8:00AM A52.00001 Regularization of tunneling rates in quantum chaotic systems LOUIS PECORA, Naval Research Laboratory — Prototypical systems of two potential wells separated by a tunneling barrier exhibit the unexpected and counter-intuitive results that regular, non-chaotic systems have tunneling rates that fluctuate with energy dramatically over several orders of magnitude whereas the fully chaotic wells have orders of magnitude smaller fluctuations. All calculations were found from the Schrodinger equation using the Boundary Element Method. A random, plane wave theory explains the magnitude of the average tunneling rates as well as their fluctuations. We show that we can tune the amount of variance in tunneling rates by changing the shape of the quantum wells implying possible device design capabilities for nanodevices that operate in the electron ballistic regime.

8:36AM A52.00002 Relativistic quantum Darwinism in Dirac fermion and graphene systems XUAN NI, Arizona State University, LIANG HUANG, Arizona State University; Lanzhou University, Gansu, China, YING-CHENG LAI, Arizona State University, LOUIS PECORA, Naval Research Laboratory — We solve the Dirac equation in two spatial dimensions in the setting of resonant tunneling, where the system consists of two symmetric cavities connected by a finite potential barrier. The shape of the cavities can be chosen to yield both regular and chaotic dynamics in the classical limit. We find that certain pointer states about classical periodic orbits can exist, which are signatures of relativistic quantum Darwinism (RQD). These localized states suppress quantum tunneling, and the effect becomes less severe as the underlying classical dynamics in the cavity is chaotic, leading to regularization of quantum tunneling. Qualitatively similar phenomena have been observed in graphene. A physical theory is developed to explain relativistic quantum Darwinism and its effects based on the spectrum of complex eigenenergies of the non-Hermitian Hamiltonian describing the open cavity system.

8:48AM A52.00003 Relativistic quantum chaos—an analytic Dirac equation approach1 LIANG HUANG, HONGYA XU, School of Physical Science and Technology, Lanzhou University, YING-CHENG LAI, School of Electrical, Computer, and Energy Engineering, Arizona State University — Relativistic quantum chaos has attracted much attention since the discovery of graphene in 2004. Using graphene billiard as an apparatus of relativistic quantum particles, relativistic quantum scars, level spacing statistics, and relativistic quantum scattering have been widely investigated recently. However, since graphene has two non-equivalent Dirac points which can be coupled together by various processes, it has been wondered that whether the observed phenomena are inherent to the relativistic movement or caused by the discrete graphene lattice structure and boundary terminations. Based on Berry et al.’s work on neutrino billiards, we developed a conformal transformation method to solve the 2D Dirac equation in a confined region resembling chaotic billiards in the classical limit. This method solves both the eigen-energies and the eigen-wavefunctions of the 2D massless Dirac fermions. Level spacing statistics and relativistic quantum scars for a heart-shaped billiard are investigated and comparisons with graphene billiards are made.

1This work was supported by AFOSR under Grant No. FA9550-09-1-0026 and NSF of China under Grant No. 11005053.

9:00AM A52.00004 Using Local Perturbations To Manipulate and Control Pointer States in Quantum Dot Systems, RICHARD AKIS, GIL SPEYER, DAVID FERRY, Arizona State University, ROLAND BRUNNER, University of Leoben, Austria — Recently, scanning gate microscopy (SGM) was used to image scarred wave functions in an open InAs quantum dot[1]. The SGM tip provides a local potential perturbation and imaging is performed by measuring changes in conductance. Scarred wave functions, long associated with quantum chaos, have been shown in open dots to correspond to pointer states[2], eigenstates that survive the decoherence process that occurs via coupling to the environment. Pointer states modulate the conductance, yielding periodic fluctuations and the scars, normally thought unstable, are stabilized by quantum Darwinism [3]. We shall show that, beyond probing states, pointer states can be manipulated by local perturbations. Particularly interesting effects occur in coupled quantum dot arrays, where a pointer state localized in one dot can be shifted into another with a perturbation in a completely different part of the system. These nonlocal effects may perhaps be exploited to give such systems an exotic functionality. [1] A. M. Burke, R. Akis, T. E. Day, Gil Speyer, D. K. Ferry, and B. R. Bennett, Phys. Rev. Lett. 104, 176801 (2010). [2] D. K. Ferry, R. Akis, and J. P. Bird, Phys. Rev. Lett. 104, 176801 (2004). [3] R. Brunner, R. Akis,D. K. Ferry, F. Kuchar, and R. Meisels, Phys. Rev. Lett. 101, 024102 (2008).

9:12AM A52.00005 Periodic Orbit Scar in Propagation of Wave Packet, MITSUYOSHI TOMIYA, HIROYOSHI TSUYUKI, SHOICHI SAKAMOTO, Faculty of Science and Technology, Seikei University, ERIC HELLER, Department of Physics, Harvard University — The scar-like enhancement is found in the accumulation of the time-evolving wave packet in stadium billiard. The time-average of the absolute square of the time-evolving wave functions in the stadium billiard is investigated numerically and semiclassically. Nowadays nano- or subnano-sized devices are getting more and more available. This kind of dynamical properties is essential, when the devices actually work. The enhancement appears along an unstable periodic orbit, when the Gaussian wave packet is launched as the initial state along the orbit. Introducing the window function which is closely related to the eigenfunction expansion coefficients of the wave packet, the localization around the periodic orbit is clarified by the semiclassical approximation that it is due to essentially the same mechanism of the scar states in stationary states. The “smoothed” window function is well estimated by the intensity spectrum in Prof. Heller’s theory of the long-time semiclassical dynamics. The key parameters that determine its shape are actually classical quantities: the size of the initial wave packet and the Lyapunov exponent.

9:24AM A52.00006 Chaotic Ionization of Bidirectionally Kicked Rydberg Atoms, KORANA BURKE, Boston University, KEVIN MITCHELL, UC Merced, SHUZHENG YE, F. BARRY DUNNING, BRENDAN WYKER, Rice University — A highly excited quasi one-dimensional Rydberg atom is exposed to periodic alternating electric field pulses. The ionization of this system is governed by a geometric structure of phase space called a homoclinic tangle and its tunnelwave. We present and explain the results from an experiment designed to probe the structure of the phase space tangle. We create time-dependent Rydberg wave packets, subject them to alternating applied electric fields (kicks), and measure the survival probability. We show that the survival probability of the electron depends not only on the initial electron energy, but also on the phase space position of the electron relative to the tunnelwave inside the turnstile. After one period of the applied field, while that portion outside the turnstile ionizes after multiple kicking periods. Finally, we use the turnstile geometry to explain the dependence of the survival probability on the kicking period. This procedure describes a very robust yet simple way to control chaotic ionization of an atomic system.

