogenation into H2O. For the OOH dissociation pathway, the hydrogenation of O2 to OOH is the rate-limiting step with a rather small barrier energy of 0.66 eV. The current results indicate that the Si-P-G is a novel metal-free catalyst for ORR, and which is comparable to that of the Pt catalyst.  

M1.00343 Lattice-Boltzmann-based Simulations of Diffusiohoresis  
Joshua Castiglione, Jennifer Kreft Pearce, Roger Williams University — We present results from a lattice-Boltmann-base Brownian Dynamics simulation on diffusiohoresis and the separation of particles within the system. A gradient in viscosity that simulates a concentration gradient in a dissolved polymer allows us to separate various types of particles by their deformability. As seen in previous experiments, simulated particles with a higher deformability react differently to the polymer matrix than those with a lower deformability. Therefore, the particles can be separated from each other. This simulation, in particular, was intended to model an oceanic system where the particles of interest were zooplankton, phytoplankton and microplastics. The separation of plankton from the microplastics was achieved.
M1.00344 Electro-responsive supramolecular graphene oxide hydrogels for active bacteria adsorption and removal, BIN XUE, YI CAO, WEI WANG, Nanjing Univ — Bacteria are major contaminants in drinking water and healthcare products. Bacteria contamination may cause severe health problems, including food poisoning and diseases. Currently water sterilization and purification methods to remove contaminated bacteria are mainly based on the size-exclusion mechanism. In order to completely remove all bacteria in water, the pore sizes of the membranes or cartilages should be comparable to the size of bacteria, which inevitably leads to high cross-membrane water pressure and slow purification speed. Moreover, the membranes can easily get clogged. Therefore it is highly demanded to develop efficient methods and novel materials for water purification. Recently, Cui and coworker have introduced a bacteria inactivation method with high efficiency and fast purification speed based on a kind of complex materials made of silver nanofibers, carbon nanotubes and cotton, operating in an electric field. With the help of electric field, the bacteria can be efficiently killed when passing through the membrane even the pore sizes are larger than bacteria. Inspired by their work, here we report a proof-of-principle demonstration of bacteria removal using electro-responsive hydrogels.

M1.00345 From Compartamentalized to Agent-based Models of Epidemics, CHARLES MACAL, Argonne National Laboratory — Supporting decisions in the throes of an impending epidemic poses distinct technical challenges arising from the uncertainties in modeling disease propagation processes and the need for producing timely answers to policy questions. Compartmental models, because of their relative simplicity, produce timely information, but often do not include the level of fidelity of the information needed to answer specific policy questions. Highly granular agent-based simulations produce an extensive amount of information on all aspects of a simulated epidemic, yet complex models often cannot produce this information in a timely manner. We propose a two-phased approach to addressing the tradeoff between model complexity and the speed at which models can be used to answer questions about an impending outbreak. In the first phase, in advance of an epidemic, ensembles of highly granular agent-based simulations are run over the entire parameter space, characterizing the space of possible model outcomes and uncertainties. Meta-models are derived that characterize model outcomes as dependent on uncertainties in disease parameters, data, and structural relationships. In the second phase, envisioned as during an epidemic, the meta-model is run in combination with compartmental models, which can be run very quickly. Model outcomes are compared as a basis for establishing uncertainties in model forecasts.

M1.00346 Analytical vacuum force, atmospheric pressure dispute, HAN YONGQUAN, 15611860790 — Typically, the gap gas molecules 10^{-9} \text{ m}, since the center speed of the tornado is over 100 \text{ m/s}, it divided by the speed of a tornado, the gap of the gas molecules becomes 10^{-11} \text{ m}. Equivalent to the gap when there is no tornado that the gas molecules allow radiation to pass through, equivalent to the gap is reduced gas molecules 100 times by a tornado. There is no change in the Earth’s radiate, the Earth’s radiation is reduced to one percent of the original intensity by the radiation through the tornado periphery into the center of the tornado. According to the APS Division of Nuclear Physics in APS -2013 Fall Meeting - Event - Gravitational radiation theory http://meetings.aps.org/Meeting/DNP13/Session/FB.8, which I published, the gravity will be reduced to the original gravity percentage one. Watsepspot by the Earth’s gravity to become the original one percent. Cause the external of the tornadoes atmospheric pressure is constant, the height waterspot should support column height atmospheric pressure is 100 times, that height waterspot may reach nearly kilometers.

M1.00347 Observation of anomalous dielectric properties in low-dimensional spin 1/2 $\alpha$-Cu$_2$V$_2$O$_7$ magnetic system, YU-JEN CHEN, KAKARLA-DEVI CHANDRASEKHAR, KO-JUNG FAN, Department of Physics, National Sun Yat-Sen University, JIUNN-YUAN LIN, Institute of Physics, National Chiao Tung University, JENN-MIN LEE, JIN-MING CHEN, National Synchrotron Radiation Research Center, HUNG-DUEN YANG, Department of Physics, National Sun Yat-Sen University — Recently, low-dimensional magnetic systems have received much attention from both theoretical and experimental physics point of view due to their fascinating physical properties. In general, Cu$_2$V$_2$O$_7$ can stabilize at least two sibling polymorphs named as $\alpha$ and $\beta$ phases. In $\alpha$ phase, Cu$_2$V$_2$O$_7$ is crystallized in orthorhombic with Ddd2 space groups. The complex magnetic exchange interaction between the Cu-O-Cu ion within the intra and interchain creates the Dzyaloshinksi-Joriya interaction that leads to weak ferromagnetism below the magnetic transition temperature $T_N = 34 \text{ K}$. In this study, we present the results of multiple dielectric anomalies observed in the low dimensional spin 1/2 $\alpha$-Cu$_2$V$_2$O$_7$ magnetic system. The observed dielectric signature can be ascribed to the complex magnetic interaction $\alpha$-Cu$_2$V$_2$O$_7$. Further, the chemical doping effect on the magnetic and multiferroic properties of $\alpha$-Cu$_2$V$_2$O$_7$ is underway.

M1.00348 Quantum antiferromagnetic Heisenberg half-odd integer spin model as the entanglement Hamiltonian of the Affleck-Kennedy-Lieb-Tasaki valence bond solid states, GUANG-MING ZHANG, Tsinghua University, Beijing — Applying a symmetric bulk bipartition to the one-dimensional Affleck-Kennedy-Lieb-Tasaki valence bond solid (VBS) states for the integer spin-S Haldane gapped phase, we can create an array of fractionalized spin-S/2 edge states with the super unit cell $l$ in the reduced bulk system, and the topological properties encoded in the VBS wave functions can be revealed. The entanglement Hamiltonian (EH) with $l = \text{even}$ corresponds to the quantum antiferromagnetic Heisenberg spin-S/2 model. For the even integer spins, the EH still describes the Haldane gapped phase. For the odd integer spins, however, the EH just corresponds to the quantum antiferromagnetic Heisenberg spin-S/2 model with spinon excitations, characterizing the critical point separating the topological Haldane phase from the trivial gapped phase. Our results thus demonstrate that the topological bulk property not only determines its fractionalized edge states, but also the quantum criticality associated with the topological phase, where the elementary excitations are precisely those fractionalized edge degrees of freedom confined in the bulk of the topological phase.

M1.00349 The flexibility of Daubechies wavelets for Linear Scaling DFT calculations, LUIGI GENOVESE, STEPHAN MOHR, Commissariat l’Energie Atomique et aux nergies Alternatives, LAURA ELISABETH RATCLIFF, Argonne National Laboratory, DAMIEN CALISTE, THIERRY DEUTSCH, Commissariat l’Energie Atomique et aux nergies Alternatives, STEFAN GOEDECKER, Basel University — In recent works, we presented the linear scaling version of the BigDFT code [1] based on Daubechies wavelets, where a minimal set of localized support functions is optimized in situ. Our linear scaling approach is able to generate support functions for systems in various boundary conditions, like isolated, surface and periodic cases, and it is based on a algorithm which is universally applicable, requiring only moderate amount of computing resources. We will present how the flexibility of this approach is helpful in providing a basis that is optimally tuned to the chemical environment surrounding each atom. In addition than providing a basis useful to project Kohn-Sham orbitals informations like atomic charges and partial density of states, it can also be reused as-is, i.e. without reoptimization, for charge-constrained DFT calculations within a fragment approach [3]. We demonstrate the interest of this approach to express highly precise and efficient basis useful to project Kohn-Sham orbitals informations like atomic charges and partial density of states, it can also be reused as-is, i.e. without reoptimization, for charge-constrained DFT calculations within a fragment approach [3].

1 This work is funded by Six talent peaks project in Jiangsu Province, the National Natural Science Foundation of China (Nos. 11304156, 11334004, 31170813, 81421091 and 91127020), the 973 Program of China (No. 2012CB921801 and 2013CB834100), the Priority Ac...
M1.00350 Interdependent Lattice Networks in High Dimensions. STEVEN LOWINGER, GABRIEL CWILICH, SERGEY BULDYREV, Yeshiva University — We study the mutual percolation of two interdependent lattice networks following the procedure outlined by Buldyrev et al. We studied lattices of dimensions 2, 3, 4, 5 and 6. We imposed that the length of interdependent links connecting the nodes from one lattice to the other be less than a certain value, r. We find that for each dimension, \( D < 6 \), there is a value of \( r = r_1 > 1 \) such that for \( r \geq r_1 \), the cascading failures occur as a discontinuous first order transition, while for \( r < r_1 \), the system undergoes a continuous second order transition, as in the classical percolation theory. \( r_1 \) represents the dimension of the lattice increases. For \( D = 6 \), \( r_1 = 1 \), which is the same as in random regular (RR) graphs with the same degree (coordination number) of nodes. \( D = 6 \) is the upper critical dimension for classical percolation, the point at which the critical exponents of the lattice model become identical to those of RR graphs. We found that in all dimensions the maximal vulnerability of the networks, as a function of \( r \), is achieved at a distance of \( r = r_{\text{max}} > r_1 \), but for \( r > r_{\text{max}} \) the vulnerability starts to decrease as \( r \to \infty \). However, the decrease becomes less significant as the dimension increases and becomes negligible for \( D = 6 \). Results on how the parameters of the transition scale with the size of the system will be presented. [1] Catastrophic cascade of failures in interdependent networks, Buldyrev, Parshani, Paul, Stanley & Havlin, Nature 464, 1025-1028 (15 April 2010)

M1.00351 Behavioral analysis of the escape response in larval zebrafish. RUOPEI FENG, KIRAN GIRDHAR, YANN CHEMLA, MARTIN GRUEBELE, Univ of Illinois - Urbana — The behavior of larval zebrafish is of great interest because the limited number of locomotor neurons in larval zebrafish couples with its rich repertoire of movements as a vertebrate animal. Current research uses a priori-selected parameters to describe their swimming behavior while our lab has built a parameter-free model based on singular value decomposition analysis to characterize it. Our previous work has analyzed the free swimming of larval zebrafish and presented a different picture from the current classification of larval zebrafish locomotion. Now we are extending this work to the studies of their escape response to acoustic stimulus. Analysis has shown intrinsic difference in the locomotion between escape response and free swimming.

M1.00352 Synchronization modulation of Na/K pumps on Xenopus oocytes. FENGFEI LIANG, JASON MAST, WEI CHEN, Univ of South Florida — We developed a new technique named synchronization modulation to electrically synchronize and modulate the Na/K pump molecules by a specially designed oscillating electric field. This technique is based on the theory of energy-trap in quantum physics as well as the concept of electronic synchrotron accelerator. As a result, the Na-pumps are all entrapped into the positive half-cycle of the applied electric field and consequently, all of the K-transporters are entrapped into the negative half cycle of the field. To demonstrate the process of the pump synchronization and modulation, we use Xenopus oocytes as a platform and introduce two-electrode whole-cell voltage clamp in measurement of pump current. Practically, we first synchronize the pump molecules running at the same pace (rate and phase) by a specially designed oscillation electric field. Then, we carefully maintain the pump synchronization status and gradually change the field frequency (decrease and increase) to modulate the pump molecules to newer pumping rate. The result shows a separation of the inward Na current from the outward K current and about 10 times increase of the total (inward plus outward) pump current from the net outward current from the random paced pump molecules. Also, the ratio of the modulated total pump current with synchronized total pump current is consistent with the ratio of their field frequencies.

M1.00353 Kinetic inductance parametric up-converter. ADITYA KHER, California Institute of Technology, PETER DAY, NASA Jet Propulsion Laboratory, BYEONG HO EOM, JONAS ZMUIDZINAS, California Institute of Technology, H. G. LEDUC, NASA Jet Propulsion Laboratory — We describe a novel class of devices based on the nonlinearity of the kinetic inductance of a superconducting thin film. By placing a current-dependent inductance in a microwave resonator, small currents can be measured through their effect on the resonator’s frequency. By using a high-resistivity material for the film and nanowires as kinetic inductors, we can achieve a large coefficient of nonlinearity to improve device sensitivity. We demonstrate a current sensitivity of 8 pA/Hz^{1/2}, making this device useful for transition edge sensor readout and other cutting-edge applications. An advantage of these devices is their natural ability to be multiplexed in the frequency domain, enabling large detector arrays for TES-based instruments. A traveling-wave version of the device, consisting of a thin-film microwave transmission line, is also sensitive to small currents as they change the phase length of the line due to their effect on its inductance. We demonstrate a current sensitivity of 5 pA/Hz^{1/2} for this version of the device, making it also suitable for TES readout and other applications. It has the advantage of multi-GHz bandwidth and greater dynamic range, offering a different approach to the resonator version of the device.

M1.00354 Atomic study on the generation and gliding properties of pyramidal dislocations in magnesium. HIDEO KABURAKI, MITSUHIRO ITAKURA, MASATAKE YAMAGUCHI, Japan Atomic Energy Agency — Plastic deformation of magnesium and its alloys is attracting great interest as one of the candidate materials for energy-conserving lightweight structural metals. The generation of non-basal pyramidal dislocations near the c-axis direction is the key to enhancing plasticity in these highly anisotropic hcp magnesium materials. However, the fundamental understanding of the generation and gliding properties of pyramidal dislocations is still not clear because of the large Burgers vector. Using the molecular dynamics method, we have successfully generated a corrugated structure. We also found that both dislocations can easily cross-slip to other slip planes. In particular, it is observed that the core of the gliding pyramidal type I screw dislocation cross-slips to other slip planes. The detailed processes of cross-slip are elucidated in the presentation.

M1.00355 Outdoor concert hall sound design: idea and possible solutions. YANG-HANN KIM, JUNG-MIN LEE, Korea Adv Inst of Sci & Tech, WANJUNG KIM, HWAN KIM, NARU-EMS co. Ltd., JUNG-WOO CHOI, Korea Adv Inst of Sci & Tech, SEMYUNG WANG, Gwangju Inst of Sci & Tech — Sound design of outdoor concert halls needs to satisfy two contradictory objectives: good sound reproduction within the hall, as well as the minimization of external sound radiation. Outdoor concert hall usually has open space, therefore good sound for the listeners can be bad sound for its neighborhood. It would be a good attempt to have a virtual sound wall that can reflect all sound, therefore making a relatively quiet zone in the outside. This attempt can be possible if we could generate an acoustically bright zone inside and a dark (quite) zone outside. Earlier work [Choi, J.-W. and Kim, Y.-H. (2002). J. Acoust. Soc. Am. 111, 1695–1700], at least, assures it is possible for a selected region and frequencies. Simulations show that it is possible for a two-dimensional case. Experimental verification has been also tried. The discrepancies have been explained in terms of the number of loudspeakers, their spatial distributions, spacing with regard to wavelength. The dependency of its performances with respect to the size of bright and dark zone scaled by wavelength of interest has also been explained.
M1.00356 Multiscale modeling of nanostructured ZnO based devices for optoelectronic applications: Dynamically-coupled structural fields, charge, and thermal transport processes.\textsuperscript{1}, ABDULMUIN ABDULLAH, SAAD ALQAHTANI, MD REZAUL KARIM NISHAT, SHAikh AHMED, Southern Illinois University at Carbondale, SIU NANO-ELECTRONICS RESEARCH GROUP TEAM — Recently, hybrid ZnO nanostructures (such as ZnO deposited on ZnO-oligos, Si, GaN, polymer, conducting oxides, and organic compounds) have attracted much attention for their possible applications in optoelectronic devices (such as solar cells, light emitting and laser diodes), as well as in spintronics (such as spin-based memory, and logic). However, efficiency and performance of these hybrid ZnO devices strongly depend on an intricate interplay of complex, nonlinear, highly stochastic and dynamically-coupled structural fields, charge, and thermal transport processes at different length and time scales, which have not yet been fully assessed experimentally. In this work, we study the effects of these coupled processes on the electronic and optical emission properties in nanostructured ZnO devices. The multiscale computational framework employs the atomistic valence force-field molecular mechanics, models for linear and non-linear polarization, the 8-band $sp^3$-s* tight-binding models, and coupling to a TCAD toolkit to determine the terminal properties of the device. A series of numerical experiments are performed (by varying different nanoscale parameters such as size, geometry, crystal cut, composition, and electrostatics) that mainly aim to improve the efficiency of these devices.

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M1.00357 ZnO nanowire-based CO sensor, MON-SHU HO, Physics Department, National Chung Hsing University, WEI-HAO CHEN, Institute of Electronics Engineering, National Tsing Hua University, YU-LIN CHEN, Physics Department, National Chung Hsing University, MENG-FAN CHANG, Institute of Electronics Engineering, National Tsing Hua University — This study applied ZnO nanowires to the fabrication of a CO gas sensor operable at room temperature. Following the deposition of a seed layer by spin coating, an aqueous solution method was used to grow ZnO nanowires. This was followed by the self-assembly of an electrode array via dielectrophoresis prior to the fabrication of the CO sensing device. The material characteristics were analyzed using FE-SEM, EDS, GIXRD, FE-TEM, and the measurement of photoluminescence (PL). Our results identified the ZnO nanowires as a single crystalline wurtzite structure. Extending the growth period from 30 min to 360 min led to an increase in the length and diameter of the nanowires. After two hours, the ZnO nanowires received a preferred crystal orientation of [002]. Sensor chips were assembled using 60 pairs of electrodes with gaps of 2μm, over which were laid nanowires to complete the sensing devices. The average sensing response was 48.37 s and the average recovery time was 65.61 s, with a sensing response magnitude of approximately 6.8% at room temperature.

M1.00358 Neutron Imaging Studies of In Situ Growth of Neutron and Gamma Detector Materials, NICHOLAS STRANGE, CHRISTOPHER CRAIN, FATEMA WAHIDA, ZACH STROUPE, J.Z. LARESE, University of Tennessee — The studies described here are aimed at addressing the critical need to develop dependable crystal growth techniques of solid-state materials used as radiation detectors for both national security and medical applications. We present our activities using pulsed neutron, radiographic imaging and simultaneous diffraction techniques to examine the synthesis of both CZT and CLYC with the goal of identifying the conditions that favor the production of defect free materials. Using a pulsed neutron beam and time of flight detection methods, we exploit the penetrating power and wavelength dependence of neutron absorption to perform measurements during crystal growth. Furthermore, solid boules can be examined either inside the furnace or free standing. The objective of these studies include the validation/improvement of the modeling studies of CLYC and CZT growth behavior, the development of new/improved furnace design, and the identification of optimum growth techniques that enable the production of large boules of defect free, single crystalline materials in a timely/cost effective manner. We provide our preliminary results that include the experiential setup at LANSCE and sample neutron radiographic and synchrotron based IR images of CZT flat solid plates.

M1.00359 Investigation of Natural Bombyx mori Silk Fibroin Proteins Using INS, CHRISTOPHER CRAIN, NICHOLAS STRANGE, J.Z. LARESE, Univ of Tennessee, Knoxville — The mechanical properties of many protein comprised biomaterials are a direct reflection of their component (i.e. Peptide) interacting ions such as F-actin in muscles, tubulin in the cytoskeleton of cells, viral capsids, and silk. Porter and Vollrath underscored the two main factors that are critical for understanding the high mechanical strength of silks: the nanoscale semi-crystalline folding structure, which gives it exceptional toughness and strength, and the degree of hydration of the disordered fraction, which acts to modify these properties. Understanding and controlling these two principal factors are the key to the functionality of protein elastomers, and render silk an ideal model material for (bio)material design. We will describe our investigation of electrospun silk of the Bombyx mori (silk worm), using Inelastic Neutron Scattering (INS). These techniques were used to investigate the microscopic dynamics of the dry and hydrated protein.

M1.00360 Study of the nanosurface properties by analyzing its absorption and scattering cross-section. IRINA BARIAKHTR, Boston College — The interest to study the nanoparticles absorbed on the dielectric or semiconductor substrate is caused by the multiple practical applications of these systems such as nanosensors, electronic devices and lately in PV elements for improving of their efficiency [1, 2]. The author suggests a method of examining the properties of the nanosurface with the absorbed nanoparticle by calculating the absorption and scattering of the electromagnetic field by such system based on construction of its effective electric susceptibility. It was built based on the Green’s function approach [3]. The computer simulations show good correspondence with the theory. It was shown that this approach can be applied to investigate the optical absorption and scattering on the nanoparticles on the substrate to be used in PV engineering. 1. Schaadt, D. M., Feng, B., Yu, E. Appl. Phys. Lett. 86 (6): 063106 (2005) 2. K. R. Catchpole and A. Polman, Opt. Express 16, 21793-21800 (2008) 3. I. Bariakhtr, Y. Demidenko, S. Kriuchchen, V. Vozovski, Surf. Sci. 323 (1995).

M1.00361 Controlling Spin State of Magnetic Molecules by Oxygen Binding Studied Using Scanning Tunneling Microscopy, SOON-HYEONG LEE, Korea University, YUN HEE CHANG, KAIST, HOWON KIM, KYUNG MIN KIM, Korea University, YONG-HYUN KIM, KAIST, SE-JONG KAHNG, Korea University — Binding and unbinding between molecular oxygen and metallo-porphyrin is a key process for oxygen delivery in respiration. It can be also used to control spin state of magnetic metallo-porphyrin molecules. Controlling and sensing spin states of magnetic molecules in such reactions at the single molecule level is essential for spintronic device applications. Here, we demonstrate that spin states of metallo-porphyrin on surfaces can be controlled over by binding and unbinding of oxygen molecule, and be sensed using scanning tunneling microscopy and spectroscopy. Kondo localized state of metallo-porphyrin showed significant modification by the binding of oxygen molecule, implying that the spin state was changed. Our density functional theory calculation results explain the observations with the hybridization of unpaired spins in d and $*$ orbitals of metallo-porphyrin, respectively. This study opens up ways to control molecular spin state and Kondo effect by means of molecular binding and unbinding reactions on surfaces.

M1.00362 Spotting the Gel Point of Photopolymers by Examining NMR Relaxation, JAC KLEE, GRETCHEN HOFMEISTER, MARTHA-ELIZABETH BAYLOR, Carleton College — Spotting when a polymer goes from liquid to solid during polymerization is necessary when working with certain optically cured polymers used to fabricate optofluidic devices that contain both optical and microfluidic features. Through the use of nuclear magnetic resonance (NMR) it may be possible to determine when the transition from liquid to solid, called the gel point, occurs. In examining the proton longitudinal relaxation time for one species of monomers in our polymer mix, our data shows as the polymer cures the relaxation time increases. By examining this data we were able to extract a time to gel point that was within the margin of error of the theoretical gel point of our materials. Hence we were able to extend the gel point.

$*_{orbitals}$
M1.00363 Observation of Voltage Oscillations in VO$_2$ with Negative Differential Resistance. 
DAE-JOON KANG, HYOUNG WOO YANG, GARAM BAE, Department of Physics, Sungkyunkwan University, Republic of Korea — Many strongly correlated electron systems exhibit complex nonlinear behaviors with electric fields. The origin of the electrical instabilities is closely related to a negative differential resistance (NDR). Here, we report electrical characteristics of two-terminal devices based on vanadium dioxide (VO$_2$) thin films fabricated on c-cut sapphire substrates, exhibiting NDR behavior in their I-V characteristics that may work as a voltage oscillator of high efficiency. We show that the NDR behavior can be better understood in the context of metal-insulator phase transition. Furthermore, we found that the source voltage and frequency affect greatly the NDR behaviors, which is indicated by an evident shift of oscillation voltage from 10 V to 1 V. Based on the experimental results, with the source voltage and the frequency systematically varied, the mechanism of the oscillation was found to be the ascribed to an alternate occurrence of an electric-field-induced resistance switching in the MIT of VO$_2$. We discuss herein, the origin and potential applications of NDR based devices in detail and investigated the voltage oscillation behaviors of VO$_2$ to elucidate the underlying physics of its metal-insulator transition behavior.

M1.00364 Cloisite 30B as Nanoclay Compatible for Polysulfone/Polyimide Blend Films. 
ALI AMMAR, Akron Univ, AHMED ELZATAHRY, MARIAM AL-MAAEDDEQ, Qatar Univ, ABDULLAH ALENIZI, King Saud Univ, KARIM ALAMGIR, Akron Univ — Polysulfone (PSF) and polyimide (PI) are used in many applications including membranes for gas separation and water purification. The phase separation issues limit the blend application of these polymers. We studied the effect of nanoclay and Cloisite 30B had on (PSF/PI) films. This was done in order to examine the compatibility effects of clay on phase separation behavior, mechanical strength, and structure properties. The addition of weight percentage of organoclay strongly compatibilized the blend phases for all compositions, decreasing the scale of blend phase separation by a factor of 5-10. Interestingly, the net phase separated domain area converged to the 50% blend composition in all cases. This is attributed to a high degree of exfoliation and degradation of nanoclay particles within the PSF/PI matrix as well as interfacial regions, independent of the blend composition. AFM confirmed these optically observed compatibilization effects by quantitative reduction of aspect ratio (width/height) of surface phase separated domains. The surface free energies of the films decreased by adding Clo30B. This has led us to conclude that there is a changing of surface topography, which conforms to the contact angle. PSF/PI films showed decreasing in thermal stability due to the surfactant modification of Clo30B.

M1.00365 Electronic state modulation of iron selenide by intercalating copper. 
KAYA KOBAYASHI, Y ITO, F NAGAI, S MATSUMOTO, T KAMBE, Y BENINO, T NAMBA, Okayama University — FeSe is one of the iron-based superconductors that have the simplest structure. Its superconducting properties are easily modified by chemical and mechanical method, such as alkali metal intercalation and thinning down to monolayer. The synthesis of copper intercalation by melt method brought the structural change of the system in increasing the copper amount. To investigate the superconducting property of the system, we synthesized copper intercalated FeSe single crystal. The decrease of superconducting transition temperature observed here is discussed in relation to its modulation on to electronic state of iron.

M1.00366 Boson Sampling with Trapped Ions. 
KATHERINE COLLINS, Univ of Maryland-College Park, KENNETH WRIGHT, CHRISTOPHER RICKERD, CHRISTOPHER MONROE. Univ of Maryland-College Park and Joint Quantum Institute — A classical computer is limited in its ability to solve certain types of problems. A quantum computer might be able to solve some of these problems more efficiently. Calculating the permanent of an NxN matrix is an example of a problem that cannot be efficiently solved by a classical computer. Computing the permanent of an NxN matrix can be related to compute an NxN permanent through boson sampling represents a physical device that can evaluate a problem not efficiently solvable by a classical system. Some experiments have already demonstrated boson sampling with photons for a small number of bosonic modes, but it is difficult to increase the number of bosons in such experiments. One way to demonstrate a larger-scale boson sampling problem is to use the phonon excitations of a trapped ion chain. We present our progress towards experimentally demonstrating boson sampling with trapped ions.


M1.00367 Block Copolymer-Based Supramolecular Elastomers with High Extensibility and Large Stress Generation Capability. 
ATSUSHI NORO, MIKIHIRO HAYASHI, Nagoya University — We prepared block copolymer-based supramolecular elastomers with high extensibility and large stress generation capability. Reversible addition fragmentation chain transfer polymerizations were conducted under normal pressure and high pressure to synthesize several large molecular weight polystyrene-b-[poly(butyl acrylate)-co-polyacrylamide]-b-polystyrene (S-Ba-S) block copolymers. Tensile tests revealed that the largest S-Ba-S with middle block molecular weight of 3140k achieved a breaking elongation of over 2000% with a maximum tensile stress of 3.6 MPa and a toughness of 28 MJ/m$^3$ while the reference sample without any middle block hydrogen bonds, polystyrene-b-poly(butyl acrylate)-b-polystyrene with almost the same molecular weight, was merely viscous and not self-standing. Hence, incorporation of hydrogen bonds into a long soft middle block was found to be beneficial to attain high extensibility and large stress generation capability probably due to concerted combination of entropic changes and internal potential energy changes originating from the dissociation of multiple hydrogen bonds by elongation.

1 This work was supported by JSPS KAKENHI Grant Numbers 1302357, 24065305, 15K13785, and 23655213 for M.H. and A.N. A.N. also expresses his gratitude for Tanaka Rubber Science & Technology Award by Enokagaku-Shinko Foundation, Japan.

M1.00368 Continued Growth on Graphene Edges. 
ZHENGTANG LUO, Hong Kong Univ of Sci & Tech — Previously, we have shown that the large-size single crystal graphene can be obtained by suppressing the nucleation density during Chemical Vapor Deposition (CVD) growth. Here we demonstrate that the graphene single crystal can be amplified by a continued growth method. In this process, we used a mild oxidation step after the first-growth, which lead to the observed formation of oxides at the vicinity of graphene edges, which allows the graphene growth at seed edges due to reduced activation energy. Consequently, we successfully grown a secondary single-crystal graphene structures with the same lattice structure, orientation on the graphene edges. This amplification method would enable the production of graphene electronics with controlled properties.

KAMIL WALCZAK, Pace University — We examine heat transport carried by acoustic phonons in molecular junctions composed of organic molecules coupled to two thermal baths of different temperatures. The phononic heat flux and its dynamical noise properties are analyzed within the scattering (Landauer) formalism with transmission probability function for acoustic phonons calculated within the method of atomistic Green’s functions (AGF technique). The perturbative computational scheme is used to determine nonlinear corrections to phononic heat flux and its noise power spectral density with up to the second order terms with respect to temperature difference. Our results show the limited applicability of ballistic Fourier’s law and fluctuation-dissipation theorem to heat transport in quantum systems. We also derive several noise-signal relations applicable to nanoscale heat flow carried by phonons, but valid for electrons as well. We also discuss the extension of the perturbative transport theory to higher order terms in order to address a huge variety of problems related to finite size and time effects, which may occur at nanoscale and at strongly non-equilibrium conditions with high-intensity heat fluxes.

1 This work was supported by Pace University Start-up Grant.
M1.00370 Spectroscopic study of some diatomic molecules via the proper quantization rule. B. FALAYE, IPN, Mexico City, Mexico — Spectroscopic techniques are very essential tools in studying electronic structures, spectroscopic constants and energetic properties of diatomic molecules. These techniques are also required for parametrization of new methods based on theoretical analysis and computational calculations. In this research, we apply the proper quantization rule in spectroscopic study of some diatomic molecules by solving the Schrödinger equation with two solvable quantum molecular systems-Tietz-Wei and shifted Deng-Fan potential models for their approximate nonrelativistic energy states via an appropriate approximation to the centrifugal term. We show that the energy levels can be determined from its ground state energy. The beauty and simplicity of the method applied in this study is that, it can be applied to any exactly as well as approximately solvable models. The validity and accuracy of the method is tested with previous techniques via numerical computation for $H_2$ and CO diatomic molecules. The result also include energy spectrum of 5 different electronic states of NO and 2 different electronic state of ICl.

M1.00371 “Dual Society Ever Precedes through Trevor SWAN & Wassily Leontief”1, WH-MAS SoloD, Prodi of Physics UI, Depok 16424- INDONESIA — “Dual Society” introduced by E.F. Schumacher are classified as non-stable society who easy to be shaken by politics uncertainties. Robert J. Barro & X. Sala-i-Martín: “Convergence” states: “a key economic issue is whether poor countries or regions tend to grow faster than ones. For growth models from Roy Forbes Herrod & EuseyDomar, three assumptions described by Eduardo Ley are (U-23091): (i) output is proportional to capital, (ii) Investment ex ante equals saving & (iii) saving proportional to output. Underlines Trevor SWAN, developing countries differ significantly among themselves. Economic growth models comprises Herrod-Domar growth model, Solow growth model & endogenous growth model. Further, for five stages of economic growth from Rostov of Leontief technology, ever retrieves the Jens Beckert: “Institutional Isomorphism revisited: Convergence & Divergence in Institutional Change” instead Frumkin’s “Institutional Isomorphism & Public Sector Organizations”.


M1.00373 “From Fundamental Motives to Rational Expectation Equilibrium[REE, henceworth] of Indeterminacy”1, WH-MAS SoloD,SSI2, Prodi of Physics UI, Depok 16424- INDONESIA — For “Principle of Indeterminacy” from Heisenberg states: “one of the fundamental cornerstone of quantum mechanics is the Heisenberg uncertainty principle”. whereas canonically conjugate quantities can be determined simultaneously only with a characteristic indeterminacy[M. Arelavo Aguilar, et.al]. Accompanying Alfred North Whitehead conclusion in “The Aims of Education” that mathematical symbols are artificial before new meanings given, two kinds of fundamental motives: (i) expectation-expectation, (ii) expectation-certainty inherently occurs with determinacy properties of rational expectation equilibrium(REE, henceworth)- Guido Ascari & Tizano Ropele: “Principle of Indeterminacy”1, Kiel Institute, June 2007. Furthers, relative price expression can be compare of their expectation-certainty inherently occurs with determinacy properties of rational expectation equilibrium(REE, henceworth)."Institutional Isomorphism revisited: Convergence & Divergence in Institutional Change" instead Frumkin’s “Institutional Isomorphism & Public Sector Organizations”.

M1.00374 Can we judge an oxide by its cover? The case of the metal/oxide interface from first principles1, MAYTAL CASPY TORKER, Department of Materials Science and Engineering — Metal/oxide interfaces appear in a wide variety of disciplines including electronics, corrosion, electrochemistry, and catalysis. Specifically, covering a metal-oxide with a metal is often thought to enhance solar energy absorption and to improve photocatalytic activity. For example, the platinum/hematite (Pt/α-Fe$_2$O$_3$) interface has demonstrated improved functionality. In order to advance our understanding of how metal coverage over an oxide helps performance, we characterize the geometry and electronic structure of the Pt/α-Fe$_2$O$_3$ interface. We investigate the interface using density functional theory +U, and find a stable crystallographic orientation relationship that agrees with experiment. Furthermore, there are significant changes in the electronic structure of α-Fe$_2$O$_3$ as a result of Pt coverage. We therefore suggest the concept of “judging” the electronic properties of an oxide only with its cover. Specifically, covering Fe$_2$O$_3$ with Pt reduces carrier effective mass and creates a continuum of states in the band gap. The former could be beneficial for catalytic activity, while the latter may cause surface recombination. In order to circumvent this problem, we suggest putting metal coverage behind the oxide and far from the electrolyte in a photoelectrochemical device in order to quickly collect electron carriers and avoid recombination with vulnerable holes accumulating as a result of catalysis at the surface. Reference: O. Neufeld and M. Caspary Toroker, “Can we judge an oxide by its cover? The case of platinum over alpha-Fe$_2$O$_3$ from first principles”, Phys. Chem. Chem. Phys. 17, 24129 (2015).

M1.00375 Carbon nanotube transistor based high-frequency electronics, MICHAEL SCHRÖTER, Technical University Dresden — At the nanoscale carbon nanotubes (CNTs) have higher carrier mobility and carrier velocity than most incumbent semiconductors. Thus CNT based field-effect transistors (FETs) are being considered as strong candidates for replacing existing MOSFETs in digital applications. In addition, the predicted high intrinsic transit frequency and the more recent finding of ways to achieve highly linear transfer characteristics have inspired investigations on analog high-frequency (HF) applications. High linearity is extremely valuable for an energy efficient usage of the frequency spectrum, particularly in mobile communications. Compared to digital applications, the much relaxed constraints for CNT placement and lithography combined with already achieved operating frequencies of at least 10 GHz for fabricated devices make an early entry in the low GHz HF market more feasible than in large-scale digital circuits. Such a market entry would be extremely beneficial for funding the development of production CNTFET based process technology. This talk will provide an overview on the present status and feasibility of HF CNTFET technology will be given from an engineering point of view, including device modeling, experimental results, and existing roadblocks.
M1.00376 Gate Opening Transition of Zeolitic Imidazolate Framework – 8 in Xenon adsorption and Carbon Monoxide Adsorption. DINUKA H GALLABA, ALDO D MIGONE, Department of Physics, Southern Illinois University, Carbondale IL 62901, KARIM SAPIA, HONNY VILLAROLE, Universidad Nacional de San Luis, San Luis 5700, Argentina. — Zeolitic Imidazolate Framework – 8 (ZIF-8) is a porous metal-organic framework material that shows flexibility in adsorbing larger molecules. We have investigated Xe adsorption on ZIF-8 for temperatures in the range between 95K and 157.5 K and we are exploring CO adsorption between 80K and 110K. ZIF-8 is known to undergo a structural (“gate-opening”) transition when sorbent loading increases. We report on this gate-opening phenomenon for Xe and CO on ZIF-8. The gate-opening transition appears as a sub-step at higher loadings in the adsorption isotherm data. For Xe the sub-step disappeared for temperatures above 145 K. All isotherms below this temperature clearly show the extra step. Gate-opening occurs as a result of the re-orientation of the organic linkers in ZIF-8. This re-orientation increases the size of the apertures in the structure, consequently allowing more molecules or atoms to adsorb into the ZIF-8 (which produces the additional sub-step). The isosteric heat of adsorption as a function of loading, and, the energy associated with the structural transition were determined from the adsorption data. We also report on the kinetics of sorption for Xe on ZIF-8: there are two rates that dominate the sorption kinetics on ZIF-8. We report on the values of the rates as a function of sorbent loading.

M1.00377 Majorana fermion mean field study of two-dimensional inequivalent bipartite kondo lattice. SAYED ALI AKBAR GHORASHI, Department of physics and Texas center for superconductivity, University of Houston, RUI WANG, Texas center for superconductivity, university of Houston, CHIN-SEN TING, Department of physics and Texas center for superconductivity, University of Houston — We study the antiferromagnetic kondo lattice in a bipartite square lattice using Majorana fermion representation mean field theory. In different sublattice, we introduce different kondo coupling interaction between the local moment and the conduction electrons, and discuss the possible phases of ground state. It is shown that for weak coupling regime there is more competition between two sublattices local moment interactions. Next, we turn on an equal ferromagnetic Heisenberg interaction for both sublattices and we show possible competition and cooperation between these three interactions. Finally, to gain more physical insights we investigate static magnetic susceptibility for different ratios of couplings.

M1.00378 A universal scaling law for the evolution of granular gases. MATHIAS HUMMEL, JAMES CLEWETT, MARCO G. MAZZA, Max Planck Institute for Dynamics and Self-Organization — Dry, freely evolving granular materials in a dilute gaseous state coalesce into dense clusters only due to dissipative interactions. This clustering exhibits a scale-free dynamics but the clustered state becomes observable when the Mach number is approximately of O(1). Our results provide a method to determine the age of a granular gas and predict the macroscopic appearance of clusters.

M1.00379 Development, Selection, and Validation of Tumor Growth Models. AMIR SHAHRORADIA, ERNESTO LIMA², J. TINSLEY ODEN³, The University of Texas at Austin — In recent years, a multitude of different mathematical approaches have been taken to develop multiscale models of solid tumor growth. Prime successful examples include the lattice-based, agent-based (off-lattice), and phase-field approaches, or a hybrid of these models applied to multiple scales of tumor, from subcellular to tissue level. Of overriding importance is the predictive power of these models, particularly in the presence of uncertainties. This presentation describes our attempt at developing lattice-based, agent-based and phase-field models of tumor growth and assessing their predictive power through new adaptive algorithms for model selection and model validation embodied in the Occam Plausibility Algorithm (OPAL), that brings together model calibration, determination of sensitivities to outputs, parameter variances, and calculation of model plausibilities for model selection.

1Institute for Computational Engineering and Sciences
2Institute for Computational Engineering and Sciences
3Institute for Computational Engineering and Sciences

M1.00380 Evidence for quantization and topological states in spin Hall conductivity of low-dimensional systems. SEBASTIAN KUEFNER, LARS MATTHES, JUERGEN FURTHMUeller, FRIEDHELM BECHSTEDT, FSU Jena — Ab initio relativistic band structure calculations are performed for the frequency-dependent spin Hall conductivity of two-dimensional atomically thin crystals and one-dimensional nanoribbons. We study the influence of topology, quantization and topological edge states. As model systems, fully halogenated germanene, Gel, and its zigzag nanoribbons are investigated. Gel represents a topological insulator due to strong spin-orbit interaction and, hence, band inversion. We demonstrate the quantization of the static spin Hall conductivity. It is hardly influenced by temperature variation but significantly by Fermi level shift. The frequency dependence of the conductivity is governed by the band-structure details. Topological edge states influence the conductivity mainly for vanishing frequencies.

M1.00381 Ultrafast spectroscopy of exciton and exciton dynamics in mono and few layers of WS2. SUDIKSHA KHADKA, SHROUQ ALEITHAN, MAX LIVSHITS, JEFFREY J. RACK, MARTIN KORDESCH, ERIC STINAFF, Ohio University — Single layer of Transitional metal dichalcogenides (MX2) are 2D semiconductors that have a direct band gap in visible spectrum and fill the gap in between 2D metallic and insulating materials. They have possible application in optoelectronic devices, photovoltaics and photodetection, molecular sensing, ‘valleytronics’, and flexible transparent electronics. Tungsten Disulphide (WS2), one of the member of MX2 family, has a direct band gap of 2.2 eV and a large valley splitting of about 0.4 eV. Here we present a detailed study of exciton states and their decay mechanisms in mono and few layer WS2 using femto-second transient absorption spectroscopy. We report a new peak at 3.010.1 eV which is assigned to the break in the band gap. The mechanism behind the excitonic transition is still under debate. Recently, work on larger aluminum nanoparticles (18nm) embedded in an insulating Al2O3 matrix showed an onset of the superconducting transition as high as three times that of bulk aluminum. In this situation, the Al grains are electrically disconnected and in a regime far removed from that of the granular films. We compare the two situations through electronic and thermal measurements in order to help elucidate the mechanism behind the enhancements. S. Pracht, et al., arXiv:1508.04270v1 [cond-mat.supr-con] (2015). G. Deutscher, New Superconductors From Granular to High Tc, New Jersey: World Scientific, 2006, p. 72-74. V. N. Smolyaninova, et al., Sci. Rep. 5, 15777 (2015).

1Funding by NSF DMR 1410665
Manipulating individual defects in graphene/BN heterostructures: a first-principles study

LEDE XIANG, ANGELO RUBIO, Univ of the Basque Country — Recent experiments have demonstrated the possibility of manipulating defects in insulating hexagonal boron nitride (hBN) within a graphene/hBN heterostructure using scanning tunneling microscopy, opening a new pathway of manipulating individual defects of insulators at the nanoscopic scale. With first principle calculations, we are able to simulate this process and elucidate the relevant physics in experiments. Moreover, we calculate the band level alignments between graphene and possible defects states in hBN. Thus, we identify different defects observed in experiments and provide important reference for future experiments and applications.
can explain this relationship and examine the limits that the physical aspects of transcription place on gene expression.

LEVINE, Rice Univ — The ability to watch biochemical events at the single-molecule level has increasingly revealed that stochasticity plays a leading role in many.

and the recent experimental observation that geometric confinement of human embryonic stem cells is sufficient to recapitulate much of germ layer patterning.

TEIMOURI, ANATOLY B. KOLOMEISKY, Rice University — We present a quantitative model that explains the scaling of BMP4 gradients during gastrulation.

relations that optimally transmit information. Using E. coli chemotaxis as an example, we conclude that its pathway is compatible with an optimal information.

separation into input, channel, and output is not always clear in biological systems. Output might feed back into the input, and the channel, made by proteins,

fast and reliably. These decisions are inherently affected by noise at all levels of the signaling pathway, and cells are often modeled as an input-output device.

To enhance the accuracy of secondary structure calculations, improved methods in the fitting of absorbance spectra are needed. In this talk, we will explore the.

changes in the macroscopic properties of the liquid or in its structural properties. Different density functionals produce answers that differ by as much as 35% in.

M1.00391 Study of correlations from Ab-Initio Simulations of Liquid Water1. ADRIAN SOTO, MARIVI FERNANDEZ-SERRA, Stony Brook University, DEUYU LU, SHINJAE YOO, Brookhaven National Lab — An accurate understanding of the dynamics and the structure of H2O molecules in the liquid phase is of extreme importance both from a fundamental and from a practical standpoint. Despite the successes of Molecular Dynamics (MD) with Density Functional Theory (DFT), liquid water remains an extremely difficult material to simulate accurately and efficiently because of fine balance between the covalent O-H bond, the hydrogen bond and the attractive the van der Waals forces. Small errors in those produce dramatic changes in the macroscopic properties of the liquid or in its structural properties. Different density functionals produce answers that differ by as much as 35% in ambient conditions, with none providing quantitative results in agreement with experiment at different mass densities [J. Chem Phys. 139, 194502(2013)]. In order to understand these differences we perform an exhaustive scanning of the geometrical coordinates of MD simulations and study their statistical correlations with the simulation output quantities using advanced correlation analyses and machine learning techniques.

Wednesday, March 16, 2016 2:30PM - 5:18PM –
Session P39 DBIO GSNP: Information Processing in Cellular Signaling and Gene Regulation
342 - Andrew J. Mugler, Purdue University

2:30PM P39.00001 Towards a predictive theory for genetic regulatory networks. GASPER TKACIK, IST Austria — When cells respond to changes in the environment by regulating the expression levels of their genes, we often draw parallels between these biological processes and engineered information processing systems. One can go beyond this qualitative analogy, however, by analyzing information transmission in biochemical ‘hardware’ using Shannon’s information theory. Here, gene regulation is viewed as a transmission channel operating under restrictive constraints set by the size of the cell and intracellular noise. We present a series of results demonstrating that a theory of information transmission in genetic regulatory circuits feasibly yields non-trivial, testable predictions. These predictions concern strategies by which individual genetic regulatory elements, e.g., promoters or enhancers, read out their signals; as well as strategies by which small networks of genes, independently or in spatially coupled settings, respond to their inputs. These predictions can be quantitatively compared to the known regulatory networks and their function, and can elucidate how reproducible biological processes, such as embryonic development, can be orchestrated by networks built out of noisy components. Preliminary successes in the gap gene network of the fruit fly Drosophila indicate that a full ab initio theoretical prediction of a regulatory network is possible, a feat that has not yet been achieved for any real regulatory network. We end by describing open challenges on the path towards such a prediction.

3:06PM P39.00002 Theory of optimal information transmission in E. coli chemotaxis pathway. GABRIELE MICALI, ROBERT G. ENDRES, Imperial College London — Bacteria live in complex microenvironments where they need to make critical decisions fast and reliably. These decisions are inherently affected by noise at all levels of the signaling pathway, and cells are often modeled as an input-output device that transmits extracellular stimuli (input) to internal proteins (channel), which determine the final behavior (output). Increasing the amount of transmitted information between input and output allows cells to better infer extracellular stimuli and respond accordingly. However, in contrast to electronic devices, the separation into input, channel, and output is not always clear in biological systems. Output might feed back into the input, and the channel, made by proteins, normally interacts with the input. Furthermore, a biological channel is affected by mutations and can change under evolutionary pressure. Here, we present a novel approach to maximize information transmission: given cell-external and internal noise, we analytically identify both input distributions and input-output relations that optimally transmit information. Using E. coli chemotaxis as an example, we conclude that its pathway is compatible with an optimal information transmission device despite the ultrasensitive rotary motors.

3:18PM P39.00003 BMP4 density gradient in disk-shaped confinement. BEHN AZ BOZORGUI, HAMID TEIMOURI, ANATOLY B. KOLOMEISKY, Rice University — We present a quantitative model that explains the scaling of BMP4 gradients during gastrulation and the recent experimental observation that geometric confinement of human embryonic stem cells is sufficient to recapitulate much of germ layer patterning. Based on a assumption that BMP4 diffusion rate is much smaller than the diffusion rate of its inhibitor molecules, our results confirm that the length-scale which defines germ layer territories does not depend on system size.

3:30PM P39.00004 Mechanical Feedback and Arrest in Gene Expression. STUART SEVIER, HERBERT LEVINE, Rice Univ — The ability to watch biochemical events at the single-molecule level has increasingly revealed that stochasticity plays a leading role in many biological phenomena. One important and well know example is the noisy “bursty” manner of transcription. Recent experiments have revealed relationships between the level and noise in gene expression hinting at deeper stochastic connections. In this talk we will discuss how the mechanical nature of transcription can explain this relationship and how the limits that the physical aspects of transcription place on gene expression.
3:42PM P39.00005 Information processing in multi-step signaling pathways, AMBHI GANESAN, IBM, ARCHER HAMIDZADEH, Yale University, JIN ZHANG, UCSD, ANDRE L'ÈVCHENKO, Yale University — Information processing in complex signaling networks is limited by a high degree of variability in the abundance and activity of biochemical reactions (biological noise) operating in living cells. In this context, it is particularly surprising that many signaling pathways found in eukaryotic cells are composed of long chains of biochemical reactions, which are expected to be subject to accumulating noise and delayed signal processing. Here, we challenge the notion that signaling pathways are insulated chains, and rather view them as parts of extensively branched networks, which can benefit from a low degree of interference between signaling components. We further establish conditions under which this pathway organization would limit noise accumulation, and provide evidence for this type of signal processing in an experimental model of a calcium-activated MAPK cascade. These results address the long-standing problem of diverse organization and structure of signaling networks in live cells.

3:54PM P39.00006 Towards Predictive Modeling of Information Processing in Microbial Ecosystems With Quorum-Sensing Interactions, TAHIR YUSUFALY, JAMES BOEDICKER, University of Southern California — Bacteria communicate using external chemical signals in a process known as quorum sensing. However, the efficiency of this communication is reduced by both limitations on the rate of diffusion over long distances and potential interference from neighboring strains. Therefore, having a framework to quantitatively predict how spatial structure and biodiversity shape information processing in bacterial colonies is important, both for understanding the evolutionary dynamics of natural microbial ecosystems, and for the rational design of synthetic ecosystems with desired computational properties. As a first step towards these goals, we implement a reaction-diffusion model to study the dynamics of a LuxI/LuxR quorum sensing circuit in a growing bacterial population. The spatiotemporal concentration profile of acyl-homoserine lactone (AHL) signaling molecules is analyzed, and used to define a measure of physical and functional signaling network connectivity. From this, we systematically investigate how different initial distributions of bacterial populations influence the subsequent efficiency of collective long-range signal propagation in the population. We compare our results with known experimental data, and discuss limitations and extensions to our modeling framework.

4:06PM P39.00007 Thermodynamics of nuclear transport, CHING-HAO WANG, PANKAJ MEHTA, Department of Physics, Boston University, Boston, MA 02215, MICHAEL ELBAUM, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel — Molecular transport across the nuclear envelope is important for eukaryotes for gene expression and signaling. Experimental studies have revealed that nuclear transport is inherently a nonequilibrium process and actively consumes energy. In this work we present a thermodynamics theory of nuclear transport for a major class of nuclear transporters that are mediated by the small GTPase Ran. We identify the molecular elements responsible for powering nuclear transport, which we term the “Ran battery” and find that the efficiency of transport, measured by the cargo nuclear localization ratio, is limited by competition between cargo molecules and RanGTP to bind transport receptors, as well as the amount of NTF2 (i.e. RanGDP carrier) available to circulate the energy flow. This picture complements our current understanding of nuclear transport by providing a comprehensive thermodynamics framework to decipher the underlying biochemical machinery.

4:18PM P39.00008 Vector Encoding in Biochemical Networks, GARRETT POTTER, BO SUN, Oregon State University — Encoding of environmental cues via biochemical signaling pathways is of vital importance in the transmission of information for cells in a network. The current literature assumes a single cell state is used to encode information, however, recent research suggests the optimal strategy utilizes a vector of cell states sampled at various time points. To elucidate the optimal sampling strategy for vector encoding, we take an information theoretic approach and determine the mutual information of the calcium signaling dynamics obtained from fibroblast cells perturbed with different concentrations of ATP. Specifically, we analyze the sampling strategies under the cases of fixed and non-fixed vector dimension as well as the efficiency of these strategies. Our results show that sampling with greater frequency is optimal in the case of non-fixed vector dimension but that, in general, a lower sampling frequency is best from both a fixed vector dimension and efficiency standpoint. Further, we find the use of a simple modified Ornstein-Uhlenbeck process as a model qualitatively captures many of our experimental results suggesting that sampling in biochemical networks is based on a few basic components.

4:30PM P39.00009 Deciphering the Minimal Algorithm for Development and Information-gene, ZHIYUAN LI, Princeton Center for Theoretical Science, Princeton University, CHAO TANG, Center for Quantitative Biology, Peking University, HAO LI, Dept. of Biochemistry and Biophysics and California Institute for Quantitative Biosciences, University of California, San Francisco — During development, cells with identical genomes acquire different fates in a highly organized manner. In order to decipher the principles underlying development, we used C.elegans as the model organism. Based on a large set of microscopy imaging, we first constructed a “standard worm” in silico: from the single zygotic cell to about 500 cell stage, the lineage, position, cell-cell contact and gene expression dynamics are quantified for each cell in order to investigate principles underlying these intensive data. Next, we reverse-engineered the possible gene-gene/cell-cell interaction rules that are capable of running a dynamic model recapitulating the early fate decisions during C.elegans development. we further formalized the C.elegans embryogenesis in the language of information generation. Analysis towards data and model uncovered the global landscape of development in the cell fate space, suggested possible gene regulatory architectures and cell signaling processes, revealed diversity and robustness as the essential trade-offs in development, and demonstrated general strategies in building multicellular organisms.

4:42PM P39.00010 Reliable Signal Transduction, ROY WOLLMAN, Dept of Chemistry and Biochemistry, University of California, San Diego — Stochasticity inherent to biochemical reactions (intrinsic noise) and variability in cellular states (extrinsic noise) degrade information transmitted through signaling networks. We analyzed the ability of temporal signal modulation - that is dynamics - to reduce noise-induced information loss. In the extracellular signal-regulated kinase (ERK), calcium (Ca(2+)), and nuclear factor kappa-B (NF-κB) pathways, response dynamics resulted in significantly greater information transmission capacities compared to nondynamic responses. Theoretical analysis demonstrated that signaling dynamics has a key role in overcoming extrinsic noise. Experimental measurements of information transmission in the ERK network under varying signal-to-noise levels confirmed our predictions and showed that signaling dynamics mitigate, and can potentially eliminate, extrinsic noise-induced information loss. By curbing the information-degrading effects of cell-to-cell variability, dynamic responses substantially increase the accuracy of biochemical signaling networks.

Wednesday, March 16, 2016 2:30PM - 5:30PM – Session P40 GSNP GSOFT: More Geometry and Dynamics: Wrinkling, Folding, Snapping, etc. 343 - Dominic Vella, Oxford University
2:30PM P40.00001 Rolling Wrinkles on Elastic Substrates, MICHAEL IMBURGIA, ALFRED CROSBY, Univ of Mass - Amherst. The mechanics of rolling contact between an elastomer layer and a thin film present unique opportunities for taking advantage of elastic instabilities, such as surface wrinkling, to create patterned surfaces. Here we present a plate-to-roller(P2R) geometry to laminate a thin film onto an elastomer layer in order to induce surface wrinkling. First, a poly(dimethylsiloxane)(PDMS) layer is draped around a roller and pressed into contact with a poly(styrene)(PS) film supported on a plate. Once rolling begins, the PS film preferentially laminates onto the PDMS layer. During this process, the deformation of the PDMS layer can induce wrinkling when the contact load exceeds a critical value. Wrinkle feature size consists of amplitudes of 0.3 - 1µm and wavelengths of 15 - 20µm. Wrinkle amplitude can be controlled by contact load and roller curvature, as well as the mechanical properties and thickness of the film and elastomer. We develop semi-empirical equations to describe the effect of contact load and roller curvature on the wrinkle aspect ratio. Finite-element modeling of an elastomer layer in rolling contact with a rigid plate is used to support experimental results. Using these models, wrinkle-based technologies such as optoelectronics and enhanced adhesives can be envisioned.

2:42PM P40.00002 Slow frictional waves, KRISHNUK VISWANATHAN, Purdue University, NARAYAN SUNDARAM, Indian Institute of Science, SRINIVASAN CHANDRASEKAR, Purdue University. Stick-slip, manifest as intermittent tangential motion between two dry solid surfaces, is a friction instability that governs diverse phenomena from automobile brake squeals to earthquakes. We show, using high-speed in situ imaging of an adhesive polymer interface, that low velocity stick-slip is fundamentally one of three kinds, corresponding to passage of three different surface waves separation pulses, slip pulses and the well-known Schallamach waves. These waves, traveling much slower than elastic waves, have clear distinguishing properties. Separation pulses and Schallamach waves involve local interface separation, and propagate in opposite directions while slip pulses are characterized by a sharp stress front and do not display any interface detachment. A change in the stick-slip mode from separation to slip pulse is effected simply by increasing the normal force. Together, these three waves constitute all possible stick-slip modes in adhesive friction and are shown to have direct analogues in muscular locomotory waves in soft bodied invertebrates. A theory for slow wave propagation is also presented which is capable of explaining the attendant interface displacements, velocities and stresses.

2:54PM P40.00003 Poking around: how indentation reveals wrinkly isometries, DOMINIC VELLA, University of Oxford, HAMID EBRAMI, Northeastern University, JOSEPH PAULSEN, Syracuse University, ASHKAN VAZIRI, Northeastern University, NARAYANAN MENON, BENNY DAVIDOVITCH, UMass Amherst. When deforming extremely thin objects, deformation via stretching is relatively expensive. It is therefore natural to seek deformations that preserve lengths, or isometries. Two common examples of such isometries in mechanics are the 'd-cone' (for a plate) and 'mirror buckling' (for a shell). I will show two examples for which the presence of a weak tension means that these isometries are not obtained experimentally. Instead, the systems in question wrinkle and tend to new 'wrinkly isometries': isometries that are only available to a wrinkled object.

3:06PM P40.00004 Curvature-induced stiffness and the spatial variation of wavelength in wrinkled sheets, NARAYANAN MENON, JD PAULSEN, EVAN HOHFELD, HUNTER KING, JIANGSHUI HUANG, THOMAS RUSSELL, ZHANLONG QIU, BENNY DAVIDOVITCH, U of Massachusetts, Amherst, DOMINIC VELLA, Mathematical Institute, Oxford University. Natural wrinkle patterns often inhabit surfaces of curved substrates, and typically are spatially nonuniform. However, the unified understanding of wrinkle wavelength [1] in terms of a competition between the bending energy of a sheet and the stiffness provided by the tension or potential energy of the supporting substrate, applies only to nearly-planar, parallel, and spatially uniform wrinkle patterns. We describe theory and experiment that extend this understanding in two major directions. The first is to show that the local variation of the wavelength may be treated as a distinct term in the substrate stiffness. The second is to demonstrate in two very different settings that the local value of the wavelength is determined by the local stiffness of the subphase. Both results are encapsulated in a simple, local law for the wavelength that has greatly expanded applicability. We acknowledge support from the WM Keck Foundation. 1. Cerda, E., & Mahadevan, L. (2003). Physical review letters, 90, 074302.

3:18PM P40.00005 Geometry-driven folding transitions in floating thin films, JOSEPH D. PAULSEN, Syracuse University, VINCENT DÉMERY, PCT-ESPCI, France, K. BUGRA TOGA, Eastman Chemical Company, ZHANLONG QIU, BENNY DAVIDOVITCH, THOMAS P. RUSSELL, NARAYANAN MENON, Univ of Mass - Amherst. When a thin elastic sheet is compressed, it forms wrinkles to gather excess material, while deforming the fluid or solid substrate by only a small amount. Upon further compression, the sheet may fold, in order to lower the mechanical energy of the system. We here present a folding transition that is independent of the mechanical properties of the sheet. We study the deformations of a thin polymer film that has an annular shape, floating on a planar air-water interface. By controlling the concentration of a surfactant outside the film, we vary the tension pulling on the annular boundary of the annulus. The competition between the bending energy and the tension of the subphase on the geometry of the sheet, but is independent of its bending rigidity. Our results are consistent with a simple geometric principle: the sheet adopts the unstrained shape that minimizes the interfacial energy of the exposed liquid. Finally, we consider the application of this geometric principle to the folding of a floating indented film.

3:30PM P40.00006 Ribbon curling, ANNE JUEL, University of Manchester, UK, CHRIS PRIOR, University of Durham, UK, JULIEN MOUSSOU, ENS Paris, France, BUDDHAPRIYA CHAKRABARTI, University of Durham, UK, OLIVER JENSEN, University of Manchester, UK. The procedure of curling a ribbon by running it over a sharp blade is commonly used when wrapping presents. Despite its ubiquity, a quantitative explanation of this everyday phenomenon is still lacking. We address this using experiment and theory, and examine the dependence of ribbon curvature on blade curvature, the longitudinal load imposed on the ribbon and the speed of pulling. Experiments in which a ribbon is drawn steadily over a blade under a fixed load show that the ribbon curvature is generated over a restricted range of loads, the curvature/loid relationship can be non-monotonic, and faster pulling (under a constant imposed load) results in less tightly curled ribbons. We develop a theoretical model that captures these features, building on the concept that the ribbon under the imposed deformation undergoes differential plastic stretching across its thickness, resulting in a permanently curved shape. The model identifies factors that optimize curling and clarifies the physical mechanisms underlying the ribbon's nonlinear response to an apparently simple deformation.

3:42PM P40.00007 Periodic Buckling Patterns On Constrained Elastic Shells, JOEL MARTHELOT, ANNA LEE, PIERRE-THOMAS BRUN, FRANCISCO LOPEZ JIMENEZ, PEDRO M. REIS, MIT. Thin spherical shells range from nanometer-sized viruses to space vehicles. A pressure differential between the inner and outer part of the shell can result in the buckling and catastrophic failure of the structure. We revisit this classic buckling problem, depressing thin elastic shells, which are arrested from within by a concentric spherical mandrel. As a result, buckling is constrained to occur within the gap between the two. Above a critical pressure, dimples appear sequentially on the surface of the shell to form a robust periodic pattern. We perform precision desktop experiments to construct the bifurcation diagram of the process, and explore a range of geometric and material properties. A scaling analysis enables us to rationalize the dependence of the size of the dimples on both the radius of the shell and the radial gap between the shell and the inner rigid mandrel. Moreover, we characterize the process of nucleation and progression of the dimpled pattern front. Particular emphasis is given to the patterns obtained in the strongly nonlinear post-buckling regime where a network of sharp ridges forms.
Similar phenomena were seen in nonlinear equations of motion representing various non-mechanical systems. Compression. "Reputable" finite element and finite difference codes could not reliably predict deformation of an aluminum beam under a transverse pressure and formed a folded six-corner star. In another test, an impulsively stretched rod buckled and obtained a final shape similar to that of a rod under static axial tension limit, by applying a bending modulus dependent term to the tension dominated scale. The simulation results also highlight the residual compressive singular expansion, which previous studies relied on, becomes ill-defined. To reveal the morphology in the zero-tension limit, we employ numerical simulations based on a naive estimate of the elastic timescales. To explain this discrepancy, the natural conclusion has been drawn that some other effect, such as viscoelasticity, must play a role. We demonstrate here that purely elastic systems may show similar 'slow' dynamics during snap-through. This behaviour is due to a remnant (or 'ghost') of the snap-through bifurcation underlying the instability, analogously to bottleneck phenomena in 1-D dynamical systems. This slowness is a generic consequence of being close to bifurcation — it does not require dissipation. We obtain scaling laws for the length of the delay and compare these to numerical simulations and experiments on real samples.
Inertial Granular Flows


Experiment were non-Gaussian velocity distributions and a violation of the equipartition of kinetic energy in the steady state. Rotational degrees of freedom starting from a homogeneous state. Experimentally, such a gas in 3D can only be realized with strong external forcing or in microgravity. We have recently to picture, but still insufficiently understood. Numerous theoretical treatments have been performed, favorably with spherical grains and periodic boundaries.

Sandra Wegner, Torsten Trittel, Ralf Stannarius, Institute of Experimental Physics and Mars, Otto von Guericke University Magdeburg — We study a peculiar, anomalous weakening in wet sand brought about by the addition of small amounts of fine silt. The effect has been observed in uncontrolled field experiments, which we reproduce in the lab. Samples consist of sand from a local state park with a broad grain-size distribution between 300-600 microns, to which we add controlled amounts of silt, with a size distribution between 25-75 microns. Moisture contents range from 0-15% (by mass); we find our samples unable to hold much more than 15%. Samples are formed into free-standing cylinders and loaded from above until collapse. Mass fraction of silt varies from 0-20%, spanning the range observed in coastal sands. Results are compared with dynamic deflection moduli found in the field, and possible mechanisms are discussed.

2:42PM P43.00002 Enhanced Flow of Granular Material

George M. McMurtry, Scott Franklin, Charles Bachmann, Rochester Institute of Technology — We study a peculiar, anomalous weakening in wet sand brought about by the addition of small amounts of fine silt. The effect has been observed in uncontrolled field experiments, which we reproduce in the lab. Samples consist of sand from a local state park with a broad grain-size distribution between 300-600 microns, to which we add controlled amounts of silt, with a size distribution between 25-75 microns. Moisture contents range from 0-15% (by mass); we find our samples unable to hold much more than 15%. Samples are formed into free-standing cylinders and loaded from above until collapse. Mass fraction of silt varies from 0-20%, spanning the range observed in coastal sands. Results are compared with dynamic deflection moduli found in the field, and possible mechanisms are discussed.

2:54PM P43.00003 Solid-liquid like phase transition in a confined granular suspension

Nakia Sakai, Frederic Lecheneault, Mokhtar Adda Bedia, Laboratoire de Physique Statistique - Ecole Normale Superieure, Paris — We present an experimental study of a liquid-solid like phase transition in a two-dimensional granular media. Particles are placed in a vertical Hele-Show cell filled with a denser solution of cesium-chloride. Thus, when the cell is rotated around its axis, hydrostatic pressure exerts a centripetal force on the particles which confines them towards the center. This force is in competition with gravity, thus by modifying the rotation rate, it is possible to transform continuously and reversibly the sample from a disordered loose state to an ordered packed state. The system presents many similarities with thermal systems at equilibrium like density and interface fluctuations, and the transition between the two phases goes through a coexistence state, where there is nucleation and growth of locally ordered domains which are captured by the correlation length of the hexatic order parameter. We discuss the possibility to extend the grand-canonical formalism to out-of-equilibrium systems, in order to uncover a state equation between the density and the pressure in the medium.

3:06PM P43.00004 Forces and Flows in Non-Newtonian Suspensions

Melody Lim, Jonathan Barres, Robert Behringer, Duke University — Above a certain solid mass fraction, suspensions of dense granular particles in water exhibit non-Newtonian behavior, including impact-activated solidification. Although it has been suggested that solidification depends on interactions with the suspension boundary, quantitative experiments on the boundary forces have not been reported. In the present experiments, we determine the magnitude and timings of impactor-driven events in both the boundaries and body of the suspension using high-speed video, tracer particles, and photoelastic container boundaries. We observe a shock-like propagation in the cornstarch suspension during impact. The dynamics of the shockfront are strongly correlated to those of the intruder. We also observe a second extremely fast shockfront, associated with the propagation of forces to the boundaries of the suspension. The dynamics of this shockfront do not depend on the intruder dynamics, but are correlated to the volume fraction of cornstarch particles in the suspension. The observed shockfront propagates at a speed which is faster than the sound speed in the experiment container.

3:18PM P43.00005 Cooling of 3D Granular Gases: Experiments in Microgravity

Kirsten Harth, Sandra Wegner, Torsten Trittel, Ralf Stannarius, Institute of Experimental Physics and Mars, Otto von Guericke University Magdeburg — Granular gases are ensembles of macroscopic grains, which move randomly and interact through inelastic collisions. This non-equilibrium statistical system is easy to picture, but still insufficiently understood. Numerous theoretical treatments have been performed, favorably with spherical grains and periodic boundaries, starting from a homogeneous state. Experimentally, such a gas in 3D can only be realized with strong external forcing or in microgravity. We have recently demonstrated that the use of elongated grains facilitates the realization of 3D experiments beyond the Knudsen regime (1). Main findings in a sounding rocket experiment were non-Gaussian velocity distributions and a violation of the equipartition of kinetic energy in the steady state. Rotational degrees of freedom are under-excited. When the excitation is stopped, energy is dissipated, the granular gas is "cooling". We present the first quantitative study of the cooling of a granular gas, based on a 3D data evaluation, from drop tower experiments. The evolution of the kinetic energy in translational and rotational degrees of freedom is compared to Haff’s law and recent numerical studies. Additionally, we analyze velocity and density distributions.


3:30PM P43.00006 ABSTRACT WITHDRAWN —

3:42PM P43.00007 Flying in a sandstorm: granular flow dynamics around an intruder

Yasin Karim, Eric Corwin, University of Oregon — Using high-speed imaging and direct force measurements, we study the flow dynamics around an intruder in a quasi-two-dimensional granular gas. We also vary the geometry of the intruder and explore how changing the curvature, for instance, affects the lift force. For a given angle of attack, an intruder with a straighter side facing the flow experiences higher lift than one with a more convex side. We use particle image velocimetry to measure flow fields and correlate them with our direct force measurements to elaborate on how granular gas flows respond to changes in intruder geometry.
3:54PM P43.00008 Collisional Model of the Stopping Force of 3D Granular Impact\textsuperscript{1} , CACEY STEVENS, JONATHAN BARES, ROBERT BEHRINGER, Department of Physics, Duke University — A dense granular packing can cause a free-falling intruding object to come to an abrupt stop as its momentum is dissipated to the grains. An empirical force law has been widely accepted to describe this process; it characterizes the stopping force as the sum of depth-dependent friction and velocity-dependent inertial drag\textsuperscript{2}. However, a complete interpretation of this force, incorporating grain-scale interactions during impact, remains unresolved. Here, the momentum transfer is proposed to occur through sporadic collisions with clusters of high force-carrying grains at the intruder’s surface\textsuperscript{3}. To test this model in 3D impact experiments, we determine the forces acting on an intruder decelerating through a dense granular medium using high-speed video of its trajectory. By attaching a rod to the intruder and observing its motion from perpendicular angles, we obtain all translational and rotational dynamics. We vary the shape of the impeding object to infer intruder-grain interactions from its consequent path. As a result, we connect the inertial drag to the effect of intruder shape and rotation based on the collisional model.

\textsuperscript{1}Supported by Duke University Provost’s Postdoctoral Program and NASA grant NNX15AD38G

\textsuperscript{2}H. Katsuragi et al, Nat. Phys. 3, 6 (2007)

\textsuperscript{3}Y. Takehara et al EPL 92, 44003 (2010), A. Clark et al, PRE 89, 012011 (2014)

4:06PM P43.00009 Real-time magnetic resonance imaging of highly dynamic granular phenomena , ALEXANDER PENN, Laboratory for Energy Science and Engineering, ETH Zurich and Institute for Biomedical Engineering, University and ETH Zurich, KLAAS P. PRUESSMANN, Institute for Biomedical Engineering, University and ETH Zurich, CHRISTOPH MILLER, Laboratory for Energy Science and Engineering, ETH Zurich — Probing non-intrusively the interior of three-dimensional granular systems is a challenging task for which a number of imaging techniques have been applied including positron emission particle tracking, X-ray tomography and magnetic resonance imaging (MRI). A particular advantage of MRI is its versatility allowing quantitative velocimetry through phase contrast encoding and tagging, arbitrary slice orientations and the flexibility to trade spatial for temporal resolution and vice versa during image reconstruction. However, previous attempts to image granular systems using MRI were often limited to (pseudo-) steady state systems due to the poor temporal resolution of conventional imaging methodology. Here we present an experimental approach that overcomes previous limitations in temporal resolution by implementing a variety of methodological advances, viz. parallel data acquisition through tailored multiple receiver coils, fast gradient readouts for time-efficient data sampling and engineered granular materials that contain signal sources of high proton density. Achieving a spatial and temporal resolution of, respectively, 2 mm × 2 mm and 50 ms, we were able to image highly dynamic phenomena in granular media such as bubble coalescence and granular compaction waves.

4:18PM P43.00010 Investigation of the effect of wall friction on the flow rate in 2D and 3D Granular Flow\textsuperscript{3} , BRENDA CARBALLO-RAMIREZ, MOLLIE PLEAU,NALINI EASWAR, Smith College, SUMIT BIRWA, TCIS Hyderabad, NEIL SHAH, SHUBHA TEVAR, University of Massachusetts — We have measured the mass flow rate of spherical steel spheres under gravity in vertical, straight-walled 2 and 3-dimensional hoppers, where the flow velocity is controlled by the opening size. Our measurements focus on the role of friction and its placement along the walls of the hopper. In the 2D case, an increase in the coefficient of static friction from $\mu = 0.2$ to 0.6 is seen to decrease the flow rate significantly. We have changed the placement of frictional boundaries/regions from the front and back walls of the 2D hopper to the side walls and floor to investigate the relative importance of the different regions in determining the flow rate. Fits to the Beverloo equation show significant departure from the expected exponent of 1.5 in the case of 2D flow. In contrast, 3D flow rates do not show much dependence on wall friction and its placement. We compare the experimental data to numerical simulations of gravity driven hopper granular flow with varying frictional walls constructed using LAMMPS\textsuperscript{*}. * http://lammps.sandia.gov

\textsuperscript{3}Supported by NSF MRSEC DMR 0820506

4:30PM P43.00011 Normal coefficient of restitution of wet particles\textsuperscript{3} , KAI HUANG, THOMAS MUELLER, INGO REHBERG, Experimentalphysik V, University of Bayreuth — The normal coefficient of restitution (COR) for a spherical particle bouncing on a wet surface is investigated experimentally. The dependence of the COR on the impact velocity and various particle and liquid properties will be presented and discussed in terms of dimensionless numbers that characterize the interplay between inertial, viscous, and surface forces. At a fixed ratio of the liquid film thickness $\delta$ to the particle diameter $D$, the wet COR is found to be inverse proportional to the Stokes number $St$, which measures the inertia of the particle to the viscous force from the liquid. This relation provides a convenient way of predicting wet COR with two fit parameters. Finally, we rationalize the observations with a model that considers possible sources of energy dissipation associated with a wet impact.

\textsuperscript{3}KH and TM acknowledge the support from the DFG through Grant No. HU1939/2-1

4:42PM P43.00012 Long-term behavior of granular chains held between walls is really equilibrium\textsuperscript{1} , MICHELLE PRZEDBORSKI, Brock University, SURAJIT SEN, State University of New York at Buffalo, THAD HARROUN, Brock University — Granular chains have been the focus of a number of studies, in part due to their numerous applications, ranging from shock absorption and vibration reduction to energy localization. Force impulses to an unloaded granular chain result in a propagating solitary wave (SW), analogous to a soliton of the Korteweg-de Vries equation. When SWs collide with a boundary or another SW, secondary solitary waves (SSWs) are produced as grains break contact. A consequence of this process is the transition from a non-ergodic, SW dominant, phase to the stable “quasi-equilibrium” (QE) phase, thought to be distinct from true thermodynamic equilibrium due to the absence of equipartitioning of energy. We show that, in the absence of energy dissipation, when granular systems are allowed to evolve to extremely long times, the number of SSWs becomes sufficiently large that the system actually approaches a true equilibrium phase. In this extreme-time limit, energy in fact becomes equipartitioned among all grains, and we illustrate how the specific heat and kinetic energy fluctuations can be predicted by the generalized equipartition theorem, regardless of the degree of the interaction potential. This opens up the possibility that granular systems should be treated by equilibrium statistical mechanics.

\textsuperscript{1}This work was supported by a Vanier Canada Graduate Scholarship

4:54PM P43.00013 Experimental observations of root growth in a controlled photoelastic granular material , SERGE MORA, JONATHAN BARES, LMGC Montpellier, JEAN-YVES DELENNE, INRA-UMR-IATE Montpellier, THIERRY FOURCAUD, CIRAD-UMR-AMAP Montpellier — The mechanism of root growth in soil is a key issue to understand both how to improve plant development and how to stabilize grounds. However, no experimental studies have been carried out to directly observe root development and surrounding stress while imposing specific grain configurations or mechanical loading. We present a novel set-up which permits to observe the development of chickpea root networks in a 2D granular material made of bidisperse photoelastic discs while imposing the position of the grains, the intergranular spacing and the nature of the system confinement: (i) open cell, (ii) confined cell (iii) sheared cell. In the experimental apparatus several root development cells are treated in parallel to increase the statistical meaning of the observations. Evolution of the root network is followed as well as position and pressure inside each disc by mean of a camera and classical photoelastic techniques. Preliminary results will be presented.
5:06PM P43.00014 Topological interlocking provides stiffness to stochastically micro-cracked materials beyond the transport percolation limit . ANIRBAN PAL, CATALIN PICU, Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytech Institute, MARIAN V. LUPULESCU, New York State Museum, Research and Collections — We study the mechanical behavior of two-dimensional, stochastically microcracked continua in the range of crack densities close to, and above the transport percolation threshold. We show that these materials retain stiffness up to crack densities much larger than the transport percolation threshold, due to topological interlocking of sample sub-domains. Even with a linear constitutive law for the continuum, the mechanical behavior becomes non-linear in the range of crack densities bounded by the transport and stiffness percolation thresholds. The effect is due to the fractal nature of the fragmentation process and is not linked to the roughness of individual cracks. We associate this behavior to that of talc-ilomite, a sandstone that exhibits unusual flexibility.

Thursday, March 17, 2016 8:00AM - 11:00AM – Session R3 DCMP GSOFT GSNP: Glass and Jamming Transitions Ballroom III - Sydney Nagel, University of Chicago

8:00AM R3.00001 The Gardner Transition: A new approach for understanding low-temperature glasses . PATRICK CHARBONNEAU, Duke University — Recent theoretical advances in the mean-field theory of glasses predict the existence deep in the glass phase of a novel phase transition, a so-called Gardner transition. This transition signals the emergence of a complex free energy landscape composed of a marginally stable hierarchy of sub-basins within a broad glass metastasis. It is thus the onset of marked changes in thermal and transport properties of glasses, and ultimately leads to the unusual critical behavior at jamming. The Gardner transition itself is immediately related to a diverging (i) characteristic relaxation time, (ii) caging susceptibility and (iii) correlation length of the caging heterogeneity as well as aging, even in well-thermalized glasses. We have detected some of these signatures both in a mean-field model and in standard hard-sphere glass formers. We find the results to quantitatively agree with theory in the former and qualitatively so in the latter, which suggest that the transition should be detectable in a wide array of numerical and experimental systems. Interestingly, although the Gardner transitions is primarily associated with structural glass formers, we also find features of the transition in crystals of polydisperse particles once the landscape becomes rough.

8:36AM R3.00002 Scaling theory for the jamming transition1. ANDREA J. LIU, University of Pennsylvania, Department of Physics and Astronomy — The existence of a critical jamming transition, which marks the onset of rigidity in athermal packings of spheres, suggests that universal physics underlies the origin and nature of rigidity in disordered solids ranging from glasses to foams and granular materials. The jamming transition was originally proposed as a zero-temperature critical point in a non-equilibrium phase diagram in packing density and shear stress. Many studies have documented critical phenomena near the jamming transition, including power-law scaling, diverging length scales and scaling collapse, and theories have been developed to understand these phenomena. However, a number of confusing features have precluded a unified critical scaling analysis of the transition. Here we resolve these issues to present a scaling ansatz for the jamming critical point in terms of density and shear stress. The theory predicts new exponents that we verify with numerical simulations.

9:12AM R3.00003 Frustration by Shape-Designed Local Polymorphism: A Near-Equilibrium Colloidal Glass of Hard Kites , THOMAS MASON, University of California- Los Angeles — We study glass formation in uniform Brownian dispersions of hard colloidal polygonal platelets having the shape of 72-degree achiral kites, fabricated using optical stepper lithography. These kites are confined to a plane through roughness-controlled depletion attractions, and they diffuse in two-dimensions as we very slowly raise the particle density in the system. Although the densest packing of these kites is a crystalline lattice that fully tiles the plane, remarkably, we observe that the kites do not crystallize even for such quasi-static osmotic compression. By contrast, we have previously shown that such slow compression does cause crystallization of Brownian systems of other convex 2D lithographic shapes, such as squares and rhombs. Instead, the system of kites forms a disordered glass that undergoes an ergodic to non-ergodic transition, both in a rotational and a translational sense, while remaining near-equilibrium, as we measure by video particle tracking. We show that the high diversity of few-particle local polymorphic configurations (LPCs) of kites, related to our choice of angles and lengths in the designed shape, is responsible for suppressing long range spatial order and consequently favors glass formation instead. The prevalence and diversity of 5-particle LPCs, such as the pentagonal star, frustrate crystallization because these pentagonal LPCs are topologically different than the one 4-particle LPC that corresponds to the space-filling crystal. We anticipate that this mechanism of glass formation through shape-dependent frustration by diverse and incommensurate LPCs will also be relevant for molecular systems in three dimensions.

9:48AM R3.00004 Solution of the dynamics of high-dimensional liquids , JORGE KURCHAN1, LPS-ENS 24 rue Lhomond, 75231 Paris — The dynamics of a liquid composed of particles with spherically symmetric potentials has been solved exactly in limit of high dimensions d. The calculation is long but straightforward. At high density, an ergodicity-breaking glass transition is found. This computation allows one to assess the validity of approximation schemes such as Mode-Coupling Theory. As a by-product, because our calculation is, if not rigorous, elementary, an improvement in the bound for sphere packings in large dimensions is now at hand.

10:24AM R3.00005 Spinodals with Disorder: from Avalanches in Random Magnets to Glassy Dynamics , GIULIO BIROLI, IPHT CEA Saclay and LPS ENS Paris — We revisit the phenomenon of spinodals in the presence of quenched disorder and develop a complete theory for it. We focus on the spinodal of an Ising model in a quenched random field (RFIM), which has many applications in many areas from materials to social science. By working at zero temperature in the quasi-statically driven RFIM, thermal fluctuations are eliminated and one can give a rigorous content to the notion of spinodal. We show that the spinodal transition is due to the depinning and the subsequent expansion of rare droplets. We work out the critical behavior, which, in any finite dimension, is very different from the mean-field one: the characteristic length diverges exponentially and the thermodynamic quantities display very mild non-analyticities much like in a Griffith phenomenon. Thanks to the recently established connection between the spinodal of the RFIM and glassy dynamics, our results allow us to conclusively assess the physical content and the status of the dynamical transition predicted by the mean-field theory of glass-forming liquids.
imaging, mutants, and drug applications, we construct the phase diagram of M. xanthus high cell density the formation of fruiting bodies is a phase separation process. From experimental data that combines single-cell tracking, population-scale of aggregation for comparison to experiments.

Using 2D molecular dynamics simulations, we map the phase behavior in the space of Péclet number and local density and examine the kinetics may play an important role. We have adapted self-propelled particle models to include cell reversal and motility suppression resulting from sporulation observed direction. The first stage of fruiting body formation is characterized by the aggregation of cells on a surface into round mesoscopic structures. Experiments collective behaviors including streaming, swarming, and generation of fruiting bodies. A striking feature of M. xanthus is that it periodically reverses its motility in a cycle of a microfluidic device and then changes the local density and cell motility.

Due to the non-uniform distribution of the pitch of a helix subject to viscous drag, linear and nonlinear behavior is identified along the contour length of a single helix. When a polymer solution is used for the viscous flow, an interesting multiscale problem arises and the typical polymer size needs to be compared not only to the global size of the helix, but also to the dimensions of the ribbon.

The moving frame as well as differential equations that can be interpreted as effective constitutive relations encoding the effect that the second strand has on the first as the braid deforms under the action of end loads. Simple analytical cases are discussed first and used as starting solutions in parameter continuation studies to compute classes of both open and closed (linked or knotted) braid solutions.

Deformation and transport of micro-fibers and helices in viscous flows.

Wrinkles, loops, and topological defects in twisted ribbons.

Phase separation dynamics during Myxococcus xanthus fruiting body formation.

Phase separation model of Myxococcus xanthus aggregation.
8:24AM R35.00003 Thermodynamics of the motility-induced phase separation. ALEXANDRE SOLON, Massachusetts Institute of Technology, USA, JOACHIM STENHAMMAR, Lund University, Sweden, MICHAEL CATES, University of Cambridge, UK, JULIEN TAILLEUR, Université Paris Diderot, France — Self-propelled particles are known to accumulate in regions of space where their velocity is lowered. In addition, if their velocity diminishes when the local density increases (for example due to crowding effects), a positive feedback loop leads to the now well-established motility-induced phase separation (MIPS) between a dense immobile phase and a dilute motile phase. Understanding the phase equilibrium of MIPS is still a matter of debate. Although, depending on the models used to study the transition, a chemical potential or a pressure can be defined, these quantities do not play their usual thermodynamic role. In particular, the usual common tangent or equal-area constructions fail in these systems. Indeed, we will show that describing the phase equilibrium of MIPS necessitates generalized thermodynamics that include non-equilibrium contributions. This approach allows us to predict correctly the phase diagram of MIPS and to gain insight into the thermodynamics of active systems. It also sheds light on the (in)equivalence of statistical ensembles for these systems, paving the way for more efficient computational studies.

8:36AM R35.00004 Epithelial gap closure governed by forces and geometry. BENOIT LADOUX, Mechatronics Institute (Singapore) and Institut Jacques Monod (CNRS, France) — The closure of gaps within epithelia is crucial to maintain the integrity and the homeostasis of the tissue during wound healing or cell extrusion processes. Cells mediate gap closure through either the assembly of multicellular actin-based contractile cables (purse-string contraction) or the protrusive activity of border cells into the gap (cell crawling). I will present experimental data and numerical modeling that show how these mechanisms can mutually interact to promote efficient epithelial gap closure and how mechanical constraints can regulate these mechanisms. I will first present how geometrical constraints dictate mechanisms of epithelial gap closure. We determine the importance of tissue shape during closure and the role of curvature of cell boundaries in this process. An essential difference between the two closure mechanisms is that cell crawling always pulls the edge of the tissue forward (i.e. towards the gap) while purse string pulls the edge forward or backwards depending on the local geometry. Our study demonstrates how the interplay between these two mechanisms is crucial for closing gaps and wounds, which naturally come in arbitrary shapes. Then I will focus on epithelial closure mechanism during cell extrusion. Within confluent cell layers, cellular motions coupled between neighbors are tightly regulated by the packing density of the epithelium inducing drastic changes in the dynamics of these tissues. I will show how cell density and tissue mechanics regulate the extrusion of cells within a confluent epithelial cell sheet, simultaneously measuring collective movements and traction forces. Epithelial packing and collective cell dynamics dictate the modes of cellular extrusions from lamellipodia crawling of the neighboring cells at low densities to coordinated actin-based contractile purse-string mechanism at higher density.

9:12AM R35.00005 Self-Driven Jamming of Growing Microbial Populations, CARL SCHRECK, MORGAN DELARUE, PAWEL GNEIWES, OSKAR HALLATSCHEK, University of California, Berkeley — When cells grow in confined spaces, they assemble into dense populations that interact both chemically and physically. Although in recent years scientists have uncovered a previously hidden layer of mechanical regulation in mammalian tissues that impacts gene expression and development, little is known about the consequences of mechanical constraints on single-celled microbes. This is largely due to a lack of appropriate culturing techniques and accurate computational models. Using physically explicit computer models that are developed alongside microfluidic experiments, we address two fundamental questions: (1) what structures self-assemble in confined geometries due to the cell growth and division process? and (2) how do those structures and associated stresses feed back on to cell physiology? We find that microbial growth in confinement can lead to jamming, heterogeneous stress fields, and intermittent flow that in turn result in spatially and temporally heterogeneous physiological responses. With computer simulations, we further explore the differences between this ‘active’ flow that is driven internally by cell growth and ‘inactive’ flow, such as shear and hopper flow, that is driven externally.