9:36AM A52.00007 Quantized Intrinsically Localized Modes1, PETER RISEBOROUGH, Physics Department — We have calculated the quantized n = 2 breather spectra of both the β and the α Fermi-Pasta-Ulam lattices. The breather spectra are composed of resonances in the two-phonon continuum and branches of infinitely long-lived excitations. The non-linear attributes of these excitations become more pronounced at elevated temperatures. The calculated n = 2 breather and the resonance of the β-lattice hybridize and exchange identity at the zone boundary, and are in reasonable agreement with the results of previous authors using the number conserving approximation. However, by contrast the breather spectrum of the α-lattice couples resonantly with the single-phonon spectrum and cannot be calculated within a number conserving approximation. Furthermore we show that, for sufficiently strong non-linearity, the α-lattice breathers can be observed directly through the single-phonon inelastic neutron scattering spectrum. As the temperature is increased, the single-phonon dispersion relation for the α-lattice becomes progressively softer as the lattice instability is approached. We compare our theoretical results with the recent experimental observation of breathers in NaI by Manley et al. 

1US Department of Energy, Office of Basic Energy Sciences, Materials Science, Grant DEFG02-84ER4587
9:48AM A52.00008 Using quantum chaos to control the production of bipartite entangled states  , LOCK CHEW, Nanyang Technological University, NING CHUNG, National University of Singapore — Recently, we have shown that it is possible for the entanglement dynamics to depend on the global classical dynamical regime instead of the local classical behavior. We observe that as the corresponding classical system becomes more chaotic, the rate of entanglement production increases with the emergence of larger entanglement entropy in the steady state. This suggests that quantum chaos can be used to control the generation of highly entangled quantum states, which are typically more robust against the effects of decoherence from the environment. Furthermore, the dependence of our system on the global classical dynamical regime indicates that the mode of production is insensitive to errors in the preparation of the initial separable coherent states. In this talk, I will present our recent results of using the additional control of quantum squeezing to further enhance the entanglement of the dynamically generated quantum states. I will show that the concomitant application of quantum squeezing leads to a more entangled state at a faster production rate relative to squeezing without quantum chaos.

10:00AM A52.00009 Entanglement Entropy and Entanglement Spectrum for Two-Dimensional Classical Spin Configuration , HIROAKI MATSUEDA, Sendai National College of Technology — In quantum spin chains at criticality, two types of scaling for the entanglement entropy exist: one comes from conformal field theory (CFT), and the other is for entanglement support of matrix product state (MPS) approximation. On the other hand, quantum spin-chain models can be mapped onto two-dimensional (2D) classical ones. Motivated by the scaling and the mapping, we introduce new entanglement entropy for 2D classical spin configuration as well as entanglement spectrum, and examine their basic properties in the Ising and the three-state Potts models on the square lattice. They are defined by the singular values of the reduced density matrix for a Monte Carlo snapshot. We find scaling relations of the entropy analogous to the CFT and the MPS results. At criticality, the spin configuration is fractal, and various sizes of ordered clusters coexist. Then, the original snapshot can be decomposed into a set of images, and they have different length scales, respectively. This is the origin of the scaling. Based on these observations as well as calculation of the entanglement spectrum, we conclude that the amount of information of only one snapshot at criticality is equal to that of 1D quantum critical systems.

10:12AM A52.00010 Fluctuation theorem for a double quantum dot coupled to a point-contact elec trometer , YASUHIRO UTSUMI, Department of Physics Engineering, Faculty of Engineering, Mie University, DMITRI GOLUBEV, MICHAEL MARTHAHLER, GERD SCHÖN, KARLSRUHE INSTITUTE OF TECHNOLOGY, GERMANY COLLABORATION — We study the fluctuation theorem in a double-electron spin-valley tunneling regime. We consider single-electron transport through a double quantum dot (DQD) monitored by a capacitively coupled quantum point-contact (QPC) electrometer. In this setup it is possible to perform a direction resolved real-time electron counting experiment. We derive the full counting statistics for the coupled DQD - QPC system and obtain the joint probability distribution of the charges transferred through the DQD and the QPC. We show that the joint probability distribution satisfies the fluctuation theorem for 4-terminal system. For two-terminal DQD, the effective temperature should be introduced to recover the fluctuation theorem. The system can be described by a master equation with tunneling rates depending of the counting fields and satisfying a generalized local detailed-balance relation. Furthermore, we derive universal relations between the non-linear corrections to the current and noise, which can be verified in experiment.

10:24AM A52.00011 Electromagnetic fluctuations in non-equilibrium: Casimir forces and heat transfer  , MATTHIAS KRUGER, MIT, Department of Physics, 77 Massachusetts Ave, Cambridge, MA 02139, THORSTEN EMIG, Laboratoire de Physique Theorique et Modesles Statistiques, CNRS UMR 8626, Universite Paris-Sud, 91405 Orsay cedex, France, GIUSEPPE BIMONTE, Dipartimento di Scienze Fisiche, Universita di Napoli Federico II, Complesso Universitario MSA, Via Cintia, I-80126 Napoli, Italy and INFN Sezione, VLADYSLAV GOLYK, ALEXANDER MCCAULEY, MEHRAN KARDAR, MIT, Department of Physics, 77 Massachusetts Ave, Cambridge, MA 02139 — It is well known that quantum Casimir forces play an important role in micro- or nanostructures. Recently, the role of temperature in thermal non-equilibrium raised theoretical as well as experimental interest. If the objects are held at different temperatures, the interactions depend on all temperatures in the system, and show many effects which are absent in equilibrium. Additionally, the objects exchange thermal energy by electromagnetic fields, known as radiative heat transfer, which is fundamentally different from macroscopic cases described by the well known laws of Planck or Stefan-Boltzmann and which can be studied in a non-linear context. We discuss recent theoretical progress describing such effects, and illustrate the dependence of both quantities on the temperatures as well as the distances of the objects.

8:00AM A53.00001 The dependence of fragility of glass forming liquids on interparticle interactions and density  , SRIKANTH SASTRY, SHILADITYA SENGUPTA, Jawaharlal Nehru Centre for Advanced Scientific Research, FREDERIC AFFOUARD, FILIPE VASCONCELOS, Universite Lille, JNCASR COLLABORATION — The fragility of a glass forming liquid quantifies the rapidity of the change in viscosity and relaxation times, and is an important material property. We study the influence of interparticle interactions on the fragility of a set of model glass formers using computer simulations. We consider both the kinetic fragility, given by the temperature variation of relaxation times, and the thermodynamic fragility obtained by the temperature variation of the configurational entropy. The Adam-Gibbs relation describes the temperature variation of relaxation times in terms of the variation of the configurational entropy, and thus we expect the kinetic and thermodynamic fragilities to be consistent with each other. However, we have found that the kinetic fragility increases with increasing softness of the interaction potential, with thermodynamic fragility showing the opposite trend. We rationalize our results by considering the full form of the Adam-Gibbs relation, which involves knowledge in addition of the high temperature activation energies, and explore the role of relevant ideas on the scaling of temperature and density in systems exhibiting behavior akin to those with inverse power law interactions.