9:24AM R35.00006 Cell Size Clues for the Allee Effect in Vegetative Amoeba Suspension Culture, CARL FRANCK, BRENDA RAPPASO, XIAONING WANG, IGOR SEGOTA, Cornell University — That cells proliferate at higher rates with increasing density helps us appreciate and understand the development of multicellular behavior through the study of dilute cell systems. However, arduous cell counting with a microscope reveals that in the model eukaryote, Dictostelium discoideum this transition is difficult to ascertain and thereby further explore despite our earlier progress (Phys. Rev. E 77, 041905, (2008)). Here we report preliminary evidence that the slow proliferation phase is well characterized by reduced cell size compared to the wide distribution of cell sizes in the familiar exponential proliferation phase of moderate densities. This observation is enabled by a new system for characterizing cells in stirred suspension cultures. Our technique relies on quickly acquiring magnitude distributions of detected flashes of laser light scattered in situ by cell targets.

9:36AM R35.00007 Manipulation of long-term dynamics in a colloidal active matter system using speckle light fields, ERCAG PINCE, SABAREESH K.P. VELU, AGNESE CALLEGARI, PARVIZ ELAHI, Bilkent University, SYLVAIN GIGAN, Université Pierre et Marie Curie, GIOVANNI VOLPE, Bilkent University, GIORGIO VOLPE, University College London — Particles undergoing a hopping flow, that is driven externally.

9:48AM R35.00008 A Density-Independent Flocking Transition in Confluent Tissues, MICHAEL CZAJKOWSKI, Syracuse Univ, DAPENG BI, Rockefeller Univ, M. LISA MANNING, M. CRISTINA MARCHETTI, Syracuse Univ — Some of us recently demonstrated a density-independent solid-liquid transition in confluent tissues controlled by cell motility and a cell shape parameter measuring the interplay of cortical tension and cell-cell adhesion. An important insight of this work is that the rigidity and dynamics of cell layers depends sensitively on cell shape. To explore the influence of cell shape on collective states, we have constructed continuum equations that couple a scalar field describing cell-shape anisotropy to cell polarization. The model displays a density independent transition to a polarized state of elongated cells driven by a cellular shape-index parameter. We map out the phase diagram using linear stability analysis and numerical solution of the nonlinear hydrodynamic equations. The proposed transition constitutes a density-independent flocking transition.

1We acknowledge support from The Simons Foundation and NSF-DGE-1068780
10:00AM R35.00009 Multicellular contractility contributes to the emergence of mesothelioma nodules. ANDRAS CZIROK, University of Kansas Medical Center — Malignant pleural mesothelioma (MPM) nodules arise from the mesothelial lining of the pleural cavity by a poorly understood mechanism. We demonstrate that macroscopic multicellular aggregates, reminiscent of the MPM nodules found in patients, develop when MPM cell lines are cultured at high cell densities for several weeks. Surprisingly, the nodule-like aggregates do not arise by excessive local cell proliferation, but by myosin II-driven cell contractility. Contractile nodules contain prominent actin cables that can span several cells. Several features of the in vitro MPM nodule development can be explained by a computational model that assumes uniform and steady intercellular contractile forces within a monolayer of cells, and a mechanical load-dependent lifetime of cell-cell contacts. The model behaves as a self-tensioned Maxwell fluid and exhibits an instability that leads to pattern formation. Altogether, our findings suggest that inhibition of the actomyosin system may provide a hitherto not utilized therapeutic approach to affect MPM growth.

10:12AM R35.00010 Cilia driven flow networks in the brain. YONG WANG, MPI Dynamics and Self-Organization, REGINA FAUBEL, MPI biophysical Chemistry, CHRISTIAN WESTENDORF, MPI Dynamics and Self-Organization, GREGOR EICHELE, MPI biophysical Chemistry, EBERHARD BODENSCHATZ, MPI Dynamics and Self-Organization. Neurons exchange soluble substances via the cerebrospinal fluid (CSF) that fills the ventricular system. The walls of the ventricular cavities are covered with motile cilia that constantly beat and thereby induce a directional flow. We recently discovered creating the third ventricle genes, a complex trait pattern leading to reduced areas of the ventricular volume and substraction of transport pathways along the walls. Transient and daily recurrent alterations in the cilia beating direction lead to changes in the flow pattern. This has consequences for delivery of CSF components along the near wall flow. The contribution of this cilia-induced flow to overall CSF flow remains to be investigated. The state-of-art lattice Boltzmann method is adapted for studying the CSF flow. The 3D geometry of the third ventricle at high resolution was reconstructed. Simulation of CSF flow without cilia in this geometry confirmed that the previous idea about unidirectional flow does not explain how different components of CSF can be delivered to their various target sites. We study the contribution of the cilia-induced flow pattern to overall CSF flow and identify target areas for site-specific delivery of CSF-constituents with respect to the temporal changes.

10:24AM R35.00011 Collective motion of motile cilia: from human airways to model systems. PIETRO CICUTA, LUIGI FERIANI, MAURIZIO CHIOCCHIOLI, JURIJ KOTAR, University of Cambridge — Mammalian airways are a fantastic playground of nonlinear phenomena, from the function of individual active filaments, to the emerging collective behaviour, to the rheology of the mucus solution surrounding cilia. We have been investigating the fundamental physics of this system through a variety of model system approaches, both experimental and computational. In the last year we have started measurements on living human cells, observing cilia shape during beating, and measuring speed and coherence of the collective dynamics. We report on significant differences in the collective motion in ciliated cell carpets from a variety of diseases, and we attempt to reconcile the collective dynamical properties to the properties of individual filaments and the mechanics of the environment.

10:36AM R35.00012 Active matter clusters at interfaces. KATHERINE COPENHAGEN, Univ of California - Merced, AJAY GOPINATHAN, University of California - Merced — Collective and directed motility or swarming is an emergent phenomenon displayed by many self-organized assemblies of active biological matter such as clusters of embryonic cells during tissue development and flocks of birds. Such clusters typically encounter very heterogeneous environments. What happens when a cluster encounters an interface between two different environments has implications for its function and fate. Here we study this problem by using a mathematical model of a cluster that treats it as a single cohesive unit whose movement depends on the nature of the local environment. We find that low speed clusters which exert forces but no active torques, encountering an interface with a moderate difference in properties can lead to refraction or even total internal reflection of the cluster. For large speeds and clusters with active torques, they show more complex behavior, becoming trapped at the interface and deviating from the predictable refraction and reflection of the low velocity clusters. Our results show a wide range of behaviors that occur when collectively moving active biological matter moves across interfaces and these insights can be used to control motion by patterning environments.

Thursday, March 17, 2016 8:00AM - 11:00AM — Session R36 GSNP GSOFT: Continuum Descriptions of Discrete Materials II 339 - Paul Umbanhowar, Northwestern University

8:00AM R36.00001 Dynamic shear jamming in dense suspensions. IVO PETERS, University of Southampton, SAYANTAN MAJUMDAR, HEINRICHJAEGER, University of Chicago — Shear a dense suspension of cornstarch and water hard enough, and the system seems to solidify as a result. Indeed, previous studies have shown that a jamming front propagates through these systems until, after interaction with boundaries, a jammed solid spans across the system. Because these fully jammed states are only observed if the deformation is fast enough, a natural question to ask is how this phenomenon is related to the discontinuous shear thickening (DST) behavior of these suspensions. We present a single experimental setup in which we on the one hand can measure the rheological flow curves, but on the other hand also determine if the suspension is in a jammed state. This we do by using a large-gap cylindrical Couette cell, where we control the applied shear stress using a rheometer. Because our setup only applies shear, the jammed states we observe are shear-jammed, and cannot be a result of an overall increase in packing fraction. We probe for jammed states by dropping small steel spheres on a large-gap cylindrical Couette cell, where we control the applied shear stress using a rheometer. Because our setup only applies shear, the jammed states we observe are shear-jammed, and cannot be a result of an overall increase in packing fraction. We probe for jammed states by dropping small steel spheres on the surface of the suspension, and identify elastic responses. Our experiments reveal a clear distinction between the onset of DST and Shear-Jammed states, which have qualitatively different trends with packing fraction close to the isotropic jamming point.

8:12AM R36.00002 Rheological behavior of partially-wet granular matter. RAMIN GHELICHI, Postdoctoral Associate, KEN KAMRIN, Assistant Professor. KAMRIN GROUP TEAM — The topic of wet granular material modeling is an open area of study. In this talk we present a comprehensive continuum model for wet granular matter, which is informed by a novel Discrete Element Method (DEM), which tracks the fluid content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the content coating each grain as well as a variable fluid-bridge volume.
8:24AM R36.00003 Effect of friction on shear jamming\(^1\), DONG WANG, JONATHAN BARES, Duke University, JOSHUA DJIKSMAN, Wageningen University, JIE REN, Merck & Co, HU ZHENG, Hohai University, ROBERT BEHRINGER, Duke University — Shear jamming of granular materials was first found for systems of frictional disks, with a static friction coefficient $\mu \approx 0.6$ (Bi et al. Nature (2011)). Jamming by shear is obtained by starting from a zero-stress state with a packing fraction $\phi$ between $\phi_J$ (isotropic jamming) and a lowest $\phi_J^\text{shear}$ for shear jamming. This phenomenon is associated with strong anisotropy in stress and the contact network in the form of force chains, which are stabilized and/or enhanced by the presence of friction. Whether shear jamming occurs for frictionless particles is under debate. The issue we address experimentally is how changing friction affects shear jamming. By applying a homogeneous simple shear, we study the effect of friction by using photoelastic disks either wrapped with Teflon to reduce friction or with fine teeth on the edge to increase friction. Shear jamming is still observed; however, the difference $\phi_J - \phi_J^\text{shear}$ is smaller with lower friction. We also observe larger fluctuations due to initial configurations both at the lowest and the highest friction systems studied. Ongoing work is to use particles made of gelatin to reduce the friction coefficient to the order of 0.01.

\(^1\)We acknowledge support from NSF Grant DMR1206351, NASA Grant NNX15AD38G and the William M. Keck Foundation

8:36AM R36.00004 Frictionless Shear Jamming, a finite-size phenomenon, MARCO BAITY-JESI, Universidad Complutense de Madrid, CARL GOODRICH, Harvard University, JAMES SETHNA, Cornell University, ANDREA LIU, University of Pennsylvania — Athermal frictionless spheres jam as their density is increased. A few years ago, it was shown that at sufficiently high density, an initially unjammed system of frictional particles can jam under shear. Here we study shear jamming in packings of frictionless particles, and show that it is a finite-size effect with scalings that can be understood within a generalized scaling theory.

8:48AM R36.00005 Slow Relaxations in Fluid-Driven Granular Flows, CARLOS ORTIZ, DOUGLAS DURIAN, DOUGLAS JEROLMACK, Univ of Pennsylvania — Particles in a pack may appear frozen, but exhibit very slow dynamics (creep). To probe long-time dynamics, we construct an annular channel that mimics an infinitely-long river channel. We drive the packs with a laminar flow and record dynamics by laser scanned particle tracking. The dynamics of “bed load” grains near the surface exhibit relatively fast shear and their velocity profile as a function of depth can be well-described by a local $\mu(r)$-rheology. However, grains deep in the pack, which appear frozen by eye, exhibit slow creep dynamics that are not captured by the local model. This transition between bed load and creep occurs at a critical value of the local relaxation time. We find that the timescale for heterogeneous dynamics increases monotonically as a function of depth, but the length scale characterized by the domain size of the heterogeneities achieves a maximum at the transition to creeping. We explore the relation between the important length and time scales of the flow in the creep phase using nonlocal rheology.

9:00AM R36.00006 Flow of interacting colloidal suspensions through a narrow channel, RAUL CRUZ HIDALGO, SARA ARIETALEANIZ, University of Navarra, IGNACIO PAGONABARRAGA, University of Barcelona — In this work we numerically study the constitutive behavior of interacting colloidal suspensions at intermediate and high concentrations. The influence of the interaction potential strength on the system’s response is examined, in suspensions flowing through narrow channels at low Reynold’s numbers. Using Lattice Boltzmann methods, we analyze the rheological response of a colloidal suspension once the steady state is established. In dilute suspensions we always recover a newtonian behavior. At higher volume fractions, the range and strength of the interaction potential has a stronger impact in the behavior of the suspension. While for short range potentials, the non-newtonian response mostly depends on colloid concentration and confinement distance, for a Lennard-Jones potential we identify two rheological responses depending on the potential strength, $\xi$ and $\xi'$, at a given concentration. For weak $\xi'$, the effective viscosity $\eta_{eff}$ increases until a minimum is reached. On the contrary, at large values of $\xi'$, the effective viscosity $\eta_{eff}$ decreases until a minimum is reached. A dimensionless indicator of the comminution intensity is also formulated. The theory was inspired by noting that the local kinetic energy of shear strain rate plays a role analogous to the local kinetic energy of eddies in turbulent flow.

9:12AM R36.00007 Impact Fragmentation and Crushing of Concrete and Other Solids Due to Kinetic Energy of High Shear Strain Rate, ZDENEK BAZANT, KEDAR KIRANE, Northwestern University — While numerous studies have dealt with dynamic crack propagation, they have not led to a macroscopic continuum model usable in FE analysis. Recent work on such a model is reviewed. The key idea is that comminution under high-rate shear is driven by the release local kinetic (rather than strain) energy of the shear strain rate field in forming finite-size fragments. At strain rates $>10^3$/s, this energy exceeds the maximum possible elastic strain energy by orders of magnitude. It is found that the particle size scales as the $-2/3$ power of the shear strain rate and as the $2/3$ power of interface fracture energy, and the released and dissipated kinetic energy as the $2/3$ power of the shear strain rate. These results explain the long debated phenomenon of “dynamic overstress”. In FE simulations, this kinetic energy of strain rate field can be dissipated either by equivalent viscosity or by the work of increased strength limits. In simulating the impact of missiles into concrete walls, both approaches give nearly equivalent results. A dimensionless indicator of the comminution intensity is also formulated. The theory was inspired by noting that the local kinetic energy of shear strain rate plays a role analogous to the local kinetic energy of eddies in turbulent flow.

9:24AM R36.00008 Explanation of nonlocal granular fluidity in terms of microscopic fluctuations, QIONG ZHANG, KEN KAMRIN, Massachusetts Inst of Tech-MIT — A recently proposed granular constitutive law has shown capability to predict nonlocal granular rheology using a variable denoted granular fluidity. This work is aimed at finding the microscopic physical meaning of fluidity in terms of fluctuation of normalized shear stress and fluctuation of velocity. We try to predict the fluidity as a function of the fluctuation of normalized shear stress, and also test Eyring equation and kinetic theory based on the theoretical prediction proposed in other work. We find a consistent definition for the fluidity to be proportional to the product of the velocity fluctuations and some function of packing fraction divided by the average diameter of the grains. This definition shows predictive ability in multiple geometries for which flow behavior is nonlocal. It is notable that the fluidity is well-defined as a function of kinematic state variables, as one would hope for a quantity of this nature.

9:36AM R36.00009 Mesoscale poroelasticity of heterogeneous media, SIAVASH MONFARED, HADRIEN LAUBIE, Massachusetts Inst of Tech-MIT, FARHANG RADJAI \(^1\), Universite de Montpellier, ROLAND PELLENQ, FRANZ-JOSEF ULM, Massachusetts Inst of Tech-MIT — Poroelastic behavior of heterogeneous media is revisited. Lattice Element Method (LEM) is used to model interaction between solid constituents due to a pressurized pore space. Exploring beyond mean-field based theories in continuum microporomechanics, local textural variations and their contribution to the global anisotropic poroelastic behavior of real multiphase porous media are captured. To this end, statistical distributions of mesoscale poroelastic coefficients from numerical simulations on X-ray microscopy scans of two different organic-rich shales with different microtextures are presented. The results are compared with predictions using mean-field based tools of continuum micromechanics. The textural dependency of strain localization and stress chain formation captured in this framework promises a powerful tool for modeling poroelastic response of complex porous composites and a path to incorporate local textural and elastic variations into a continuum description.

\(^1\)Visiting Scientist, CNRS-MIT, MIT
John Marko, Northwestern University

**9:48AM R36.00010 Low-frequency oscillations in vibrated granular columns.** NICOLAS RIVAS, Helmholz Institute Erlangen-Nuremberg, ANTHONY THORNTON, KIT WINDOWS-YULE, University of Twente, DAVE PARKER, University of Birmingham, STEFAN LUDING, University of Twente — We present simulations, experiments and theoretical treatments of vertically vibrated granular media. The systems considered are quasi-one-dimensional. This column geometry makes it possible to study collective oscillations of the grains with a characteristic frequency that is much lower than the frequency of energy injection (LFOs). Using event-driven molecular dynamics simulations we see that LFOs become slower and more pronounced as the shaking of the container increases. Experimental observations, using the positron emission particle tracking technique, agree well with the simulated data. The conditions necessary for the existence of LFOs are derived from a granular continuum model, which is able to relate the column density profile with the measured characteristic frequencies.

**10:00AM R36.00011 Continuum model and simulation of segregating rods.** RICHARD M. LUEPTOW, Northwestern University, YONGZHI ZHAO, Zhejiang University, PAUL B. UMBANHOWAR, Northwestern University — Most studies of segregation of flowing granular materials focus on spherical particles, even though particles are often non-spherical in practical granular systems. Here we focus on the segregation of rod-like (cylindrical) particles of the same diameter but different lengths using continuum theory and DEM simulations based on super-ellipsoids. In the flowing layer of a bounded heap flow, a bidisperse mixture of long and short rods segregates such that the shorter rods percolate toward the lower portion of the flowing layer while longer rods rise toward the upper portion of the flowing layer, much like smaller spherical particles segregate from larger spherical particles. The rods tend to deposit on the underlying bed of particles in the heap such that they are aligned with the flow with the smaller rods deposited upstream of the larger rods due to segregation. The percolation velocities related to segregation for long and short rods depend on the local shear rate and the concentration of the other particle species, just as is the case for small and large spherical particles. Using this percolation velocity and an appropriate value for collisional diffusion, the advection-diffusion-segregation continuum model successfully predicts the segregation of rod-like particles.

**10:12AM R36.00012 Flow and packing properties of frictional shapes from spheres to cubes.** LEONARDO E. SILBERT, Southern Illinois University, K. MICHAEL SALERNO, DAN S. BOLINTINEANU, JEREMY B. LECHMAN, GARY GREST, Sandia National Laboratories — Though grains in many applications are aspherical and rough, many computational studies of granular flow and packing focus on ideal spherical particles, often without friction. Following Latham [1], we optimally represent arbitrary shapes using overlapping spheres of different sizes. We use discrete element simulations to study the packing and flow of frictional granular superquadric (superball) shapes ranging from spheres to cubes. When packing particles, friction becomes more important as particle shape becomes more angular. This leads to a larger density change between frictional and frictionless packings. Friction and shape are also important to granular flow. For a planar-shear flow different shapes have similar flow behavior in the zero-friction limit. However, with increasing friction particle shape couples to the tangential frictional forces and becomes more important. Flow results are compared with continuum theories of granular materials. Results from simulations of anisotropic particles and mixtures of shapes will also be discussed.


**10:24AM R36.00013 Scaling Relations for Wheeled Locomotion in Granular Media.** JAMES SLONAKER, KEN KAMRIN, MIT — Vehicular wheel design for use on granular material has not currently been perfected. Resistive Force Theory (RFT) is a reduced-order empirical model for granular drag, which shows promise to help simulate and understand locomotion processes to design more efficient wheels. Here we explore the fundamental relations derived from RFT and their experimental validation. Similar to the non-dimensional scaling relations in fluid mechanics, the relative simplicity of RFT asserts that only one material parameter, the “granule-structure coefficient”, is required, which reduces the complexity of the non-dimensional groups implied by the system. Therefore, wheels with differing input design parameters like size, mass, shape and even gravity, can be tested and their performance related to each other in predictable ways. We experimentally confirmed these relations by testing with 3D printed wheel geometries in a controlled sand bed.

**10:36AM R36.00014 Scaling of heat transfer in granular material.** YOHANNES, Rutgers University, HEATHER EMADY, Arizona State University, INGRID PARDES, MAHAM GLASSER, FERNANDO MUZZIO, ALBERTO CUATINO, Rutgers University — Several industrial processes involve granular solids, such as powders, in devices such as rotating drums, to bring about a desired chemical and/or physical transformation. This heat transfer process can significantly improve the quality of the end product and efficiency. However, there is a lack of predictive models, for example, to manufacturing scale productions. We used discrete element method (DEM) based simulations to study the evolution of the distribution and average of the particles’ temperature, particularly for the purpose of scale-up from laboratory scale experiments to manufacturing scale productions. We identified timescales relevant to the heat transfer process and developed a relationship between these timescales and temperature of particles. We also found that the evolution of the temperature distribution, since different particles are expected to have different heat transfer rates, can be predicted based on these timescales. These findings can be used to predict the required time to heat up all particles to the desired temperature.

**10:48AM R36.00015 Structural evolution of Colloidal Gels under Flow.** ARMAN BOROMAND, JOAO MAIA, Case Western Reserve University, SAFA JAMALI, Massachusetts Institute of Technology — Colloidal suspensions are ubiquitous in different industrial applications ranging from cosmetic and food industries to soft robotics and aerospace. Owing to the fact that mechanical properties of colloidal gels are controlled by its microstructure and network topology, we trace the particles in the networks formed under different attraction potentials and try to find a universal behavior in yielding of colloidal gels. Many authors have implemented different simulation techniques such as molecular dynamics (MD) and Brownian dynamics (BD) to capture better picture during phase separation and yielding mechanism in colloidal system with short-ranged attractive force. However, BD neglects multi-body hydrodynamic interactions (HI) which are believed to be responsible for the second yielding of colloidal gels. We envision using dissipative particle dynamics (DPD) with modified depletion potential and hydrodynamic interactions, as a coarse-grain model, can provide a robust simulation package to address the gel formation process and yielding in short ranged-attractive colloidal systems. The behavior of colloidal gels with different attraction potentials is not well understood due to multi-body hydrodynamic interactions (HI) which are believed to be responsible for the second yielding of colloidal gels. We envision using dissipative particle dynamics (DPD) with modified depletion potential and hydrodynamic interactions, as a coarse-grain model, can provide a robust simulation package to address the gel formation process and yielding in short ranged-attractive colloidal systems. The behavior of colloidal gels with different attraction potentials is not well understood due to multi-body hydrodynamic interactions (HI) which are believed to be responsible for the second yielding of colloidal gels.

**Thursday, March 17, 2016 8:00AM - 11:00AM**

Session R39 DBIO DPOLY GSNP: Physics of Genome Organization: from DNA to Chromatin
8:00AM R39.00001 New insights into chromatin folding and dynamics from multi-scale modeling1. WILMA OLSON, Rutgers, the State University of New Jersey — The dynamic organization of chromatin plays an essential role in the regulation of gene expression and in other fundamental cellular processes. The underlying physical basis of these activities lies in the sequential positioning, chemical composition, and intermolecular interactions of the nucleosomes—the familiar assemblies of roughly 150 DNA base pairs and eight histone proteins—found on chromatin fibers. We have developed a mesoscale model of short nucleosomal arrays and a computational framework that make it possible to incorporate detailed structural features of DNA and histones in simulations of short chromatin constructs with 3-25 evenly spaced nucleosomes. The correspondence between the predicted and observed effects of nucleosome composition, spacing, and numbers on long-range communication between regulatory proteins bound to the ends of designed nucleosome arrays lends credence to the model and to the molecular insights gleaned from the simulated structures. We have extracted effective nucleosome-nucleosome potentials from the mesoscale simulations and introduced the potentials in a larger scale computational treatment of regularly repeating chromatin fibers. Our results reveal a remarkable influence of nucleosome spacing on chromatin flexibility. Small changes in the length of the DNA fragments linking successive nucleosomes introduce marked changes in the local interactions of the nucleosomes and in the spatial configurations of the fiber as a whole. The changes in nucleosome positioning influence the statistical properties of longer chromatin constructs with 100-10,000 nucleosomes. We are investigating the extent to which the ‘local’ interactions of regularly spaced nucleosomes contribute to the corresponding interactions in chains with mixed spacings as a step toward the treatment of fibers with nucleosomes positioned at the sites mapped at base-pair resolution on genomic sequences.

1Support of the work by USPHS R01 GM 34809 is gratefully acknowledged.

8:36AM R39.00002 Mitotic chromosome compaction via active loop extrusion1. ANTON GOLOBORODKO, MAXIM IMAKAEV, Massachusetts Inst of Tech-MIT, JOHN MARKO, Northwestern University, LEONID MIRNY, Massachusetts Inst of Tech-MIT, MIT-NORTHEASTERN TEAM — During cell division, two copies of each chromosome are segregated from each other and compacted more than hundred-fold into the canonical X-shaped structures. According to earlier microscopic observations and the recent Hi-C study, chromosomes are compacted into arrays of consecutive loops of ~100 kilobases. Mechanisms that lead to formation of such loop arrays are largely unknown. Here we propose that, during cell division, chromosomes can be compacted by enzymes that extrude loops on chromatin fibers. First, we use computer simulations and analytical modeling to show that a system of loop-extruding enzymes on a chromatin fiber self-organizes into an array of consecutive dynamic loops. Second, we model the process of loop extrusion in 3D and show that, coupled with the topo II strand-passing activity, it leads to robust compaction and segregation of sister chromatids. This mechanism of chromosomal condensation and segregation does not require additional proteins or specific DNA markup and is robust against variations in the number and properties of such loop extruding enzymes.

8:48AM R39.00003 Multiscale modeling of three-dimensional genome, BIN ZHANG, PETER WOLYNES, Rice University — The genome, the blueprint of life, contains nearly all the information needed to build and maintain an entire organism. A comprehensive understanding of the genome is of paramount interest to human health and will advance progress in many areas, including life sciences, medicine, and biotechnology. The overarching goal of my research is to understand the structure-dynamics-function relationships of the human genome. In this talk, I will present our efforts in moving towards that goal, with a particular emphasis on studying the three-dimensional organization, the structure of the genome under conditions of interphase and metaphase. Specifically, I will discuss the reconstruction of genome structures at both interphase and metaphase by making use of data from the latest experiments. Computationally modeling of chromatin fiber at atomic level from first principles will also be presented as our effort for studying the genome structure from bottom up.


9:12AM R39.00005 Elucidate Chromatin Folding at the Mesoscale, XIANGYUN QIU, George Washington Univ — Knowledge of the three-dimensional structure of chromatin, an active participant of all gene-directed processes, is required to decode its (epi)genetics-structure-function relationships. Albeit often simplified as “beads-on-a-string”, chromatin possesses daunting complexity in its intricate intra- and inter-nucleosome interactions, as well as the myriad ways of molecules acting on it. On the other hand, the folding of chromatin from an extended chain of nucleosomes is highly constrained, e.g., by rather bulky nucleosomes and semi-rigid linker dsDNAs. Further given the well-defined nucleosome and dsDNA structures at the nanometer scale, this creates an opportunity for low-resolution structural methods such as small angle scattering to obtain mesoscale structures of chromatin, which can be further refined computationally to yield atomic structures of chromatin. Here we present results from our recent studies of recombinant nucleosome arrays with solution small angle x-ray scattering (SAXS) and ensemble structure modeling.

9:24AM R39.00006 Formation of chromosomal domains in interphase by loop extrusion, GEOFFREY FUDENBERG, MIT — While genomes are often considered as one-dimensional sequences, interphase chromosomes are organized in three dimensions with an essential role for regulating gene expression. Recent studies have shown that Topologically Associating Domains (TADs) are fundamental structural and functional building blocks of human interphase chromosomes. Despite observations that architectural proteins, including CTCF, demarcate and maintain the borders of TADs, the mechanisms underlying TAD formation remain unknown. Here we propose that loop extrusion underlies the formation of TADs. In this process, cis-acting loop-extruding factors, likely cohesins, form progressively larger loops, but stall at TAD boundaries due to interactions with boundary proteins, including CTCF. This process dynamically forms loops of various sizes within but not between TADs. Using polymer simulations, we find that loop extrusion can produce TADs as determined by our analyses of the highest-resolution experimental data. Moreover, we find that loop extrusion can explain many diverse experimental observations, including: the preferential orientation of CTCF motifs and enrichments of architectural proteins at TAD boundaries; TAD boundary deletion experiments; and experiments with knock-down or deletion of CTCF, cohesins, and cohesin-loading factors. Together, the emerging picture from our work is that TADs are formed by rapidly associating, growing, and dissociating loops, presenting a clear framework for understanding interphase chromosomal organization.

Robustness of nucleosome patterns in the presence of DNA sequence-specific free energy landscapes and active remodeling

Johannes Nuebler, Physik-Department, Technische Universität München — Proper positioning of nucleosomes in eukaryotic cells is important for transcription regulation. When averaged over many genes, nucleosome positions in coding regions follow a simple oscillatory pattern, which is described by a surprising degree of accuracy by a simple one-dimensional gas model for particles interacting via a soft-core repulsion. The quantitative agreement is surprising given that nucleosome positions are known to be determined by a complex interplay of mechanisms including DNA sequence-specific nucleosome stability and active repositioning of nucleosomes by remodeling enzymes. We rationalize the observed robustness of the simple oscillatory pattern by showing that the main effect of several known nucleosome positioning mechanisms is a renormalization of the particle interaction. For example, disorder from sequence-specific affinities leads to an apparent softening, while active remodeling can result in apparent softening for directional sliding or apparent stiffening for clamping mechanisms. We suggest that such parameter renormalization can explain the apparent difference of nucleosome properties in two yeast species, S. cerevisiae and S. pombe.

The role of nucleosome positions on chromatin structure: A multi-scale approach

Joshua Lequieu, Andres Cordero, Juan J. de Pablo, University of Chicago — Nucleosomes compose the basic unit of chromatin, and their locations are central to the regulation and compaction of eukaryotic genomes. In this work, we examine the coupling between different length scales within chromatin by examining the influence of nucleosome positions on three-dimensional chromatin structure. First, using a detailed molecular model of DNA and proteins, we predict the one-dimensional positioning of nucleosomes and the repositioning mechanisms of nucleosomal DNA. We demonstrate that this mechanism is strongly dependent on DNA sequence and that DNA slides around the histone proteins by either a screw-like or loop-like rearrangement. Next, we couple this detailed model to a coarsened model of chromatin and examine the impact of DNA sequence on chromatin’s three-dimensional structure. We show that both the locations of nucleosomes and the mechanisms by which they move have a significant impact on higher-order chromatin structure and that variations in DNA sequence lead to “open” or “closed” regions of chromatin. This approach represents an efficient tool towards understanding the higher order structure of chromatin and how various aspects of chromatin structure are coupled together.

Chromatin extrusion explains key features of loop and domain formation in wild-type and engineered genomes

Adrian Sandborn, Suhas Rao, Stanford, Su-Chen Huang, Neva Durand, Miriam Huntley, Andrew Jewett, Ivan Bochkov, Dharmaráj Chinnappan, Ashok Cutkosky, Jian Li, Kristopher Geeting, Doug McKenna, Elena Stamenova, Baylor College of Medicine, Andreas Giritke, Alexandre Melnikov, Eric Landers, Broad Institute, Erez Aiden, Baylor College of Medicine — Our recent kilobase-resolution genome-wide maps of DNA self-contacts demonstrated that mammalian genomes are organized into domains and loops demarcated by the DNA-binding protein CTCF. Here, we combine these maps with new Hi-C, microscopy, and genome-editing experiments to study the physical structure of chromatin fibers, domains, and loops. We find that domains are inconsistent with equilibrium and fractal models. Instead, we use physical simulations to study two models of genome folding. In one, intermonomer attraction during condensation leads to formation of an anisotropic “tension globule.” In the other, CTCF and cohesin act together to extrude unknotted loops. Both models are consistent with the observed domains and loops. However, the extrusion model explains a far wider array of observations, such as why the CTCF-binding motifs at pairs of loop anchors lie in the convergent orientation. Finally, we perform 13 genome-editing experiments examining the effect of altering CTCF-binding sites on chromatin folding. The extrusion model predicts in silico the experimental maps using only CTCF-binding sites. Thus, we show that it is possible to disrupt, restore, and move loops and domains using targeted mutations as small as a single base pair.

Kinetic roughening: how directionality changes the game

Nuno Araujo, Universidade de Lisboa — The nonequilibrium evolution of growing interfaces has attracted many experimental and theoretical studies over decades. One of the most popular theoretical approaches considers kinetic discrete models to describe particle aggregation on substrates. Albeit simple, these models are expected to contain the relevant physics. Inspired by recent advances in the production of functionalized colloidal particles, with attractive patches on their surface, we have proposed a stochastic model to study the effect of directionality and selective pairwise interactions on the kinetics of aggregation. We find a nontrivial dependence of the bulk and surface properties on the strength and flexibility of the patch-patch interactions, and on the spatial-patch distribution. For three-patch particles, sustained growth is only observed for a finite-range of the distance between patches, yielding two absorbing phase transitions and a tricritical flexibility. For four-patch particles with two distinct patches, i.e. strong and weak bonds, and sufficiently different bonding probabilities, the scaling properties of the interface crossover from the universality class of Kardar-Parisi-Zhang to the critical class of Kardar-Parisi-Zhang with quenched disorder. The latter is observed for an extended range of the parameters revealing the presence of a self-organized critical mechanism. Implications of our findings beyond functionalized particles are also discussed.

Exactly solvable models of growing interfaces: the Arcetri models

Xavier Durang, Korean Institute for Advanced Study, Malte Henkel, Université de Lorraine, France — Motivated by an analogy with the spherical model of a ferromagnet, the Arcetri models present new universality classes for the growth of interfaces, distinct from the common Edwards-Wilkinson and Kardar-Parisi-Zhang universality classes. Those models are obtained by treating and replacing the non-linear term in the noisy Burgers equation or the KPZ equation by a mean spherical condition. We studied the observability of such constraints on the Edwards-Wilkinson (EW) interface.
1:00AM R40.00004 Random field disorder at an absorbing state transition in one and two dimensions1, HATEM BARGHATHI, THOMAS VOJTA, Missouri S&T — We investigate the behavior of nonequilibrium phase transitions under the influence of disorder that locally breaks the symmetry between two symmetrical macroscopic absorbing states. In equilibrium systems such “random-field” disorder destroys the phase transition in low dimensions by preventing spontaneous symmetry breaking. In contrast, we show here that random-field disorder fails to destroy the nonequilibrium phase transition of the one- and two-dimensional generalized contact process. Instead, it hampers the dynamics in the symmetry-broken phase. Specifically, the dynamics in the one-dimensional case is described by a Sinai walk of the domain walls between two different absorbing states. In the two-dimensional case, we map the dynamics onto that of the well studied low-temperature random-field Ising model. We also study the critical behavior of the nonequilibrium phase transition and characterize its universality class in one dimension. We support our results by large-scale Monte-Carlo simulations and discuss the applicability of our theory to other systems.

1This work was supported by the NSF under Grants No. DMR-1205803

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9:12AM R40.00005 Leveraging large fluctuations for stochastic control in uncertain environments1, IRA SCHWARTZ2, Naval Research Lab, CHRISTOFFER HECKMAN, University of Colorado, M. ANI HSIEH, Drexel University — We present the development of a stochastic control strategy that leverages the environmental dynamics and uncertainty to navigate in a stochastic fluidic environment. We assume that the domain is composed of the union of a collection of disjoint regions, each bounded by Lagrangian coherent structures (LCSs). We analyze a passive particle’s noise-induced transition between adjacent LCS-bounded regions and show how most probable escape trajectories with respect to the transition probability between adjacent LCS-bound regions can be determined. Additionally, we show how the likelihood of transition can be controlled through minimal actuation. The result is an energy efficient navigation strategy that leverages the inherent uncertainty of the surrounding flow field for controlling sensors in a noisy fluidic environment. We experimentally validate the proposed control strategy and show that the single vehicle control parameter exhibits a predictable exponential scaling with respect to the escape times and is effective even in situations where the structure of the flow is not fully known and control effort is costly.

1IBS supported by ONR nos. F1ATA01098G001, N0001412WX-20083. MAH by ONR award numbers N000141211019 and N0001413-10731.
2Nonlinear Systems Dynamics Section, Code 6792, Washington, DC 20375 USA

9:24AM R40.00006 Flux line non-equilibrium relaxation kinetics following current quenches in disordered type-II superconductors1, HARSHWARDHAN CHATURVEDI, HIBA ASSI, Department of Physics, Virginia Tech, ULRICH DOBRAMYSY, The Gurdon Institute, University of Cambridge, U.K., MICHEL PLEIMLING, UWE TAUBER, Department of Physics, Virginia Tech — We investigate the relaxation dynamics of magnetic vortex lines in disordered type-II superconductors following rapid changes in the external driving current by means of Langevin molecular dynamics simulations for an elastic line model. A system of driven interacting flux lines in a sample with randomly distributed point pinning centers is initially relaxed to a moving non-equilibrium steady state. The current is then instantaneously decreased, such that the final stationary state resides either still in the moving regime, or in the pinned Bragg glass phase. The ensuing non-equilibrium relaxation kinetics of the vortices is studied in detail by measuring the mean flux line gyration radius and the two-time transverse height autocorrelation function. The latter allows us to investigate the physical aging properties for quenches from the moving into the glassy phase, and to compare with non-equilibrium relaxation features obtained with different initial configurations.

1Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

9:36AM R40.00007 Local temperatures and voltages in quantum systems far from equilibrium1, ABHAY SHASTRY, CHARLES STAFFORD, University of Arizona, DEPARTMENT OF PHYSICS COLLABORATION — We show that the local measurement of temperature and voltage for a quantum system in steady state, arbitrarily far from equilibrium, with arbitrary interactions within the system, is unique when it exists. This is interpreted as a consequence of the second law of thermodynamics. We further derive a necessary and sufficient condition for the existence of a solution. In this regard, we find that a solution occurs whenever there is no net population inversion. However, when there is a net population inversion, we may characterize the system with a (unique) negative temperature. These results provide a firm mathematical foundation for our measurement protocol, and sound meaning to such measurements in the thermodynamic sense.

1Research supported by the US Department of Energy, grant DE-SC 0006699
trajectories in the system phase space. At long times, the area tensor scales linearly with time, with a coefficient that precisely vanishes when the system satisfies the associated Langevin equation. To better characterize fluctuation loops, we study the time-dependent area tensor that is swept out by individual stochastic optimal fluctuation pathways, and construct corresponding fluctuation loops. Analytical results agree closely with suitably averaged simulation results based on own noise source and, generally, the effective noise strengths of different elements are not equal. Using a stochastic Hamiltonian approach, we determine the

AKHIL GHANTA, JOHN NEU, Duke University — Understanding the spatio-temporal structure of most probable fluctuation pathways to rarely occurring states in a non-integrable quantum spin chain, CHENG-JU LIN, OLEXEI MOTRUNICH, Caltech — Eigenstate Thermalization Hypothesis provides one picture of thermalization in a quantum system by looking at individual eigenstates. However, it is also important to consider how local observables reach equilibrium values dynamically. Quench protocol is one of the settings to study such questions. A recent numerical study [Banuls, Cirac, and Hastings, Phys. Rev. Lett. 106, 050405 (2011)] of a nonintegrable quantum Ising model with longitudinal field under such quench setting found different behaviors under different initial quantum states. One particular case termed weak thermalization regime showed apparently persistent oscillations of some observables. Here we provide an explanation of such oscillations. We use perturbation theory near the ground state of the model, and identify the oscillation frequency as the quasiparticle mass. With this quasiparticle picture, we can then address the long-time behavior of the oscillations.

10:00AM R40.00009 How can an autonomous quantum Maxwell demon harness correlated information?, ADRIAN CHAPMAN, AKIMASA MIYAKE, Univ of New Mexico, CQUIC THERMODYNAMICS TEAM — We study an autonomous quantum system, which exhibits refrigeration under an information-work tradeoff like a Maxwell demon. The system becomes correlated as a single demon qubit interacts sequentially with memory qubits while in contact with two heat reservoirs of different temperatures. Using strong subadditivity of the von Neumann entropy, we derive a global Clausius inequality to show thermodynamical advantages from access to correlated information. It is demonstrated, in a matrix product density operator formalism, that our demon can simultaneously realize refrigeration against a thermal gradient and erasure of information from its memory, which is impossible without correlations. The phenomenon can be even enhanced by the presence of quantum coherence.

1The work was supported in part by National Science Foundation grants PHY-1212445 and PHY-1521016.

10:12AM R40.00010 Fano-Andreev effect in Quantum Dots in Kondo regime, PEDRO ORELLANA, ANA MARIA CALLE, MONICA PACHECO, Universidad Tecnica Federico Santa Maria, VICTOR APEL, Universidad Catlica del Norte — In the present work, we investigate the transport through a T-shaped double quantum dot system coupled to two normal leads and to a superconducting lead. We study the role of the superconducting lead in the quantum interferometric features of the double quantum dot and by means of a slave boson mean field approximation at low temperature regime. We inquire into the influence of intradot interactions in the electronic properties of the system as well. Our results show that Fano resonances due to Andreev bound states are exhibited in the transmission from normal to normal lead as a consequence of quantum interference and proximity effect. This Fano effect produced by Andreev bound states in a side quantum dot was called Fano-Andreev effect, which remains valid even if the electron-electron interaction are taken into account, that is, the Fano-Andreev effect is robust against e-e interactions even in Kondo regime.

1We acknowledge the financial support from FONDECYT program Grants No. 3140053 and 11400571

10:24AM R40.00011 Quantum critical temperature of a modulated oscillator, VITTORIO PEANO, University of Erlangen-Nurnberg, LINGZHEN GUO, MICHAEL MARTHALER, Karlsruhe Institute of Technology, MARK DYKMAN, Michigan State University — We show that the rate of switching between the vibrational states of a modulated nonlinear oscillator is characterized by a quantum critical temperature $T_c \propto h^2$. Above $T_c$ there emerges a quantum crossover region where the switching rate displays a steep and characteristic temperature dependence, followed by a qualitatively different temperature dependence for higher $T$. In contrast to the crossover between tunneling and thermal activation in equilibrium systems, here the crossover occurs between different regimes of switching activated by quantum fluctuations. The results go beyond the standard real-time instanton technique of the large-deviation theory.

10:36AM R40.00012 The interplay between universal scaling laws and vortex clustering in two-dimensional quantum turbulence, AUDUN SKAUGEN, LUIZA ANGHELUTA, Univ of Oslo — The relationship between vortex dynamics and the turbulent energy spectrum is an active research topic in quantum turbulence of superfluids and Bose-Einstein condensates. The energy spectra in quantum turbulence exhibit a Kolmogorov -5/3 scaling law, analogous to classical turbulence. Recent developments show that in two-dimensional quantum flows, this energy spectrum corresponds to an inverse energy cascade, which is realized by clustering of like-signed quantized vortices. We investigate numerically the statistics of quantized vortices in two-dimensional quantum turbulence using the Gross-Pitaevskii equation. We find that a universal -5/3 scaling law in the turbulent energy spectrum is intimately connected with the vortex statistics, such as number fluctuations and velocity, which also show a similar scaling behavior. The -5/3 scaling law appearing in the power spectrum of the vortex number is consistent with a scenario of isolated vortices passively advected by a turbulent superfluid velocity, which is again generated by like-signed vortex clusters. The velocity probability distribution of clustered vortices is also sensitive to spatial correlations, and exhibits a power-law tail with a -5/3 exponent that we can predict analytically from the point vortex model.