Monday, February 27, 2012 8:00AM - 11:00AM — Session A53 GSNP: Disordered and Glassy Systems I 153B

8:00AM A53.00001 The dependence of fragility of glass forming liquids on interparticle interactions and density  , SRIKANTH SASTRY, SHILADITYA SENGUPTA, Jawaharlal Nehru Centre for Advanced Scientific Research, FREDERIC AFFOUARD, FILIPE VASCONCELOS, Universite Lille, JNCASR COLLABORATION — The fragility of a glass forming liquid quantifies the rapidity of the change in viscosity and relaxation times, and is an important material property. We study the influence of interparticle interactions on the fragility of a set of model glass formers using computer simulations. We consider both the kinetic fragility, given by the temperature variation of relaxation times, and the thermodynamic fragility obtained by the temperature variation of the configurational entropy. The Adam-Gibbs relation describes the temperature variation of relaxation times in terms of the variation of the configurational entropy, and thus we expect the kinetic and thermodynamic fragilities to be consistent with each other. However, we have found that the kinetic fragility increases with increasing softness of the interaction potential, with thermodynamic fragility showing the opposite trend. We rationalize our results by considering the full form of the Adam-Gibbs relation, which involves knowledge in addition of the high temperature activation energies, and explore the role of relevant ideas on the scaling of temperature and density in systems exhibiting behavior akin to those with inverse power law interactions.
8:12AM A53.00002 Frequency and Wavevector Dependence of the Atomic Level Stress-Stress Correlation Function in a Model Supercooled Liquid. VALENTIN A. LEVASHOV, JAMES R. MORRIS, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — Temporal and spatial correlations among the local atomic level stress stresses were studied for a model liquid iron by molecular dynamics simulation [PRL 106,115703]. Integration over time and space of the shear stress correlation function \( F(r,t) \) yields viscosity via Green-Kubo relation. The stress correlation function in time and space \( F(r,t) \) was Fourier transformed to study the dependence on frequency, \( E \), and wave vector, \( Q \). The results, \( F(Q,E) \), showed damped shear stress waves propagating in the liquid for small \( Q \) at high and low temperatures. We also observed additional diffuse feature that appears as temperature is reduced below crossover temperature of potential energy landscape at relatively low frequencies at small \( Q \). We suggest that this additional feature might be related to dynamic heterogeneity and boson peaks. We also discuss a relation between the time-scale of the stress-stress correlation function and the alpha-relaxation time of the intermediate self-scattering function \( S(Q,E) \).

1This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering

8:24AM A53.00003 Measuring Dynamical Facilitation in Supercooled Liquids and Related Materials. YAE LELMATAD, Center for Soft Matter, Physics Department, New York University, New York NY USA, AARON KEYS, Chemistry Department, University of California, Berkeley, CA USA and Lawrence Berkeley National Laboratory, Berkeley, CA USA — We provide a physical interpretation for excitation dynamics in kinetically constrained lattice models in the context of supercooled liquids and granular materials. Several physical quantities such as instanton times, onset temperatures, and particle displacement fields are derived. These quantities are used to interpret measurements of dynamical facilitation previously performed for atomic and molecular supercooled liquids and granular materials. We show that these previous measurements provide strong evidence that dynamical facilitation plays a key role in glassy materials.

8:36AM A53.00004 Excitations are localized and relaxation is hierarchical in glass-forming liquids. AARON KEYS, LESTER HEDGES, Lawrence Berkeley National Laboratory, JUAN GARRAHAN, University of Nottingham, SHARON GLOTZER, University of Michigan, DAVID CHANDLER, University of California, Berkeley — For several atomistic models of glass formers, at conditions below their glassy dynamics onset temperatures, \( T_o \), we use importance sampling of trajectory space to study the structure, statistics and dynamics of excitations responsible for structural relaxation. Excitations are detected in terms of persistent particle displacements of length \( a \). At supercooled conditions, for \( a \) of the order of or smaller than a particle diameter, we find that excitations are associated with correlated particle motions that are sparse and localized, occupying a volume with an average radius that is temperature independent and no larger than a few particle diameters. We show that the statistics and dynamics of these excitations are facilitated and hierarchical. Excitation energy scales grow logarithmically with \( a \). Excitations at one point in space facilitate the birth and death of excitations at neighboring locations, and space-time excitation structures are microcosms of heterogeneous dynamics at larger scales. This nature of dynamics becomes increasingly dominant as temperature \( T \) is lowered. We show that slowing of dynamics upon decreasing temperature below \( T_o \) is the result of a decreasing concentration of excitations and concomitant growing hierarchical length.

8:48AM A53.00005 Anomalous properties of liquids for a family of models with short range tetrahedral interactions. SERGEY BULDYREV, Yesiva University, GIANCARLO FRANZESE, University of Barcelona — Liquids with tetrahedral symmetry of the first coordination shell often display anomalous thermodynamic and dynamic behavior. The main reason for these anomalies is that pressurizing such liquids leads to the disordering of this local symmetry by the particles migrating from the second to the first coordination shell. This in some case may lead to the increase of entropy upon pressurizing and consequently to the volume increase upon cooling. Molecular simulations of various models with tetrahedral symmetry are able to reproduce this anomalous behavior. We study a family of simple models in which we can gradually change the degree of tetrahedrality and investigate the associated changes of the phase diagram by discrete molecular dynamics. A molecule in these models consist of a hard sphere and four point particles attached to the center of the hard sphere by directional bonds arranged in tetrahedral geometry. Each of these four particles has a narrow attractive well, we find that excitations are associated with correlated particle motions that are sparse and localized, occupying a volume with an average radius that is temperature independent and no larger than a few particle diameters. We show that the statistics and dynamics of these excitations are facilitated and hierarchical. Excitation energy scales grow logarithmically with \( a \). Excitations at one point in space facilitate the birth and death of excitations at neighboring locations, and space-time excitation structures are microcosms of heterogeneous dynamics at larger scales. This nature of dynamics becomes increasingly dominant as temperature \( T \) is lowered. We show that slowing of dynamics upon decreasing temperature below \( T_o \) is the result of a decreasing concentration of excitations and concomitant growing hierarchical length.