10:48AM R40.00013 Fluctuation loops in a noise-driven linear circuit model, STEPHEN TEITSWORTH, AKHIL GHANTA, JOHN NEU, Duke University — Understanding the spatio-temporal structure of most probable fluctuation pathways to rarely occurring states is a central problem in the study of noise-driven, non-equilibrium dynamical systems. When the underlying system does not possess detailed balance, the optimal fluctuation pathway to a particular state and relaxation pathway from that state may combine to form a loop-like structure in the system phase space which we call a fluctuation loop. Here, we study fluctuation loops in a linear circuit model consisting of coupled RC elements, where each element is driven by its own noise source and, generally, the effective noise strengths of different elements are not equal. Using a stochastic Hamiltonian approach, we determine the optimal fluctuation pathways, and construct corresponding fluctuation loops. Analytical results agree closely with suitably averaged simulation results based on the associated Langevin equation. To better characterize fluctuation loops, we study the time-dependent area tensor that is swept out by individual stochastic trajectories in the system phase space. At long times, the area tensor scales linearly with time, with a coefficient that precisely vanishes when the system satisfies detailed balance.

Thursday, March 17, 2016 8:00AM - 10:48AM –
Session R43 GSNP: Nonlinear Dynamics in Networks I
Coupled Oscillators

of semi-passive oscillators. To obtain a bound tighter than those previously reported. We extend both analyses to a homogeneous FN network with heterogeneous inputs and show how inputs. We first apply a passivity-based Lyapunov analysis to undirected networks of homogeneous FitzHugh-Nagumo (FN) oscillators with homogeneous inputs synchronization, we investigate synchronous firing patterns in arbitrary networks of neuronal oscillators coupled through gap junctions with heterogeneous external inputs. Studies of synchronization in networks of neuronal oscillators offer insight into neuronal ensemble behavior in the brain. Systematic means to understand how network structure and external input affect synchronization in network models have the potential to improve methods for treating synchronization-related neurological disorders such as epilepsy and Parkinson’s disease. To elucidate the complex relationships between network structure, external input, and synchronization, we investigate synchronous firing patterns in arbitrary networks of neuronal oscillators coupled through gap junctions with heterogeneous external inputs. We first provide a deeper understanding of how to synchronize heavy jet lag symptoms. [1] Y. Yamaguchi, T. Suzuki, Y. Mizoro, H. Kori, K. Okada, Y. Chen, J.M. Fustin, F. Yamazaki, N. Mizuguchi, J. Zhang, X. Dong. G. Tsujimoto, Y. Okuno, M. Doi, H. Okamura: Mice Genetically Deficient in Vasopressin V1a and V1b Receptors Are Resistant to Jet Lag. Science 342, pp. 85-90 (2013).

Moreover, when intercellular interaction is weaker, this desynchrony is suppressed and the recover from jet lag is considerably accelerated. Our mathematical simplicity, this model can reproduce important dynamical properties of the SCN. For example, this model reproduces the desynchrony of oscillators after jet lag. Strikingly, we find that increasing the noise level in the input to the individual neurons form a complex network and interact with each other using various types of neurotransmitters. The rhythmic gene expressions of individual cells in the called the suprachiasmatic nucleus (SCN). The SCN consists of a population of neurons, each of which exhibit circadian (i.e., approximately 24 h) gene expression. Thus, the synchronization of the network rhythms differs qualitatively from that of individual oscillators. Therefore, changing the noise level in the input to the individual subnetworks can become synchronized and each subnetwork can exhibit coherent oscillatory dynamics, e.g., an ING-rhythm. In the absence of coupling between the networks the rhythms will in general have different frequencies. We investigate the interaction between these different rhythms. Strikingly, we find that increasing the noise level in the input to the individual neurons can synchronize the rhythms of the two networks, even though the inputs to different neurons are uncorrelated, sharing no common component. A heuristic phase model for the coupled network showed that this synchronization hinges on the fact that only a fraction of the neurons may spike in a given cycle. Thus, the synchronization of the network rhythms differs qualitatively from that of individual oscillators.

Supported by NSF-CMMI 1435358

9:00AM R43.00004 A simple experimental realization of the Sakaguchi-Kuramoto model. DAVID MERTENS, ZHUWEI ZENG, LARS ENGLISH, Dickinson College — We explore the collective phase dynamics of Wien-bridge oscillators coupled resistively. The dynamics of these oscillators were recently shown to follow Sakaguchi’s modification to the Kuramoto model. In this talk we outline the steps of that analysis. We then examine results for a variety of experimentally obtained coupling arrangements, including all-to-all and some-to-all. In particular, we provide evidence for the emergence of synchronized clusters, a finite-size effect that is not accounted for in the traditional theories for the Sakaguchi-Kuramoto model.

9:12AM R43.00005 Experimental studies of a chain of Sakaguchi-Kuramoto oscillators. HANYU MA, DAVID MERTENS, LARS ENGLISH, Dickinson College, HANYU MA TEAM, LARS ENGLISH COLLABORATION, DAVID MERTENS COLLABORATION — The collective phase dynamics of Wien-bridge oscillators, coupled resistively, were recently shown to follow the Sakaguchi-Kuramoto model. In this talk we present experimental findings for the dynamics of rings of oscillators. For identical speeds and uni-directional nearest-neighbor coupling, we find that the system quickly approaches a steady state of identical nearest-neighbor phase offsets. We then present the effects of adding disorder to the natural speeds. We also discuss the case of bi-directional coupling, in which case chimera behavior is expected.

9:24AM R43.00006 Title: Chimeras in small, globally coupled networks: Experiments and stability analysis. JOSEPH D. HART, University of Maryland, College Park, KANIKI BANSAL, None, THOMAS E. MURPHY, RAJRASHI ROY, University of Maryland, College Park — Since the initial observation of chimera states, there has been much discussion of the conditions under which these states emerge. The emphasis thus far has mainly been to analyze large networks of coupled oscillators; however, recent studies have begun to focus on the opposite limit: what is the smallest system of coupled oscillators in which chimeras can exist? We experimentally observe chimeras and other partially synchronous patterns in a network of four globally-coupled chaotic opto-electronic oscillators. By examining the equations of motion, we demonstrate that symmetries in the network topology allow a variety of synchronous states to exist, including cluster synchronous states and a chimera state. Using the group theoretical approach recently developed for analyzing cluster synchronization, we show how to derive the variational equations for these synchronous patterns and calculate their linearity stability. The stability analysis gives good agreement with our experimental results. Both experiments and simulations suggest that these chimera states often appear in regions of multistability between global, cluster, and desynchronized states.

9:36AM R43.00007 ABSTRACT WITHDRAWN

9:48AM R43.00008 Emerging hierarchies in dynamically adapting webs. ELENI KATIFORI, University of Pennsylvania, JOHANNES GRAUER, Max-Planck Institute for Dynamics and Self-Organization, MARCELO MAGNASCO, CARL MODES, Rockefeller University — Transport networks play a key role across four realms of eukaryotic life: slime molds, fungi, plants, and animals. In addition to the developmental algorithms that build them, many also employ adaptive strategies to respond to stimuli, damage, and other environmental changes. We model these adapting network architectures using a generic dynamical system on weighted graphs and find in simulation that these networks ultimately develop a hierarchical organization of the final weighted architecture accompanied by the formation of a system-spanning backbone. We quantify the hierarchical organization of the networks by developing an algorithm that decomposes the architecture to multiple scales and analyzes how the organization in each scale relates to that of the scale above and below it. The methodologies developed in this work are applicable to a wide range of systems including the slime mold physarum polycelphalum, human microvasculature, and force chains in granular media.
10:00AM R43.00009 Hybrid percolation transition in complex networks, BYUNG NAM KAHNG, Seoul National University — Percolation has been one of the most applied statistical models. Percolation transition is one of the most robust continuous transitions known thus far. However, recent extensive researches reveal that it exhibits diverse types of phase transitions such as discontinuous and hybrid phase transitions. Here hybrid phase transition means the phase transition exhibiting natures of both continuous and discontinuous phase transitions simultaneously. Examples include k-core percolation, cascading failures in interdependent networks, synchronization, etc. Thus far, it is not manifest if the critical behavior of hybrid percolation transitions conforms to the conventional scaling laws of second-order phase transition. Here, we investigate the critical behaviors of hybrid percolation transitions in the cascading failure model in inter-dependent networks and the restricted Erdos-Renyi model. We find that the critical behaviors of the hybrid percolation transitions contain some features that cannot be described by the conventional theory of second-order percolation transitions.

10:12AM R43.00010 Phase Transitions in Networks of Memristive Elements, FORREST SHELDON, MASSIMILIANO DI VENTRA, Univ of California - San Diego — The memory features of memristive elements (resistors with memory), analogous to those found in biological synapses, have spurred the development of neuromorphic systems based on them (see, e.g., [1]). In turn, this requires a fundamental understanding of the collective dynamics of networks of memristive systems. Here, we study an experimentally-inspired model of disordered memristive networks in the limit of a slowly ramped voltage and show through simulations that these networks undergo a first-order phase transition in the conductivity for sufficiently high values of memory, as quantified by the memristive ON/OFF ratio. We provide also a mean-field theory that reproduces many features of the transition and particularly examine the role of boundary conditions and current- vs. voltage-controlled networks. The dynamics of the mean-field theory suggest a distribution of conductance jumps which may be accessible experimentally. We finally discuss the ability of these networks to support massively-parallel computation. Work supported in part by the Center for Memory and Recording Research at UCSD. [1] Y.V. Pershin and M. Di Ventra, Proc. IEEE, 100, 2071 (2012).

10:24AM R43.00011 ABSTRACT WITHDRAWN

10:36AM R43.00012 A network model of human aging: Limits, errors, and information, SPENCER FARRELL, ARNOLD MITNITSKI, KENNETH ROCKWOOD, ANDREW RUTENBERG, Dalhousie University — The Frailty Index (FI) quantifies human aging using the fraction of accumulated age-related deficits. The FI correlates strongly with mortality and accumulates non-linearly and stochastically with age. Clinical data shows a nearly universal limit of FI ≤ 0.7. We computationally model an aging population using a network model of interacting deficits. Deficits damage and repair at rates that depend upon the average damage of connected nodes. The model is parametrized to fit clinical data. We find that attribution errors, especially false negative, allow the model to recover the frailty limit. Mutual information allows us to assess how well the FI can predict mortality. Mutual information provides a non-parametric measure of how the FI predicts mortality. We find that attribution errors have a small effect on the mutual information when many deficits are included in the model. The mutual information of our model and of the clinical data are comparable.

Thursday, March 17, 2016 11:15AM - 1:51PM

Session S35 DBIO GSOFT GSNP: Active Matter: Collective Phenomena in Living Systems IV

11:15AM S35.00001 Fluid flows created by swimming bacteria drive self-organization in confined suspensions, ENKELEIDA LUSHI, Brown University, HUGO WIOLAND, Institut Jacques Monod, Paris 7 Diderot , RAYMOND GOLDSTEIN, DAMTP, University of Cambridge — Concentrated suspensions of micro-swimmers can display intricate self-organized spatiotemporal patterns on scales larger than those of the individual motile units. The collective dynamics of swimming microorganisms exhibits a complex interplay with the surrounding fluid: the motile cells stir the fluid, which in turn can reorient and advect them. This feedback loop can result in long-range interactions between the cells. We present a computational model that takes into account these cell-fluid interactions and cell-cell forces and that predicts counterintuitive cellular order driven by long-range flows. The predictions are confirmed by new experiments with Bacillus Subtilis bacteria. Simulations and experiments show that if the micro-swimmers are confined inside thin cylindrical chambers the suspension self-organizes into a stable swirling vortex. If the micro-swimmers are confined in thin racetracks, a persistent unidirectional stream can emerge. Both these phenomena emerge as a result of the complex interplay between the swimmers, the specific confining boundaries and the fluid flow.

11:27AM S35.00002 Fluid flow in monolayers: Cells under pressure, KYLE SCHULZE, STEVEN ZEHNDER, GREG SAWYER, THOMAS ANGELINI, University of Florida — Number density fluctuations are intimately tied to collective behavior in particulate soft matter and active matter systems, including tissue cell monolayers. In cell monolayers, there is no free space between cells, so density fluctuations must involve either out of plane motion, or cell volume fluctuations. Recent work has shown that cells fluctuate in volume to accommodate collective density fluctuations, and that fluid moves between cells in this process. However, measurements of the resistance to this flow with controlled applied pressures have never been performed. Here we apply pressure to local regions in cell monolayers with an indentation instrument mounted on an inverted microscope. While simultaneously measuring contact area, indentation depth, and applied force as a function of time we determine a compression modulus and a permeability of cells. We find that cells are highly permeable, and that cytoskeleton-generated stresses are large enough to drive fluid from cell to cell as they spontaneously fluctuate in volume.

11:39AM S35.00003 Hydrodynamic interactions and their role on the dynamics of bacterial predators, HOSSEIN JASHNSAZ, Physics Department, IUPUI, Indianapolis, IN 46202, MOHAMMED AL JUBOORI, Biomedical Engineering, IUPUI, Indianapolis, IN 46202, COREY WEISTUCH, Department of Applied Mathematics and Statistics, Stony Brook University, Stony Brook, NY 11794, TYLER NGUYEN, Stark Neurosciences Research Institute, IUSM, Indianapolis, IN 46202, NICK MILLER, Biomedical Engineering, IUPUI, Indianapolis, IN 46202, VIK-TORIA MEYERHOFF, Mechanical Engineering, IUPUI, Indianapolis, IN 46202, KYLE PROCTOR, BRYAN MCCOY, Biological Chemistry, IUPUI, Indianapolis, IN 46202, STEVE PRESSE, Physics Department, IUPUI, Indianapolis, IN 46202 — We consider the effects of hydrodynamics on the behavior of bacterial predators searching for bacterial prey. Experimentally, we find that bacterial predators respond to external flow fields in addition to responding to their own self-generated flow fields neighboring surfaces and finite boundaries. We will discuss the implications of this finding on bacterial hunting strategies. 

1 SP acknowledges the NSF (MCB 1412259) and a Graduate Student Imaging Research Fellowship from the IUPUI Office of the Vice Chancellor for Research.
characterizing active fluids using concepts drawn from classical thermodynamics.

12:03PM S35.00005 Discontinuous fluidization transition in dense suspensions of actively deforming particles, ELSEN T JHUNG, Univ of Cambridge, LUDOVIC BERTHIER, CNRS, Universite Montpellier — Collective dynamics of self-propelled particles at high density have been shown to display a glass-like transition with a critical slowing down of 2 to 4 orders of magnitude. In this talk, we propose a new mechanism of injecting energy or activity via volume fluctuations. We uncover an anomalous coupling between the translational and rotational degrees of freedom that is strictly prohibited in the classical Brownian diffusion.

12:15PM S35.00006 Superfluid-like dynamics in active vortex fluids, JONASZ SLOMKA, JORN DUNKEL, Massachusetts Inst of Tech-MIT — Active biological fluids exhibit rich non-equilibrium dynamics and share striking similarities with quantum fluids, from vortex formation and magnetic ordering to superfluid-like behavior. Building on universality ideas, we have recently proposed a generalization of the Navier–Stokes equations that captures qualitatively the active bulk flow structures observed in bacterial suspensions. Here, we present new numerical simulations that explicitly account for boundary and shear effects. The theory successfully reproduces recent experimental observations of bacterial suspensions, including a superfluid-like regime of nearly vanishing shear viscosity. Our simulations further predict a geometry-induced 'quantization' of viscosity and the existence of excited states capable of performing mechanical work. It is plausible that these results generalize to a broad a class of fluids that are subject to an active scale selection mechanism.

12:27PM S35.00007 Swarming in viscous fluids: three-dimensional patterns in swimmer- and force-induced flows, YAO-LI CHUANG, MARIA R. D’ORSOGNA, Dept. of Mathematics, CSUN & Dept. of Biomathematics, UCLA, TOM CHOU, Dept. of Biomathematics UCLA & Dept. of Mathematics, UCLA — Mathematical models of self-propelled interacting particles have reproduced various fascinating “swarming” patterns observed in natural and artificial systems. The formulation of such models usually ignores the influence of the surrounding medium in which the particles swarm. Here we develop from first principles a three-dimensional theory of swarming particles in a viscous fluid and investigate how the hydrodynamic coupling among the particles may affect their collective behavior. Specifically, we examine the hydrodynamic coupling among self-propelled particles interacting through “social” or “mechanical” forces. We discover that new patterns arise as a consequence of different interactions and self-propulsion mechanisms. Examples include flocks with proteolate or oblate shapes, intermittent mills, recirculating peloton-like structures, and jet-like flows that kinetically destabilize mill-like structures. Our results reveal possible mechanisms for three-dimensional swarms to kinetically control their collective behaviors in fluids.

12:39PM S35.00008 Numerical study of the hydrodynamic interactions in an Ecoli suspension, XINLIANG XU, LIPENG LAI, Beijing Computational Science Research Center, YI PENG, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota — The active suspension of Ecoli displays many interesting non-equilibrium phenomena, e.g. “swarming” at high bacterial concentrations, and viscosity change under simple shear. To understand the microscopic mechanism underlying these phenomena requires detailed knowledge about the hydrodynamics within the suspension. Here we numerically study in detail the hydrodynamic interactions between a bacterium and an ellipsoid tracer at small separations, where the tracer can no longer be treated as a point-like particle that creates no disturbance to local flow field. We observed a significant drop in bacterium swimming velocity, in agreement with previous experimental study.

12:51PM S35.00009 Anomalous diffusion of an ellipsoid in quasi-2D active fluids, YI PENG, OU YANG, CHAO TANG, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota — Enhanced diffusion of a tracer particle is a unique feature in active fluids. Here, we studied the diffusion of an ellipsoid in a free-standing film of E. coli. Particle diffusion is linearly enhanced at low bacterial concentrations, whereas a non-linear enhancement is observed at high bacterial concentrations due to the giant fluctuation. More importantly, we uncover an anomalous coupling between the translational and rotational degrees of freedom that is strictly prohibited in classical Brownian diffusion. Combining experiments with theoretical modeling, we show that such an anomaly arises from the stretching flow induced by the force dipole of swimming bacteria. Our work illustrates a novel universal feature of active matter and transforms the understanding of fundamental transport processes in microbiological systems.

1:03PM S35.00010 Non-monotonic size-dependent particle diffusion in active fluids, ALISON PATTESON, Univ of Pennsylvania, ARVIND GOPINATH, University of California, Merced, PAULO ARRATIA, University of Pennsylvania — We experimentally investigate the effect of particle size on the motion of passive polystyrene spheres in suspensions of Escherchia coli. Using particles covering a range of sizes from 0.6 to 39 microns, we probe particle dynamics at both short and long time scales. In all cases, the particles exhibit super-diffusive ballistic behavior at short times before eventually transitioning to diffusive behavior. Surprisingly, the long-time hydrodynamic effective diffusivity exhibits a peak in particle size; an anomalous response that is fundamentally different from classical thermal diffusion. Consistent with recent theory, we find that the active contribution to particle diffusion is controlled by a dimensionless parameter, the Peclet number. We propose a minimal model that allows us to predict the requirements for a peak in the diffusivity as well as the magnitude of the peak as a function of particle size and bacterial concentration. Our results have broad implications on characterizing active fluids using concepts drawn from classical thermodynamics.

3Chemical Engineering and Material Science department
2Chemical Engineering and Material Science department
1:15PM S35.00011 Hydrodynamics of spinning bacteria at a surface, RACHEL BENNETT, Univ of Pennsylvania, RAMIN COLESTANIAN, University of Oxford — Bacteria tethered to a surface by their flagellum show a variety of different spinning behaviors, including different angles made with the surface and rotation velocities. We have developed a hydrodynamic model to show that the different behaviors arise from several factors including the degree of flagellar constraint, the shape of the bacterium, the flexibility of the flagellar hook and the motor torque. Our minimal model produces the wide variety of behaviors observed in experiments and successfully predicts the detachment angle for bacteria with three different body curvatures.

1:27PM S35.00012 Mobile wedges in an active turbulent bath, ANDREAS KAISER, ANDREY SOKOLOV, Argonne Nati Lab, HARTMUT LOWEN, Heinrich-Heine Universitat Dusseldorf, IGOR S. ARONSON, Argonne Nati Lab — The motion of micro-wedges in a turbulent bacterial bath is explored using computer simulations with explicit modeling of the bacteria and experiments. We demonstrate that collective turbulentike motion in a bacterial bath can power and steer the directed transport of mesoscopic carriers through the suspension. We will show that both polar ordering and swirl shielding inside the wedge yield an optimal transport velocity. Finally, we show the behavior of several wedges exposed to a bacterial bath.

1:39PM S35.00013 Entrainment dominates the interaction of microalgae with micron-sized objects, RAPHAEL JEANNERET, VASILY KANTSLER, MARCO POLIN, University of Warwick — Swimming microorganisms usually navigate through fluids containing a variety of microparticles, with which they inevitably interact with important biological and ecological implications. Regarding the prokaryotic realm, it has been shown that the colloidal dynamics within bacterial suspensions is well described by a persistent random walk. As to the other major class of microorganisms, the eukaryotes, much less is known. By directly tracking polystyrene colloids in baths of the model puller-type alga Chlamydomonas reinhardtii, a pioneering work [1] has shown that they still behave diffusively asymptotically with diffusivities linearly increasing with the concentration. The values reported as well as the distribution of displacements having exponential tails are well explained theoretically when considering the hydrodynamic far-field contribution of the algae. However nothing has yet been described regarding the short range interactions that inevitably exist. In this work we show, by means of 3 different experiments, that the coarse-grained dynamics of the colloids is in fact dominated by very rare but large jumps due to entrainment by the algae leading to a total effective diffusion an order of magnitude higher than previously reported. [1] Leptos et al, PRL 103, 198103 (2009).

Thursday, March 17, 2016 11:15AM - 2:15PM — Session S39 DBIO DPOLY GSNP: Physics of Genome Organization: from DNA to Chromatin

11:15AM S39.00001 Inferring the locations of DNA bound proteins from Hi-C data, PAU FARRE, ELDON EMBERLEY, Simon Fraser University — Eukaryotic DNA can be found in either a tightly packed state (heterochromatin) or an open conformation (euchromatin). Certain proteins that bind to the DNA are responsible for setting up these two types of states. They interact with each other, and generate spatially separated compartments in the DNA through the formation of loops. In this talk I will present a combination of analytic and simulation results for the effects of protein-protein interactions on the large-scale 3D structure of chromatin. Using these findings we have developed a maximum-likelihood method for inferring the distribution of DNA bound factors that can help refine and make new predictions for the locations of proteins responsible of structuring the chromosome.

11:27AM S39.00002 Coalescence Model for Crumpled Globules Formed in Polymer Collapse, GUY BUNIN, MEHRAN KARDAR, Massachusetts Inst of Tech-MIT — The rapid collapse of a polymer, due to external forces or changes in solvent, yields a long-lived “crumpled globule.” The conjectured fractal structure shaped by hierarchical collapse dynamics has proved difficult to establish, even with large simulations. To unravel this puzzle, we study a coarse-grained model of in-falling spherical blobs that coalesce upon contact. Distances between pairs of monomers are assigned upon their initial coalescence, and do not “equilibrate” subsequently. Surprisingly, the model reproduces quantitatively the dependence of distance on segment length, suggesting that the slow approach to scaling is related to the wide distribution of blob sizes.

11:39AM S39.00003 Probing nuclear dynamics and architecture using single-walled carbon nanotubes, YOON JUNG, JUNANG LI, NIKTA FAKHRI, Department of Physics, Massachusetts Institute of Technology — Chromatin is a multiscale dynamic architecture that acts as a template for many biochemical processes such as transcription and DNA replication. Recent developments such as Hi-C technology enable an identification of chromatin interactions across an entire genome. However, a single cell dynamic view of chromatin organization is far from understood. We discuss a new live cell imaging technique to probe the dynamics of the nucleus at a single cell level using single-walled carbon nanotubes (SWNTs). SWNTs are non-perturbing rigid rods (diameter of 1 nm and length of roughly 100 nm) that fluoresce in the near infrared region. Due to their high aspect ratio, they can diffuse in tight spaces and report on the architecture and dynamics of the nucleoplasm. We develop 3D imaging and tracking of SWNTs in the volume of the nucleus using double helix point spread function microscopy (DH-PSF) and discuss the capabilities of the DH-PSF for inferring the 3D orientation of nanotubes based on vectorial diffraction theory.

11:51AM S39.00004 Fractionation of Exosomes and DNA using Size-Based Separation at the Nanoscale, BENJAMIN WUNSCH, JOSHUA SMITH, IBM Research Labs, CHAO WANG, Arizona State University, STACEY GIFFORD, MARKUS BRINK, ROBERT BRUCE, GUSTAVO SOLOVITZKY, IBM Research Labs, ROBERT AUSTIN, Princeton University, YANN ASTIER, IBM Research Labs — Exosomes, a key target of liquid biopsies, are nano-vesicles found in nearly all biological fluids. Exosomes are secreted by eukaryotic and prokaryotic cells alike, and contain information about their originating cells, including surface proteins, cytoplasmic proteins, and nucleic acids. One challenge in studying exosome morphology is the difficulty of sorting exosomes by size and surface markers. Common separation techniques for exosomes include ultracentrifugation and ultraltracentrifugation, for preparation of large volume samples, but these techniques often show contamination and significant heterogeneity between preparations. To date, deterministic lateral displacement (DLD) pillar arrays in silicon have proven an efficient technology to sort, separate, and enrich micron-scale particles including human parasites, eukaryotic cells, blood cells, and circulating tumor cells in blood; however, the DLD technology has never been translated to the true nanoscale, where it could function on bio-colloids such as exosomes. We have fabricated nanoscale DLD (nanoDLD) arrays capable of rapidly sorting colloids down to 20 nm in continuous flow, and demonstrated size sorting of individual exosome vesicles and dsDNA polymers, opening the potential for on-chip biomolecule separation and diagnosis.

12:03PM S39.00005 The impact of non-uniform capsid charge density on virus assembly, SIYU LI, GONCA ERDEMCI-TANDOGAN, University of California, riverside, JEF WAGNER, Lawrence University, ROYA ZANDI, University of California, riverside — Many spherical viruses efficiently encapsulate their genome into shells (capsids) with icosahedral symmetry. Under many circumstances, this process is spontaneous and is primarily driven by the electrostatic interaction between positively charged capsid proteins and negatively charged genome. Through the free energy minimization of a generic potential, we calculate the optimal encapsulated genome length. In this talk, I will present our results due to a non-uniform charge distribution on the shell and its impact on the optimal size of encapsulated genome.

1This work was supported by the National Science Foundation through Grant No. DMR-13-10687.
and HHMI International Student Fellowship. 1
metabolites. The simplicity of the uncovered coordination mechanism and starvation sensing suggests that it may be widely applicable in a variety of gene
and cell-cycle parameters with decreased growth rate in starvation conditions enable cells to indirectly detect starvation without the need for evaluating specific
imbalance is detected by the sporulation network to produce cell-cycle coordinated pulses of the sporulation master regulator Spo0A\textasciitilde P. This pulsed response
between the two bases as \(-3/2\) and \(-4/3\) in the molten and glass phases, respectively. In this study, we characterize the full probability distributions of pair
phase and a weakly disordered, high-temperature molten phase. The probability of two bases pairing in these phases have been shown to scale with the distance
between the two bases as \(-3/2\) and \(-4/3\) in the molten and glass phases, respectively. In this study, we characterize the full probability distributions of pair
binding both near and far from the critical point rather than just the behavior of their means studied before. We anticipate that this approach allows one to
more closely probe the nature of the phase transition and better measure the system's critical exponents close to and at its critical point.

12:15PM S39.00006 Single molecule fluorescence studies of transition paths in DNA hairpin folding 1, KATHERINE TRUEX, HOI SUNG CHUNG, JOHN LOUIS, WILLIAM EATON, National Institutes of Health — DNA hairpins are the simplest structures for investigating fundamental aspects of nucleic acid folding mechanisms. For two-state hairpins, all of the mechanistic information on how the hairpin folds is contained in the transition path (TP), the rare event in single molecule trajectories when the free energy barrier between folded and unfolded states is actually crossed. The only previous experimental study of TPs in nucleic acids used optical tweezer measurements and Szabo’s analytical theory for diffusive barrier crossing to reconstruct the free energy surface for an indirect determination of average TP times (Neupane et al. PRL 2012). We used confocal single molecule FRET and maximum likelihood analysis of photon trajectories to determine an upper bound of 2.5 \(\mu\)s for the average TP time of a DNA hairpin (Truex et al., PRL 2015), compared to the value of 4 \(\mu\)s predicted by Neupane et al., providing an important test of energy landscape theory. Current experiments are aimed at eventually characterizing structural changes during TPs, which will provide a very demanding test of mechanisms predicted by both theoretical models and simulations.

12:27PM S39.00007 The Molecular Atlas Project 1, JESSE SILVERBERG, PENG YIN, Wyss Institute for Biologically Inspired Engineering, Harvard University — The promise of super-resolution microscopy is a technology to discover new biological mechanisms that occur at smaller length scales than previously observable. However, with higher-resolution, we generally lose the larger spatial context of the image itself. The Molecular Atlas Project (MAP) directly asks how these competing interests between super-resolution imaging and broader spatially contextualized information can be reconciled. MAP enables us to acquire, visualize, explore, and annotate proteomic image data representing 7 orders of magnitude in length ranging from molecular (nm) to tissue (cm) scales. This multi-scale understanding is made possible by combining multiplexed DNA-PAINT, a DNA nanotechnology approach to super-resolution imaging, with “big-data” strategies for information management and image visualization. With these innovations combined, MAP enables us to explore cell-specific heterogeneity in ductal carcinoma for every cell in a cm-sized tissue section, analyze organoid growth for advances in high-throughput tissue-on-a-chip technology, and examine individual synapses for connectome mapping over extremely wide areas. Ultimately, MAP is a fundamentally new way to interact with multiscale biophysical data.

12:39PM S39.00008 simulation of the DNA force-extension curve 1, GREGORY SHINABERRY, IVAN MIKHAYLOV, ALEXANDER BALAEFF, University of Central Florida — A molecular dynamics simulation study of the force-extension curve of double-stranded DNA is presented. Extended simulations of the DNA at multiple points along the force-extension curve are conducted with DNA end-to-end length constrained at each point. The calculated force-extension curve qualitatively reproduces the experimental one. The DNA conformational ensemble at each extension shows that the famous plateau of the force-extension curve results from B-DNA melting, whereas the formation of the earlier-predicted novel DNA conformation called “zip-DNA” takes place at extensions past the plateau. An extensive analysis of the DNA conformational ensemble in terms of base configuration, backbone configuration, solvent interaction energy, etc., is conducted in order to elucidate the physical origin of DNA elasticity and the main interactions responsible for the shape of the force-extension curve.

12:51PM S39.00009 Characterization of the full base pairing probability distribution in RNA secondary structure folding1, WILLIAM BAEZ, Ohio State University, KAY WIJSE, CNRS-LPTENS, RALF BUNDSCHUH, Ohio State University — Below the denaturation temperature of RNA, its secondary structures can exist in one of two phases: a strongly disordered, low-temperature glass phase and a weakly disordered, high-temperature molten phase. The probability of two bases pairing in these phases have been shown to scale with the distance between the two bases as \(-3/2\) and \(-4/3\) in the molten and glass phases, respectively. In this study, we characterize the full probability distributions of pair binding both near and far from the critical point rather than just the behavior of their means studied before. We anticipate that this approach allows one to more closely probe the nature of the phase transition and better measure the system’s critical exponents close to and at its critical point.

1This material is based upon work supported by the National Science Foundation under Grants No. DMR-0110545 and DMR-01410172.

1:03PM S39.00010 Gene dosage imbalance during DNA replication controls bacterial cell-fate decision1, OLEG IGOSHIN, Rice University — Genes encoding proteins in a common regulatory network are frequently located close to one another on the chromosome to facilitate co-regulation or coupled gene expression to growth rate. Contrasting with these observations, here we demonstrate a functional role for the arrangement of Bacillus subtilis sporulation network genes on opposite sides of the chromosome. We show that the arrangement of two sporulation network genes, one located close to the origin, the other close to the terminus leads to a transient gene dosage imbalance during chromosome replication. This imbalance is detected by the sporulation network to produce cell-cycle coordinated pulses of the sporulation master regulator Spo0A\textasciitilde P. This pulsed response allows cells to decide between sporulation and continued vegetative growth during each cell-cycle spent in starvation. Furthermore, changes in DNA replication and cell-cycle parameters with decreased growth rate in starvation conditions enable cells to indirectly detect starvation without the need for evaluating specific metabolites. The simplicity of the uncoupled coordination mechanism and starvation sensing suggests that it may be widely applicable in a variety of gene regulatory and stress-response settings.

1This work is supported by National Science Foundation grants MCB-1244135, EAGER-1450867, MCB-1244423, NIH NIGMS grant R01 GM088428 and HHMI International Student Fellowship.

1:39PM S39.00011 Torque-induced buckling behavior in stretched intertwined DNAs1, SUMITABHA BRAHMACHARI, JOHN F. MARKO, Northwestern Univ — Two intertwined DNA molecules (a DNA ‘braid’) is a common occurrence in the cell and is a relevant substrate for the study of topoisomerase and recombination enzymes. Single molecule experiments have observed the signature of a buckling transition in braids under tensile and torsional stress. We present a free energy model for braided DNA to investigate the mechanical properties of these structures. Our model is based on the semi-flexible polymer model for double helix DNA and is in quantitative accord with the experiments. We identify coexistence of a force-extended state with a plectonemically buckled state, which is reminiscent of single supercoiled DNA behavior. However, the absence of an intrinsic twist modulus in braided DNA results in unique mechanical properties such as non-linear torque in the extended state. At the buckling transition, we predict a jump in the braid extension due to the plectoneme end loop which acts as a nucleation barrier. We investigate the effect of salt concentration on the mechanical response of braids, e.g. we find that buckling starts at a lower linking number for lower salt concentration, the opposite of what is seen for single supercoiled DNAs. Also, concentrations less than 20 mM monovalent salt favor formation of multiple plectoneme domains.

1NSF grant: DMR-9734178
1:51PM S39.00012 Sequence Heterogeneity Accelerates Protein Search for Targets on DNA\(^1\). ALEXEY SHVETS, ANATOLY KOLOMEISKY, Rice Univ — The process of protein search for specific binding sites on DNA is fundamentally important since it marks the beginning of all major biological processes. We present a theoretical investigation that probes the role of DNA sequence symmetry, heterogeneity and chemical composition in the protein search dynamics. Using a discrete-state stochastic approach with a first-passage events analysis, which takes into account the most relevant physical-chemical processes, a full analytical description of the search dynamics is obtained. It is found that, contrary to existing views, the protein search is generally faster on DNA with more heterogeneous sequences. In addition, the search dynamics might be affected by the chemical composition near the target site. The physical origins of these phenomena are discussed. Our results suggest that biological processes might be effectively regulated by modifying chemical composition, symmetry and heterogeneity of a genome.

\(^1\)The work was supported by the Welch Foundation (Grant C-1559), by the NSF (Grant CHE-1360979), and by the Center for Theoretical Biological Physics sponsored by the NSF (Grant PHY-1427654).

2:03PM S39.00013 SA1 and TRF1 synergistically bind to telomeric DNA and promote DNA-DNA pairing. HONG WANG, JIANGGUO LIN, PRESTON COUNTRYMAN, HAI PAN, North Carolina State University, PARMINDER KAUR TEAM, ROBERT RIEHN TEAM, PATRICIA OPRESKO TEAM, JANE TAO TEAM, SUSAN SMITH TEAM — Impaired telomere cohesion leads to increased aneuploidy and early onset of tumorigenesis. Cohesion is thought to occur through the entrapment of two DNA strands within tripartite cohesion ring(s), along with a fourth subunit (SA1/SA2). Surprisingly, cohesion rings are not essential for telomere cohesion, which instead requires SA1 and shelterin proteins including TRF1. However, neither this unique cohesion mechanism at telomeres or DNA-binding properties of SA1 is understood. Here, using single-molecule fluorescence imaging of quantum dot-labeled proteins on DNA we discover that while SA1 diffuses across multiple telomeric and non-telomeric regions, the diffusion mediated through its N-terminal domain is slower at telomeric regions. However, addition of TRF1 traps SA1 within telomeric regions, which form longer DNA-DNA pairing tracts than with TRF1 alone, as revealed by atomic force microscopy. Together, these experimental results and coarse-grained molecular dynamics simulations suggest that TRF1 and SA1 synergistically interact with DNA to support telomere cohesion without cohesin rings.

Thursday, March 17, 2016 11:15AM - 2:15PM —
Session S40 GSNP: Systems with Large Fluctuations and Strong Correlations II

11:15AM S40.00001 First-Passage Statistics of Extreme Values, ELI BEN-NAIM, Los Alamos National Laboratory — Theoretical concepts from nonequilibrium statistical physics such as scaling and correlations are used to analyze first-passage processes involving extreme values. The focus of this talk is statistics of the running maxima, defined as the largest variable in a sequence of random variables. In particular, the running maxima of multiple independent sequences of stochastic variables are compared. The probability that these maxima remain perfectly ordered decays algebraically with the number of random variables, and the decay exponent characterizing this decay is nontrivial. Exact solutions for the scaling exponents will be discussed for uncorrelated variables as well as Brownian trajectories which are correlated. Relevance of such statistical measures for analysis of empirical data will be discussed as well.

11:51AM S40.00002 Emergence of universal statistics from conserved topological features of underlying network dynamics, SRIVIDYA IYER-BISWAS, Department of Physics, Purdue University — In this talk I will discuss how universal statistics emerge from conserved topological features of underlying network dynamics. I will indicate how dynamical phase transitions between different network structures also encode universal statistics. I will connect these results with our single-cell experiments on C. crescentus cells.

12:03PM S40.00003 Anomalous Dimension in a Two-Species Reaction-Diffusion Model, JOSHUA HELLERICK, BENJAMIN VOLLMAYR-LEE, Bucknell University — We consider particles (A) diffusing in the presence of traps (B), which themselves are diffusing and reacting, i.e., the two-species reaction-diffusion model \(A + B \rightarrow B + B \rightarrow (0, B)\). We introduce a simulation technique that provides the full probability distribution of particles for a given realization of the trap dynamics. Previous renormalization group analysis predicted that the density of A particles decays as \(\theta^{-\theta}\), where \(\theta\) is a nontrivial, universal exponent for \(d < 2\). We compare our results with these predictions, and also demonstrate the scaling of the correlation functions. We discover an anomalous dimension in the particle-particle correlation function, described by \(G_{AA}(0) \sim t^\theta\), and we report our measurements for this new exponent.

12:15PM S40.00004 Non-equilibrium steady states of stochastic processes with intermittent resetting, STEPHAN EULE, Max-Planck-Institute, JAKOB METZGER, Rockefeller University — Stochastic processes that are randomly reset to an initial condition serve as a showcase to analytically investigate non-equilibrium steady states. Here we study such processes for which the time between the resets is random and drawn from a generic waiting time distribution. We obtain the general solution for the stationary state and quantify the temporal relaxation of the process in terms of its moments. Our results are applied to analyze the efficiency of constrained random search processes. For a fixed mean reset time, we show that the search efficiency can be optimized by adapting the shape of the waiting time distribution.

12:27PM S40.00005 Persistent Probability Currents in Non-equilibrium Steady States\(^1\), ROYCE ZIA, Iowa State and Virginia Tech, ANDREW MELLOR, MAURO MÖBILIA, University of Leeds, BAYLOR FOX-KEMPER, Brown University, JEFFREY WEISS, University of Colorado at Boulder — For many interesting phenomena in nature, from all life forms to the global climate, the fundamental hypothesis of equilibrium statistical mechanics does not apply. Instead, they are perhaps better characterized by non-equilibrium steady states, evolving with dynamical rules which violate detailed balance. In particular, such dynamics leads to the existence of non-trivial, persistent probability currents - a principal characteristic of non-equilibrium steady states. In turn, they give rise to the notion of ‘probability angular momentum’. Observable manifestations of such abstract concepts will be illustrated in two distinct contexts: a heterogeneous nonlinear voter model and our ocean heat content.

\(^1\)Supported in part by grants from the Bloom Agency (Leeds, UK) and the US National Science Foundation: OCE-1245944. AM acknowledges the support of EPSRC Industrial CASE Studentship, Grant No. EP/L50550X/1.
For randomly accelerated particles we detected, and were able to analyze in detail (PRL 113, 184101 (2014)), the phenomenon of weak-ergodicity breaking (WEB), i.e. the inequivalence of ensemble- and time-averaged mean-squared displacements (MSD). These results, including their aging time dependence, are relevant for anomalous chaotic diffusion in Hamiltonian systems, for passive tracer transport in turbulent flows, and many other systems showing momentum diffusion. There are, however, several related models, such as the integrated random excursion model, or, space-time correlated Lévy walks and flights, with similar statistical behavior. We compare the WEB related properties of these models and find surprising differences although, for equivalent parameters, all of them are supposed to lead to the same ensemble-averaged MSD. Our findings are relevant for distinguishing possible models for the anomalous diffusion occurring in experimental situations.

We discuss the effect of disordered confinement on anomalous diffusion. We treat confinement in conjunction with ordinary diffusion and with anomalous diffusions associated with aging and with correlated displacements. In particular, we compute the altered anomalous exponents. Finally, we relate these results to previous work and show that they shed light on the nature of diffusion on percolation clusters.

Aging time dependence, are relevant for anomalous chaotic diffusion in Hamiltonian systems, for passive tracer transport in turbulent flows, and many other weak-ergodicity breaking (WEB), i.e. the inequivalence of ensemble- and time-averaged mean-squared displacements (MSD). These results, including their aging time dependence, are relevant for anomalous chaotic diffusion in Hamiltonian systems, for passive tracer transport in turbulent flows, and many other systems showing momentum diffusion. There are, however, several related models, such as the integrated random excursion model, or, space-time correlated Lévy walks and flights, with similar statistical behavior. We compare the WEB related properties of these models and find surprising differences although, for equivalent parameters, all of them are supposed to lead to the same ensemble-averaged MSD. Our findings are relevant for distinguishing possible models for the anomalous diffusion occurring in experimental situations.

Supported by the European Research Council (ERC), project MHetScale (617511), (Grant No. 2009 SGR 597), ERC AdG Osyris, and Spanish Ministry Projects (FOQUS (FIS2013-46768-P) and No. MAT2011-22887)

Research is supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-FG02-09ER46613.

1:03PM S40.00008 Non-equilibrium dynamics of the complex Ginzburg-Landau equation. WEIGANG LIU, UWE TAUBER, Virginia Tech — The complex Ginzburg-Landau equation combines the quantum many-particle nonlinear Schrödinger equation with the time-dependent Ginzburg-Landau equation to model A relaxational dynamics. It arises in quite diverse contexts that include spontaneous pattern formation out of equilibrium, chemical oscillations, multi-mode lasers, thermal convection in binary fluids, cyclic population dynamics, and driven-dissipative Bose-Einstein condensates. Indeed, the complex Ginzburg-Landau equation exhibits a remarkably rich phase diagram with intriguing dynamics. We employ detailed numerical studies as well as analytical tools such as the perturbative renormalization group and the spherical model limit to study the non-equilibrium coarsening and critical aging scaling for the complex Ginzburg-Landau equation following quenches from an initial disordered configuration to either one of the ordered phases or the critical point.

1:27PM S40.00010 Ligand binding kinetics in surface plasmon resonance devices: A Monte Carlo simulation analysis. JACOB CARROLL, UWE TAUBER, Virginia Tech — Surface plasmon resonance (SPR) chips are widely used to measure association and dissociation rates for the binding kinetics between two species of chemicals, e.g., cell receptors and ligands. It is commonly assumed that ligands are spatially well mixed in the SPR region, and hence a mean-field rate equation description is appropriate. This approximation however ignores the spatial fluctuations as well as temporal correlations induced by multiple local rebinding events, which become prominent for slow diffusion rates. We report detailed Monte Carlo simulations of ligand binding kinetics in an SPR cell subject to laminar flow. We extract the binding and dissociation rates by means of the techniques frequently employed in experimental analysis, where the input simulation values. These results underscore the crucial quantitative importance of spatio-temporal correlations in binary reaction kinetics in SPR cell geometries.