9:00AM A53.00006 Stretched-exponential relaxation and hidden power laws in a solidifying 2D liquid. ALEXANDER PATASHINSKI, Northwestern University, RAFAŁ ORLIK, Orlik-software LLC, Poland, ANTONI MITUS, Polytechnic University, Wrocław, Poland, BARTOSZ GRZYBOWSKI, MARK RATNER, Northwestern University — In a 2D Lennard-Jones liquid, the number of particles keeping their memorized nearest neighbors is found to decay stretched-exponentially; the probability for a particle to keep the same nearest neighbors for a time \( t \) can be fitted with a power law. Using the lists of nearest neighbors (nn-lists) as a topological order parameter, we studied the dynamics of the structure underlying these signature features of complexity in materials. The \( nn \)-changes randomly appear along the boundaries of better ordered blocks at a time scale of the order of particle vibration period; these boundaries, and the shapes of the blocks, perform a next time-scale random motion. Particles diffusion includes periods of slow and fast diffusion. We discuss the feedback interactions between \( nn \)-changes, block boundaries motion, and orientation relaxation in the system.

9:12AM A53.00007 Sheared athermal soft-particle suspensions near jamming: dependence of effective diffusion on packing density and system size. KAMRAN KARIMI, CRAIG MALONEY, Carnegie Mellon University — We perform numerical simulations to study diffusion in a model bi-disperse frictionless athermal soft-particle suspension of disks in two dimensions (2D) using the so-called “mean field” version of Durian’s bubble model. We measure the effective transverse diffusion coefficient \( D_{eff} \) in shear flows at various volume fraction \( \phi \) and shearing rate \( \dot{\gamma} \). For \( \dot{\gamma} > \dot{\gamma}_c \), where \( \dot{\gamma}_c \) is identified with the random close packing limit, in the quasi-static limit, \( D_{eff} \) shows a pronounced linear system size dependence with very weak dependence on \( \phi \). For \( \dot{\gamma} < \dot{\gamma}_c \), \( D_{eff} \) in the quasi-static limit, increases with increasing \( \dot{\gamma} \) and shows very small system size dependence. We discuss how the behavior of \( D_{eff} \) is related to non-trivial correlations in the spatial structure of the displacement fields at long times in the Fickian regime.

3This work was supported by the Non-equilibrium Energy Research Center (NERC) which is an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0000989
9:24AM A53.00008 Decoupling of Rotational and Translational Diffusion in Supercooled Colloidal Fluids1, KAZEM V. EDMOND2, Emory University, MARK T. ELSESSER3, New York University, GARY L. HUNTER, Emory University, HYUNJOO PARK, DAVID J. PINE, New York University, ERIC R. WEEKS, Emory University — Using high-speed confocal microscopy, we directly observe the three-dimensional rotational dynamics of rigid clusters of microspheres suspended in dense colloidal suspensions. The clusters are highly ordered packings of fluorescently-labeled PMMA particles, fabricated using a recently developed emulsification technique. Our colloidal suspensions serve as an excellent model of hard spheres, perhaps the simplest system with a glass transition, while the clusters probe the system's local rotational and translational dynamics. Far from the colloidal liquid's glass transition temperature both translational motion of the clusters are purely Brownian. However, in the liquid's supercooled regime, we observe a decoupling between the two types of motion: as the glass transition is approached, rotational diffusion slows down even more than translational diffusion. The nature of the decoupling is in good agreement with theoretical predictions and experiments with molecular glass formers. Our observation supports the notion that supercooled liquids are not merely liquids with large viscosities but that diffusion takes place by fundamentally changed mechanisms.

1NSF Grant No. CHE-0910707
2Currently at the Center for Soft Matter Research at New York University.
3Currently at the University of North Carolina.

9:36AM A53.00009 Thermodynamics versus network topology of network glasses, LE YAN, MATTHIEU WYART, Center for Soft Matter Research, Physics Department, New York University — Under cooling, the thermodynamics and the dynamics of super-cooled liquids are strongly correlated. The thermal evolutions of these quantities, characterizing the liquid fragility, depend greatly on the specific liquid considered. To date, there is no understanding of what controls these properties at a microscopic level. In chalcogendie glasses, the coordination of the covalent network can be changed continuously by varying their composition. Experiments show that as the coordination is increased, the jump of specific heat varies non-monotonically and is minimal at coordination near the Maxwell threshold where the covalent network becomes rigid. At such a composition the liquid is strong. We introduce a simplified model for the thermal evolution of networks that captures this observation.

9:48AM A53.00010 Elastic properties of compressed emulsions, IVANE JORJADZE, JASNA BRUJIC, NYU — Visualizing the packing of a dense emulsion in 3D as a function of the external pressure allows us to characterize the geometry and the local stress distribution inside this jammed system. We first calculate the first two orders of the pressure and average coordination number over two orders of magnitude in density. We find deviations from theoretical exponents due to the non-affine motion of the particles. Second, we observe that the distribution of forces changes from a broad exponential at the jamming point to a narrower Gaussian-like distribution under high compression. Finally, we calculate the density of states of the measured force network in the approximation of a harmonic potential. Close to jamming, the number of low frequency modes is high, while the application of pressure shifts the distribution to higher frequencies, indicative of a rigid network. The confocal images reveal the structural features associated with the low frequency modes as well as their localization within the packing. These data are then compared with published results from numerical simulations.

10:00AM A53.00011 Glassy Dynamics of Charge Density Waves in Chromium1, HYEKYUNG KIM, JONATHAN LOGAN, University of Chicago, OLEG SHPYRKO, University of California San Diego, ERIC ISAACS, Argonne National Laboratory; University of Chicago — Charge-density waves provide theoretically tractable systems for exploring longstanding questions posed by the physics of elastic media in the presence of quenched disorder. Interaction of quenched pinning fields and phase elasticity of CDWs results in a complex energetic landscape of metastable states, which in turn gives rise to "glassy" phenomena such as aging and hysteresis. Using synchrotron x-rays we have observed aging of CDW order parameter Q in bulk chromium following thermal quench to out-of-equilibrium configuration. Although temperature stabilization occurs in under two minutes, Q relaxes exponentially over the course of hours toward metastable configurations that depend on sample history.

1Argonne National Laboratory; University of Chicago

10:12AM A53.00012 Local collapse of the atomic cage in a liquid flow, TAKUYA IWASHITA, TAKESHI EGAMI, University of Tennessee — The local structure of a model glass under steady shear was studied by molecular dynamics simulation for both high (T>Tg) and low (T=Tg) temperature ranges. The local structure was presented in terms of the anisotropic pair-density function (PDF). We found that the local structure was strained over a limited range of distances, and the length-scale of the strained region was dependent on the strain rate, extrapolating to zero at a critical strain rate. A strong correlation between the local collapse, represented by cutting of the atomic bond, and the structural strain in the PDF was found. At low temperatures, local failure happens in a serrated manner, caused mechanically by shear. At high temperatures, the local failure occurs more randomly, which is governed by thermal fluctuation. An anomalous behavior was observed as temperature approaches Tg. The results suggest that except for the supercooled state above Tg, local failure occurs by cutting of a single bond. Only in the supercooled state multiple bonds have to be cut for flow to occur. A possible relation to the dynamic heterogeneity is discussed.