1:39PM S40.00011 Thermodynamic and Information Entropy in Electroconvection. JOHN CRESSMAN, George Mason University, MARCUS DAUM, George Institute of Technology, DAVID PATRICK, George Mason University, RORY CERBUS, WALTER GOLDBURG, University of Pittsburgh — Transitions in driven systems often produce wild fluctuations that can be both detrimental and beneficial. Our fundamental understanding of these transitions is inadequate to permit optimal interactions with systems ranging from biology, to energy generation, to finance. Here we report on experiments performed in electroconvection liquid crystals where we abruptly change the electrical forcing across the sample from a state below defect turbulence into a state of defect turbulence. We simultaneously measure the electrical power flow through the liquid crystal as well as image the structure in the system. We can simultaneously track the evolution of the thermodynamic and information entropies. Our experiments demonstrate that there are strong correlations between the fluctuations in these two entropic measures however they are not exact. We will discuss these discrepancies as well as the relevance of large transient fluctuations in non-equilibrium transitions as well as their entropy evolution in general.

1:51PM S40.00012 Low dissipation in non-equilibrium control: sampling the ensemble of efficient protocols. GRANT ROTSKOFF, Univ of California - Berkeley, TODD GINGRICH, Massachusetts Institute of Technology, GAVIN CROOKS, Lawrence Berkeley National Laboratory, PHILLIP GEISSLER, Univ of California - Berkeley — Designing schemes to efficiently control fluctuating, non-equilibrium systems is problem of fundamental importance and tremendous practical interest. A number of optimization techniques have proven fruitful in the pursuit of optimal control, but these approaches focus on the singular goal of finding the exact, optimal protocol. Here, we investigate the diversity of protocols that achieve low dissipation with a Monte Carlo path sampling algorithm. Akin to Boltzmann weighting configurations in Metropolis Monte Carlo, each protocol is exponentially biased by its mean dissipation. We show that the ensemble of low dissipation protocols can be sampled exactly in the Gaussian limit and that the method continues to robustly generate low dissipation protocols, even as the external control drives the system far from equilibrium.

2:03PM S40.00013 Geometry of dissipative evolution equations. CELIA REINA, University of Pennsylvania — The modeling of continuum dissipative evolution equations remains a challenge and is primarily based on phenomenological constitutive relations. In this talk we present some connections between the geometry of dissipative gradient flows, the principle of maximum entropy production, large deviation principles for stochastically augmented evolution equations and fluctuation-dissipation relations.
Quantifying Stability in Complex Networks: From Linear to Basin Stability

JÜRGEN KURTHS, Humboldt University — The human brain, power grids, arrays of coupled lasers and the Amazon forest are all characterized by multistability. The likelihood that these systems will remain in the most desirable of their many stable states depends on their stability against significant perturbations, particularly in a state space populated by undesirable states. Here we claim that the traditional linearization-based approach to stability is in several cases too local to adequately assess how stable a state is. Instead, we quantify it in terms of basin stability, a new measure related to the volume of the basin of attraction. Basin stability is non-local, nonlinear and easily applicable, even to high-dimensional systems. It provides a long-sought-after explanation for the surprisingly regular topologies of neural networks and power grids, which have eluded theoretical description based solely on linear stability.

Specifically, we employ a component-wise version of basin stability, a nonlinear inspection scheme, to investigate how a grid’s degree of stability is influenced by certain patterns in the wiring topology. Various statistics from our ensemble simulations all support one main finding: The widespread and cheapest of all connection schemes, namely dead ends and dead trees, strongly diminish stability. For the Northern European power system we demonstrate that the inverse is also true. ‘Healing’ dead ends by addition of transmission lines substantially enhances stability. This indicates a crucial smart-design principle for tomorrow’s sustainable power grids: add just a few more lines to avoid dead ends. Further, we analyse the particular function of certain network motifs to promote the stability of the system. Here we uncover the impact of so-called detour motifs on the appearance of nodes with a poor stability score and discuss the implications for power grid design. Moreover, it will be shown that basin stability enables uncovering the mechanism for explosive synchronization and understanding of evolving networks.


Control of State Transitions in Complex and Biophysical Networks

ADILSON MOTTER, DANIEL WELLS, WILLIAM KATH, Northwestern University — Noise is a fundamental part of intracellular processes. While the response of biological systems to noise has been studied extensively, there has been limited understanding of how to exploit it to induce a desired cell state. Here I will present a scalable, quantitative method based on the Freidlin-Wentzell action to predict and control noise-induced switching between different states in genetic networks that, conveniently, can also control transitions between stable states in the absence of noise. I will discuss applications of this methodology to predict control interventions that can induce lineage changes and to identify new candidate strategies for cancer therapy. This framework offers a systems approach to identifying the key factors for rationally manipulating network dynamics, and should also find use in controlling other classes of complex networks exhibiting multi-stability. Reference: D. K. Wells, W. L. Kath, and A. E. Motter, Phys. Rev. X 5, 031036 (2015).

Quantifying Stability in Complex Networks: From Linear to Basin Stability

MOTTER, Northwestern University — Networks of coupled dynamical subsystems are increasingly used to represent complex natural and engineered systems. The overall behavior of the systems depends crucially on the network structure depicting how the nodes are linked with each other. It is usually possible to measure the dynamics of the individual nodes but difficult, if not impossible, to directly measure the interactions or links between the nodes. For most systems of interest, the links are directional in that one node affects the dynamics of the other but not vice versa. Moreover, the strength of interaction can vary for different links. Reconstructing directed and weighted networks from dynamics is one of the biggest challenges in network research. We have studied directed and weighted networks modelled by noisy dynamical systems with nonlinear dynamics and developed a method that reconstructs the links and their directions using only the dynamics of the nodes as input. Our method is motivated by a mathematical result derived for dynamical systems that approach a fixed point in the noise-free limit. We show that our method gives good reconstruction results for several directed and weighted networks with different nonlinear dynamics.

This work was supported by NSF grant PHY 1205840.
12:51PM S43.00007 Hamiltonian-Based Model to Describe the Nonlinear Physics of Cascading Failures in Power-Grid Networks, YANG YANG, ADILSON MOTTER, Department of Physics and Astronomy, Northwestern University — A local disturbance to the state of a power-grid system can trigger a protective response that disables some grid components, which leads to further responses, and may finally result in large-scale failures. In this talk, I will introduce a Hamiltonian-like model of cascading failures in power grids. This model includes the state variables of generators, which are determined by the nonlinear swing equations and power-flow equations, as well as the on/off status of the network components. This framework allows us to view a cascading failure in the power grid as a phase-space transition from a fixed point with high energy to a fixed point with lower energy. Using real power-grid networks, I will demonstrate that possible cascade outcomes can be predicted by analyzing the stability of the system’s equilibria. This work adds an important new dimension to the current understanding of cascading failures.

1:03PM S43.00008 Cascading Failures in Flow-Driven Networks Induced by Multiple Initiators, ALAA MOUSSAWI, NOEMI DERSZY, XIN LIN, BOLESLAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — Flow-driven networks are particularly prone to cascading failures. These failures are non self-averaging and this makes them very difficult to predict or subdue [1, 2]. Previous work has suggested that uniformly increasing edge or node capacities may lead to larger failures [1]. This suggests that some nodes/edges may act as fuses and mitigate cascading failures. We investigate this idea, and analyze how properties of the initiators of the cascade influence its outcome. We also discuss how stochastic node capacity allocation can be utilized to mitigate cascades induced by multiple initiators. We demonstrate the efficacy of these strategies on random geometric graphs (RGG) and the UCTE European electrical power transmission network, with capacities allocated in a fashion similar to the industry standard. [1] A. Asztalos, S. Sreenivasan, B.K. Szymanski, and G. Korniss, “Cascading Failures in Spatially Embedded Random Networks”, PLOS ONE 9(1): e84563 (2014). [2] Bernstein et al., ACM SIGMETRICS Performance Eval. Rev. 40, 33-37 (2012).

1:15PM S43.00009 Cascading processes on multiplex networks: Impact of weak layers, KYU-MIN LEE, KWANG-IL GOH, Korea University — Many real-world complex systems such as biological and socio-technological systems consist of manifold layers in multiplex networks. The multiple network layers give rise to the nonlinear effect for the emergent dynamics of systems. Especially, the weak layers plays the significant role in nonlinearity of multiplex networks, which can be neglected in single-layer network framework overlaying all layers. Here we present a simple model of cascades on multiplex networks of heterogeneous layers. The model is simulated on the multiplex network of international trades. We found that the multiplex model produces more catastrophic cascading failures which were the result of collective behaviors from coupling layers rather than the simple summation effect. Therefore risks can be systematically underestimated in simply overlaid network system because the impact of weak layers is overlooked. Our simple theoretical model would have some implications to investigate and design optimal real-world complex systems.

1:27PM S43.00010 Long-term Failure Prediction based on an ARP Model of Global Risk Network, XIN LIN, ALAA MOUSSAWI, BOLESLAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — Risks that threaten modern societies form an intricately interconnected network. Hence, it is important to understand how risk materializations in distinct domains influence each other. In the paper, we study the global risks network defined by World Economic Forum experts in the form of Stochastic Block Model. We model risks as Alternating Renewal Processes with variable intensities driven by hidden values of exogenous and endogenous failure probabilities. Based on the expert assessments and historical status of each risk, we use Maximum Likelihood Evaluation to find the optimal model parameters and demonstrate that the model considering network effects significantly outperforms the others. In the talk, we discuss how the model can be used to provide quantitative means for measuring interdependencies and materialization of risks in the network. We also present recent results of long-term predictions in the form of predicted distributions of materializations over various time periods. Finally we show how the simulation of ARPs enables us to probe limits of the predictability of the system parameters from historical data and ability to recover hidden variable.

1:39PM S43.00011 Hybrid dynamics in delay-coupled swarms with “mothership” networks, JASON HINDES, IRA SCHWARTZ, U.S. Naval Research Laboratory — Swarming behavior continues to be a subject of immense interest because of its centrality in many naturally occurring systems in biology and physics. Moreover, the development of autonomous mobile agents that can mimic the behavior of swarms and be engineered to perform complex tasks without constant intervention is a very active field of practical research. Here we examine the effects on delay-coupled swarm pattern formation from the inclusion of a small fraction of highly connected nodes, “motherships”, in the swarm interaction network. We find a variety of new behaviors and bifurcations, including new hybrid motions of previously analyzed patterns. Both numerical and analytic techniques are used to classify the dynamics and construct the phase diagram. The implications for swarm control and robustness from topological heterogeneity are also discussed.

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Thursday, March 17, 2016 11:15AM - 2:15PM –
Session S55 DBIO GSNP: Inference in Biophysics
University of Pennsylvania

11:15AM S55.00001 Genetic networks and the flow of positional information in embryonic development, WILLIAM BIALEK, Princeton University — When we study a biological system, we make inferences about the underlying mechanisms and dynamics. But biological systems themselves must also solve inference problems, as when our brains draw conclusions about the world given (often quite limited) data from our eyes and ears. My colleagues and I have been exploring both of these inference problems as they play out in the first hours of development of the fruit fly embryo. In this system, the concentrations of particular molecules encode the position of each cell in the embryo, and these concentrations are the inputs of a genetic network. Putting ourselves in the place of the cells, we have been able to read the code, building a dictionary that maps gene expression levels back into estimates of position. If our dictionary really is the one used by the embryo, then mutants should build predictably distorted body plans, and preliminary results show quantitative agreement with these predictions. Independent of their role as carriers of information, we can also analyze the patterns of gene expression to draw inferences about the underlying network. Finally, it is possible that the network architecture and parameters have been chosen to optimize the flow of information, and we see signatures of this optimization. Joint work with CG Callan, JO Dubuis, T Gregor, D Krotov, M Petkova, TR Sokolowski, G Tkacik, AM Walczak, and EF Wieschaus.
Spring of 2011.

the propagation of a sudden change or collapse, and we show that catastrophe hopping is consistent with the outbreak of protests observed during the Arab

them. Here our focus is on abrupt changes in networks, due both to phase transitions and to jumping between bi-stable equilibria. We begin with an overview

of California, Davis — Collections of interdependent networks are at the core of modern society, spanning physical, biological and social systems. Simple

static counterparts, with the former enjoying dramatic and simultaneous reductions in all costs of control. This is true despite the fact that temporality tends

failed) state. Second, I will show that nonlinearity in the form of time-varying dynamics unexpectedly makes temporal networks easier to control than their

require us to drive a system to—or keep it in—a desired state. This process is complicated by the nonlinear dynamics inherent to most real systems, which

habitats, spatial scales, and taxonomic groups. A systematic pattern of failure is observed, however, for ecosystems either losing species following disturbance

or diversifying in evolutionary time; I show that this problem may be remedied with a stochastic-dynamic extension of the theory.

Northeastern University, Center for Complex Network Research — The proper functioning and reliability of many man-made and natural systems is fundamentally

more vulnerable compared to non embedded networks. In particular, small localized attacks may lead to cascading failures and catastrophic consequences. Thus,

independent networks embedded in space are significantly

and the theory suggests an optimal repairing strategy of system of systems. I will also show that interdependent networks embedded in space are significantly

they cause dependent nodes in other networks to also fail. This is also the case when some nodes like certain locations play a role in two networks –multiplex.

In reality, many real-networks, such as power grids, transportation and communication infrastructures interact and depend on other networks. I will present a

framework for studying the vulnerability and the recovery of networks of interdependent networks. In interdependent networks, when nodes in one network fail,

they depend on other networks to also fail. This is also the case when some nodes like certain locations play a role in two networks –multiplex. This may happen recursively and can lead to a cascade of failures and to a sudden fragmentation of the system. I will present analytical solutions for the critical threshold and the giant component of a network of n interdependent networks. I will show that the general theory has many novel features that are not present in the classical network theory. The recovery of components is possible global spontaneous recovery of the networks and hysteresis phenomena occur in the theory and the theory suggests an optimal repairing strategy of system of systems. I will also show that interdependent networks embedded in space are significantly

more vulnerable compared to non embedded networks. In particular, small localized attacks may lead to cascading failures and catastrophic consequences. Thus,


3:06PM S55.00003 Fock spaces for modeling macromolecular complexes, JUSTIN KINNEY, Cold Spring Harbor Laboratory — Large macromolecular complexes play a fundamental role in how cells function. Here I describe a Fock space formalism for mathematically modeling these complexes. Specifically, this formalism allows ensembles of complexes to be defined in terms of elementary molecular “building blocks” and “assembly rules.” Such definitions avoid the massive redundancy inherent in standard representations, in which all possible complexes are manually enumerated. Methods for systematically computing ensembles of complexes from a list of components and interaction rules are described. I also show how this formalism readily accommodates coarse-graining. Finally, I introduce diagrammatic techniques that greatly facilitate the application of this formalism to both equilibrium and non-equilibrium biochemical systems.

Thursday, March 17, 2016 2:30PM - 5:30PM –

Session V3 GSNP: Complex Network Dynamics Ballroom III - Adison Motter, Northwestern University


1DTRA, ONR, Israel Science Foundation

3:06PM V3.00002 The Life-Changing Magic of Nonlinearity in Network Control, SEAN CORNELIUS, Northeastern University, Center for Complex Network Research — The proper functioning and reliability of many man-made and natural systems is fundamentally tied to our ability to control them. Indeed, applications as diverse as ecosystem management, emergency response and cell reprogramming all, at their heart, require us to drive a system to—or keep it in—a desired state. This process is complicated by the nonlinear dynamics inherent to most real systems, which has traditionally been viewed as the principle obstacle to their control. In this talk, I will discuss two ways in which nonlinearity turns this view on its head, in fact representing an asset to the control of complex systems. First, I will show how nonlinearity in the form of multistability allows one to systematically design control interventions that can deliberately induce “reverse cascading failures”, in which a network spontaneously evolves to a desirable (rather than a failed) state. Second, I will show that nonlinearity in the form of time-varying dynamics unexpectedly makes temporal networks easier to control than their static counterparts, with the former enjoying dramatic and simultaneous reductions in all costs of control. This is true despite the fact that temporal features tend to fragment a network’s structure, disrupting the paths that allow the directly-controlled or “driver” nodes to communicate with the rest of the network. Taken together, these theoretical insights highlight the crucial role of nonlinearity in network control, and provide support to the idea we can control nonlinearity, rather than letting nonlinearity control us.

3:42PM V3.00003 Novel percolation transitions and coupled catastrophes, RAISSA D’SOUZA, University of California, Davis — Collections of interdependent networks are at the core of modern society, spanning physical, biological and social systems. Simple mathematical models of the structure and function of networks can provide important insights into real-world systems, enhancing our ability to steer and control them. Here our focus is on abrupt changes in networks, due both to phase transitions and to jumping between bi-stable equilibria. We begin with an overview of novel classes of percolation phase transitions that result from repeated, small interventions intended to delay the transition. These new phenomena allow us to extend percolation approaches to modular networks, Brownian motion, and cluster growth dynamics. We then focus on abrupt transitions due to a system jumping between bi-stable equilibria, modeled as a cusp catastrophe in nonlinear dynamics. We show that when systems that each undergo a cusp catastrophe interact, we can observe a new phenomena of catastrophe-hopping leading to non-local cascading failures. Here an intermediate system facilitates the propagation of a sudden change or collapse, and we show that catastrophe hopping is consistent with the outbreak of protests observed during the Arab Spring of 2011.
4:18PM V3.00004 Interdisciplinary applications of network dynamics: From microscopic to Macroscopic. HAVOONG JEONG, KAIST, Korea — Everything touches everything. We are living in a connected world, which has been modeled successfully by complex networks. Ever since, network science becomes new paradigm for understanding our connected yet complex world. After investigating network structure itself, our focus naturally moves to dynamics of/on the network because our connected world is not static but dynamic. In this presentation, we will briefly review the historical development of network science and show some applications of network dynamics ranging from microscopic (metabolic engineering, PNAS, 104 13638) to macroscopic scale (price of anarchy in transportation network, Phys.Rev.Lett. 101 128701).

1Supported by National Research Foundation of Korea through Grant No. 2011-0028908

4:54PM V3.00005 Rank Dynamics. CARLOS GERSHENSON, Universidad Nacional Autonoma de Mexico — Studies of rank distributions have been popular for decades, especially since the work of Zipf. For example, if we rank words of a given language by use frequency (most used word in English is the, rank 1; second most common word is of, rank 2), the distribution can be approximated roughly with a power law. The same applies for cities (most populated city in a country ranks first), earthquakes, metabolism, the Internet, and dozens of other phenomena. We recently proposed rank diversity to measure how ranks change in time [1], using the Google Books Ngram dataset. Studying six languages between 1800 and 2009, we found that the rank diversity curves of languages are universal, adjusted with a sigmoid on log-normal scale. We are studying several other datasets (sports, economies, social systems, urban systems, earthquakes, artificial life). Rank diversity seems to be universal, independently of the shape of the rank distribution. I will present our work in progress towards a general description of the features of rank change in time, along with simple models which reproduce it. [1]Cocho G, Flores J, Gershenson C, Pineda C, Sanchez S (2015) Rank Diversity of Languages: Generic Behavior in Computational Linguistics. PLoS ONE 10(4): e0121898.http://dx.doi.org/10.1371/journal.pone.0121898

Thursday, March 17, 2016 2:30PM - 5:30PM —
Session V35 DBIO GSOFT GSNP: Active Matter: Collective Phenomena in Living Systems V

2:30PM V35.00001 Questioning the activity of active matter: the case of bird flocks. THIERRY MORA, ALEKSANDRA WALCZAK, Ecole normale superieure and CNRS, LORENZO DEL CASTELLO, University of Rome and CNR, FRANCESCO GINELLI, University of Aberdeen, STEFANIA MELILLO, LEONARDO PARISI, MASSIMILIANO VIALE, ANDREA CAVAGNA, IRENE GIARDINA, University of Rome and CNR — Animal flocking is a natural instance of active matter. What makes flocks active is the rearrangement of neighborhoods, which constantly remodels the network of interactions between individuals in the group, keeping the system out of equilibrium. Despite the predicted importance of this reshuffling, its true impact for natural flocks is not well understood. Here we analyse films of flocks of starlings with a novel statistical inference technique based on dynamical maximum entropy to measure the parameters of flock alignment - alignment strength, interaction range, and noise. We show that birds align their flight orientations faster than they change neighbors. In the statistical mechanics sense, this means that flocks remain adiabatically in equilibrium, allowing for a rigorous analogy with equilibrium systems of interacting spins, and we show that an inference method based on equilibrium assumptions gives fully consistent results.

2:42PM V35.00002 Linear response to leadership, effective temperature and decision making in flocks. DANIEL PEARCE, LUCA GIOMI, Univ of Leiden — The Vicsek model is the prototypical system for studying collective behavior of interacting self propelled particles (SPPs). It has formed the basis for models explaining the collective behavior of many active systems including flocks of birds and swarms of insects. To the standard Vicsek model we introduce a small angular torque to a subset of the particles and observe how this effects the direction of polarisation of the entire swarm. This is analogous to a few informed birds trying to lead the rest of a large flock by initiating a turn. We find a linear response to this perturbation and fluctuations that are in agreement with fluctuation dissipation theorem. This allows the identification of an effective temperature for the Vicsek model that follows a power law with the noise amplitude. The linear response can also be extended to the process of decision-making, wherein flocks must decide between the behaviors of two competing subgroups of individuals.

2:54PM V35.00003 Fluctuation Spectra Underlie the Behavior of Non-equilibrium Systems . ALPHA LEE, Harvard University, DOMINIC VELLA, University of Oxford, JOHN WETTLaUFer, Yale University — A diverse set of important physical phenomena, ranging from hydrodynamic turbulence to the collective behaviour of bacteria, are intrinsically far from equilibrium. Despite their ubiquity, there are few general theoretical results that describe these non-equilibrium steady states. Here we argue that a generic signature of non-equilibrium systems is nontrivial fluctuation spectra. Based on this observation, we derive a general relation for the force exerted by a non-equilibrium system on two embedded walls. We find that for a narrow, unimodal spectrum, the force depends solely on the width and the position of the peak in the fluctuation spectrum, and will oscillate between repulsion and attraction. We demonstrate the generality of our framework by examining two apparently disparate examples: the Maritime Casimir effect and recent simulations of active Brownian particles. A key implication of our work is that important non-equilibrium interactions are encoded within the fluctuation spectrum. In this sense the noise becomes the signal.

3:06PM V35.00004 Visual perturbations and the collective dynamics of fish schools. JULIA GIANNINI, JAMES PUCKETT, Gettysburg College — We investigate the dynamics of the collective behaviors exhibited in a laboratory fish school. Using an artificial light gradient that varies both spatially and temporally, we investigate the competition between individual locomotion and local polarization arising from social interactions between individuals. We will discuss how our work informs current agent-based models of the interplay between social interactions and heterogeneous environments.

3:18PM V35.00005 The influence of following on bidirectional flow through a doorway1. AMY GRAVES, RACHEL DIAMOND, EDUARD SAAKASHVILI, Swarthmore College — Pedestrian dynamics is a subset of the study of self-propelled particles. We simulate two species of pedestrians undergoing bidirectional flow through a narrow doorway. Using the Helbing-Monfr-Farkas-Vicsek Social Force Model, our pedestrians are soft discs that experience psychosocial and physical contact forces. We vary the following parameter which determines the degree to which a pedestrian matches its direction of movement to the average of nearby, same-species pedestrians. Current density, efficiency and statistics of bursts and lags are calculated. These indicate that choosing different following parameters for each species affects the efficacy of transport - greater following being associated with lower efficacy. The information entropy associated with velocity and the long time tails of the complementary CDF of lag times are additional indicators of the dynamical consequences of following during bidirectional flow.

1Acknowledgement is made to the donors of the ACS Petroleum Research Fund, and the Vandervelde-Cheung Fund of Swarthmore College
We then compare the results with visualizations of 2D aggregations. In this talk, we will present data pertaining to the aggregation of individual ants contributes non-trivially to the bulk material properties of the aggregation. We have measured some of these properties using experimentally.

We identify the size as being proportional to an inverse effective temperature and thus the system can exhibit a mesoscopic transition between order and disorder. We combine experiments and theory to characterize the collective transport. The ants are modeled as binary Ising spins, representing the two roles ants can do that, we introduce a simple model of self-propelled hard disks moving in 2D carrying an internal variable which follows a Kuramoto dynamics. We find that, the presence of sterically interactions give rise to an optimal self-propulsion for synchronization as a consequence of the parameters of the model. However, the presence of sterically interactions plays an important role for the performance of mobile systems. We single out several dynamic regimes controlled by different processes that we describe. We analyse the relaxation of the system and show that synchronization proceeds through a mechanism that, despite being out-of-equilibrium, verifies the dynamical scaling hypothesis.

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1Supported by NIH grant 1R01HD070038.

3:42PM V35.00007 To be decided by speaker, MADAN RAO, National Centre for Biological Sciences(TIFR) — No abstract available.

4:18PM V35.00008 Critical phenomena in active matter1, MATTEO PAOLUZZI, M CRISTINA MARCHETTI, Syracuse Univ, CLAUDIO MAGGI COLLABORATION, UMBERTO MARINI BETTOLLO MARCONI COLLABORATION, NICOLETTA GNAN COLLABORATION — A collection of active agents can organize in phases with structural properties remarkably similar to those of ordinary materials, such as active gases, liquids and glasses. These phases are formed, however, out of equilibrium, where the machinery of equilibrium statistical mechanics cannot be applied. It has recently been shown that models of particles with Gaussian colored noise can capture some of the nonequilibrium behavior of active Brownian particles, including motility-induced phase separation. By using the Unified Gaussian Colored Noise Approximation (UCNA) it has been possible to obtain an equilibrium-like probability distribution function and an effective free energy for active Brownian particles. Here we employ UCNA to examine the effect of colored noise on mean-field order-disorder transitions. Starting with a $\alpha^4$ Landau model that undergoes a second-order phase transition as a function of a tuning parameter, we calculate the shift in transition due to colored noise as a function of the noise amplitude and correlation time $\tau$. We find that the transition line exhibits reentrance as a function of $\tau$. The mean-field theoretical predictions are compared with Molecular Dynamics simulations of active Lennard-Jones particles.

1We acknowledge support from NSF-DMR-1305184.

4:30PM V35.00009 Long-range Acoustic Interactions in Insect Swarms: An Adaptive Gravity Model, DAN GORBONOS, REUVEN IANCONESCU, Department of Chemical Physics, The Weizmann Institute of Science, JAMES G. PUCKETT, Department of Physics, Gettysburg College, RUI NI, Department of Mechanical and Nuclear Engineering, The Pennsylvania State University, NICHOLAS T. OUELLETTE, Department of Civil and Environmental Engineering, Stanford University, NIR S. GOV, Department of Chemical Physics, The Weizmann Institute of Science — The collective motion of groups of animals emerges from the net effect of the interactions between individual members of the group. In many cases, such as birds, fish, or ungulates, these interactions are mediated by sensory stimuli that predominantly arise from nearby neighbors. But not all stimuli in animal groups are short range. Here, we consider mating swarms of midges, which interact primarily via long-range acoustic stimuli. We exploit the similarity in form between the decay of acoustic and gravitational sources to build a model for swarm behavior. By accounting for the adaptive nature of the midges acoustic sensing, we show that our adaptive gravity model makes mean-field predictions that agree well with experimental observations of laboratory swarms. Our results highlight the role of sensory mechanisms and interaction range in collective animal behavior. The adaptive interactions that we present here open a new class of equations of motion, which may appear in other biological contexts.

4:42PM V35.00010 Synchronization of self-propelled units carrying an internal oscillator, DEMIAN LEVIS, IGNACIO PAGONABARRAGA, ALBERT DIAZ-GUILERA, Univ de Barcelona — We address the question of how self-propulsion, and the dynamical patterns emerging from it, affects the synchronization of motile physical entities, like moving cells synchronizing their intracellular genetic oscillators. In order to do that, we introduce a simple model of self-propelled hard disks moving in 2D carrying an internal variable which follows a Kuramoto dynamics. We find that, in the absence of particle-particle interactions, self-propulsion promotes the synchronization of the particles up to a saturation threshold that we identify with the parameters of the model. However, the presence of sterically interactions give rise to an optimal self-propulsion for synchronization as a consequence of the coupling between the oscillators and the topology of the underlying network, arising from particle interactions, plays an important role for the performance of mobile systems. We single out several dynamic regimes controlled by different processes that we describe. We analyse the relaxation of the system and show that synchronization proceeds through a mechanism that, despite being out-of-equilibrium, verifies the dynamical scaling hypothesis.

5:06PM V35.00012 Dynamics of fire ant aggregations, MICHAEL TENNEINBAUM, DAVID HU, ALBERTO FERNANDEZ-NEVES, Georgia Inst of Tech — Fire ant aggregations are an inherently active system. Each ant harvests its own energy and can convert it into motion. The motion of individual ants contributes non-trivially to the bulk material properties of the aggregation. We have measured some of these properties using plate-plate rheology, where the response to an applied external force or deformation is measured. In this talk, we will present data pertaining to the aggregation behavior in the absence of any external force. We quantify the aggregation dynamics by monitoring the rotation of the top plate and by measuring the normal force. We then compare the results with visualizations of 2D aggregations.
3:06PM V39.00004 Using chaos to model random symbols for improved unsupervised information processing1, SUMONA MUKHOPADHYAY2, HENRY LEUNG3, Department of Electrical and Computer Engineering, University of Calgary — We present theoretical analyses that may allow strengthening the connection between chaotic dynamical system and information processing. The analytical and empirical studies prove that computing with chaos and nonlinear characterization of information improves unsupervised information processing. Traditional supervised techniques for information retrieval from noisy environment achieve optimal performance. However, the need for training symbols is an inefficient strategy. We prove that with a chaotic generator as an information source, unsupervised performance is close to that of supervised with a white Gaussian noise. This suggests that chaotic symbol processing can be used to improve unsupervised information processing. Our results show that chaotic symbol processing can be used to achieve optimal performance in unsupervised information processing.

1This research is supported by Alberta Innovates Technology Futures doctoral scholarship
2PhD student
3Professor

3:18PM V39.00005 Anatomy of a Spin: The Information-Theoretic Structure of Classical Spin Systems, RYAN JAMES, VIKRAM VIJAYARAGHAVAN, JAMES CRUTCHFIELD, Univ of California - Davis — Collective organization in matter plays a significant role in its expressed physical properties. Typically, it is detected via an order parameter, appropriately defined for a given system’s observed emergent patterns. Recent developments in information theory suggest how to quantify collective organization in a system and phenomenon-agnostic way: decompose the system’s thermodynamic entropy density into a localized entropy, that solely contained in the dynamics at a single location, and a bound entropy, that stored in space as domains, clusters, excitations, or other emergent structures. We compute this decomposition and related quantities explicitly for the nearest-neighbor Ising model on the 1D chain, the Bethe lattice with coordination number k = 3, and the 2D square lattice, illustrating its generality and the functional insights it gives near and away from phase transitions. In particular, we consider the roles that different spin motifs play (cluster bulk, cluster edges, and the like) and how these affect the dependencies between spins.
3:30PM V39.00006 Global Characterization of Model Parameter Space Using Information Topology. MARK TRANSTRUM, Brigham Young University — A generic parameterized model is a mapping between parameters and data and is naturally interpreted as a prediction manifold embedded in data space. In this interpretation, known as Information Geometry, the Fisher Information Matrix (FIM) is a Riemannian metric that measures the identifiability of the model parameters. Varying the experimental conditions (e.g., times at which measurements are made) alters both the FIM and the geometric properties of the model. However, several global features of the model manifold (e.g., edges and corners) are invariant to changes in experimental conditions as long as the FIM is not singular. Invariance of these features to changing experimental conditions generates an “Information Topology” that globally characterizes a model’s parameter space and reflects the underlying physical principles from which the model was derived. Understanding a model’s information topology can give insights into the emergent physics that controls a system’s collective behavior, identify reduced models and describe the relationship among them, and determine which parameter combinations will be difficult to identify for various experimental conditions.

1EPSCoR capacity building grant and UNI summer fellowship

3:42PM V39.00007 Statistical Physics of High Dimensional Inference. MADHU ADVANI, SURYA GANGULI, Stanford University — To model modern large-scale datasets, we need efficient algorithms to infer a set of $P$ unknown model parameters from $N$ noisy measurements. What are fundamental limits on the accuracy of parameter inference, given limited measurements, signal-to-noise ratios, prior information, and computational tractability requirements? How can we combine prior information with measurements to achieve these limits? Classical statistics gives incisive answers to these questions as the measurement density $\alpha \to \frac{N}{P} \to \infty$. However, modern high-dimensional inference problems, in fields ranging from bio-informatics to economics, occur at finite $\alpha$. We formulate and analyze high-dimensional inference analytically by applying the replica and cavity methods of statistical physics where data serves as quenched disorder and inferred parameters play the role of thermal degrees of freedom. Our analysis reveals that widely cherished Bayesian inference algorithms such as maximum likelihood and maximum a posteriori are suboptimal in the modern setting, and yields new tractable, optimal algorithms to replace them as well as novel bounds on the achievable accuracy of a large class of high-dimensional inference algorithms.

3:54PM V39.00008 Compression and regularization with the information bottleneck. DJ STROUSE, Princeton University, DAVID SCHWAB, Northwestern University — Compression fundamentally involves a decision about what is relevant and what is not. The information bottleneck (IB) by Tishby, Pereira, and Bialek formalized this notion as an information-theoretic optimization problem and proposed an optimal tradeoff between throwing away as many bits as possible, and selectively keeping those that are most important. The IB has also recently been proposed as a theory of sensory gating and predictive computation in the retina by Palmer et al. Here, we introduce an alternative formulation of the IB, the deterministic information bottleneck (DIB), that we argue better captures the notion of compression, including that done by the brain. As suggested by its name, the solution to the DIB problem is a deterministic encoder, as opposed to the stochastic encoder that is optimal under the IB. We then compare the IB and DIB on synthetic data, showing that the IB and DIB perform similarly in terms of the IB cost function, but that the DIB vastly outperforms the IB in terms of the DIB cost function. Our derivation of the DIB also provides a family of models which interpolates between the DIB and IB by adding noise of a particular form. We discuss the role of this noise as a regularizer.

4:06PM V39.00009 A novel method for the precise determination of step times and sizes in counting large numbers of photobleaching events. CONSTANTINOS TSEKOURAS, STEVE PRESSE, Indiana University - Purdue University Indianapolis — Counting of photobleaching steps is of importance in the investigation of many open problems in biophysics. Current methods of counting photo-bleaching steps does not directly account for fluorophore photophysical behaviors such as fluorophore self-quenching, blinking and flickering. Our Bayesian approach to the counting problem allows for fluorophore blinking and reactivation as well as for multiple simultaneous photobleaching events and is neither computational resource- nor time- heavy. We detail the methods applicability and limitations and present examples of application in photobleach event counting.

4:18PM V39.00010 Assessing the limits of hidden Markov model analysis for multi-state particle tracks in living systems. DYLAN YOUNG, Clarkson Univ — Particle tracking offers significant insight into the molecular mechanics that govern the behavior of living cells. The analysis of molecular trajectories that transition between different motive states, such as diffusive, driven and tethered models, is of considerable importance, with even single trajectories containing significant amounts of information about a molecule’s environment and its interactions with cellular structures such as the cell cytoskeleton, membrane or extracellular matrix. Hidden Markov models (HMM) have been widely adopted to perform the segmentation of such complex tracks, however robust methods for failure detection are required when HMMs are applied to individual particle tracks and limited data sets. Here, we show that extensive analysis of hidden Markov model outputs using data derived from multi-state Brownian dynamics simulations can be used for both the optimization of likelihood models, and also to generate custom failure tests based on a modified Bayesian Information Criterion. In the first instance, these failure tests can be applied to assess the quality of the HMM results. In addition, they provide critical information for the successful design of particle tracking experiments where trajectories containing multiple mobile states are expected.

4:30PM V39.00011 Inferring phenomenological models of Markov processes from data. CATALINA RIVERA, ILYA NEMENMAN, Emory Univ — Microscopically accurate modeling of stochastic dynamics of biochemical networks is hard due to the extremely high dimensionality of the state space of such networks. Here we propose an algorithm for inference of phenomenological, coarse-grained models of Markov processes describing the network dynamics directly from data, without the intermediate step of microscopically accurate modeling. The approach relies on the linear nature of the Chemical Master Equation and uses Bayesian Model Selection for identification of parsimonious models that fit the data. When applied to synthetic data from the Kinetic Proofreading process (KPR), a common mechanism used by cells for increasing specificity of molecular assembly, the algorithm successfully recovers the known coarse-grained description of the process. This phenomenological description has been notice previously, but this time it is derived in an automated manner by the algorithm.

4:42PM V39.00012 Probing self similar structures by studying the frequency of directional changes. ALI Tabei, University of Northern Iowa, STANISLAV BUROV, Bar Ilan University, ANDREW MILBRANDT, KYLE SPURGEON, University of Northern Iowa — It has been shown that in two and higher dimension, when the time series of individual particle trajectories exist, the distribution of relative angles of motion between successive time intervals of random motions provides information about stochastic processes, which is beyond the information obtained from measuring squared displacement. We show that this distribution is a useful measure, which provides supplementary information about the structural properties of the media that a random walker is diffusing. We compare the behavior of this measure for common self-similar structures. We show that the distribution of relative angles is a good measure to discriminate different complex structural geometries.
4:54PM V39.00013 Diffusion, Backward In Time: A Universal Inversion Scheme, DERVIS VURAL, VU NGUYEN, University of Notre Dame — A sugar cube placed in a cup of tea will erode and eventually dissolve. Given the initial shape of the sugar block, it is trivial to predict its final distribution. However, the opposite problem of determining the initial state, given a final one is extremely difficult. A surprising number of seemingly unrelated topics in biology are the same one in disguise: Inverting diffusion on a network. Here we present a method that will identify the origin of a stochastic biological diffusion process, regardless of the forward model. We will then discuss potential implications to evolution, neuroscience, aging biology, and epidemiology.

5:06PM V39.00014 Inferring biological dynamics in heterogeneous cellular environments, STEVE PRESS, IU PUI — In complex environments, it often appears that biomolecules such as proteins do not diffuse normally. That is, their mean square displacement does not scale linearly with time. This anomalous diffusion happens for multiple reasons: proteins can bind to structures and other proteins; fluorophores used to label proteins may flicker or blink making it appear that the labeled protein is diffusing anomalously; and proteins can diffuse in differentially crowded environments. Here we describe methods for learning about such processes from imaging data collected inside the heterogeneous environment of the living cell. Refs. “Inferring Diffusional Dynamics from FCS in Heterogeneous Nuclear Environments” Konstantinos Tsekouras, Amanda Siegel, Richard N. Day, Stee Press*, Biophys. J., 109, 7 (2015). “A data-driven alternative to the fractional Fokker-Planck equation” Steve Press*, J. Stat. Phys.: Th. and Exptm., P07009 (2015).

5:18PM V39.00015 Discovering cell types in flow cytometry data with random matrix theory, YANG SHEN, Chemical Physics Graduate Program, University of Maryland, ROBERT NUSSENBLATT, Laboratory of Immunology, National Eye Institute, National Institutes of Health, WOLFGANG LOSERT1, Chemical Physics Graduate Program, University of Maryland — Flow cytometry is a widely used experimental technique in immunology research. During the experiments, peripheral blood mononuclear cells (PBMC) from a single patient, labeled with multiple fluorescent stains that bind to different proteins, are illuminated by a laser. The intensity of each stain on a single cell is recorded and reflects the amount of protein expressed by that cell. The data analysis focuses on identifying specific cell types related to a disease. Different cell types can be identified by the type and amount of protein they express. To date, this has most often been done manually by labelling a protein as expressed or not while ignoring the amount of expression. Using a cross correlation matrix of stain intensities, which contains both information on the proteins expressed and their amount, has been largely ignored by researchers as it suffers from measurement noise. Here we present an algorithm to identify cell types in flow cytometry data which uses random matrix theory (RMT) to reduce noise in a cross correlation matrix. We demonstrate our method using a published flow cytometry data set. Compared with previous analysis techniques, we were able to rediscover relevant cell types in an automatic way.

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Thursday, March 17, 2016 2:30PM - 5:42PM –
Session V40 GSNP GSOFT DBIO: Robophysics: Physics Meets Robotics I 343 - Chen Li, Johns Hopkins University

2:30PM V40.00001 Geometric mechanics for modelling bioinspired robots locomotion: from rigid to continuous (soft) systems, FREDERIC BOYER, MATHIEU POREZ, Ecole des Mines de Nantes, FEDERICO RENDA, Khalifa University — This talk presents recent geometric tools developed to model the locomotion dynamics of bio-inspired robots. Starting from the model of discrete rigid multibody systems we will rapidly shift to the case of continuous systems inspired from snakes and fish. To that end, we will build on the model of Cosserat media. This extended picture of geometric locomotion dynamics (inspired from fields’ theory) will allow us to introduce models of swimming recently used in biorobotics. We will show how modeling a fish as a one-dimensional Cosserat medium allows to recover and extend the Large Amplitude Elongated Body theory of J. Lighthill and to apply it to an eel-like robot. In the same vein, modeling the mantle of cephalopods as a two dimensional Cosserat medium will build a basis for studying the jet propelling of a soft octopus like robot.

2:42PM V40.00002 Geometric Mechanics Reveals Optimal Complex Terrestrial Undulation Patterns, CHAOHUI GONG, Carnegie Mellon University, HENRY ASTLEY, PERRIN SCHIEBEL, Georgia Institute of Technology, JIN DAI, MATTHEW TRAVERS, Carnegie Mellon University, DANIEL GOLDMAN, Georgia Institute of Technology, HOWIE CHOSET, Carnegie Mellon University, CMU TEAM, GT TEAM — Geometric mechanics offers useful tools for intuitively analyzing biological and robotic locomotion. However, utility of these tools were previously restricted to systems that have only two internal degrees of freedom and in uniform media. We show kinematics of complex locomotors that make intermittent contacts with substrates can be approximated as a linear combination of two shape bases, and can be represented using two variables. Therefore, the tools of geometric mechanics can be used to analyze motions of locomotors with many degrees of freedom. To demonstrate the proposed technique, we present studies on two different types of snake gaits which utilize combinations of waves in the horizontal and vertical planes: sidewinding (in the sidewinder rattlesnake C. cerastes) and lateral undulation (in the desert specialist snake C. occipitalis). C. cerastes moves by generating posteriorly traveling body waves in the horizontal and vertical directions, with a relative phase offset equal to ±π, while C. occipitalis maintains a π/2 offset of a frequency doubled vertical wave. Geometric analysis reveals these coordination patterns enable optimal movement in the two different styles of undulatory terrestrial locomotion. More broadly, these examples demonstrate the utility of geometric mechanics in analyzing realistic biological and robotic locomotion.

2:54PM V40.00003 Optimal bipedal interactions with dynamic terrain: synthesis and analysis via nonlinear programming, CHRISTIAN HUBICKI, DANIEL GOLDMAN, AARON AMES, Georgia Institute of Technology — In terrestrial locomotion, gait dynamics and motor control behaviors are tuned to interact efficiently and stably with the dynamics of the terrain (i.e. terradynamics). This controlled interaction must be particularly thoughtful in bipeds, as their reduced contact points render them highly susceptible to falls. While bipedism under rigid terrain assumptions is well-studied, insights for two-legged locomotion on soft terrain, such as sand and dirt, are comparatively sparse. We seek an understanding of how biological bipeds stably and economically negotiate granular media, with an eye toward imbuing those abilities in bipedal robots. We present a trajectory optimization method for controlled systems subject to granular intrusion. By formulating a large-scale nonlinear program (NLP) with reduced-order resistive force theory (RFT) models and jamming cone dynamics, the optimized motions are informed and shaped by the dynamics of the terrain. Using a variant of direct collocation methods, we can express all optimization objectives and constraints in closed-form, resulting in rapid solving by standard NLP solvers, such as IPOPT. We employ this tool to analyze emergent features of bipedal locomotion in granular media, with an eye toward robotic implementation.
3:06PM V40.00004 Geometric Mechanics for Continuous Swimmers on Granular Material. JIN DAI, Carnegie Mellon Univ, HOSSEIN FARAJI, Oregon State University, PERRIN SCHIEBEL, Georgia Institute of Technology, CHAOHUI GONG, MATTHEW TRAVERS, Carnegie Mellon Univ, ROSS HATTON, Oregon State University, DANIEL GOLDMAN, Georgia Institute of Technology, HOWIE CHOSET, Carnegie Mellon Univ, THE BIOROBOTICS LAB COLLABORATION, LABORATORY FOR ROBOTICS AND APPLIED MECHANICS (LRAM) COLLABORATION, COMPLEX RHEOLOGY AND BIOMECHANICS LAB COLLABORATION — Animal experiments have shown that Chironomus occipitalis (N=10) effectively undulates on granular substrates. A uniaxial oscillator exhibits a particular serpenoid waveform, which can be approximated by a series of helices in a very viscous fluid. Furthermore, all snakes tested used a narrow subset of all available waveform parameters, measured as the relative curvature equal to 5.00, and number of waves on the body equal to 1.0. We used a physical model (snake robot) to empirically explore the space of serpenoid motions, which is linearly spanned with two independent continuous serpenoid basis functions. The empirical derived height function map, which is a geometric mechanics tool for analyzing movements of cyclic gaits, showed that displacement per gait cycle increases with amplitude at small amplitudes, but reaches a peak value of 0.55 body-lengths at relative curvature equal to 6.0. This work signifies that with shape basis functions, geometric mechanics tools can be extended for continuous swimmers.

3:18PM V40.00005 A Cosserat-based formulation for elastic, axisymmetric shells with implications to the pulsed-jetting propulsion of soft-bodied aquatic vehicles. FEDERICO RENDA, Khalifa University Robotics Institute, Khalifa University, FRANCESCO GIORGIO-SERCHI, Southampton Marine and Maritime Institute, University of Southampton, FREDERIC BOYER1, Institut de Recherche en Communication et Cybernétique de Nantes, Ecole des Mines de Nantes — We take the cue from recent development in geometric-based modelling in order to describe the dynamics of a novel soft-structured aquatic vehicle. The Cosserat-like formulation for an axisymmetric, elastic shell subject to concentrated dynamic loadings lends itself to the case of this new vehicle, recently designed by the authors, which consists of a shell of rubber-like materials undergoing segments of motion and inflation in order to propel itself in water via pulsed-jetting. The experiments performed on the existing robotic prototypes are used for the validation of the geometric model. This is eventually employed for deriving an accurate measure of the efficiency of propulsion which explicitly accounts for the elastic energy involved during the propulsion routine. The model yields a-priori estimations of swimming efficiency based on vehicle specifications and mode of actuation. These provide invaluable information for both design optimization and control, as well as a means to study the biomechanics of soft-bodied aquatic organisms.

1 Presenting author

3:30PM V40.00006 Reverse engineering the euglenoid movement: from unicellular swimmers to bio-inspired robots. ANTONIO DESIMONE, GIOVANNI NOSELLI, SISSA-International School for Advanced Studies, MARINO ARROYO, Universitat Politècnica de Catalunya — Euglenids are unicellular organisms living in freshwater, which are capable of moving either by beating a flagellum, or by executing dramatic shape changes. These are accomplished thanks to a complex structure made of interlocking pellicle strips, microtubules, and motor proteins. Relative sliding of the pellicle strips, suitably orchestrated, can cause the propagation of a bulge along the body, hence generating a propulsive force. We study the mechanisms by which the sliding of pellicle strips leads to shape control and locomotion, by means of both theory (through the mechanics of active surfaces and its coupling to computational fluid dynamics for the surrounding fluid) and experimental observations. Moreover, we implement them into a new concept of a surface with programmable shape, obtained by assembling 3D-printed strips in a construct mimicking the biological template. We explore the range of possible geometries achievable by actuating these surfaces, to assess their potential in soft robotics applications. The subtle balance between constraints and flexibility leads to a wide variety of shapes that can be obtained with relatively simple controls, similar to the notion of morphological computation in biological systems.

3:42PM V40.00007 Robotics and Biology: Let's get Physical. HOWIE CHOSET, Carnegie Mellon University — Our research group investigates the core fundamentals of locomotion as it exists in biology and as it applies to locomoting robotic systems. Initially, our work advanced techniques found in geometric mechanics to design cyclic controllers, often called gaits, for snake robots, highly articulated mechanisms that can thread through tightly packed spaces to access locations people cannot. We had considerable success in designing snake robot gaits, but found our systems stymied in terrains characterized by sandy substrates. Sandy terrains and other granular media pose a challenge to snake robots because it is unclear how the mechanism interacts with environment: we cannot simply assume the robot is on hard-ground nor in a fluid. Simulating granular interactions can prove to be computationally intractable for real-time use on the robots. Therefore, we developed experimental tools that allowed us to sieve out models of the locomoting systems operating on granular media. We were then able to bring these models into harmony with the elegant formulation of our geometric mechanics approach. This allowed us to derive adaptive controllers for our snake robots in sandy terrains, and enabled us to gain deeper insight into how biological systems move over similar terrains as well.

4:18PM V40.00008 Bio-inspired robot design for viscous fluids. GRACE MA, TYLER LIPMAN, SUNGHWAN JUNG, Virginia Tech — Many modern micro-robots are designed for biomedical applications to transport drugs to targets or to operate tests in the body for diagnosis. However, most micro-robots simply mimic the morphology and the propulsive mechanism of micro-organisms without understanding the underlying physics of low-Reynolds number flows, and how it can be applied to non-Newtonian fluids. The keyword here is viscous. Bacteria, flagellated micro-organisms capable of propelling themselves, can have been observed in micro-organisms; the stresslet and source-dipole swimming. The stresslet model (e.g. E. coli) uses a rotating helical appendage, whereas the source-dipole swimmer (e.g. Paramecium) creates surface velocity for propulsion. Using this principle, we designed a robot to swim in very viscous fluids either by rotating a helix or creating surface velocity, simply by changing the orientation of the appendage. Further, we will discuss the performance of this robot (swimming speed and rotation speed) with respect to the number, winding angle, and radius of helices in a very viscous fluid.

4:30PM V40.00009 A microfluidic two-pump system inspired by liquid feeding in mosquitoes. ANDREW MARINO, Virginia Tech, ANGELA GOAD, Carroll County High School, MARK STREMLER, JOHN SOCHA, SUNGHWAN JUNG, Virginia Tech — Mosquitoes feed on nectar and blood using a two-pump system in the head—a smaller ciliary pump in lieu with a larger a pharyngeal pump, with a valve in between. To suck, mosquitoes transport the liquid (which may be a multi-component viscous fluid, blood) through a long micro-channel, the proboscis. In the engineering realm, microfluidic devices in biomedical applications, such as lab-on-a-chip technology, necessitate implementing a robust pump design to handle clogging and increase flow control compared to a single-pump system. In this talk, we introduce a microfluidic pump design inspired by the mosquito’s two-pump system. The pumping performance (flow rate) in presence of impurities (air bubbles, soft clogs) is quantified as a function of phase difference and volume expansion of the pumps, and the elasticity of the valve.

4:42PM V40.00010 Propulsion of a two-sphere swimmer. DAPHNE KLOTSA, Department of Applied and Physical Sciences, University of North Carolina at Chapel Hill, KYLE BALDWIN, RICHARD HILL, ROGER BOWLEY, MICHAEL SWIFT, School of Physics and Astronomy, University of Nottingham, UK — We describe experiments and simulations demonstrating the propulsion of a neutrally-buoyant macroscopic swimming robot that consists of a pair of spheres attached by a spring, immersed in a vibrating fluid. The vibration of the fluid induces relative motion of the spheres which, for sufficiently large amplitudes, can lead to motion of the center of mass of the two spheres. We find that the swimming speed obtained from both experiment and simulation agree and collapse onto a single curve if plotted as a function of the streaming Reynolds number, suggesting that the propulsion is related to streaming flows. This appears to be a critical onset value of the streaming Reynolds number for swimming to occur. We observe a change in the swimming speed obtained from both experiment and simulation agree and collapse onto a single curve if plotted as a function of the streaming Reynolds number, suggesting that the propulsion is related to streaming flows.
5:06PM V40.00012 Bipedal locomotion in granular media . MARK KINGSBURY, TINGNAN ZHANG, DANIEL GOLDMAN, Georgia Inst of Tech — Bipedal walking, locomotion characterized by alternating swing and double support phase, is well studied on ground where feet do not penetrate the substrate. On granular media like sand however, intrusion and extrusion phases also occur. In these phases, relative motion of the two feet requires that one or both feet slip through the material, degrading performance. To study walking in these phases, we designed and studied a planarized bipedal robot (1.6 kg, 42 cm) that walked in a fluidized bed of poppy seeds. We also simulated the robot in a multi-body software environment (Chrono) using granular resistive force theory (RFT) to calculate foot forces. In experiment and simulation, the robot experienced slip during the intrusion phase, with the experiment presenting additional slip due to motor control error during the double support phase. This exaggerated slip gave insight (through analysis of ground reaction forces in simulation) into how slip occurs when relative motion exists between the two feet in the granular media, where the foot with higher relative drag forces (from its instantaneous orientation, rotation, relative direction of motion, and depth) remains stationary. With this relationship, we generated walking gaits for the robot to walk with minimal slip.

5:18PM V40.00013 Obstacle traversal and self-righting of bio-inspired robots reveal the physics of multi-modal locomotion . CHEN LI, RONALD FEARING, ROBERT FULL, University of California, Berkeley — Most animals move in nature in a variety of locomotor modes. For example, to traverse obstacles like dense vegetation, cockroaches can climb over, push across, reorient their bodies to maneuver through slits, or even transition among these modes forming diverse locomotor pathways; if flipped over, they can also self-right using wings or legs to generate body pitch or roll. By contrast, most locomotion studies have focused on a single mode such as running, walking, or jumping, and robots are still far from capable of life-like, robust, multi-modal locomotion in the real world. Here, we present two recent studies using bio-inspired robots, together with new locomotion energy landscapes derived from locomotor-environment interaction physics, to begin to understand the physics of multi-modal locomotion. (1) Our experiment of a cockroach-inspired legged robot traversing grass-like beam obstacles reveals that, with a terradynamically “streamlined” rounded body like that of the insect, robot traversal becomes more possible by accessing locomotor pathways that overcome lower potential energy barriers. (2) Our experiment of a cockroach-inspired self-righting robot further suggests that body vibrations are crucial for exploring locomotion energy landscapes and reaching lower barrier pathways. Finally, we posit that our new framework of locomotion energy landscapes holds promise to better understand and predict multi-modal biological and robotic movement.

5:30PM V40.00014 Swarming Bristle-Bots: Exploring Properties of Active Matter . MARTIN B. FORSTNER, DAMIAN BEASOCK, Syracuse University — Active Matter describes an ubiquitous class of non-equilibrium systems that encompasses a diverse range of phenomena in the living and non-living realm. Examples are microscopic bio-filaments and their associated motor proteins, flocks of birds and fish, vibrated rods and disks, or nanoscale colloids actuated by catalytic activity on their surface. What unifies these systems is that they are all composed of self-driven units. In consequence, these systems are not driven into non-equilibrium by energy input at their boundary, but by local energy injection. As fascinating as these systems are, there are currently barely any laboratory systems that allow for controlled experiments in dry active matter. That is, systems not immersed in a fluid that can be observed without specialized equipment. Here we present a two-dimensional ‘active matter’ system consisting of hundreds of macroscopic (~0.05 m) long, modified, commercially available bristle-bots. We show that this swarm of toys classifies as active matter as it exhibits properties such as dynamic phase separation. Because of their straightforward implementation, their size and controllability, such swarms can not only answer scientific questions, but they have great potential as educational tools in teaching labs and classrooms.

Thursday, March 17, 2016 2:30PM - 5:30PM —
Session V43 GSNP: Wave Chaos: Theory and Applications 346 - Gabriele Gradoni, University of Nottingham

2:30PM V43.00001 Modeling Transmission Line Networks Using Quantum Graphs1 . TRYSTAN KOCH, THOMAS ANTONSEN, Univ of Maryland-College Park — Quantum graphs—one dimensional edges, connecting nodes, that support propagating Schrödinger wavefunctions—have been studied extensively as tractable models of wave chaotic behavior (Smilansky and Gnutzmann 2006, Berkolaiko and Kuchment 2013). Here we consider the electrical analog, in which the graph represents an electrical network where the edges are transmission lines (Hul et. al. 2004) and the nodes contain either discrete circuit elements or intricate circuit elements best represented by arbitrary scattering matrices. Including these extra degrees of freedom at the nodes leads to phenomena that do not arise in simpler graph models. We investigate the properties of eigenfrequencies and eigenfunctions on these graphs, and relate these to the statistical description of voltages on the transmission lines when driving the network externally. The study of electromagnetic compatibility, the effect of external radiation on complicated systems with numerous interconnected cables, motivates our research into this extension of the graph model.

1Work supported by the Office of Naval Research (N00014130474) and the Air Force Office of Scientific Research.

2:42PM V43.00002 Experimental Study of Quantum Graphs with Microwave Networks1 . ZIYUAN FU, TRYSTAN KOCH, THOMAS ANTONSEN, EDWARD OTT, STEVEN ANLAGE, University of Maryland. College Park. WAVE CHAOS TEAM — An experimental setup consisting of microwave networks is used to simulate quantum graphs. The networks are constructed from coaxial cables connected by T junctions. The networks are built for operation both at room temperature and superconducting versions that operate at cryogenic temperatures. In the experiments, a phase shifter is connected to one of the network bonds to generate an ensemble of quantum graphs by varying the phase delay. The eigenvalue spectrum is found from S-parameter measurements on one-port graphs. With the experimental data, the nearest-neighbor spacing statistics and the impedance separation. Because of their straightforward implementation, their size and controllability, such swarms can not only answer scientific questions, but they have great potential as educational tools in teaching labs and classrooms.

1We acknowledge support under contract AFOSR COE Grant FA9550-15-1-0171.
2:54PM V43.00003 Numerical and experimental studies of the elastic enhancement factor of 2D open systems. LESZEK SIRKO, MALGORZATA BIAŁOUS, VITALII YUNKO, SZYMON BAUCH, MICHAŁ LAWNICZAK, Institute of Physics Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warszawa, Poland — We present the results of numerical and experimental studies of the elastic enhancement factor \( W \) for microwave rough and rectangular cavities simulating two-dimensional chaotic and partially chaotic quantum billiards in the presence of moderate absorption strength. We show that for the frequency range \( \nu = 15.0 - 18.5 \) GHz, in which the coupling between antennas and the system is strong enough, the values of \( W \) for the microwave rough cavity lie below the predictions of random matrix theory and on average they are above the theoretical results of V. Sokolov and O. Zhislov, Phys. Rev. E, 91, 052917 (2015). We also show that the enhancement factor \( W \) of a microwave rectangular cavity coupled to the external channels of microstrip cavities, simulating a partially chaotic quantum billiard [1], calculated by applying the Potter-Rosenzweig model with \( \kappa = 2.8 \pm 0.5 \) is close to the experimental one. Our numerical and experimental results suggest that the enhancement factor can be used as a measure of internal chaos which can be especially useful for systems with significant openness or absorption. [1] M. Lawniczak, M. Białous, V. Yanko, S. Bauch, and L. Sirko, Phys. Rev. E 91, 032925 (2015).

3:06PM V43.00004 Statistical Model of Wave Transport in Systems with Coexisting Chaotic and Regular Phase Space Regions. EDWARD OTT, University of Maryland — We study the statistics of the input-output properties of wave systems in which ray trajectories that are regular and chaotic coexist (i.e., ‘mixed systems’). The transport is expressed as a summation over eigenmodes (energy states) where the eigenmodes can typically be classified as either regular or chaotic. By appropriate characterization of regular and chaotic contributions, we obtain predictions for the transport as characterized by impedance or scattering matrices. We test these predictions by comparison with numerical calculations for a specific example. [Collaborators: M.-J. Lee, T.M. Antonsen, and K. Ma]

3:42PM V43.00005 Radiation of complex and noisy sources within enclosures. GABRIELE GRADONI, STEPHEN CREAKH, GREGOR TANNER, University of Nottingham — Predicting the radiation of complex electromagnetic sources inside semi-open cavities and resonators with arbitrary geometry is a challenging topic both for physics and for engineering. We have exploited a Perron-Frobenius operator to propagate field-field correlation functions of complex and extended sources in free-space. The formula is based on a phase-space picture of the electromagnetic field, using the Wigner distribution function, and naturally captures evanescent as well as diffracted waves. This approach can be extended to study the propagation of field-field correlation functions within cavities, with the ray-dynamical map given by the geometry of the cord connecting a point of the boundary to another. While ray methods provide an efficient way to predict average values of the correlation matrix elements, the use of random matrix theory approaches allows efficient characterization of statistical fluctuations around these averages. Universal relations are derived and tested in the presence of dissipation for quantum maps and billiard systems. The use of this formalism is discussed in the contexts of open systems with surface roughness. The theory and achieved results are of interest in the simulation of next-generation of wireless communications.

3:54PM V43.00006 FDTD simulations of the losses in complex electromagnetic cavities. FRANCO MOGLIE, LUCA BASTIANELLI, VALTER MARIANI PRIMIANI, Universita’ Politecnica delle Marche - DII, Ancona, EMC TEAM — The simulations of complex electromagnetic cavities like reverberation chambers (RC) require a massive parallel computer to accurately account the complex three dimensional geometry. A parallel finite-difference time-domain (FDTD) code optimized for a massive parallel computer could lose its efficiency if the losses are concentrated in some part of the computation volume. For example, the simulation of the finite conductivity of the cavity metallic walls requires a significant overcharge for the computer processors that handle the boundary part of the global computational domain. Our in-house parallel FDTD code replaces the volumetric losses in every cell of the grid instead of the Ohmic losses on the walls. In this contribution, we evaluate the difference in the field distribution inside the cavity due to this replacement. Moreover, we compare the common RC statistics like the number of stirrer uncorrelated positions and the field uniformity, and the resources required for the two methods are reported and discussed. Finally, the numerical results are labeled with a volume of 60 m\(^3\) and plated steel walls in the frequency range 0.2-1.0 GHz, that includes the transition from the undermoded to the overmoded region.

4:06PM V43.00007 Conductance and Transmittance of waves through a chaotic cavity (or, equivalently, quantum dot) results in regularization of tunneling rates. LOUIS PECORA, DONG HO WU, CHRISTOPHER KIM, Naval Research Lab — Tunneling rates in closed, double well quantum or wave systems in two dimensions or higher are radically different between wells with classically regular or chaotic behavior [1]. Wells with regular dynamics have tunneling rates that fluctuate by several orders of magnitude as a function of energy or frequency. Wells with chaotic dynamics have fluctuations smaller than one order of magnitude (a regularization of the fluctuations). We examine a more realistic experimental system, a single well with two channels with tunneling barriers at their junctions with the wells. Former theories for conductance in quantum dots will not apply here. We developed a theory, which uses proper boundary conditions at the barriers and yields the scattering matrix. Results show that the transmission rates fluctuate by orders of magnitude in the regular-shaped well, but are greatly reduced (regularized) for the chaotic-shaped well. We will show experimental results that test these theoretical findings for microwave transmission through a chaotic-shaped cavity, which is made of copper and has two ports with tunneling barriers. [1] Chaos regularization of quantum tunneling rates, L. M. Pecora, H. Lee, D-H. Wu, T. Antonsen, M-J. Lee, and E. Ott, Phys. Rev. E 83, 065201(R) (2011)

4:18PM V43.00008 Time Reversed Electromagnetics as a Novel Method for Wireless Power Transfer. ANU CHALLA, ECE Department, University of Maryland, STEVEN M. ANLAGE, Physics and ECE Departments, University of Maryland, TESLA TEAM — Taking advantage of ray-chaotic enclosures, time reversal has been shown to securely transmit information via short-wavelength waves between two points, yielding noise at all other sites. In this presentation, we propose a method to adapt the signal-focusing technique to electromagnetic signals in order to transmit energy to portable devices. Relying only on the time-reversal invariance properties of waves, the technique is unencumbered by the inversely-proportional-to-distance path loss or precise orientation requirements of its predecessors, making it attractive for power transfer applications. We inject a short microwave pulse into a complex, wave-chaotic chamber and collect the resulting long time-domain signal at a designated transceiver. The signal is then time reversed and emitted from the collection site, collapsing as a time-reversal replica of the initial pulse at the injection site. When amplified, this reconstruction is robust, as measured through metrics of peak-to-peak voltage and energy transfer ratio. We experimentally demonstrate that time reversed collapse can be made on a moving target, and propose a way to selectively target devices through nonlinear time-reversal.

3Work supported by the UK Engineering and Physical Sciences Research Council

1Work supported by the UK Engineering and Physical Sciences Research Council

4University of Maryland Gemstone Team TESLA: Frank Cangialosi, Anu Challa, Tim Furman, Tyler Grover, Patrick Healey, Ben Philip, Brett Potter, Scott Roman, Andrew Simon, Liangcheng Tao, Alex Tabatabai
4:30PM V43.00009 Enhancement of coherent terahertz beam with chaotic electrodes in a photoconductive antenna, DONALD HO WU, BENJAMIN GRABER, LOUIS PECORA, CHRISTOPHER KIM, U.S. Naval Research Laboratory — We investigated terahertz beam emission from photoconductive antennas containing various shapes of electrodes. With a pair of curved (e.g. concave shape) electrodes it appears that electrons (mostly thermal electrons) follow chaotic trajectories, which keep the electrons away from the surface plasma so that the surface plasma can coherently oscillates without being disrupted by thermal electrons, resulting in a slightly increased coherent terahertz power. For an emitter with a pair of ripple electrodes, the classical Poincaré surface section map using Birkhoff coordinate tends to exhibit chaotic sea and KAM islands if the ripple amplitude becomes comparable to the electrode gap, indicating considerable electron bunching in between the ripple electrodes. Our data show that, when the bunched electrons are stimulated by terahertz pulses, the emitter produces additional spontaneous coherent terahertz beams, which is known as Dicke effect. We will discuss details of our experiments and results.

4:42PM V43.00010 Controlling and enhancing high frequency collective electron dynamics in superlattices by chaos-assisted miniband transport, MARK FROMHOLD, MARK GREENAWAY, NATALIA ALEXEEVA, University of Nottingham, ALEXANDER BALANOV, Loughborough University, OLEG MAKAROVSKY, AMALIA PATANE, University of Nottingham, MARAT GAIFULLIN, FEO KUSMARTSEV, Loughborough University — We show in both measurements and calculations that a tilted magnetic field can transform the structure and THz dynamics of charge domains in a biased semiconductor superlattice (SL) [1]. In SLs, at critical field values, when the Bloch frequency equals the cyclotron frequency corresponding to the magnetic field component along the SL axis, the semiclassical electron motion changes abruptly from localized stable trajectories to unbounded chaotic paths, which propagate rapidly through the SL. This delocalisation of the electron creates a series of sharp resonant peaks in drift velocity-field characteristics, which were detected in previous DC current-voltage measurements. We show that these additional peaks can create multiple propagating charge domains, shaped by both the strength and tilt angle of the magnetic field. As a result, the tilted magnetic field generates AC currents whose magnitude and frequencies are far higher than with no magnetic field applied. Chaos-assisted single-electron transport induced by the interplay between cyclotron and Bloch motion therefore provides a mechanism for controlling the collective dynamics of miniband electrons, and thus enhancing the high frequency response of SLs. References: [1] N. Alexeeva et. al. Phys. Rev. Lett. 109, 024102 (2012)

4:54PM V43.00011 Light transport in dense composite media: role of near-field coupling, ROXANAirezvani NARAGHI, CREOL and Department of Physics, University of Central Florida, SERGEY SUKHOV, CREOL, University of Central Florida, JUAN JOS SENZ, Condensed Matter Physics Center, Universidad Autonoma de Madrid and Donostia International Physics Center, Paseo Manuel Lardizabal 4, ARISTIDE DOGARIU, CREOL, University of Central Florida — In scattering media, optical waves comprise both homogeneous and evanescent components. At very high concentrations of scatterers, particles are located in close proximity and interact through evanescent near fields. Thus, in this regime the energy is not only carried by propagating waves but it also evolves through evanescent coupling between individual scatterers. We have shown that in dense composite media additional transmission channels open because of these near-field interactions between close proximity scatterers and, consequently, a new regime of transport emerges. This is clearly beyond simple descriptions of scatterers acting independently of their environment and framed in terms of far-field characteristics such as Mie cross-sections. We will show that, because in the dense media the energy can transfer through both diffusion and evanescent channels, the total transmittance is $T = T_{CS} + T_{NF} = 1/L(r_{CS} + r_{NF})$. Correcting the total transmission in this manner is appealing because it is done in terms of physically meaningful and measurable quantities such a near-field (NF) scattering cross-section $\sigma_{NF}$.

5:06PM V43.00012 Complexity of knotting in chaotic 3D eigenfunctions, ALEXANDER TAYLOR, MARK DENNIS, University of Bristol — Quantised vortices occur generically in disordered 3D complex scalar fields, forming a geometrically complex and statistically random large scale tangle even in systems with very different origins of complexity such as turbulent superfluids, optical volume speckle, the quantum eigenfunctions of chaotic 3D cavities, and liquid crystal phases. Although all such systems are random and fractal on large scales [1], it has previously been established that topological measures such as the probability of vortices knotting or linking with one another are sensitive to the local physics. We use the wave chaos as a universal model system with just one physical lengthscale, the wavelength, beyond which its vortices are Brownian. To access finite-volume realisations of wavefields, vortices are traced numerically in three different random degenerate eigenfunction systems, each approximating the random isotropic limit but with different constraints and symmetries that significantly impact topological statistics even at high energies. By a simple mode counting argument, we observe that the probability of a generic eigenfunction containing a knotted vortex line reaches 50% by around its 1000-3000th mode.

5:18PM V43.00013 Supersymmetric sigma model of disordered, isotropic, elastic media, DOUGLAS PHOTIADIS, Naval Research Laboratory — The supersymmetry method proposed by Efetov in 1983 has been enormously successful at describing a broad range of phenomena involving disorder, providing a framework for understanding and going beyond the successes of random matrix theory and allowing a calculation of the slowing of diffusion as the Anderson transition is approached. The original model described the propagation of a scalar wave in a disordered medium, and subsequent work extended these ideas to classical waves, optical or elastic, with the approximation that the wave propagation can be similarly described by a scalar theory. Such a theory cannot however account correctly for scattering between different polarizations. A direct attempt to derive a supersymmetric model describing elastic waves results in a non-renormalizable field theory, and poses substantial difficulties. We have obtained a supersymmetric sigma model by considering the dual model which describes a generalized superstress field. The model enables one to fully account for the different wave types and polarizations in the medium. We will present our recent results in this area, including model predictions for the obtained diffusion constants, and the effects of renormalization to first order.

This research was funded by the Office of Naval Research.

Thursday, March 17, 2016 2:30PM - 5:30PM – Session V55 DBIO GSNP DPOLY: DNA Physics and Chromatin Organization Hilton Baltimore

Holiday Ballroom 6 - Alexandre V. Morozov, Rutgers University
Detecting early-warning signals of critical transitions for complex systems

JOHN MARKO, Northwestern University — I will discuss micromechanics experiments that our group has used to analyze protein-DNA interactions and chromosome organization. In single-DNA experiments we have found that a feature of protein-DNA complexes is that their dissociation rates can depend strikingly on bulk solution concentrations of other proteins and DNA segments; I will describe experiments which demonstrate this effect, which can involve tens-fold changes in off-rates with submicromolar changes in solution concentrations. Second, I will discuss experiments aimed at analyzing large-scale human chromosome structure: we isolate metaphase chromosomes, which in their native form behave as remarkably elastic networks of chromatin. Exposure to DNA-cutting restriction enzymes completely eliminates this elasticity, indicating that there is not a mechanically contiguous protein “scaffold” from which the chromosome gains its stability. I will show results of siRNA experiments indicating that depletion of condensin proteins leads to destabilization of chromosome mechanics, indicating condensin’s role as the major chromatin “cross-linker” in metaphase chromosomes. Finally I will discuss similar experiments on human G1 nuclei, where we use genetic and chemical modifications to separate the contributions of the nuclear lamina and chromatin to the mechanical stiffness of the nucleus as a whole.

This work was supported by the NSF DMR-1206146 and the NIH (GM105847, CA193419).

I’d like to present my talk from my laptop (movies)

Detecting early-warning signals of critical transitions for complex systems

LEONID MIRNY, MIT — Chromosome Conformation Capture technique (Hi-C) provides comprehensive information about frequencies of spatial interactions between genomic loci. Inferring 3D organization of chromosomes from these data is a challenging biophysical problem. We develop a top-down approach to biophysical modeling of chromosomes. Starting with a minimal set of biologically motivated interactions we build ensembles of polymer conformations that can reproduce major features observed in Hi-C experiments. I will present our work on modeling organization of human metaphase and interphase chromosomes. Our works suggests that active processes of loop extrusion can be a universal mechanism responsible for formation of domains in interphase and chromosome compaction in metaphase.

Detecting early-warning signals of critical transitions for complex systems

JANE KONDEV, Brandeis University — Various functions performed by chromosomes involve long-range communication between DNA sequences that are tens of thousands of bases apart along the genome, and microns apart in the nucleus. In this talk I will discuss experiments and theory relating to two distinct modes of long-range communication in the nucleus, chromosome looping and protein hopping along the chromosome, both in the context of DNA-break repair in yeast. Yeast is an excellent model system for studies that link chromosome conformations to their function as there is ample experimental evidence that yeast chromosome conformations are well described by a simple, random-walk polymer model. Using a combination of polymer physics theory and experiments on yeast cells, I will demonstrate that loss of polymer entropy due to chromosome looping is the driving force for homology search during repair of broken DNA by homologous recombination. I will also discuss the spread of histone modifications along the chromosome and away from the DNA break point in the context of simple physics models based on chromosome looping and kinase hopping, and show how combining physics theory and cell-biology experiment can be used to dissect the molecular mechanism of the spreading process. These examples demonstrate how combined theoretical and experimental studies can reveal physical principles of long-range communication in the nucleus, which play important roles in regulation of gene expression, DNA recombination, and chromatin modification.

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This work was supported by the NSF DMR-1206146 and the NIH (GM105847, CA193419).

I’d like to present my talk from my laptop (movies)
8:36AM X35.00002 The evolution of lossy compression, SARAH MARZEN, University of California, Berkeley, SIMON DEDEO, Indiana University, Bloomington — In complex environments, there are costs to both ignorance and perception. An organism needs to track fitness-relevant information about its world, but the more information it tracks, the more resources it must devote to memory and processing. As a first step towards understanding this tradeoff, we use rate-distortion theory to study large, unstructured environments with fixed, randomly-drawn penalties for stimulus confusion (“distortions”). We find that two different environments will have nearly identical rate-distortion functions (but very different codebooks) when distortions are drawn from the same distribution, suggesting an interesting weak universality. We further identify two distinct regimes for organisms in these structured environments: a high-fidelity regime where perceptual costs grow linearly with environmental complexity, and a low-fidelity regime where perceptual costs are, remarkably, independent of the number of environmental states. This last result suggests that evolution will drive organisms to the threshold between the high- and low-fidelity regimes. In dynamic environments of rapidly-increasing complexity, well-adapted organisms will find themselves able to make, just barely, the most subtle distinctions in their environment.

8:48AM X35.00003 Dynamics of neuroendocrine stress response: bistability, timing, and control of hypocortisolism, MARIA D'ORSOGNA, California State University at Northridge, TOM CHOU, LAE KIM, UCLA — The hypothalamic-pituitary-adrenal (HPA) axis is a neuroendocrine system that regulates numerous physiological processes. Disruptions in its activity are correlated with stress-related diseases such as post-traumatic stress disorder (PTSD) and major depressive disorder. We characterize “normal” and “diseased” states of the HPA axis as basins of attraction of a dynamical system describing the inhibition of peptide hormones, corticotropin-releasing hormone (CRH) and adrenocorticotropic hormone (ACTH), by circulating glucocorticoids such as cortisol (CORT). Our model includes ultradian oscillations, CRH self-upregulation of CRH release, and distinguishes two components of negative feedback by cortisol on circulating CRH levels: a slow direct suppression of CRH synthesis and a fast indirect effect on CRH release. The slow regulation mechanism mediates external stress-driven transitions between the stable states in novel, intensity, duration, and timing-dependent ways. We find that the timing of traumatic events may be an important factor in determining if and how the hallmarks of depressive disorders will manifest. Our model also suggests a mechanism whereby exposure therapy of stress disorders may act to normalize downstream dysregulation of the HPA axis.

9:00AM X35.00004 Dynamics of blood flow in a microfluidic ladder network, JEEVAN MADDALA, JEVGENIA ZILBERMAN-RUDENKO, OWEN MCCARTY, Oregon Health and Science University — The dynamics of a complex mixture of cells and proteins, such as blood, in perturbed shear flow remains ill-defined. Microfluidics is a promising technology for improving the understanding of blood flow under complex conditions of shear; as found in stent implants and in tortuous blood vessels. We model the fluid dynamics of blood flow in a microfluidic ladder network with dimensions mimicking venules. Interaction of blood cells was modeled using multigiant framework, where cells of different diameters were treated as spheres. This model served as the basis for predicting transition regions, collection pathways, re-circulation zones and residence times of cells dependent on their diameters and device architecture. Based on these insights from the model, we were able to predict the clot formation configurations at various locations in the device. These predictions were supported by the experiments using whole blood. To facilitate platelet aggregation, the devices were coated with fibrillar collagen and tissue factor. Blood was perfused through the microfluidic device for 9 min at a physiologically relevant venous shear rate of 600 s$^{-1}$. Using fluorescent microscopy, we observed flow transitions near the microfluidic intersections and at the areas of blood flow obstruction, which promoted larger thrombus formation. This study of integrating model predictions with experimental design, aids in defining the dynamics of blood flow in microvasculature and in development of novel biomedical devices.

9:12AM X35.00005 Identifying driving gene clusters in complex diseases through critical transition theory, NATHANIEL WOLANYK, The Department of Physics University of Alabama at Birmingham, XUJING WANG, NHLB1, NIH, MARTIN HESSNER, Medical College of Wisconsin, SHOUGuO GAO, YE CHEN, NHLB1, NIH, SHuang JIA, Medical College of Wisconsin — A novel approach of looking at the human body using critical transition theory has yielded positive results: clusters of genes that act in tandem to drive complex disease progression. This cluster of genes can be thought of as the first part of a large genetic force that pushes the body from a curable, but sick, point to an incurable diseased point through a catastrophic bifurcation. The data analyzed is time course microarray blood assay data of 7 high risk individuals for Type 1 Diabetes who progressed into a clinical onset, with an additional larger study requested to be presented at the conference. The normalized data is 25,000 genes strong, which were narrowed down based on statistical metrics, and finally a machine learning algorithm using critical transition metrics found the driving network. This approach was created to be repeatable across multiple complex diseases with only progression time course data needed so that it would be applicable to identifying when an individual is at risk of developing a complex disease. Thusly, preventative measures can be enacted, and in the longer term, offers a possible solution to prevent all Type 1 Diabetes.

9:24AM X35.00006 Finding the role of time-delays in complex systems, WEI LIN, School of Mathematical Sciences and Centre Computational Systems Biology, Fudan University — Time delays are omnipresently observed in many nature and artificial systems including physical, biological, and chemical systems. Naturally, two kinds of questions arise: How to identify the time delays when a certain amount of datasets are obtained from the same distribution, and how to identify the models that are suitable for unstructured complex systems with time delays that are played in the critical transition of coupled network systems. In this talk, we introduce recent works that address the previous two questions, and show the significance of time delays in dealing with various biological systems.

9:36AM X35.00007 Detecting critical state before phase transition of complex systems by hidden Markov model, RUI LIU, PEI CHEN, YONGJUN LI, South China University of Technology, LUONAN CHEN, Shanghai Institutes for Biological Sciences — Identifying the critical state or pre-transition state just before the occurrence of a phase transition is a challenging task, because the state of the system may show little apparent change before this critical transition during the gradual parameter variations. Such dynamics of phase transition is generally composed of three stages, i.e., before-transition state, pre-transition state, and after-transition state, which can be considered as three different Markov processes. Thus, based on this dynamical feature, we present a novel computational method, i.e., hidden Markov model (HMM), to detect the switching point of the two Markov processes from the before-transition state (a stationary Markov process) to the pre-transition state (a time-varying Markov process), thereby identifying the pre-transition state or early-warning signals of the phase transition. To validate the effectiveness, we apply this method to detect the signals of the imminent phase transitions of complex systems based on the simulated datasets, and further identify the pre-transition states as well as their critical modules for three real datasets, i.e., the acute lung injury triggered by phosgene inhalation, MCF-7 human breast cancer caused by heregulin, and HCV-induced dysplasia and hepatocellular carcinoma.

$^3$The work is supported by NNSF of China [Grant No. 11322111 and 61273014] and SCMS.
9:48AM X35.00008 Identification of driving network of cellular differentiation from single sample time course gene expression data . YE CHEN, The National Heart, Lung, and Blood Institute (NHBLI), NATHANIEL WOLANYK, University of Alabama at Birmingham, TUNC ILKER, SHOUGUO GAO, XUJING WANG, The National Heart, Lung, and Blood Institute (NHBLI) — Methods developed based on bifurcation theory have demonstrated their potential in driving network identification for complex human diseases, including the work by Chen, et al. Recently bifurcation theory has been successfully applied to model cellular differentiation. However, there one often faces a technical challenge in driving network prediction: time course cellular differentiation study often only contains one sample at each time point, while driving network prediction typically require multiple samples at each time point to infer the variation and interaction structures of candidate genes for the driving network. In this study, we investigate several methods to identify both the critical time point and the driving network through examination of how each time point affects the autocorrelation and phase locking. We apply these methods to a high-throughput sequencing (RNA-Seq) dataset of 42 subsets of thymocytes and mature peripheral T cells at multiple time points during their differentiation (GSE48138 from GEO). We compare the predicted driving genes with known transcription regulators of cellular differentiation. We will discuss the advantages and limitations of our proposed methods, as well as potential further improvements of our methods.

10:00AM X35.00009 Experimental and theoretical description of higher order periods in cardiac tissue action potential duration . CONNER HERNDON, FLAVIO FENTON, ILIJA UZELAC, Georgia Tech — Much theoretical, experimental, and clinical research has been devoted to investigating the initiation of cardiac arrhythmias by alternans, the first period doubling bifurcation in the duration of cardiac action potentials. Although period doubling above alternans has been shown to exist in many mammalian hearts, little is understood about their emergence or behavior. There currently exists no physiologically correct theory or model that adequately describes and predicts their emergence in stimulated tissue. In this talk we present experimental data of period 2, 4, and 8 dynamics and a mathematical model that describes these bifurcations. This model extends current cell models through the addition of memory and includes spatiotemporal nonlinearities arising from cellular coupling by tissue heterogeneity.

10:12AM X35.00010 Theory of advection-driven long range biotic transport . OLEG KOGAN, KEVIN O’KEEFFE, Cornell University, DAVID SCHNEIDER, United States Department of Agriculture, Cornell University, CHRISTOPHER MYERS, Cornell University — We consider a new reaction-transport framework, and apply it to the problem of advection-driven biotic transport. The are two compartments - the growth layer, coupled to a separate, advective layer. Density fronts propagate in both layers. Crucially, the downwind front speed goes to a finite value as the coupling goes to zero. We next include diffusion in the growth layer, and study the competition between the advective and diffusive transport mechanisms. Advection wins for small diffusion and cannot be ignored, no matter how weak is the coupling. When coupling is not small, both mechanisms work cooperatively, without a clear winner. A further surprise is the existence of a critical diffusion constant at which the front speed is independent of the interlayer coupling.

10:24AM X35.00011 Geometric phase transition in the cellular network of the pancreatic islets may underlie the onset of type 1 diabetes . XUJING WANG, NHBLI, NIH — Living systems are characterized by complexity in structure and emergent dynamic orders. In many aspects the onset of a chronic disease resembles phase transition in a dynamic system: quantitative changes accumulate largely unnoticed until a critical threshold is reached, which causes abrupt qualitative changes of the system. In this study we investigate this idea in a real example, the insulin-producing pancreatic islet \( \beta \)-cells and the onset of type 1 diabetes. Within each islet, the \( \beta \)-cells are electrically coupled to each other, and function as a network with synchronized actions. Using percolation theory we show how normal islet function is intrinsically linked to network connectivity, and the critical point where the islet cellular network loses site percolation, is consistent with laboratory and clinical observations of the threshold \( \beta \)-cell loss that causes islet functional failure. Numerical simulations confirm that the islet cellular network needs to be percolated for \( \beta \)-cells to synchronize. Furthermore, the interplay between site percolation and bond strength predicts the existence of a transient phase of islet functional recovery after disease onset and introduction of treatment, potentially explaining a long time latency phenomenon in the clinical study of type 1 diabetes: the honeymoon phenomenon. Based on these results, we hypothesized that the onset of T1D may be the result of a phase transition of the islet \( \beta \)-cell network. We further discuss the potential applications in identifying disease-driving factors, and the critical parameters that are predictive of disease onset.

Friday, March 18, 2016 8:00AM - 11:00AM — Session X40 GSNP: General Statistical and Nonlinear Physics 343 - Flavio Fenton

8:00AM X40.00001 Chaotic dynamics of a candle oscillator . MARY ELIZABETH LEE, Georgia Inst of Tech, GREG BYRNE, FDA, FLAVIO FENTON, Georgia Inst of Tech — The candle oscillator is a simple, fun experiment dating to the late nineteenth century. It consists of a candle with a rod that is transverse to its long axis, around which it is allowed to pivot. When both ends of the candle are lit, an oscillatory motion will initiate due to different mass loss as a function of the flame angle. Stable oscillations can develop due to damping when the system has friction between the rod and the base where the rod rests. However, when friction is minimized, it is possible for chaos to develop. In this talk we will show periodic orbits found in the system as well as calculated, maximal Lyapunov exponents. We show that the system can be described by three ordinary differential equations (one each for angle, angular velocity and mass loss) that can reproduce the experimental data and the transition from stable oscillations to chaotic dynamics as a function of damping.

8:12AM X40.00002 Spike Bursts from an Excitable Optical System1 . JOSE R RIOS LEITE, EDISON JR ROSERO, WENDSON A S BARBOSA, Depto. Fisica- Univ. Fed. de Pernambuco-Recife, JORGE R TREDICCE, INLN-Univ de Nice-Sophie Antipolis -France — Diode Lasers with double optical feedback are shown to present power drop spikes with statistical distribution controllable by the ratio of the two feedback times. The average time between spikes and the variance within long time series are studied. The system is shown to be excitable and present bursting of spikes — Diode Lasers with double optical feedback are shown to present power drop spikes with statistical distribution controllable by the ratio of the two feedback.

8:24AM X40.00003 Singular probability distribution of a parametric oscillator driven by Poisson noise . PAVEL M. POLULIN, Michigan State University, PANPAN ZHOU, Hong Kong University of Science and Technology, STEVEN W. SHAW, Michigan State University, HO BUN CHAN, Hong Kong University of Science and Technology, MARK I. DYKMAN, Michigan State University — We provide the results of the theoretical and experimental studies of the probability distribution of a parametric oscillator, which is additionally driven by a Poisson-like noise. The noise consists of pulses at the vibration frequency with duration small compared to the oscillator relaxation time but long compared to the vibration period. We find that the stationary probability distribution of an oscillator quadrature can display a self-similar structure of sharp peaks, almost symmetrical with respect to the maximum, or can have a strongly asymmetric two-peak structure. The form of the distribution depends on the oscillator dynamics in the rotating frame and the rate of the noise pulses. In particular, the self-similar multi-peak structure emerges if the oscillator dynamics in the rotating frame is underdamped. The peaks have a singular power-law shape. We show that the singularity is smeared by thermal noise, which makes the peaks Gaussian near the maxima. We also discuss the frequently encountered situation where the Poisson noise describes fluctuations of the oscillator eigenfrequency. The theoretical and experimental results are in excellent agreement.
8:36AM X40.00004 Quantum Boltzmann Machine, BOHDAN KULCHYTSKYY, Univ of Waterloo, EVGENY ANDRIYASH, MOHAMMED AMIN, D-Wave Systems Inc, ROGER MELKO, Univ of Waterloo, Perimeter Institute — The field of machine learning has been revolutionized by the recent improvements in the training of deep networks. Their architecture is based on a set of stacked layers of simpler modules. One of the most successful building blocks, known as a restricted Boltzmann machine, is an energetic model based on the classical Ising Hamiltonian. In our work, we investigate the benefits of quantum effects on the learning capacity of Boltzmann machines by extending its underlying Hamiltonian with a transverse field. For this purpose, we employ exact and stochastic training procedures on data sets with physical origins.