10:24AM A53.00013 Local Perturbation of Quasi Two-Dimensional Colloidal Glasses1, KEVIN APTOWICZ, West Chester University, TIM STILL, KE CHEN, PETER YUNKER, ARJUN YODH, University of Pennsylvania — Colloids are promising and widely used model systems to investigate the phase behavior of matter at length scales and timescales accessible to optical microscopy. We utilize disordered quasi two-dimensional colloidal systems in the jammed state to study the properties of glasses. It was recently found in simulation and experiment that so-called 'soft spots', where low frequency quasi-localized modes concentrate, are the locations in glasses prone to rearrangements. Therefore, we utilize short laser pulses to perturb colloidal glasses locally. By varying the pulse intensity of the laser, the strength of the perturbation is tunable, which allows us to induce either elastic or plastic deformations in the glasses. With this experimental geometry in combination with video microscopy, we investigate the correlation between locally induced rearrangements in the colloidal glass and the location of soft spots determined from analysis of the system's vibrational eigenmodes. The dependence of the mechanical response of a glass on the local environment in terms of these dynamic heterogeneities and their persistence is discussed.

1We acknowledge financial support from Research Corporation (KBA), MRSEC DMR11-20901 (AGY), and DAAD (TS).

10:36AM A53.00014 X-ray investigation of colloidal glasses under shear, DMITRY DENISOV, TRIET DANG, Van der Waals-Zeeman Institute, University of Amsterdam, Netherlands, BERND STRUTH, Deutsches Elektronen-Synchrotron, Hamburg, Germany, PETER SCHALL, Van der Waals-Zeeman Institute, University of Amsterdam, Netherlands — Understanding glassification or dynamical arrest is one of the grand challenges of material science and is a topic of great current interest. It is a central observation in soft matter systems as well as glass forming molecular systems that - in the density or decreasing temperature - the motion of the particles or molecules slows down and eventually becomes arrested. Understanding this dynamical arrest as well as relaxations in the arrested state are fundamental problems, which to a large degree remain unanswered. We use a novel combination of rheological measurement and small angle x-ray scattering (at the synchrotron DESY in Hamburg) to study structure factor of dense suspensions under shear and during relaxation. The suspensions consist of silica particles 50nm in diameter. We observe clear changes of inter particles distances and configurations due to the different shear rates. Together with future dynamic x-ray measurements we aim to develop a universal scale-bridging understanding of dynamic arrest.
when the entire network becomes non-functional or fail gradually like in a second order transition as a greater fraction of nodes is removed in the initial attack. Euclidian space. Moreover, the network failures may occur not only to the loss of connectivity but also due to overload of nodes with high betweennes. We The dependency links are not connecting nodes at random but have tendency to connect nodes with similar degrees, or nodes which are close to each other in structural networks such as the power grid, transportation network, water supply, etc. Understanding the vulnerabilities of these systems is crucial to securing them. And modulate the degree of correlated multiplexity.

First we show how the correlated multiplexity can dramatically alter the giant component properties of multiplex random networks. Secondly we introduce an evolution model of co-evolving multiplex networks by generalizing the well-known Barabási-Albert-type model, to show how the co-evolution of network layers can induce and modulate the degree of correlated multiplexity. We present results of intentional attacks on highly loaded and high degree nodes as well as a comparison between spatially concentrated and randomly path flows on spatially embedded networks and study the model of cascading failures (Motter and Lai (2002)) triggered by the removal of a single or multiple nodes. We study the effect of spatial constraints on network resilience against cascading overloads. Specifically, we consider distributed and shortest structural networks among them; they form a multiplex network with multiple layers that can be interdependent and co-evolve. In many real-world complex systems, such multiple network layers are not randomly coupled but correlated. Such a correlated multiplexity can imprint nontrivial structural correlations in the multiplex network, which in turn can impact the dynamical processes on it. Here we present some recent results on the correlated multiplexity in multiplex networks. First we show how the correlated multiplexity can dramatically alter the giant component properties of multiplex random networks. Secondly we introduce an evolution model of co-evolving multiplex networks by generalizing the well-known Barabási-Albert-type model, to show how the co-evolution of network layers can induce and modulate the degree of correlated multiplexity.

Correlated multiplexity in random and co-evolving multiplex networks.

Supported in part by DTRA.

Cascades of overload failures in spatial networks.

supported by DTRA.

Cascades of failures in various models of interdependent networks.
9:12AM A54.00007 Robustness of a Network of Networks\textsuperscript{1}, JIANXI GAO\textsuperscript{2}, Boston University, SERGEY V. BULDYREV\textsuperscript{3}, Department of Physics, Yeshiva University, H. EUGENE STANLEY, Boston University, SHLOMO HAVLIN\textsuperscript{4}, Department of Physics, Bar-Ilan University, Israel — Network research has been focused on studying the properties of a single isolated network, which rarely exists. We develop a general analytical framework for studying percolation of $n$ interdependent networks. We illustrate our analytical solutions for three examples: (i) For any tree of $n$ fully dependent Erdős-Rényi (ER) networks, each of average degree $\bar{k}$, we find that the giant component $P_{\infty} = p\left[1-\exp(-pk_{\infty})\right]^{n}$ where $1-p$ is the initial fraction of removed nodes. This general result coincides for $n=1$ with the known second-order phase transition for a single network. For any $n > 1$ cascading failures occur and the percolation becomes an abrupt first-order transition. (ii) For a starlike network of $n$ partially interdependent ER networks, $P_{\infty}$ depends also on the topology—in contrast to case (i). (iii) For a looplike network formed by $n$ partially dependent ER networks, $P_{\infty}$ is independent of $n$.

\textsuperscript{1}We thank the DTRA (Defence Threat Reduction Agency) and the Office of Naval Research for support. 

\textsuperscript{2}JG also thanks (Grant No. 09J1408000) and (Grant No. 61004088) for support. 

\textsuperscript{3}SYB acknowledges the partial support of this research through the Dr. Bernard W. Gansin Computational Science Center at Yeshiva College. 

\textsuperscript{4}SH thanks the European EPIWORK project, Deutsche Forschungsgemeinschaft (DFG), and the Israel Science Foundation for financial support.

9:24AM A54.00008 Robustness of interdependent networks under targeted attack, XUQING HUANG, Center for Polymer Studies and Department of Physics, Boston University, JIANXI GAO, Department of Automation, Shanghai Jiao Tong University, SERGEY BULDYREV, Department of Physics, Yeshiva University, SHLOMO HAVLIN, Minerva Center and Department of Physics, Bar-Ilan University, H. EUGENE STANLEY, Center for Polymer Studies and Department of Physics, Boston University — When an initial failure of nodes occurs in interdependent networks, a cascade of failure between the networks occurs. Earlier studies focused on random initial failures. Here we study the robustness of interdependent networks under targeted attack on high or low degree nodes. We introduce a general technique which maps the targeted-attack problem in interdependent networks to the random-attack problem in a transformed pair of interdependent networks. We find that when the highly connected nodes are protected and have lower probability to fail, in contrast to single scale-free (SF) networks where the percolation threshold $p_c=0$, coupled SF networks are significantly more vulnerable with $p_c$ significantly larger than zero. The result implies that interdependent networks are difficult to defend by strategies such as protecting the high degree nodes that have been found useful to significantly improve robustness of single networks.

9:36AM A54.00009 Information Spreading in Context, DASHUN WANG, Center for Complex Network Research, Northeastern University, ZHEN WEN, HANGHANG TONG, CHING-YUNG LIN, IBM T.J. Watson Research Center, CHAOMING SONG, ALBERT-LASZLO BARABASI, Center for Complex Network Research, Northeastern University — Information spreading processes are central to human interactions. Despite recent studies in online domains, little is known about factors that could affect the dissemination of a single piece of information. In this paper, we address this challenge by combining two related but distinct datasets, collected from a large scale privacy-preserving distributed social sensor system. We find that the social and organizational context significantly impacts to whom and how fast people forward information. Yet the structures within spreading processes can be well captured by a simple stochastic branching model, indicating surprising independence of context. Our results build the foundation of future predictive models of information flow and provide significant insights towards design of communication platforms.

9:48AM A54.00010 Power-grid Network Partitioning and Cluster Optimization with Applications to Florida and Texas\textsuperscript{1}, PER ARNE RIKVOLD, IBRAHIM ABOU HAMAD, BRETT ISRAELS, Florida State University, SVETLANA V. POROSEVA, University of New Mexico — Cascading power-grid failures pose serious threats to lives and property, and it is desirable to contain them within a limited geographical area. One method to achieve this is Intentional Islanding (I3): the purposeful partitioning of a grid into weakly connected “islands” of closly connected generators and loads. If such islands can be quickly isolated, the spread of faults can be limited. An additional constraint is that generating capacity and power demand within each island should be closely balanced to ensure self-sufficiency. I3 thus corresponds to constrained community detection in a network. After a matrix-based initial agglomeration of nearby loads and generators, we implement Monte Carlo simulated annealing to simultaneously optimize load-balance and internal connectivity of the resulting islands. The optimized network of islands is treated as a new network with the first-generation islands as the new nodes (“supergenerators” and “superloads”), and the same agglomeration and MC procedures are iteratively applied, reminiscent of real-space renormalization. Applications to the Floridian [1] and Texan high-voltage grids are demonstrated.


\textsuperscript{1}Supported in part by NSF DMR-1104829.

10:00AM A54.00011 Computational Analysis of Topological Survivability of Large-Scale Engineering Networks with Heterogeneous Nodes, SVETLANA V. POROSEVA, Mechanical Engineering, University of New Mexico — The scale and complexity of modern networks, their integration, and the size of population and businesses they have impact on, make their massive damage catastrophic for the society and economy. Such damage is usually caused by adverse events and is not considered by traditional design practices. In the modern society, the likelihood of adverse events has substantially increased. Therefore, there is a need in evaluating the ability of a network to survive such damage. As the network topology is a key factor to consider, the goal of our research is to develop computational tools for quantifying its effect on the network survivability. “Selfish” algorithm will be presented that addresses computational complexity associated with the problem of generation and analysis of all fault combinations possible in a given network. The reduction of computational complexity is achieved by mapping an initial network topology with multiple sources and sinks onto a set of simpler smaller topologies with multiple sources and a single sink. Application to the Texas power grid will be considered.

10:12AM A54.00012 Cascading failures in interdependent lattice networks: from first order to second order phase transition\textsuperscript{1}, WEI LI, Center for Polymer Studies and Department of Physics, Boston University, Boston, MA 02215 USA, AMIR BASHAN, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel, SERGEY BULDYREV, Department of Physics, Yeshiva University, 500 West 185th Street, New York, New York 10033, USA, EUGENE STANLEY, Center for Polymer Studies and Department of Physics, Boston University, Boston, MA 02215 USA, SHLOMO HAVLIN, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel. — We study a system composed of two interdependent lattice networks A and B, where nodes in network A depend on a node within a certain shuffling distance $r$ of its corresponding counterpart in network B and vice versa. We find, using numerical simulation that percolation in the two interdependent lattice networks system shows that for small $r$ the phase transition is second order while for larger $r$ it is a first order.

\textsuperscript{1}We wish to thank DTRA for financial support and Dr. Robin Burk for encouraging discussions. We acknowledge the partial support of this research through the Dr. Bernard W. Gansin Computational Science Center at Yeshiva College.
10:24AM A54.00013 Cascading behaviors in random directed dependency networks1. YANQING HU, City College of New York, New City College of New York, New York, HERNAN MAKSE, City College of New York — Cascading behaviors have been studied only for some specific dependency network systems. In this paper, we present a more general and realistic network system with both random connectivity and directed dependency links. Using percolation approach, we obtain the universal boundaries among first order transition, second order transition and unstable regimes, which depend only on less than fourth moments of degree distribution and the fractions of zero and one directed dependency links. Moreover, besides the connectivity degree distribution, we also find the final state of dynamical cascading process is determined by out degree distribution of directed dependency links, and the in degree distribution only influence cascading speed.

1This work is partially supported by ONR, DFG, DTRA, EU project Epi- work and the Israel Science Foundation. Y. Hu is supported by NSF under Grant No. 60974084, 60534080.

10:36AM A54.00014 Loops in hierarchical channel networks1. ELENI KATIFORI, MARCELO MAGNASCO, Rockefeller University — Nature provides us with many examples of planar distribution and structural networks having dense sets of closed loops. An archetype of this form of network organization is the vasculature of dicotyledonous leaves, which shows a hierarchically-nested architecture. Although a number of methods have been proposed to measure aspects of the structure of such networks, a robust metric to quantify their hierarchical organization is still lacking. We present an algorithmic framework that allows mapping loop networks to binary trees, preserving in the connectivity of the trees the architecture of the original graph. We apply this framework to investigate computer generated and natural graphs extracted from digitized images of dicotyledonous leaves and animal vasculature. We calculate various metrics on the corresponding trees and discuss the relationship of these quantities to the architectural organization of the original graphs. This algorithmic framework decouples the geometric information from the metric topology (connectivity and edge weight) and it ultimately allows us to perform a quantitative statistical comparison between predictions of theoretical models and naturally occurring loop graphs.