8:48AM X40.00005 Quantum Feynman Ratchet, KETAN GOYAL, RYOICHI KAWAI, Univ of Alabama - Birmingham — As nanotechnology advances, understanding of the thermodynamic properties of small systems becomes increasingly important. Such systems are found throughout physics, biology, and chemistry manifesting striking properties that are a direct result of their small dimensions where fluctuations become predominant. The standard theory of thermodynamics for macroscopic systems is powerless for such ever fluctuating systems. Furthermore, as small systems are inherently quantum mechanical, influence of quantum effects such as discreteness and quantum entanglement on their thermodynamic properties is of great interest. In particular, the quantum fluctuations due to quantum uncertainty principles may play a significant role. In this talk, we investigate thermodynamic properties of an autonomous quantum heat engine, resembling a quantum version of the Feynman Ratchet, in non-equilibrium condition based on the theory of open quantum systems. The heat engine consists of multiple subsystems individually contacted to different thermal environments.

9:00AM X40.00006 Reversibility in Quantum Models of Stochastic Processes, DAVID GIER, University of Kansas, JAMES CRUTCHFIELD, JOHN MAHONEY, RYAN JAMES, University of California at Davis — Natural phenomena such as time series of neural firing, orientation of layers in crystal stacking and successive measurements in spin-systems are inherently probabilistic. The provably minimal classical models of such stochastic processes are $\epsilon$-machines, which consist of internal states, transition probabilities between states and output values. The topological properties of the $\epsilon$-machine for a given process characterize the structure, memory and patterns of that process. However $\epsilon$-machines are often not ideal because their statistical complexity ($C_{\epsilon}$) is demonstrably greater than the excess entropy ($E$) of the processes they represent. Quantum models ($\epsilon$-machines) of the same processes can do better in that their statistical complexity ($C_{\epsilon}$) obeys the relation $C_{\epsilon} \geq C_{Q} \geq E$. $\epsilon$-machines can be constructed to consider longer lengths of strings, resulting in greater precision. With code-words of sufficiently long length, the statistical complexity becomes time-symmetric – a feature apparently novel to this quantum representation. This result has ramifications for compression of classical information in quantum computing and quantum communication technology.

9:12AM X40.00007 Finding stability domains and escape rates in kicked Hamiltonians, ARCHISHMAN RAJU, SAYAN CHOWDHURY, DAVID RUBIN, JAMES SETHNA, Cornell University — We use an effective Hamiltonian to characterize particle dynamics and find escape rates in a one dimensional system with a periodically kicked Hamiltonian. We study a model of particles in storage rings which is given by the symplectic map where the chaos is described by the KAM theorem. Ignoring the resonances, the dynamics typically has a finite region in phase space where it is stable. Photon noise in the system leads to particle loss from this stable region. Determining this `aperture' and finding escape rates is therefore an important physical problem. We characterize the stable region in phase space using a perturbation theory developed in the context of quantum mechanics. We then derive analytical expressions for the escape rate in the small damping regime and compare them with numerical simulations. We discuss the possibility of extending the procedure to include higher dimensions and more complicated noise terms.

9:24AM X40.00008 The canonical ensemble revisited: a projection operator approach, WIM MAGNUS, Universiteit Antwerpen / Imec, FONS BROSENS, Universiteit Antwerpen, CONDENSED MATTER THEORY TEAM, THEORY OF QUANTUM SYSTEMS AND COMPLEX SYSTEMS TEAM — Constraining the particle number N in the canonical ensemble hampers the systematic calculation of the partition function $Z_N$ for non-interacting fermions and bosons, unlike in the case of the grand-canonical ensemble. Recently, we have shown that this task can be accomplished by invoking a projection operator that automatically imposes the particle number constraint in the many-particle Hilbert space. As a result, an integral representation is obtained for $Z_N$, as well as for the the two-point and four-point correlation functions. As an illustration, the Helmholtz free energy and the chemical potential are calculated for a two-dimensional electron gas typically residing in the inversion layer of a field-effect transistor.

9:36AM X40.00009 Novel dynamics and thermodynamics of a new Hamiltonian mean field model, SERGIO CURILEF, BORIS ATENAS, Universidad Catolica del Norte — Statistical systems are idealized by the hypothesis that the particles do not interact among them, or the range of interactions is short enough, reaching very fast the statistical state that we know as equilibrium. However, systems with long-range interactions are common in nature because of they are observed from the atomic scale to the astronomical scale, exhibiting some anomalies as inequivalence of ensembles, negative heat capacity, ergodicity breaking, non equilibrium phase transitions, quasi-stationarity, anomalous diffusion, etc. We present in this contribution a new Hamiltonian mean field model whose potential is inspired in the dipole-dipole interactions. The equilibrium is analytically studied in the canonical ensemble and coincides with the one obtained from molecular dynamics simulations (microcanonical ensemble). We notice, this model presents a kind of inequivalence of ensembles in long-standing states before arriving at equilibrium. However, the novelty, compared to other models presented in recent literature, is that two quasi-stationary states appear in the behavior of this system. The first quasi-stationary state decays to a second one, which is different to the first, before going to the equilibrium. We characterize them by its dynamics and thermodynamics.

3We acknowledge partial financial support by Anillo ACT-1204, VRIDT-UCN105/2015. We appreciate the computational assistance of A. Pluchino.

9:48AM X40.00010 Optimization of finite-size errors in finite-temperature calculations of unordered phases, DEEPAK IYER, Bucknell University, MARK SREDNICKI, University of California Santa Barbara, MARCOS RIGOL, Pennsylvania State University — It is common knowledge that the microcanonical, canonical, and grand canonical ensembles are equivalent in thermodynamically large systems. Here, we study finite-size effects in the latter two ensembles. We show that contrary to naive expectations, finite-size effects are exponentially small in grand canonical ensemble calculations of translationally invariant systems in unordered phases at finite temperature. Open boundary conditions and canonical ensemble calculations suffer from finite-size errors that are only polynomially small in the system size. We further show that finite-size effects are generally smallest in numerical linked cluster expansions. Our conclusions are supported by analytical and numerical analyses of classical and quantum systems.

10:00AM X40.00011 Complex Pole Approach in Thermodynamic Description of Fluid Mixtures with Small Number of Molecules, TIMUR ASLYAMOV, OLEG DINARIEV, Schlumberger Moscow Research — Physically consistent description of equilibrium small molecular systems requires the extension of thermodynamics. The reason is the absence of thermodynamic limit, which is mandatory for the applicability of classical thermodynamics. New theoretical method of complex pole decomposition for the statistical description of small multicomponent molecular systems is implemented. Similar approach has been previously developed and applied in nuclear physics for finite systems of nucleons. We have shown that it is transferable to matter systems with multicomponent molecular mixtures in small systems. The aim of this research is to provide new comprehensive description of small equilibrium molecular systems with numerous scientific and industrial applications for artificial and natural materials with nanoparticles. Several cases for molecular systems in small cavities are studied. In particular size-dependent additional pressure for small systems is evaluated analytically and numerically. The obtained results are in correspondence to published experimental data and molecular dynamics simulations.
show that burstiness in the naming game with committed agents shifts downwards the critical population required for consensus.

In competition between two groups (each with a different wait time distribution but the same mean), the symmetry of the system is broken and in the infinite limit becomes singular at the boundary planes. Complementing recent numerically exact results, we derive various exact analytical results for series expansion coefficients of \(v(z)\), its \(L = \infty\) scattering data for all values \(m\) of the temperature scaling field, and the low-temperature asymptotic behavior of the residual free energy and the Casimir force using a combination of boundary-operator and short-distance expansions, proper extensions of inverse scattering theory, new trace formulae, and semi-classical expansions.

10:36AM X40.00014 A Molecular Model for Chiral Symmetry Breaking, Folarin Latinwo, Frank Stillinger, Pablo Debenedetti, Princeton University — In this work, we present a new class of molecular models for chiral phenomena in condensed matter systems.

A key feature of these models is the ability of the four-site (tetramer) “molecules” to inter-convert between two distinct chiral forms (enantiomers). Given this feature, we use analytical theory and computer simulations to investigate the emergent chiral properties (including symmetry breaking) over a wide range of conditions. In particular, we consider the single-molecule level and condensed-phase behavior of our model system. Interestingly, we find that our liquid-phase predictions are in excellent agreement with recent experimental reports on chiral self-sorting in isotropic liquids. From this perspective, our model demonstrates accurate predictive capabilities, as well as a platform for understanding the microscopic origins of a variety of chiral phenomena. In a broader context, we anticipate that this class of models will be relevant to chirality-dominated areas such as the pharmaceutical industry and pre-biotic geochemistry.

10:48AM X40.00015 Thermal diffusion and colored energy dissipation in hydrogen bonded liquids. Riccardo Dettori, Department of Physics - University of Cagliari (I), Claudio Melis, Department of Physics - University of Cagliari, Michele Ceriotti, Ecole Polytechnique Federale de Lausanne (CH), Davide Donadio, Department of Chemistry - UC Davis (USA), Luciano Colombo, Department of Physics - University of Cagliari (I) — H-bonded liquids show a manifold energy dissipation dynamics due to: strong directionality of H-bonds and complexity of their network. This affects both thermal diffusion and energy dissipation mechanisms in pump-probe spectroscopy experiments. By nonequilibrium molecular dynamics (MD) simulations we investigate such phenomena in liquid methanol. While heat transport is studied by approach-to-equilibrium MD, energy dissipation is investigated by making use of a novel Generalized Langevin Equation (GLE) colored noise thermostat, which can generate a non-equilibrium frequency-resolved dynamics by using a correlated noise. The colored thermostat can thermally excite a narrow range of vibrational modes, typically the stretching mode of the OH involved in H-bonding, leaving the other degrees of freedom at the equilibrium temperature. The energy dissipation is then observed as a function of time, by probing the excitation decay and the energy transfer to other modes. In particular, by monitoring in time the different contributions to the potential energy of the system, we evaluate how energy is transferred from the excited mode to other modes of the nearby molecules and provide understanding on the dynamics of H-bonded liquids, as resulting from current experimental investigations.

Friday, March 18, 2016 8:00AM - 11:00AM – Session X43 GSNP: Statistical Mechanics of Social Systems
8:24 AM X43.00003 Comparison of human mobility patterns in different settings1, XIANGWEN WANG, MICHEL PLEMLING, Virginia Tech — The development of location tracking technologies and big-data analysis capacities makes it possible to understand human mobility patterns at the global level through the analysis of huge datasets made available by open-data communities. Working with millions of empirical world-wide GPS trajectories, we examine users’ mobility patterns in urban, rural and intermediate scenarios. Similar scaling properties are found in the analysis of several quantities, including end-to-end distance, radius of gyration, mean-squared displacement, and fixed-interval step-length. The impact of cities is elucidated by comparing mobility patterns in major cities worldwide.

8:36 AM X43.00004 Effects of long-range interactions in the one-dimensional Sznajd model JOSEPH GARCIA, University of Maine, THOMAS STONE, Husson University, SUSAN MCKAY, University of Maine — The Sznajd model is a one-dimensional, binary, voter-like model used to study consensus in systems where information flows outward from like-minded agent pairs. Here, we introduce long-range interactions to the Sznajd model, quantified by the parameter $p$ in analogy with the dynamic and static small-world rewiring parameter ($p \rightarrow 1$ is the mean-field limit, $p \rightarrow 0$ is the 1-D limit). We use Monte Carlo simulations and finite-size scaling analyses to characterize the exit probability for $p \neq 0$, finding a step function that depends on two $p$-dependent exponents. By examining the $p \rightarrow 0$ limit of these exponents, we comment on the functional form of the exit probability in one dimension, which has been an open question. We complement this limiting approach (letting $p \rightarrow 0$, which offers considerable computational speedup over the pure $p=0$ case) by also simulating the $p=0$ case via a parallel algorithm. This investigation also probes the dependence of consensus time and system magnetization on $p$.

8:48 AM X43.00005 Selection Strategies for Social Influence in the Threshold Model1, PANAGIOTIS KARAMPOURNIO蒂, BOLESŁAW SZYMANSKI, GYÖRGY KÖRNIS, Rensselaer Polytech Inst — The ubiquity of online social networks makes the study of social influence extremely significant for its applications to marketing, politics and security. Maximizing the spread of influence by strategically selecting nodes as initiators of a new opinion or trend is a challenging problem. We study the performance of various strategies for selection of large fractions of initiators on a classical social influence model, the Threshold model (TM). Under the TM, a node adopts a new opinion only when the fraction of its first neighbors possessing that opinion exceeds a pre-assigned threshold. The strategies we study are of two kinds: strategies based solely on the initial network structure (Degree-rank, Dominating Sets, PageRank etc.) and strategies that take into account the change of the states of the nodes during the evolution of the cascade, e.g. the greedy algorithm. We find that the performance of these strategies depends largely on both the network structure properties, e.g. the assortativity, and the distribution of the thresholds assigned to the nodes.

1Supported in part by ARL NS-CTA, ARO, and ONR.

9:00 AM X43.00006 Pattern Selection and Super-Patterns in Opinion Dynamics ELI BEN-NAIM, Los Alamos National Laboratory, ARND SCHEEL, University of Minnesota — We study pattern formation in the bounded confidence model of opinion dynamics. In this random process, opinion is quantified by a single variable. Two agents may interact and reach a fair compromise, but only if their difference of opinion falls below a fixed threshold. Starting from a uniform distribution of opinions with compact support, a traveling wave forms and it propagates from the domain boundary into the unstable uniform state. Consequently, the system reaches a steady state with isolated clusters that are separated by distance larger than the interaction range. These clusters form a quasi-periodic pattern where the sizes of the clusters and the separations between them are nearly constant. We obtain analytically the average separation between clusters. Interestingly, there are also very small quasi-periodic modulations in the size of the clusters. The spatial periods of these modulations are a series of integers that follow from the continued-fraction representation of the irrational average separation L.

9:12 AM X43.00007 Spatially clustered zealots in a two-dimensional voter model THOMAS STONE, Husson University, MATTHEW LUDDEN, SUSAN MCKAY, University of Maine — The voter model, solvable in all dimensions in its standard form, has been extensively used to study behavior dynamics by using the tools of statistical mechanics. Recently, much work has been focused on determining the effects of zealots in the voter model, where a zealot is an agent that maintains its opinion (akin to an Ising spin variable) no matter the local environment. Here we investigate the effects of spatially clustered zealots in the standard voter model on a two-dimensional square lattice. The clustering of zealots is quantified by the conditional probability that a zealot of the +1 state appears on an adjacent site to a randomly chosen zealot. (All zealots are of the +1 state.) We determine the functional forms of the system consensus time with respect to system size, clustering, and zealot density, and compare these findings to previous results that do not include clustering. We also discuss an interesting random walk problem that arises when one attempts to calculate how clustering affects the consensus time for fixed zealot density and system size.

9:24 AM X43.00008 Highlighting impact: Do editors’ selections identify influential papers? MANOLIS ANTONIOYIANNAKIS, (1) Columbia University (2) American Physical Society — A recent trend in scientific publishing is that journal editors highlight each week a select set among the papers published (usually) in their respective journals. The highlighted papers are deemed of higher quality, importance, or interest than the ‘average’ paper and feature prominently in the publishers’ websites. We perform a citation analysis of the highlighted papers for a number of journals from various publishers in physics. By comparing the performance of highlighted papers relative to (a) typical papers and (b) highly cited papers in their source journals and in other journals in the field, we explore whether, and to what extent, the selection process at the time of publication identifies papers that will turn out to be influential. We discuss the broader implications for research assessment.

9:36 AM X43.00009 Measuring diversity and coherence using hierarchical APS-PACS classification of sub fields of physics and their impact on citations SHIVAKUMAR JOLAD, MURALI KRISHNA ENDURI, L. VINOD REDDY, IIT Gandhinagar — American Physical Society introduced Physics and Astronomy Classification Scheme (PACS) in 1975 to classify different subfields of physics in a hierarchical tree structure. Since 1985, almost all the physical review articles include the PACS code to refer different subfields it belongs to. In this work, we define the notion of diversity of articles and authors based on the PACS codes they are associated with, using Wetzmann diversity index, from 1985-2012. We find that the fraction of authors with high diversity is increasing with time, whereas the fraction of least diversity are decreasing, and moderate diversity authors have higher tendency to switch ever to are of two kinds: strategies based solely on the initial network structure (Degree-rank).

1Supported in part by the US National Science Foundation through grant DMR-1205309.

This work is in part supported by the US National Science Foundation through grant DMR-1205309.
suggests that achieving information benefit via feedback requires dedicated systems to control gene expression noise, such as sRNA-based regulation.

At the population level, external feedback adjusts the dynamic range of the shared input to individuals' detection channels. In a quorum-sensing microbial community, wherein the internal regulator of the individual's response tracks the external cell density via an endogenously generated signal, these bacteria need to glean as much information as possible about local density. Our study is the first to physically model the flow of information in a multi-cellular system.

Despite myriad of factors that shape and influence individual choices of research subjects, we identified regularities in this dynamical process that are well captured by a simple statistical model. The results advance our understanding of scientists' behaviors during their careers and open up avenues for future studies in the science of science.

10:00AM X43.00011 A simple model for research interest evolution patterns, TAO JIA, Southwest University, China, DASHUN WANG, Pennsylvania State University, BOLESLAW SZYMANSKI, Rensselaer Polytechnic Institute — Sir Isaac Newton supposedly remarked that in his scientific career he was like "... a boy playing on the sea-shore ... finding a smoother pebble or a prettier shell than ordinary". His remarkable modesty and famous understatement motivate us to seek regularities in how scientists shift their research focus as the career develops. Indeed, despite intensive investigations on how microscopic factors, such as incentives and risks, would influence a scientist's choice of research agenda, little is known on the macroscopic patterns in the research interest change undertaken by individual scientists throughout their careers. Here we make use of over 14,000 authors' publication records in physics. By quantifying statistical characteristics in the interest evolution, we model scientific research as a random walk, which reproduces patterns in individuals' careers observed empirically. Despite myriad of factors that shape and influence individual choices of research subjects, we identified regularities in this dynamical process that are well captured by a simple statistical model. The results advance our understanding of scientists' behaviors during their careers and open up avenues for future studies in the science of science.

10:12AM X43.00012 Development of kink jams in traffic flow, DOUGLAS KURTZE, Saint Joseph's Univ — Near the threshold of absolute stability of uniform, steady traffic flow, car-following models can often be reduced to a modified Korteweg-deVries (mKdV) equation plus small corrections. The mKdV equation has a continuous family of hyperbolic-kink solutions describing boundaries between regions of different traffic densities, i.e. the edge of kink traffic jams. A simple calculation picks out the one member of this family which is consistent with the correction terms; this is usually labelled the "selected" kink. The identification of the selected kink is achieved by studying the flow of mKdV solutions which has the kink solutions as one limit and uniform flow as another, and show how the correction terms can lead to kinks developing from initially near-uniform traffic. We then clarify the meaning of the usual solvability calculation and the "selected" kink.

10:24AM X43.00013 A Langevin model for low density pedestrian dynamics, ALESSANDRO CORBETTA, Eindhoven University of Technology, CHUNG-MIN LEE, California State University Long Beach, ROBERTO BENZI, University of Rome Tor Vergata, ADRIAN MUNTEAN, Karlstad University, Sweden, FEDERICO TOSCHI, Eindhoven University of Technology — The dynamics of pedestrian crowds shares deep connections with statistical physics and fluid dynamics. Reaching a quantitative understanding, not only of the average behaviours but also of the statistics of rare fluctuations would have major impact, for instance, on the design and safety of civil infrastructures. A key feature of pedestrian dynamics is its strong intrinsic variability, that we can already observe at the single individual level. In this work we aim at a quantitative characterisation of this statistical variability by studying individual fluctuations. We consider experimental observations of low-density pedestrian flows in a corridor within a building at Eindhoven University of Technology. Few hundreds of thousands of pedestrian trajectories with high space and time resolutions have been collected via a Microsoft Kinect 3D-range sensor and automatic head tracking techniques. From these observations we model pedestrians as active Brownian particles by means of a generalised Langevin equation. With this model we can quantitatively reproduce the observed dynamics including the statistics of ordinary pedestrian fluctuations and of rarer U-turn events. Low density, pair-wise interactions between pedestrians are also discussed.

10:36AM X43.00014 A Hierarchy of Multi-Lane Driven Diffusive Systems with Unfair Resource Availability, AYSE YESIL, CEMAL YALABIK, Bilkent University — We present a model system for objects which have the ability to move along columns with the availability of a low entropy resource which is provided abundantly to a first column. The unused part of this resource is available to objects in neighbouring consecutive columns. This forms a hierarchy of multi-lane driven diffusive systems, which displays interesting dynamics. We present results from Monte Carlo simulations of the system.

1 Turkish Academy of Sciences (TUBA)

10:48AM X43.00015 Kinetic model for dilute traffic flow, ASHKAN BALOUCHI, DANA A. BROWNE, Louisiana State University, Department of Physics and Astronomy — The flow of traffic represents a many-particle non-equilibrium problem with important practical consequences. Traffic behavior has been studied using a variety of approaches, including fluid dynamics models, Boltzmann equation, and recently cellular automata (CA). The CA model for traffic flow that Nagel and Schreckenberg (NS) introduced can successfully mimic many of the known features of the traffic flow. We show that in the dilute limit of the NS model, where vehicles exhibit free flow, cars show significant nearest neighbor correlation primarily via a short-range repulsion. We introduce an approximate analytic model to describe this dilute limit. We show that the distribution of the distance between consecutive vehicles obeys a drift-diffusion equation. We compared our model with direct simulations. The steady state solution and relaxation of this model agrees well with direct simulations. We explore how this model breaks down as the transition to jams occurs.

Friday, March 18, 2016 8:00AM - 11:00AM —
Session X55 DBIO GSNP: Principles of Cell to Cell Communication Hilton Baltimore Holiday Ballroom
6 - Ned S. Wingreen, Princeton University

8:00AM X55.00001 Optimal census by quorum sensing, THIBAUD TAILLEFUMIER, Princeton University — Bacteria regulate their gene expression in response to changes in local cell density in a process called quorum sensing. To synchronize their gene-expression programs, these bacteria need to glean as much information as possible about local density. Our study is the first to physically model the flow of information in a quorum-sensing microbial community, wherein the internal regulator of the individuals response tracks the external cell density via an endogenously generated shared signal. Combining information theory and Lagrangian optimization, we find that quorum-sensing systems can improve their information capabilities by tuning circuit feedbacks. At the population level, external feedback adjusts the dynamic range of the shared input to individuals detection channels. At the individual level, internal feedback adjusts the regulators response time to dynamically balance output noise reduction and signal tracking ability. Our analysis suggests that achieving information benefit via feedback requires dedicated systems to control gene expression noise, such as sRNA-based regulation.
8:36AM X55.00002 Using memory to enforce stereotyped behavior in a bacterial community, RICHARD LOSICK, Harvard University — Bacteria communicate with each other by the exchange of chemical cues. I will describe a simple system in which bacteria form a one-dimensional community in which behavior in the community is enforced by trans-generational memory inherited from a founder cell rather than by intercellular signaling. The bacterium B. subtilis held under constant conditions of exponential phase growth switches between a unicellular, motile state and a sessile state in which individual cells are held together in a chain. I will show that cells enter the chaining state spontaneously by a stochastic mechanism involving tight binding between two proteins and remain in that state for a stereotyped number of generations due to the action of a third protein that is responsible for memory. The motile state, in contrast, is memoryless. Reconstruction of the principal features of the two states in an unrelated bacterium, E. coli, provides evidence that the three proteins are necessary and sufficient to account for the alternative behaviors. Thus, B. subtilis is capable of cell-cell communication by an epigenetic information that is transmitted to progeny cells for a characteristic number of cell divisions. We suggest that paradoxical signaling provides cell circuits with specific dynamical features that are robust to environmental perturbations.

9:12AM X55.00003 Design principles of paradoxical signaling in the immune system, YUVAL HART, Physics department, School of Engineering and Applied Sciences, Harvard University — A widespread feature of cell-cell signaling systems is paradoxical pleiotropy: the same signaling molecule can induce opposite effects in the responding cells. For example, the cytokine IL-2 can promote proliferation and death of T-cells. The role of such paradoxical signaling remains unclear. We suggest that this mechanism provides homeostatic concentration of cells, independent of initial conditions. The crux of the paradoxical mechanism is the combination of a positive and a negative feedback loops creating two stable states - an OFF state and an ON state. Experimentally, we found that CD4+ cells grown in culture with a 30-fold difference in initial concentrations reached a homeostatic concentration nearly independent of initial cell levels (ON-state). Below an initial threshold, cell density decayed to extinction (OFF-state). Mathematical modeling explained the observed cell and cytokine dynamics and predicted conditions that shifted cell fate from homeostasis to the OFF-state.

9:48AM X55.00004 The BMP Pathway is a Programmable Multi-Ligand Signal Processing System, YARON ANTEBI, Caltech — The BMP signaling pathway comprises many ligands and receptors that interact promiscuously and appear in combinations. This feature is often understood in the context of redundancy and tissue specificity, but it has remained unclear whether it enables specific signal processing capabilities. Here, we show that the BMP pathway performs a specific set of computations, including sums, ratios, and balance and imbalance detection, across the multi-dimensional space of ligand concentrations. These computations can arise directly from receptor-ligand interactions without requiring transcriptional regulation. Furthermore, cells can re-program the type of computation performed on specific ligands through changes in receptor expression, allowing different cell types to perceive distinct signals in the same ligand environment. Together, these results may help explain the prevalence of promiscuous ligand-receptor architectures across pathways and enable predictive understanding and control of BMP signaling.

10:24AM X55.00005 A positional code and anisotropic forces control tissue remodeling in Drosophila, JENNIFER ZALLEN, Sloan Kettering Institute — A major challenge in developmental biology is to understand how tissue-scale changes in organism structure arise from events that occur on a cellular and molecular level. We are using cell biological, biophysical, and quantitative live-embryo imaging approaches to understand how genes encode the forces that shape tissues, and to identify the mechanisms that modulate cell behavior in response to local forces. In many animals, the elongated head-to-tail body axis is achieved by rapid and coordinated movements of hundreds of cells. We found that in the fruit fly, these cell movements are regulated by subcellular asymmetries in the localization of proteins that generate contractile and adhesive forces between cells. Asymmetries in the force-generating machinery are in turn controlled by a positional code of spatial information provided by an ancient family of Toll-related receptors that are widely used for pathogen recognition by the innate immune system. I will describe how this spatial system systematically orients local cell movements and collective rosette-like clusters in the Drosophila embryo. Rosettes have now also been shown to shape the body axis in chicks, frogs, and mice, demonstrating that rosette behaviors are a general mechanism linking cellular asymmetry to tissue reorganization.

Friday, March 18, 2016 11:15AM - 2:15PM  
Session Y12 GSNP: Inference in Complex Networks  
308 - Adilson Motter, Northwestern University

11:15AM Y12.00001 Physics of Inference1, ZOLTAN TOROCZKAI2, Department of Physics, University of Notre Dame, USA — Jayness maximum entropy method provides a family of principled models that allow the prediction of a systems properties as constrained by empirical data (observables). However, their use is often hindered by the degeneracy problem characterized by spontaneous symmetry breaking, where predictions fail. Here we show that degeneracy appears when the corresponding density of states function is not log-concave, which is typically the consequence of nonlinear relationships between the constraining observables. We illustrate this phenomenon on several examples, including from complex networks, combinatorics and classical spin systems (e.g., Blume-Emery-Griffiths lattice-spin models). Exploiting these nonlinear relationships we then propose a solution to the degeneracy problem for a large class of systems via transformations that render the density of states function log-concave. The effectiveness of the method is demonstrated on real-world network data. Finally, we discuss the implications of these findings on the relationship between the geometrical properties of the density of states function and phase transitions in spin systems.

1Supported in part by grant No. FA9550-12-1-0405 from AFOSR/DARPA and by grant No. HDTRA 1-09-1-0039 from DTRA.

2Co-author: Szabolcs Horvat, Department of Physics, University of Notre Dame, USA and INSERM U846, Bron, France.

11:51AM Y12.00002 Nonparametric inference of network structure and dynamics, TIAGO P. PEIXOTO, University of Bremen — The network structure of complex systems determine their function and serve as evidence for the evolutionary mechanisms that lie behind them. Despite considerable effort in recent years, it remains an open challenge to formulate general descriptions of the large-scale structure of network systems, and how to reliably extract such information from data. Although many approaches have been proposed, few methods attempt to capture the statistical significance of the uncovered structures, and hence the majority cannot reliably separate actual structure from stochastic fluctuations. Due to the sheer size and high-dimensionality of many networks, this represents a major limitation that prevents meaningful interpretations of the results obtained with such nonstatistical methods. In this talk, I will show how these issues can be tackled in a principled and efficient fashion by formulating appropriate generative models of network structure that can have their parameters inferred from data. By employing a Bayesian description of such models, the inference can be performed in a nonparametric fashion, that does not require any a priori knowledge or ad hoc assumptions about the data. I will show how this approach can be used to perform model comparison, and how hierarchical models yield the most appropriate trade-off between model complexity and quality of fit based on the statistical evidence present in the data. I will also show how this general approach can be elegantly extended to networks with edge attributes, that are embedded in latent spaces, and that change in time. The latter is obtained via a fully dynamic generative network model, based on arbitrary-order Markov chains, that can also be inferred in a nonparametric fashion. Throughout the talk I will illustrate the application of the methods with many empirical networks such as the internet at the autonomous systems level, the global airport network, the network of actors and films, social networks, citations among websites, voting correlations among politicians, co-occurrence of disease-causing genes and others.
predicts a fundamental distinction between the S-phase Cdk1 trigger waves and the mitotic phase waves, which is illustrated by embryonic ablation experiments. Of the mitotic wave, while the Cdk1 positive feedback ensures an invariantly rapid onset of mitosis. Mathematical modeling captures the speed of the waves and Chk1/Wee1 pathway. The global dynamics of the mitotic signaling network illustrates a novel control principle: the S-phase activity of Cdk1 regulates the speed of microns. However, the signaling dynamics and the physical properties of chemical waves during embryonic development remain unclear. We develop FRET SIMO VERGASSOLA, Univ of California - San Diego — Mitoses in the early development of most metazoans are rapid and synchronized across the entire embryo. While diffusion is too slow, in vitro experiments have shown that waves of the cell-cycle regulator Cdk1 can transfer information rapidly across hundreds of microns. However, the signaling dynamics and the physical properties of chemical waves during embryonic development remain unclear. We develop FRET biosensors for the activity of Cdk1 and the checkpoint kinase Chk1 in Drosophila embryos and exploit them to measure waves in vivo. We demonstrate that Cdk1 chemical waves control mitotic waves and that their speed is regulated by the activity of Cdk1 during the S-phase (and not mitosis). We quantify the progressive slowdown of the waves with developmental cycles and identify its underlying control mechanism by the DNA replication checkpoint through the Chk1/Wee1 pathway. The global dynamics of the mitotic signaling network illustrates a novel control principle: the S-phase activity of Cdk1 regulates the speed of the mitotic wave, while the Cdk1 positive feedback ensures an invariantly rapid onset of mitosis. Mathematical modeling captures the speed of the waves and predicts a fundamental distinction between the S-phase Cdk1 trigger waves and the mitotic phase waves, which is illustrated by embryonic ablation experiments.

1Supported by grants of the BMBF (Future Compliant Power Grids - CoNDyNet) and by the Max Planck Society to MT.
11:51 AM Y35.00002 Collective Calcium Dynamics in Networks of Communicating Cells, TOMMY BYRD, Purdue University, GARRETT POTTER, BO SUN, Oregon State University, ANDREW MUGLER, Purdue University — Cells can sense and encode information about their environment with remarkable precision. These properties have been studied extensively for single cells, but intercellular communication is known to be important for both single- and multicellular organisms. Here, we examine calcium dynamics of fibroblast cells exposed to external ATP stimuli, and the effects of communication and stimulus strength on cells’ response. Experimental results show that increasing communication strength induces a greater fraction of cells to show oscillatory calcium dynamics, but the frequencies of oscillation do not systematically shift with ATP strength. We developed a model of calcium signaling by adding noise, communication, and cell-to-cell variability to the model of Tang and Othmer. This model reproduces cells’ increased tendency to oscillate as a function of communication strength, and frequency encoding is nearly removed at the global level. Our model therefore suggests that the propensity of cells to oscillate, rather than frequency encoding, determines the response to external ATP. These results suggest that the system lies near a critical boundary separating non-oscillatory and oscillatory calcium dynamics.


12:03PM Y35.00003 Precision of multicellular gradient sensing with cell-cell communication, ANDREW MUGLER, Department of Physics and Astronomy, Purdue University, ANDRE LEVCHENKO, Department of Biomedical Engineering and Yale Systems Biology Institute, Yale University, ILYA NEMENMAN, Departments of Physics and Biology, Emory University — Gradient sensing underlies diverse biological processes. In principle, bigger “detectors (cells or groups of cells) make better sensors, since then concentrations measured at the front and back of a detector are more different, and the gradient can be determined with higher precision. Indeed, experiments have shown that populations of cells detect gradients more precisely than single cells. However, this argument neglects the fact that information must be communicated between different parts of the detector, and the communication process introduces its own noise. Here we derive the fundamental limits to the precision of gradient sensing with cell-cell communication and temporal integration. We find that communication imposes its own sensory length scale, beyond which the precision cannot increase no matter how large the cell population grows. We also find that temporal integration couples the internal communication with the external signal diffusion, imposing an additional limit on the precision. We discuss how these limits can be improved by a strategy with two communicated molecular species, which we term 1 region excitation global inhibition. We compare our findings to experiments with communicating epithelial cells, and infer a sensor length scale of about 4 cells.

12:15PM Y35.00004 Collective synchronization of self/non-self discrimination in T cell activation, across multiple spatio-temporal scales, GREGOIRE ALTAN-BONNET, National Cancer Institute, Bethesda MD — The immune system is a collection of cells whose function is to eradicate pathogenic infections and malignant tumors while protecting healthy tissues. Recent work has delineated key molecular and cellular mechanisms associated with the ability to discriminate self from non-self agents. For example, structural studies have quantified the biophysical characteristics of antigenic molecules (those prone to trigger lymphocyte activation and a subsequent immune response). However, such molecular mechanisms were found to be highly unreliable at the individual cellular level. We will present recent efforts to build experimentally validated computational models of the immune responses at the collective cell level. Such models have become critical to delineate how higher-level integration through nonlinear amplification in signal transduction, dynamic feedback in lymphocyte differentiation and cell-to-cell communication allows the immune system to enforce reliable self/non-self discrimination at the organism level. In particular, we will present recent results demonstrating how T cells tune their antigen discrimination according to cytokine cues, and how competition for cytokine within polyclonal populations of cells shapes the repertoire of responding clones. Additionally, we will present recent theoretical and experimental results demonstrating how competition between diffusion and consumption of cytokines determine the range of cell-cell communications within lymphoid organs. Finally, we will discuss how biochemically explicit models, combined with quantitative experimental validation, unravel the relevance of new feedbacks for immune regulations across multiple spatial and temporal scales.

12:51PM Y35.00005 A generic spatial-stochastic framework for quantifying noisy information flow in multicellular systems, THOMAS SOKOLOWSKI1, GÁSPER TKÁCÍK2, IST Austria — Spatio-temporal protein signals play a crucial role in communicating information within and between cells. However, their ability to convey signals robustly is hampered by noise in gene regulation and biochemical transport, occurring at low copy numbers. While we increasingly understand distinct strategies of biochemical noise control, it remains unclear how nature orchestrates them to maximize information flow. Our recent work extends our information-theoretic framework for gene regulation to an explicitly spatial setting. We constructed a stochastic model enabling fast calculation of local means and variances in a spatially coupled gene regulatory system, which we use for rigorous quantification of information flow in an ensemble of units sensing a spatially distributed input and exchanging information via diffusion. By applying our framework to the paradigmatic Bcd-Hbk system in early fly development, we demonstrate that diffusive coupling can be of substantial benefit in encoding positional information, and uncover a novel optimal regulatory strategy relying on spatial coupling. Thanks to the generic methodology employed, our framework is universally applicable for realistic predictive modeling and data-driven inference of multicellular systems engaging in noisy communication.

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1:03PM Y35.00006 Increased dimensionality of cell-cell communication can decrease the precision of gradient sensing, TYLER SMITH, Department of Physics, Emory University, ANDRE LEVCHENKO, Department of Biomedical Engineering and Yale Systems Biology Institute, Yale University, ILYA NEMENMAN, Department of Physics, Emory University, ANDREW MUGLER, Department of Physics and Astronomy, Purdue University — Gradient sensing is a biological computation that involves comparison of concentrations measured in at least two different locations. As such, the precision of gradient sensing is limited by the intrinsic stochasticity in the concentration of a molecule in the same location. We have recently analyzed such limitations experimentally and theoretically in multicellular gradient sensing in mammmary epithelial cell organelies. For 1D chains of collectively sensing cells, the communication noise puts a severe constraint on how the accuracy of gradient sensing increases with the number of cells in the sensor. A question remains as to whether the effect of the noise can be mitigated by the extra spatial averaging allowed in sensing by 2D and 3D cellular organoids. Here we show using computer simulations that, counterintuitively, such spatial averaging decreases gradient sensing increases with the number of cells in the sensor. We explain the findings analytically and propose that a recently introduced Regional Excitation - Global Inhibition model of gradient sensing can overcome this limitation and use 2D or 3D spatial averaging to improve the sensing accuracy.

1Supported by NSF Grant PHY/1410978 and James S. McDonnell Foundation Grant 220020321

1:15PM Y35.00007 ABSTRACT WITHDRAWN —
1:27PM Y35.00008 Synthetic Quorum Sensing and Induced Aggregation in Model Microcapsule Colonies with Repressillator Feedback, HENRY SHUM, VICTOR YASHIN, ANNA BALAZS, University of Pittsburgh — We model a system of microcapsules that communicate chemically by releasing nanoparticles or signaling molecules. These signaling species bind to receptors on the shells of capsules and modulate the target shell permeability, thereby controlling nanoparticle release from the target capsule. Using the represillator regulatory network motif, whereby three species suppress the production of the next in a cyclic fashion, we show that large amplitude oscillations in nanoparticle release can emerge when many capsules are close together. This exemplifies quorum sensing, which is the ability of cells to gauge their population density and collectively initiate a new behavior once a critical density is reached. We present a physically realizable model in which the oscillations exhibited in crowded populations induce aggregation of the microcapsules, mimicking complex biological behavior of the slime mold Dictyostelium discoideum with only simple, synthetic components. We also show that the clusters can be dispersed and reformed repeatedly and controllably by addition of chemical stimuli, demonstrating possible applications in creating reconfigurable or programmable materials.

1:39AM Y37.00003 Crack Propagation in Attractive Colloidal Systems, SEAN FANCHER, ANDREW MUGLER, Department of Physics and Astronomy, Purdue University — When driven beyond yield, many amorphous solids exhibit nonlinear and dissipative processes in the material ahead of the propagating crack tip. However, the evolution of STs into a macroscopic shear band remains poorly understood. To study the process, we perform compression experiments on colloidal micropillars, are made freestanding so that shear bands can be observed directly. We find that the shear bands are characterized by a power law relationship between the velocity of the crack propagation and the energy release rate (ERR) of the system. We also find that the shear bands are highly localized and extend over long distances by secreting and absorbing a diffusive messenger molecule (paracrine signaling). In the latter case, we find that the cell spacing that optimizes precision can be large, due to a tradeoff between maintaining communication strength and reducing signal cross-correlations. This leads to the surprising result that paracrine signaling allows more precise sensing than juxtacrine signaling for sufficiently large populations, even though the cells are spaced far apart. We compare our results to recent experiments.

This research was partly supported by ImpACT program of council for science, Technology and Innovation (Cabine office government of Japan)

Friday, March 18, 2016 11:15AM - 2:15PM –
Session Y37 GSOFT GSNP: Fracture, Friction, and Deformation

11:15AM Y37.00001 Tearing Fracture of Polymer Foam Sheet, ATSUSHI TAKEI, KO OKUMURA, Ochanomizu Univ. — We study crack propagation in a sheet of polymer foam. The sheet was stretched, and an initial crack was introduced to induce the crack propagation. When the sheet width is shorter than the crack length, the energy release rate (ERR) of the system is independent of the crack length and constant during the propagation. Under the constant ERR condition, we find that the crack propagates at a constant speed. We observed the crack propagation for various values of ERR by changing the width of the sheet and the applied strain. Depending on values of ERR, the measured velocity of the crack propagation was nearly constant. We also found power laws between the velocity of the crack and the ERR. While in the literature the power law with exponent close to three (V \sim G^1) has been reported, we found that polymer foam sheets have different exponents depending on physical characteristics of polymer foam. In this presentation, we report the experimental result and its analysis.

This work is supported by a grant from the Simons Foundation (376198 to A.M.)

11:27AM Y37.00002 Effect of System Compliance on Crack Nucleation in Soft Materials, SHRUTI RATTAN, ALFRED CROSBY, UMass Amherst — Puncture mechanics in soft materials is critical for the development of new surgical instruments, robot assisted-surgery as well as new materials used in personal protective equipment. However, analytical techniques to study this important deformation process are limited. We have previously described a simple experimental method to study the resistive forces and failure of a soft gel being indented with a small tip needle. We showed that puncture stresses can be calculated by subtracting the two orders of magnitude greater than the modulus of the material and that the force response is insensitive to the geometry of the indenter at large indentation depths. Currently, we are examining the influence of system compliance on crack nucleation (e.g. puncture) in soft gels. It is well known that system compliance influences the peak force in adhesion and traditional fracture experiments; however, its influence on crack nucleation is unresolved. We find that as the system becomes more compliant, lower peak forces required to puncture a gel of certain stiffness with the same indenter were measured. We are developing scaling relationships to relate the peak puncture force and system compliance. Our findings introduce new questions with regard to the possibility of intrinsic materials properties related to the critical stress and energy for crack nucleation in soft materials.

11:39AM Y37.00004 Crack Propagation in Attractive Colloidal Systems, LAURA ROSSI, TRIET DANG, University of Amsterdam, MAXIME LEFRANC, PAUL LE FLOCH, ELISABETH BOUCHAUD, ESPCI ParisTech, PETER SCHALL, University of Amsterdam — Despite its importance, the fracture of materials, especially the regime of slow, plastic fracture, remains poorly understood. This is especially true in amorphous materials, where local inhomogeneities and structural disorder are crucial to determine the mode of failure, yet they cannot be modeled with classical homogenization methods. We use new attractive colloidal systems to study fracture at time and length scales much longer than in molecular systems. In a specific project, we focus on gels made of fluorescent pNPam microparticles aggregated via critical Casimir interactions, to analyze, at the microscopic level, nonlinear and dissipative processes in the material ahead of the propagating crack tip.

11:51AM Y37.00005 Localized Plastic Deformation in Colloidal Micropillars, DANIEL STRICKLAND, JYO LYN HOR, CARLOS ORTIZ, DAEYEON LEE, DANIEL GIANOLA, University of Pennsylvania — When driven beyond yield, many amorphous solids exhibit concentrated regions of large plastic strain referred to as shear bands. These shear bands are the result of localized, cooperative rearrangements of particles known as shear transformations (STs). STs are dilatary: their operation results in an increase of free volume and local softening that leads to spatially concentrated plasticity. However, the evolution of STs into a macroscopic shear band remains poorly understood. To study the process, we perform compression experiments on amorphous colloidal micropillars. The micropillars, which are composed of fluorescent 3 \mu m PMMA particles, are made freestanding so that shear banding instabilities are not suppressed by confining boundaries. During compression, we observe strong localization of strain in a band of the pillar. As deformation proceeds, the sheared region continues to dilate until it reaches the colloidal glass transition, at which point dilution terminates. We quantify a length scale by measuring the extent of spatial correlations in strain. This length scale decreases gradually with increasing dilution and becomes static beyond the glass transition. Our results reinforce the idea of yield as a stress-induced glass transition in amorphous solids.
12:03PM Y37.00005 Theory of rate dependent fracture size effects, ALESSANDRO TALONI, ALESSANDRO SELLERIO, STEFANO ZAPPERI, Center for Complexity and Biosystems - Physics Department, University of Milan La Stella — The idea that the solid failure can be described by means of the Kramer theory, where the intrinsic energy barrier is reduced proportionally to the applied field, first appeared in material science to treat the kinetic fracture of solids under applied stresses and dates back to '40s. Most previous works focused on the thermal dependence of the average strength or the failure time in creep experiments and did not address the survival distribution and its size dependence. To this end, we start from recent theories developed for single-molecule pulling, where the molecule core coefficient for rupture (or unbinding) is modified by the presence of an external time-dependent force, and we adjust it to a macroscopic elastic object. We generalize the extreme value theory to account for failures of materials with an explicit dependence on temperature, strain rate and size of the object. We show that in the limit of macroscopic objects, large strain rate and low temperature, thermal fluctuations are negligible and the usual extreme value theory is recovered. We provide the critical interpretation of several experiments in terms of our theory, furnishing a clearcut criterion for thermal effects to become relevant. [Phys. Rev. Applied, 024011]

12:15PM Y37.00006 Major and minor slip-events in frictional stick-slip1, GEORGIOS TSEKENIS, DEMET TATAR, SHMUEL RUBINSTEIN, DAVID WEITZ, MICHAEL AZIZ, FRANS SPAEPEN, Harvard Univ — Several universal phenomena characterize friction that are independent of the materials involved such as the logarithmic aging of the static friction coefficient and the logarithmic velocity weakening of the dynamic friction coefficient. We study dry friction between rough surfaces with programmed statistical profiles. By measuring the displacement field at the frictional interface we observe stick-slip behavior which reveals two kinds of slip: major events that tend to grow large and unbounded and minor events that usually stay small and bounded.

1Research supported by Harvard MRSEC Program under NSF contracts DMR-0820484, DMR-1420570

12:27PM Y37.00007 Tribological Properties of Nanodiamonds in Aqueous Suspensions: Effect of the Surface Charge, J. Krim, Zijian Liu, D.A. Leininger, A. Kooviland, A.I. Smirnov, North Carolina State University, O. Shendarova, International Technology Center, Raleigh, NC, D.W. Brenner, North Carolina State University — The presence of granular nanoparticulates, be they wear particles created naturally by frictional rubbing at a geological fault line or products introduced as lubricant additives, can dramatically alter friction at solid-liquid interfaces. Given the complexity of such systems, understanding system properties at a fundamental level is particularly challenging. The Quartz Crystal Microbalance (QCM) is an ideal tool for studies of material-liquid-nanoparticulate interfaces. We have employed it here to study the uptake and nanotribological properties of positively and negatively charged 5-15 nm diameter nanodiamonds dispersed in water[1] in the both the presence and absence of a macroscopic contact with the QCM electrode. The nanodiamonds were found to impact tribological performance at both nanometer and macrosopic scales. The tribological effects were highly sensitive to the sign of the charge: negatively (positively) charged particles were more weakly (strongly) bound and reduced (increased) frictional drag at the solid-liquid interface. For the macroscopic contacts, negatively charged nanodiamonds appeared to be displaced from the contact, while the positively charged ones were not. Overall, the negatively charged nanodiamonds were more stable in an aqueous dispersion for extended time periods.

1Work supported by NSF and DOE

12:39PM Y37.00008 Transition from super lubrically sliding islands to pinned monolayer, demonstrated in Xe/Cu(111) (*), ROBERTO GUERRA, International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy, ANDREA VANOSSE, CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy, ERIO TOSATTI, International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy., TRIESTE NANOFRICCTION TEAM — A molecular dynamics simulation case study of Xe on Cu(111) reveals unexpected information on the exceptionally smooth sliding state associated with incommensurate superlubricity which is argued to emerge in the large size limit of nominally incommensurate Xe islands. As coverage approaches a full monolayer, theory predicts an abrupt adhesion-driven two-dimensional density compression on the order of several per cent, implying a hysteretic jump from superlubric free islands to a pressurized sqrt(3) commensurate (and pinned, and therefore immobile) monolayer. These results match with recent quartz crystal microbalance data which show remarkably large slip times with increasing submonolayer coverage, signalling superlubricity, followed by a dramatic drop to zero for the dense commensurate monolayer [1]. Careful analysis of this variety of island sliding phenomena should be essential in future applications of friction at crystal/adsorbate interfaces. (*) Matching experimental work by M. Pierno, L. Bruschi, G. Mistura, G. Paolicelli, A. di Bona, S. Valeri. [1] M. Pierno, L. Bruschi, G. Mistura, G. Paolicelli, A. di Bona, S. Valeri, R. Guerra, A. Vanossi, E. Tosatti, Nature Nanotechnology 10, 714 (2015).

1Supported by ERC Advanced Grant N. 320796 - MODPHYSFRICT

12:51PM Y37.00009 Elastic deformations disrupt structural superlubricity in large contacts, TRISTAN A. SHARP, Johns Hopkins University, LARS PASTEWKA, Karlsruhe Institut fr Technologie, MARK O. ROBBINS, Johns Hopkins University — Force microscopy experiments observe ultra-low friction between solids with incommensurate lattice structures. This phenomenon is referred to as superlubricity and is due to a cancellation of lateral forces because surfaces sample all relative local configurations with equal probability. We use simulations to show that elasticity disrupts superlubricity in sufficiently large circular contacts. The simulations include atomic-scale geometry and reach micron-scales. For rigid solids, cancellation is complete except at the contact boundary. The static friction force per contact area, \(\tau\), falls as a power of contact radius, \(r\), and \(\tau \sim r^{-3/2}\). Elastic deformations limit this cancellation when the contact radius is larger than a characteristic length scale set by the core width of interfacial dislocations. For \(r \gg \lambda\), the static friction force per contact area, \(\tau\), approaches a constant value near the Peierls stress needed to move edge dislocations. Surprisingly, the stress in commensurate contacts drops to nearly the same value at large \(r\). We conclude that true structural lubricity does not occur in large contacts, although the constant shear stress drops rapidly with \(\tau_{\text{core}}\).

1NSF IGERT, DAAD

1:03PM Y37.00010 Subharmonic Shapiro steps in sliding colloidal monolayers, ANDREA VANOSSE, CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy, STELLA PARONUZZI, SISSA, Trieste, Italy, GALBRECE FORNASIER, NICOLA MANINI, Dipartimento di Fisica, Universita` di Milano, Italy, GIUSEPPE E. SANTORO, SISSA, Trieste, Italy, ERIO TOSATTI, SISSA & ICTP, Trieste, Italy — We examine the possibility to observe dynamical mode locking, in the form of Shapiro steps, when a time-periodic potential modulation is applied to two mutually sliding incommensurate 2D lattices. Specifically we present realistic MD simulations of a monolayer of charged colloids that are dragged by an external force over an optically generated periodic potential, where the colloidal sliding is enacted through the motion of soliton or antisoliton lines between locally commensurate domains. Clear integer Shapiro steps, with the synchronous rigid advancement of the whole monolayer, known from previous studies [1], are found. The jump between one step and the next during each AC cycle corresponds to particles jumping from one patch to the next, across the soliton boundary. We find additional smaller “subharmonic” steps. Here, the overall colloid advancement takes several AC cycles. At each cycle, different subsets of particles negotiate the soliton line between commensurate domains [2]. The wide parameter tunability of colloid monolayers makes these predictions potentially easy to access in an experimentally rich 2D geometry. [1] A. Libal et al., Phys. Rev. Lett. 96, 188301 (2006). [2] S. Paronuzzi et al., J. Phys. Cond. Matt., in press (2015)

1Supported by ERC Advanced Grant N. 320796 - MODPHYSFRICT
1:15PM Y37.00011 Superlubric-pinned Aubry transition of two dimensional monolayers in optical lattices.\(^1\), DAVIDE MANDELLI, SISSA, Trieste, ANDREA VANOSI, CNR-IOM Democritos and SISSA, Trieste, NICOLA MANINI, University of Milano, ERIO Tosatti, SISSA and ICTP, Trieste — Two-dimensional (2D) crystalline colloidal monolayers sliding over a laser-induced optical lattice “corrugation” potential emulate friction between ideal crystal surfaces. Static friction is always present when the monolayer and the optical lattices are commensurate, but when they are incommensurate the presence or absence of static friction depends upon the system parameters. In 1D, at the Aubry dynamical phase transition the static friction goes continuously from zero (superlubricity) to finite as the periodic corrugation strength is increased. We look for the Aubry-like transition in the more realistic 2D case of a monolayer in an incommensurate periodic potential using molecular dynamics simulations. Results confirm a clear and sharp 2D superlubric-pinned transition upon increasing corrugation strength. Unlike the 1D Aubry transition which is continuous, the 2D transition is first-order, with a jump of static friction. At the 2D Aubry transition there is no change of symmetry, a sudden rise of the colloid-colloid interaction energy, and a compensating drop of the colloid-corrugation energy. The observability of the superlubric-pinned colloid transition is proposed and discussed [1].

\(^1\)Supported by ERC Advanced Grant N. 320796 MODPHYSFRICT.

1:27PM Y37.00012 Superlubricity in a nutshell.\(^1\), ERIO Tosatti, SISSA and ICTP, Trieste, DAVIDE MANDELLI, SISSA, Trieste, ANDREA VANOSI, CNR-IOM Democritos and SISSA — Cold ion chains in optical lattices emulate the Frenkel-Kontorova model, whose frictional behavior depends on commensurability or incommensurability between the two lattices. In the latter and more interesting case, there are two different regimes: one with pinning and static friction, and one without pinning, called superlubric. Only in an infinite chain the two regimes exist, separated by a dynamical Aubry transition. A cold ion chain is necessarily finite and short, we nevertheless proposed that a clear remnant of that transition should persist in trapped ion chains[1]. Recent experiments showed how in fact a small number of ions suffices to demonstrate incommensuration effects, with a change of friction by orders of magnitude from matched to mismatched geometries[2]. Here we present simulation results suggesting for increasing optical lattice amplitude a clear vestigial Aubry transition for very few ions, with a weak dependence upon the ion number and a stronger one upon the relative mismatch. A properly chosen amplitude should therefore show the vestigial transition from pinning at small mismatch to superlubricity at large mismatch. Alternatively, a chain which at T=0 is pinned at all mismatches could develop an Aubry transition at finite temperature to a state of “thermally induced superlubricity”, due to the thermal smearing of the optical lattice amplitude. [1] A. Benassi et al., Nat. Comm. 2, 236 (2011). [2] A. Bylinskii et al, Science 348, 1115-1118 (2015).

1:39PM Y37.00013 An Artificial Ising System with Phononic Excitations, HAMED GAFFARI, W.ASHLEY GRIFFITH, University of Texas, PHILIP BENSON, School of Earth & Environmental Sciences, Burnaby Building, Burnaby Road, Portsmouth, M.H.B NASSERI, R.PAUL YOUNG, University of Toronto — Many intractable systems and problems can be reduced to a system of interacting spins. Here, we report mapping collective, phononic excitations from different sources of crystal vibrations to spin systems. The phononic excitations in our experiments are due to micro/nano cracking (yielding crackling noises due to lattice distortion). We develop real time mapping of the multi-array sensors to a network-space and then mapping the excitation- networks to spin-like systems. We show that new mapped system satisfies the quench (impulsive) characteristics of the Ising model in 2D classical spin systems. In particular, we show that our artificial Ising system transits between two ground states and approaching the critical point accompanies with a very short time frozen regime, inducing formation of domains separated by kinks. For a cubic-test under a true triaxial test (3D case), we map the system to a 6-spin ring under a transversal-driving field where using functional multiplex networks, the vector components of the spin are inferred (i.e., XY model). By visualization of spin patterns of the ring per each event, we demonstrate that “kinks” (as defects) proliferate when system approach from above to its critical point. We support our observations with employing recorded acoustic excitations during distortion of crystal lattices in nano-indentation tests on different crystals (silicon and graphite), triaxial loading test on rock (poly-crystal) samples and a true 3D triaxial test.

1:51PM Y37.00014 Fingerling Instability of Debonding Soft Elastic Adhesives, ELIE RAHAEL, UMR GULLIVER CNRS ESPCI Paris, FALKO ZIEBERT, Albert-Ludwigs-Universitt Freiburg, THOMAS VILMIN, UMR GULLIVER CNRS ESPCI Paris — We study the crack-front fingerling instability of an elastic adhesive tape that is peeled off a solid substrate. Our analysis is based on an energy approach using fracture mechanics and scaling laws and provides simple physical explanations for (i) the fact that the wavelength depends only on the thickness of the adhesive film and (ii) the threshold of the instability, and (iii) additionally estimates the characteristic size of the fingers.

2:03PM Y37.00015 Gluing Soft Interfaces by Nanoparticles\(^1\), ZHEN CAO, ANDREY DOBRYNNIN, Univ of Akron — Using a combination of the molecular dynamics simulations and scaling analysis we studied reinforcement of interface between two soft gel-like materials by spherical nanoparticles. Analysis of the simulations shows that the depth of penetration of a nanoparticle into a gel is determined by a balance of the elastic energy of the gel and nanoparticle deformations and the surface energy of nanoparticle/gel interface. In order to evaluate work of adhesion of the reinforced interface, the potential of mean force for separation of two gels was calculated. These simulations showed that the gel separation proceeds through formation of necks connecting nanoparticle with two gels. The shapes of the necks are controlled by a fine interplay between nanoparticle/gel surface energies and elastic energy of the neck deformation. Our simulations showed that by introducing nanoparticles at soft interfaces, the work required for separation of two gels could be 10-100 times larger than the work of adhesion between two gels without nanoparticle reinforcement. These results provide insight in understanding the mechanism of gluing soft gels and biological tissues by nano- and micro-sized particles.


11:15AM Y40.00001 Managing and capturing the physics of robotic systems, J. TIN WERFEL, Harvard University — Algorithmic and other theoretical analyses of robotic systems often use a discretized or otherwise idealized framework, while the real world is continuous-valued and noisy. This disconnect can make theoretical work sometimes problematic to apply successfully to real-world systems. One approach to bridging the separation can be to design hardware to take advantage of simple physical effects mechanically, in order to guide elements into a desired set of discrete attracting states. As a result, the system behavior can effectively approximate a discretized formalism, so that proofs based on an idealization remain directly relevant, while control can be made simpler. It is important to note, conversely, that such an approach does not make a physical instantiation unnecessary nor a purely theoretical treatment sufficient. Experiments with hardware in practice always reveal physical effects not originally accounted for in simulation or analytic modeling, which lead to unanticipated results and require nontrivial modifications to control algorithms in order to achieve desired outcomes. I will discuss these points in the context of swarm robotic systems recently developed at the Self-Organizing Systems Research Group at Harvard.
11:27 AM Y40.00002 Robot flow, clogging and jamming in confined spaces, Daria Monaenko, Vadim Linevich, Michael A.D. Goodisman, Daniel I. Goldman, Georgia Institute of Technology — We hypothesized that when a collection of robots operate in confined space, maximization of individual effort could negatively affect the collective performance by impeding the mobility of the individuals. To test our hypothesis, we built and programmed groups of 1-4 autonomous robotic diggers to construct a tunnel in a model cohesive soil. The robots’ mobility, defined in terms of the residence time (T) required for a robot to move one body-length within the tunnel, was compared between groups of maximally active robots (mode 1), groups with different levels of activity between individuals (mode 2), and maximally active robots with a “giving up” behavior (mode 3), in which the robot ceased the attempt to excavate in a crowded tunnel. In small groups of two robots, T was ∼3 sec and did not depend on the mode of operation. However, an increase in the number of robots caused an increase in T which depended upon mode. The residence time in groups of four robots in mode 1 (∼9 sec) significantly exceeded the residence time in mode 2 and 3 (∼4 sec), indicating that crowding was causing slower movement of individuals, particularly under maximum effort (mode 1). We will use our robophysical studies to discover principles of collective construction in subterranean social animals.

11:39 AM Y40.00003 Legged-locomotion on inclined granular media, Jennifer Rieser, Feifei Qian, Daniel Goldman, Georgia Institute of Technology — Animals traverse a wide variety of complex environments, including situations in which the ground beneath them can yield (e.g., dry granular media in desert dunes). Locomotion strategies that are effective on level granular media can fail when traversing a granular slope. Taking inspiration from successful legged-locomotors in sandy, uneven settings, we explore the ability of a small (15 cm long, 100 g), six-c-shaped legged robot to run uphill in a bed of 1-mm-diameter poppy seeds, using an alternating tripod gait. Our fully automated experiments reveal that locomotor performance can depend sensitively on both environmental parameters such as the inclination angle and volume fraction of the substrate, and robot morphology and control parameters like leg shape, step frequency, and the friction between the feet of the robot and the substrate. We assess performance by measuring the average speed of the robot, and we find that the robot tends to perform better at higher step frequency and lower inclination angles, and that average speed decreases more rapidly with increasing angle for higher step frequency.

11:51 AM Y40.00004 Robotic and mathematical modeling reveal general principles of appendage control and coordination in terrestrial locomotion, Benjamin McInroe, UC Berkeley, Henry Astley, Georgia Tech, ChaoHui Gong, CMU Robotics Institute, Sandy Kawano, NimbRo, Perrin Schiebel, Georgia Tech, Howie Choset, CMU Robotics Institute, Daniel I. Goldman, Georgia Tech — The transition from aquatic to terrestrial life presented new challenges to early walkers, necessitating robust locomotion on complex, flowable substrates (e.g., sand, mud). Locomotion on such substrates is sensitive to limb morphology and kinematics. Although early walker morphologies are known, principles of appendage control remain elusive. To reveal limb control strategies that facilitated the invasion of land, we study both robotic and mathematical models. Robot experiments show that an active tail is critical for robust locomotion on granular media, enabling locomotion even with poor foot placement and limited ability to lift the body. Using a granular resistive force theory model, we construct connection vector fields that reveal how appendage coordination and terrain inclination impact locomotor performance. This model replicates experimental results, showing that moving limbs/tail in phase is most effective (suggesting a locomotor template). Varying trajectory and contacts, we find gaits for which tail use can be neutral or harmful, suggesting limb-tail coordination to be a nontrivial aspect of locomotion. Our findings show that robot experiments coupled with geometric mechanics provide a general framework to reveal principles of robust terrestrial locomotion.

12:03 PM Y40.00005 Compliant Synergies in Locomotion, Matthew Travers, Howie Choset, Carnegie Mellon University, Goldman @ Georgia Tech, Physics Department Collaboration — Biological systems appear to have natural mechanisms that allow them to readily compensate for unexpected environmental variations when compared to their mechanical (i.e., robotic) counterparts. We hypothesize that the basis for this discrepancy is almost innate: what biology appears to be born with, built-in mechanisms for coordinating their many degrees of freedom, we struggle to "program." We therefore look toward biology for inspiration. In particular, we are interested in kinematic synergies, low-dimensional representations that explicitly encode the underlying structure of how systems coordinate their internal degrees of freedom to achieve high-level tasks. In this work, we derive parametric representations of kinematic synergies and present a new compliant locomotion control framework that enables the parameters to be directly controlled in response to external disturbances. We present results of this framework implemented on two separate platforms, a snake-like and hexapod robot. Our results show that, using synergies, the locomotion control of these very different systems can be reduced to simple, extremely capable, and common forms, thus offering new insights into both robotic as well as biological locomotion in complex terrains.

12:15 PM Y40.00006 Instability and maneuverability of a multi-legged robot, Shinya Aoi, Kyoto University — Our previous study showed that a centipede like multi-legged robot composed of many modules, each of which has one pair of legs, produces body undulations through a supercritical Hopf bifurcation of walking in a straight line with parallel bodies when the gait speed increases over a critical value or when the body segment joint stiffness decreases below a critical value (Aoi et al., PRE 2013, featured by Nat Phys 2013). So far, it is unclear if centipedes actively produce or resist body undulations during their locomotion and the previous study discussed the underlying mechanism responsible for the body undulations in centipede locomotion based on the robot experimental results and dynamic analysis using simplified physical model. Furthermore, centipedes produce agile locomotion despite many legs being in contact with the ground during their locomotion, which may impede their agile motions. The present study investigated the relationship between the instability of walking in a straight line and maneuverability of the robot using a quick turn task and some evaluation criteria for maneuverability.

12:27 PM Y40.00007 Are snakes particles or waves? Scattering of a limbless locomotor through a single slit, Feifei Qian, Georgia Institute of Technology, Jin Dai, ChaoHui Gong, Howie Choset, Carnegie Mellon University, Daniel Goldman, Georgia Institute of Technology — Droplets on vertically vibrated fluid surfaces can walk and diffract through a single slit by a pilot wave hydrodynamic interaction [Couter, 2006; Bush, 2015]. Inspired by the correspondence between emergent macroscale dynamics and phenomena in quantum systems, we tested if robotic snakes, which resemble wave packets, behave emergently like particles or waves when interacting with an obstacle. In lab experiments and numerical simulations we measured how a multi-module snake-like robot swam through a single slit. We controlled the snake undulation gait as a fixed serpentinoid traveling wave pattern with varying amplitude and initial phase, and we examined the snake trajectory as it swam through a slit with width d. Robot trajectories were different for undulations initially in phase or π out of phase with the slit, which changed the angle of the undulation wave to the slit edge. We also tested the case of two robots interacting with each other, which interacted sequentially with the slit with the second robot switched on at a delay of ∼3 sec after the first, causing a change in the wave angle θ after the interaction due to a complex interaction of the body wave with the slit. For fixed amplitude and large d, the snake passed through the slit with minimal interaction and theta was θ ≈ 0. For sufficiently small d, θ was finite and bimodally distributed, depending on the initial phase. For intermediate d, θ was sensitive to initial phase, and the width of the distribution of θ increased with decreasing d.
12:39PM Y40.00008 Multi-terrain locomotor interactions in flying snakes\(^1\), ISAAC YEATON, GRANT BAUMGARDNER, SHANE ROSS, JOHN SOCHA, Virginia Tech — Arboreal snakes of the genus Chrysopelea are the only known snakes to glide. To execute aerial locomotion, a snake uses one of several stereotyped jumps from a tree into the air, while simultaneously flattening its body into an aerodynamically favorable shape. Large amplitude traveling waves are propagated posteriorly during the stable glide, while landing involves body wrapping, passive body compression, and energy absorption through compliance in the landing substrate to dissipate the accumulated kinetic energy from the glide. In all of these locomotor events, from interacting with cylindrical branches, falling through the air, grasping compliant tree branches and leaves, to landing on solid ground, snakes appropriate the same body morphology and perhaps the same basic neural mechanisms. Here we discuss our use of computational models and animal experiments to understand how flying snakes interact with and locomote on and through multiple media, potentially providing principles for legless locomotor designs.

\(^1\)Supported by NSF 1351322

12:51PM Y40.00009 Aerodynamic control with passively pitching wings, NICK GRAVISH, ROBERT WOOD, Harvard University — Flapping wings may pitch passively under aerodynamic and inertial loads. Such passive pitching is observed in flapping wing insect and robot flight. The effect of passive wing pitch on the control dynamics of flapping wing flight is unexplored. Here we demonstrate in simulation and experiment the critical role wing pitching plays in yaw control of a flapping wing robot. We study yaw torque generation by a flapping wing allowed to passively rotate in the pitch axis through a rotational spring. Yaw torque is generated through alternating fast and slow upside upstroke and and downstroke. Yaw torque sensitivity depends on both the rotational spring force law and spring stiffness, and at a critical spring stiffness a bifurcation in the yaw torque control relationship occurs. Simulation and experiment reveal the dynamics of this bifurcation and demonstrate that anomalous yaw torque from passively pitching wings is the result of aerodynamic and inertial coupling between the pitching and stroke-plane dynamics.

1:03PM Y40.00010 Crucial advantages of tail use in the evolution of vertebrate terrestrial locomotion, HENRY ASTLEY, Georgia Inst of Tech, BENJAMIN MCINROE, U C Berkeley, SANDY KAWANO, National Institute for Mathematical and Biological Synthesis, RICK BLOB, Clemson University, DANIEL GOLDMAN, Georgia Inst of Tech — In the invasion of terrestrial environment, the first tetrapods faced the challenge of locomotion on flowable substrates (e.g. sand and mud), sometimes oriented at inclines. Although the morphology of many early tetrapods is known, robotic studies have revealed that effective locomotion on these substrates also depends highly upon kinematics; slight differences in movements of the same appendage can lead to success or failure. Using a model organism (the mudskipper) and a robotic physical model, we demonstrate how muscular tails provided critical locomotor advantages on granular substrates that the first invaders of land likely encountered. Mudskippers use their tails for additional propulsion with increasing frequency as the slope of the granular material increases, and the decline in locomotor performance with slope is shallow when the tail is used. Experiments with a robotic model of the mudskipper showed that, while the tail did not always provide a benefit to locomotion, use of the tail made the robot’s performance more robust, achieving effective locomotion on a wider range of slopes, limb postures and foot placements. These results suggest that, rather than simply being an inert appendage, the tails of early tetrapods were vital to their first forays into terrestrial habitats.

1:15PM Y40.00011 Mutually opposing forces during locomotion can eliminate the tradeoff between maneuverability and stability, NOAH COWAN, SHAHIN SEFATI, Johns Hopkins University, IZAAK NIEVEL, Northwestern University, EATAI ROTH, TERENCE MITCHELL, Johns Hopkins University, JAMES SNYDER, MALCOLM MACIVER, Northwestern University, ERIC FORTUNE, New Jersey Institute of Technology — A surprising feature of animal locomotion is that organisms typically produce substantial forces in directions other than what is necessary to move the animal through its environment, such as perpendicular to, or counter to, the direction of travel. The effect of these forces has been difficult to observe because they are often mutually opposing and therefore cancel out. Using a combination of robotic physical modeling, computational modeling, and biological experiments, we discovered that these forces serve an important role: to simplify and enhance the control of locomotion. Specifically, we examined a well-suited model system, the glass knifefish Eigenmannia virescens, which produces mutually opposing forces during a hovering behavior. By systematically varying the locomotor parameters of our biomimetic robot, and measuring the resulting forces and kinematics, we demonstrated that the production and differential control of mutually opposing forces is a strategy that generates passive stabilization while simultaneously enhancing maneuverability. Mutually opposing forces during locomotion are widespread across animal taxa, and these results indicate that such forces can eliminate the tradeoff between stability and maneuverability, thereby simplifying robotic and neural control.

1:27PM Y40.00012 A robotic platform for studying sea lion thrust production, MEGAN LEFTWICH, RAHI PATEL, ADITYA KULKARNI, CHEN FRIEDMAN, The George Washington University — California Sea Lions are agile swimmers and, uniquely, use their forelimbs (rather than hind flipper undulation) to generate thrust. Recently, a sea lion flipper from a deceased subject was externally scanned in high detail for muscular tails provided critical locomotor advantages on granular substrates that the first invaders of land likely encountered. Mudskippers use their tails for additional propulsion with increasing frequency as the slope of the granular material increases, and the decline in locomotor performance with slope is shallow when the tail is used. Experiments with a robotic model of the mudskipper showed that, while the tail did not always provide a benefit to locomotion, use of the tail made the robot’s performance more robust, achieving effective locomotion on a wider range of slopes, limb postures and foot placements. These results suggest that, rather than simply being an inert appendage, the tails of early tetrapods were vital to their first forays into terrestrial habitats.

1:39PM Y40.00013 Controlled locomotion of robots driven by a vibrating surface\(^1\), PAUL UMBAN-HOWAR, KEVIN M. LYNCH, Northwestern University — Robots typically derive their powers of movement from onboard actuators and power sources, but other scenarios are possible where the external environment provides part or all of the necessary forcing and control. I will discuss details of a system where the robots are just planar solid objects and the requisite driving forces originate from frictional sliding-interactions with a periodically oscillated and nominally horizontal surface. For the robots to move, the temporal symmetry of the frictional forces must be broken, which is achieved here by modulating the normal force using vertical acceleration of the surface. Independent of the initial conditions and vibration waveform, a sliding locomotor reaches a unique velocity limit cycle.

\(^1\)Supported by NSF CMMI 0700537

12:15PM Y40.00010 Crucial advantages of tail use in the evolution of vertebrate terrestrial locomotion, HENRY ASTLEY, Georgia Inst of Tech, BENJAMIN MCINROE, U C Berkeley, SANDY KAWANO, National Institute for Mathematical and Biological Synthesis, RICK BLOB, Clemson University, DANIEL GOLDMAN, Georgia Inst of Tech — In the invasion of terrestrial environment, the first tetrapods faced the challenge of locomotion on flowable substrates (e.g. sand and mud), sometimes oriented at inclines. Although the morphology of many early tetrapods is known, robotic studies have revealed that effective locomotion on these substrates also depends highly upon kinematics; slight differences in movements of the same appendage can lead to success or failure. Using a model organism (the mudskipper) and a robotic physical model, we demonstrate how muscular tails provided critical locomotor advantages on granular substrates that the first invaders of land likely encountered. Mudskippers use their tails for additional propulsion with increasing frequency as the slope of the granular material increases, and the decline in locomotor performance with slope is shallow when the tail is used. Experiments with a robotic model of the mudskipper showed that, while the tail did not always provide a benefit to locomotion, use of the tail made the robot’s performance more robust, achieving effective locomotion on a wider range of slopes, limb postures and foot placements. These results suggest that, rather than simply being an inert appendage, the tails of early tetrapods were vital to their first forays into terrestrial habitats.

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1:39PM Y40.00013 Controlled locomotion of robots driven by a vibrating surface\(^1\), PAUL UMBAN-HOWAR, KEVIN M. LYNCH, Northwestern University — Robots typically derive their powers of movement from onboard actuators and power sources, but other scenarios are possible where the external environment provides part or all of the necessary forcing and control. I will discuss details of a system where the robots are just planar solid objects and the requisite driving forces originate from frictional sliding-interactions with a periodically oscillated and nominally horizontal surface. For the robots to move, the temporal symmetry of the frictional forces must be broken, which is achieved here by modulating the normal force using vertical acceleration of the surface. Independent of the initial conditions and vibration waveform, a sliding locomotor reaches a unique velocity limit cycle at a given position. Its resulting motion can be described in terms of velocity fields which specify the robots cycle-averaged velocity as a function of position. Velocity fields with non-zero spatial divergence can be generated by combining translational and rotational surface motions; this allows the simultaneous and open-loop collection, dispersal, and transport of multiple robots. Fields and field sequences can simultaneously move multiple robots between arbitrary positions and, potentially, along arbitrary trajectories.

\(^1\)Supported by NSF CMMI 0700537
1:51PM Y40.00014 Dynamical states in the sensorimotor loop of a rolling robot, BULCSÚ SÁNDOR, TIM JAHN, LAURA MARTIN, RODRIGO ECHEVESTE, CLAUDIUS GROS, Institute for Theoretical Physics, Goethe University Frankfurt — We investigate the closed sensorimotor loop of a simple rolling robot as a dynamical system. Using the LpzRobots simulation package, we construct robots with cylindrical body, controlled by a single proprioceptual neuron with a time dependent threshold. Despite its simplicity, we obtain a rich set of rolling modes, as a result of the self-organizing processes arising through the feedback within the sensorimotor loop. These rolling modes are robust against environmental noise, since they correspond to stable limit cycle attractors. However, for certain parameters they also allow for explorative behavior via internal noise induced switching. Furthermore, we also find a region of parameters in which the motion is fully embodied, where, in engineering terms, the engine powering the motion of the robot is turned on dynamically through the feedback of its very motion.


2B. Sándor, T. Jahn, L. Martin & C. Gros, The sensorimotor loop as a dynamical system: How regular motion primitives may emerge from self-organized limit cycles, to be published, 2015

2:03PM Y40.00015 Vibration Propagation in Spider Webs1, ROSS HATTON, ANDREW OTTO, Oregon State Univ, DAMIAN ELIAS, Univ, California, Berkeley — Due to their poor eyesight, spiders rely on web vibrations for situational awareness. Web-borne vibrations are used to determine the location of prey, predators, and potential mates. The influence of web geometry and composition on web vibrations is important for understanding spiders behavior and ecology. Past studies on web vibrations have experimentally measured the frequency response of web geometries by removing threads from existing webs. The full influence of web structure and tension distribution on vibration transmission; however, has not been addressed in prior work. We have constructed physical artificial webs and computer models to better understand the effect of web structure on vibration transmission. These models provide insight into the propagation of vibrations through the webs, the frequency response of the bare web, and the influence of the spider’s mass and stiffness on the vibration transmission patterns.

1Supported by NSF-1504428.

2:15PM Y40.00016 Proprioceptive Actuation Design for Dynamic Legged locomotion1, SANGBAE KIM, PATRICK WENSING, MIT, BIOMIMETIC ROBOTICS LAB TEAM — Designing an actuator system for highly-dynamic legged locomotion exhibited by animals has been one of the grand challenges in robotics research. Conventional actuators designed for manufacturing applications have difficulty satisfying challenging requirements for high-speed locomotion, such as the need for high torque density and the ability to manage dynamic physical interactions. It is critical to introduce a new actuator design paradigm and provide guidelines for its incorporation in future mobile robots for research and industry. To this end, we suggest a paradigm called proprioceptive actuation, which enables highly- dynamic operation in legged machines. Proprioceptive actuation uses colocated force control at the joints to effectively control contact interactions at the feet under dynamic conditions. In the realm of legged machines, this paradigm provides a unique combination of high torque density, high-bandwidth force control, and the ability to mitigate impacts through backdrivability. Results show that the proposed design provides an impact mitigation factor that is comparable to other quadruped designs with series springs to handle impact. The paradigm is shown to enable the MIT Cheetah to manage the application of contact forces during dynamic bounding, with results given down to contact times of 85ms and peak forces over 450N. As a result, the MIT Cheetah achieves high-speed 3D running up to 13mph and jumping over an 18-inch high obstacle.

The project is sponsored by DARPA M3 program


11:15AM Y43.00001 Order-to-chaos transition in the hardness of random Boolean satisfiability problems, MELINDA VARGA, Department of Physics, University of Notre Dame, ROBERT SUMI, MARIA ERCSEY-RAVASZ, Faculty of Physics, Babes-Bolyai University, Romania, ZOLTAN TOROCZKAI, Department of Physics, University of Notre Dame — Transient chaos is a phenomenon characterizing the dynamics of phase space trajectories evolving towards an attractor in physical systems. We show that transient chaos also appears in the dynamics of certain algorithms searching for solutions of constraint satisfaction problems (e.g., Sudoku). We present a study of the emergence of hardness in Boolean satisfiability (k-SAT) using an analog deterministic algorithm. Problem hardness is defined through the escape rate $\kappa$, an invariant measure of transient chaos, and it expresses the rate at which the trajectory approaches a solution. We show that the hardness in random k-SAT ensembles has a wide variation approximable by a lognormal distribution. We also show that when increasing the density of constraints $\alpha$, hardness appears through a second-order phase transition at $\alpha_c$ in the random 3-SAT ensemble where dynamical trajectories become transiently chaotic, however, such transition does not occur for 2-SAT. This behavior also implies a novel type of transient chaos in which the escape rate has an exponential-algebraic dependence on the critical parameter. We demonstrate that the transition is generated by the appearance of non-solution basins in the solution space as the density of constraints is increased.

11:27AM Y43.00002 Population Annealing: Theory and Application in Spin Glasses1, JONATHAN MACHTA, Univ of Mass - Amherst, WENLONG WANG, HELMUT G. KÄTZRABER, Texas A&M University — Population annealing is an efficient sequential Monte Carlo algorithm for simulating equilibrium states of systems with rough free energy landscapes. The theory of population annealing is presented, and systematic and statistical errors are discussed. The behavior of the algorithm is studied in the context of large-scale simulations of the three-dimensional Ising spin glass and the performance of the algorithm is compared to parallel tempering. It is found that the two algorithms are similar in efficiency though with different strengths and weaknesses.

1Supported by NSF DMR-1151387, DMR-1208046 and DMR-1507506
11:39 AM Y43.00003 Bond and temperature chaos in spin glasses revealed through thermal boundary conditions1, WENLON WANG, Texas AM Univ, JONATHAN MACHTA COLLABORATION2, HELMUT G. KATZGRABER COLLABORATION3 — Spin glasses are complex systems with rugged energy landscapes that exhibit chaotic behavior. Unfortunately, despite decades of study, there is still no clear understanding of the chaotic behavior found in these systems. The use of thermal boundary conditions has become a useful approach to study such phenomena. Here we discuss how to efficiently simulate bond and temperature chaos using thermal boundary conditions and population annealing Monte Carlo. We provide a simple scaling argument for bond and temperature chaos, and present numerical results of the scaling exponents. Similarities and differences of bond chaos and temperature chaos are also discussed.

1 NSF DMR-120804
2 UMass Amherst
3 Texas AM Univ

11:51 AM Y43.00004 Can we predict the difficulty of optimization problems without solving them? HELMUT G. KATZGRABER, CHAO FANG, RICHARD LAWRENCE, OLIVER MELCHERT, HUMBERTO MUNOZ-BAUZA, ANDREW J. OCHOA, WENLON WANG, ZHENG ZHU, Texas A&M University — Surprisingly often, based on previous results of a large-scale numerical study of the equilibrium three-dimensional Edwards-Anderson Ising spin glass where it was demonstrated that autocorrelation times are directly correlated with the roughness of the free-energy landscape [Phys. Rev. E 87, 012104 (2013)], we show that a generalized spin-glass order parameter can be used as a proxy to the computational difficulty of various paradigmatic optimization problems. Our results are illustrated with different optimization algorithms, as well as optimization problems. Furthermore, we show numerical evidence that the order-parameter distribution does mirror salient features in the free-energy landscape of complex systems for moderate system sizes.

12:03PM Y43.00005 TemperSAT: A new efficient fair-sampling random k-SAT solver, CHAO FANG, ZHENG ZHU, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University — The set membership problem is of great importance to many applications and, in particular, database searches for target groups. Recently, an approach to speed up set membership searches based on the NP-hard constraint-satisfaction problem (random k-SAT) has been developed [S. Weaver et al. J SAT 8, 129 (2014)]. However, the bottleneck of the approach lies in finding the solution to a large SAT formula efficiently and, in particular, a large number of independent solutions is needed to reduce the probability of false positives. Unfortunately, traditional random k-SAT solvers such as WalkSAT are biased when seeking solutions to the Boolean formulas. By porting parallel tempering Monte Carlo to the sampling of binary optimization problems, we introduce a new algorithm (TemperSAT) whose performance is comparable to current state-of-the-art SAT solvers for large k with the added benefit that theoretically it can find many independent solutions quickly. We illustrate our results by comparing to the currently fastest implementation of WalkSAT, WalkSAT/m.

12:15PM Y43.00006 ICANP2: Isoenergetic cluster algorithm for NP-complete Problems, ZHENG ZHU, CHAO FANG, HELMUT G. KATZGRABER, Texas AM University — NP-complete optimization problems with Boolean variables are of fundamental importance in computer science, mathematics and physics. Most notably, the minimization of general spin-glass-like Hamiltonians remains a difficult numerical task. There has been a great interest in designing efficient heuristics to solve these computationally difficult problems. Inspired by the rejection-free isoenergetic cluster algorithm developed for Ising spin glasses [Phys. Rev. Lett. 115, 077201 (2015)], we present a generalized cluster update that can be applied to different NP-complete optimization problems with Boolean variables. The cluster updates allow for a wide-spread sampling of phase space, thus speeding up optimization. By carefully tuning the pseudo-temperature (needed to randomize the configurations) of the problem, we show that the method can efficiently tackle problems on topologies with a large site-percolation threshold. We illustrate the ICANP2 heuristic on paradigmatic optimization problems, such as the satisfiability problem and the vertex cover problem.

12:27PM Y43.00007 ABSTRACT WITHDRAWN —

12:39PM Y43.00008 Lower-Critical Spin-Glass Dimension from 23 Sequenced Hierarchical Models, MEHMET DEMIRTAS, Sabanci University and Cornell University, ASLI TUNCER, Istanbul Technical University, A. NIHAT BERKER, Sabanci University and MIT — The lower-critical dimension for the existence of the Ising spin-glass phase is calculated, numerically exactly, as \( d_L = 2.520 \) for a sequence of hierarchical lattices, from an essentially exact (correlation coefficient \( R^2 = 0.99999999 \)) near-linear fit to 23 different diminishing fractional dimensions. To obtain this result, the phase transition temperature between the disordered and spin-glass phases, the corresponding critical exponent \( y_T \), and the runaway exponent \( y_R \) of the spin-glass phase are calculated for consecutive hierarchical lattices as dimension is lowered.[1]


12:51PM Y43.00009 Odd q-State Clock Spin-Glass Models in Three Dimensions, Asymmetric Phase Diagrams, and Multiple Algebraically Ordered Phases, EFE ILKER, Sabanci University and Case Western Reserve University, A. NIHAT BERKER, Sabanci University and MIT — Distinctive orderings and phase diagram structures are found, from renormalization-group theory, for odd q-state clock spin-glass models in \( d = 3 \) dimensions [1]. These models exhibit asymmetric phase diagrams, as is also the case for quantum Heisenberg spin-glass models. No finite-temperature spin-glass phase occurs. For all odd \( q \geq 5 \), algebraically ordered antiferromagnetic phases [2,3] occur. One such phase is dominating and occurs for all \( q \geq 5 \); other such phases occur for \( 5 \leq q \leq 15 \). All algebraically ordered phases have the same structure, determined by an attractive finite-temperature sink fixed point where a dominant and a subdominant pair states have the only non-zero Boltzmann weights. The phase transition critical exponents quickly saturate to the high q value as previously observed for even q-state clock models [4].

Spinodals of the Ising model on the order-4 pentagonal tiling of the hyperbolic plane

HOWARD L. RICHARDS, Physics, Marshall University — In the Euclidean plane, the Ising model on a regular lattice does not have a true spinodal — that is, there is no local minimum of the free energy that persists forever (in the limit of infinitely large systems) except for the global minimum, which characterizes the stable state. However, a local minimum can persist for a very long time, so the minimum can be referred to as a “metastable” state. The manner in which the metastable state decays depends on the strength of the magnetic field and the system size; the “thermodynamic spinodal” is the transition between systems large enough to contain a single critical droplet and systems that are too small to do so, and the “dynamic spinodal” marks the transition between decay as a Poisson process to decay that is “deterministic”, meaning the standard deviation of the lifetime of the metastable state is small compared with its mean value. However, in the hyperbolic plane, true metastability exists, and evidence shows that the thermodynamic spinodal and dynamic spinodal are numerically close to the true spinodal, the field below which the metastable state cannot decay through the nucleation and growth of droplets.

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Weak confinement in the three-state Potts Field Theory

SERGEI RUTKEVICH, Univ Duisburg-Essen — Kink topological excitations are quite common in one-dimensional quantum ferromagnetic systems with the spontaneously broken discrete symmetry. Application of the external magnetic field \( h \) induces the long-range attractive force between kinks leading to their confinement. While in the Ising Field Theory the particle sector in the confinement regime contains only the two-kink bound states (“the mesons”), in the three-state Potts Field Theory (PFT) the three-kink bound states (“the baryons”) can exist as well. In the weak confinement regime, which is realized at small external magnetic fields, the meson masses in the PFT can be determined analytically in the leading order in \( h \) by means of the solution of a quantum-mechanical problem for two non-relativistic particles interacting with a linear attractive potential, and my means of the WKB method. The masses of lightest baryons in the three-state PFT were calculated by the numerical solution of a three-particle quantum-mechanical problem. The obtained mass spectra for the PFT mesons and baryons were confirmed recently by Lencs and Takács in numerical calculations based on the truncated conformal space approach.