1This work was supported in part by the NSF under Grant PHY-1058899.

Monday, February 27, 2012 11:15AM - 2:15PM
Session B51 DBIO GSNP: Focus Session: Evolutionary Systems Biology I - Evolutionary Dynamics and Rugged Fitness Landscapes

11:15AM B51.00001 Optimal lineage principle for age-structured populations. EDO KUSSELL, New York University — Populations whose individuals exhibit age-dependent growth have often been studied using temporal dynamics of age distributions. In this talk, I examine a new method that allows for the study of age-structured populations whose individuals exhibit age-dependent growth. The method provides a fundamental insight into evolutionary pressures on individuals’ aging profiles. I will describe a variational principle that enables exact results for lineage statistics, in a variety of models. I will also discuss measurements on continuously dividing bacterial populations growing in microfluidics devices.

11:51AM B51.00002 Why Do Complex Systems Age?. DERVIS VURAL, Harvard University and University of Illinois at Urbana Champaign, GREGORY MORRISON, L. MAHADEVAN, Harvard University — Aging can be defined as the increase in probability of death with time. The observation that organisms, colonies, ecosystems, as well as larger social structures age and die in very similar ways suggest that the reasons underlying aging do not depend sensitively on molecular or cellular details. In this work we argue that aging is an inevitable outcome of the neutral co-evolution of non-aging components which with time become increasingly interdependent. Starting from this hypothesis, we construct generic dependency networks and obtain mortality rate as a function of time, as well as mean life expectancy as a function of organism size, complexity and metabolic rate.

12:03PM B51.00003 Learning about evolution from sequence data. ADEL DAYARIAN, BORIS SHRAIMAN, KITP — Recent advances in sequencing and in laboratory evolution experiments have made possible to obtain quantitative data on genetic diversity of populations and on the dynamics of evolution. This dynamics is shaped by the interplay between selection acting on beneficial and deleterious mutations and recombination which reshuffles genotypes. Mounting evidence suggests that natural populations harbor extensive fitness diversity, yet most of the currently available tools for analyzing polymorphism data are based on the neutral theory. Our aim is to develop methods to analyze genomic data for populations in the presence of the above-mentioned factors which are not considered in Muller’s ratchet, mutation-recombination-selection balance and positive adaption rate — and revisit a number of observables considered in the nearly-neutral theory of evolution. In particular, we examine the coalescent structure in the presence of recombination and calculate quantities such as the distribution of the coalescent times along the genome, the distribution of haplotype block sizes and the correlation between ancestors of different loci along the genome. In addition, we characterize the probability and time of fixation of mutations as a function of their fitness effect.

12:15PM B51.00004 Population genetics inside a cell: Mutations and mitochondrial genome maintenance. SIDHARTHA GOYAL, Kavli Institute for Theoretical Physics, University of California Santa Barbara, DAN GOTTSCHLING, Fred Hutchinson Cancer Research Center — In realistic ecological and evolutionary systems natural selection acts on multiple levels, i.e. it acts on individuals as well as on collection of individuals. An understanding of evolutionary dynamics of such systems is limited in large part due to the lack of experimental systems that can challenge theoretical models. Mitochondrial genomes (mtDNA) are subjected to selection acting on cellular as well as organelle levels. It is well accepted that mtDNA in yeast Saccharomyces cerevisiae is unstable and can degrade over time scales comparable to yeast cell division time. We utilize a recent technology designed in Gottschling lab to extract DNA from populations of aged yeast cells and deep sequencing to characterize mtDNA variation in a population of young and old cells. In tandem, we developed a stochastic model that includes the essential features of mitochondrial biology that provides a null model for expected mtDNA variation. Overall, we find approximately 2% of the polymorphic loci that show significant increase in frequency as cells age providing direct evidence for organelle level selection. Such quantitative study of mtDNA dynamics is absolutely essential to understand the propagation of mtDNA mutations linked to a spectrum of age-related diseases in humans.

12:27PM B51.00005 Rare beneficial mutations can halt Muller’s ratchet. DANIEL BALICK, Physics Department, University of California, Santa Barbara, SIDHARTHA GOYAL, KITP, UCSB, ELIZABETH JERISON, Physics Department, Harvard University, RICHARD NEHER, MPI for Developmental Biology, Tubingen, BRISOR SHRAIMAN, KITP and Physics Department, UCSB, MICHAEL DESAI, Physics Department and OEB, Harvard University — In viral, bacterial, and other asexual populations, the vast majority of non-neutral mutations are deleterious. This motivates the application of models without beneficial mutations. Here we show that the presence of surprisingly few compensatory mutations halts fitness decay in these models. Production of deleterious mutations is balanced by purifying selection, stabilizing the fitness distribution. However, stochastic vanishing of fitness classes acts on multiple levels, i.e. it acts on individuals as well as on collection of individuals. An understanding of evolutionary dynamics of such systems is limited in large part due to the lack of experimental systems that can challenge theoretical models. Mitochondrial genomes (mtDNA) are subjected to selection acting on cellular as well as organelle levels. It is well accepted that mtDNA in yeast Saccharomyces cerevisiae is unstable and can degrade over time scales comparable to yeast cell division time. We utilize a recent technology designed in Gottschling lab to extract DNA from populations of aged yeast cells and deep sequencing to characterize mtDNA variation in a population of young and old cells. In tandem, we developed a stochastic model that includes the essential features of mitochondrial biology that provides a null model for expected mtDNA variation. Overall, we find approximately 2% of the polymorphic loci that show significant increase in frequency as cells age providing direct evidence for organelle level selection. Such quantitative study of mtDNA dynamics is absolutely essential to understand the propagation of mtDNA mutations linked to a spectrum of age-related diseases in humans.
These findings suggest that these generic indicators of critical slowing down can be useful in predicting catastrophic changes in population biology. Further, we test the utility of theoretically predicted warning signals by observing them in two different slowly deteriorating environments. We demonstrate the experimental observation of an increase in both the size and timescale of the fluctuations of population density near this sudden collapse. We argue that our principal finding that even analytically and numerically that, if the fitness landscape has a small highly epistatic (rough) and time-varying component, then the population genotype exhibits the naive prediction. We study genetic interactions in yeast cells by analyzing a publicly available database containing experimental growth rates of 5 million mutations and that the probability distribution of genetic interactions is a universal function. We further argue that the strength of genetic interactions depends on the ruggedness of fitness landscapes and the consequent evolutionary dynamics. Mutational pathways to drug resistance through a maximally-rugged fitness landscape, Adams Palmer, Erdal Toprak, Department of Systems Biology, Harvard Medical School, Boston, MA, USA — Natural populations must constantly adapt to the ever-changing environment. A fundamental question in evolutionary biology is whether adaptations can be reversed by returning the population to its ancestral environment. Traditionally, reverse evolution is defined as restoring an ancestral phenotype (physical characteristics such as body size), and the classic Dollo’s Law has hypothesized the impossibility of reversing complex adaptations. However, this “law” remains ambiguous unless reverse evolution can be studied at the level of genotypes (the underlying genome sequence). We measured the fitness landscapes of a bacterial antibiotic-resistance gene and analyzed the reversibility of evolution as a global, statistical feature of the landscapes. In both experiments and simulations, we find that an adaptation’s reversibility declines as the number of mutations it involves increases, suggesting a probabilistic form of Dollo’s Law at the molecular level. We also show computationally that slowly switching between environments facilitates reverse evolution in small populations, where clonal interference is negligible or moderate. This is an analog to thermodynamics, where the reversibility of a physical process is maximum when conditions are modified infinitely slowly. Clustering occurs not only in the case of assortative mating, but also in the case of asexual fission. Clustering is not observed in a control case where organisms can mate randomly. We find that the population size and the number of clusters undergo phase-transition-like behavior as the maximum mutation size is varied.

1:03PM B51.00008 Hidden Randomness between Fitness Landscapes Limits Reverse Evolution, LONGZHI TAN, STEPHEN SERENE, HUI XIAO CHAO, JEFF GORE, Massachusetts Institute of Technology — Natural populations must constantly adapt to the ever-changing environment. A fundamental question in evolutionary biology is whether adaptations can be reversed by returning the population to its ancestral environment. Traditionally, reverse evolution is defined as restoring an ancestral phenotype (physical characteristics such as body size), and the classic Dollo’s Law has hypothesized the impossibility of reversing complex adaptations. However, this “law” remains ambiguous unless reverse evolution can be studied at the level of genotypes (the underlying genome sequence). We measured the fitness landscapes of a bacterial antibiotic-resistance gene and analyzed the reversibility of evolution as a global, statistical feature of the landscapes. In both experiments and simulations, we find that an adaptation’s reversibility declines as the number of mutations it involves increases, suggesting a probabilistic form of Dollo’s Law at the molecular level. We also show computationally that slowly switching between environments facilitates reverse evolution in small populations, where clonal interference is negligible or moderate. This is an analog to thermodynamics, where the reversibility of a physical process is maximum when conditions are modified infinitely slowly.

1:15PM B51.00009 Exploring the fitness landscape of poliovirus, SIMONE BIANCO, ASHELY ACEVEDO, RAUL ANDINO, CHAO TANG, University of California San Francisco — RNA viruses are known to display extraordinary adaptation capabilities to different environments, due to high mutation rates. Their very dynamical evolution is captured by the quasispecies concept, according to which the viral population forms a swarm of genetic variants linked through mutation, which cooperatively interact at a functional level and collectively contribute to the characteristics of the population. The description of the viral fitness landscape becomes paramount towards a more thorough understanding of the virus evolution and spread. The high mutation rate, together with the cooperative nature of the quasispecies, makes it particularly challenging to explore its fitness landscape. I will present an investigation of the dynamical properties of poliovirus fitness landscape, through both the adoption of new experimental techniques and theoretical models.

1:27PM B51.00010 Scaling laws and universality for the strength of genetic interactions in yeast, ANDREA VELENICH, M.I.T., MINGJIE DAI, Harvard University, JEFF GORE, M.I.T. — Genetic interactions provide a window to the organization of the thousands of biochemical reactions in living cells. If two mutations affect unrelated cellular functions, the fitness effects of their combination can be easily predicted from the two separate fitness effects. However, because of interactions, for some pairs of mutations their combined fitness effect deviates from the naive prediction. We study genetic interactions in yeast by analyzing a publicly available database containing experimental growth rates of 5 million double mutants. We show that the characteristic strength of genetic interactions has a simple power law dependence on the fitness effects of the two interacting mutations and that the probability distribution of genetic interactions is a universal function. We further argue that the strength of genetic interactions depends only on the fitness effects of the interacting mutations and not on their biological origin in terms of single point mutations, entire gene knockouts or even more complicated physiological perturbations. Finally, we discuss the implications of the power law scaling of genetic interactions on the ruggedness of fitness landscapes and the consequent evolutionary dynamics.

1:39PM B51.00011 Speeding up Evolutionary Search by Small Fitness Fluctuations, JAKUB OTWINOWSKI, Department of Physics, Emory University, SORIN TANASE-NICOLA, Department for Cell and Molecular Biology, Uppsala University, ILYA NEMENMAN, Departments of Physics and Biology and Computational and Life Sciences Initiative, Emory University — We consider a fixed size population that undergoes a random walk on a neutral landscape. If the fitness landscape limits the evolutionary rate, we ask as a benchmark problem how far the population can go through the rugged landscape without a common tradeoff between growth and resistance. Empirical characterization of this fitness landscape has identified that ordered but sometimes indirect mutational pathways to multiple endpoints arises from near-maximal levels of sign epistasis.

1:51PM B51.00012 ABSTRACT HAS BEEN MOVED TO J42.00011 —

2:03PM B51.00013 Experimental observation of critical slowing down as an early warning of population collapse, DAAN VORSELEN, Department of Physics and Astronomy, VU University, Amsterdam, The Netherlands, LEI DAI, KIRILL KOROLEV, JEFF GORE, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — Near tipping points marking population collapse or other critical transitions in complex systems small changes in conditions can result in drastic shifts in the system state. In theoretical models it is known that early warning signals can be used to predict the approach of these tipping points (bifurcations), but little is known about how these signals can be detected in practice. Here we use the budding yeast Saccharomyces cerevisiae to study these early warning signals in controlled experimental populations. We grow yeast in the sugar sucrose, where cooperative feeding dynamics causes a fold bifurcation; falling below a critical population size results in sudden collapse. We demonstrate the experimental observation of an increase in both the size and timescale of the fluctuations of population density near this fold bifurcation. Furthermore, we test the utility of theoretically predicted warning signals by observing them in two different slowly deteriorating environments. These findings suggest that these generic indicators of critical slowing down can be useful in predicting catastrophic changes in population biology.
Simulations of Granular Particles Under Cyclic Shear, John Royer, Paul Chaikin, Center for Soft Matter Research, New York University — We perform molecular dynamics (MD) simulations of spherical grains subjected to cyclic, quasi-static shear in a 3D parallelepiped shear cell. This virtual shear cell is constructed out of rough, bumpy walls in order to minimize wall-induced ordering and has an open top surface to allow the packing to readily dilate or compact. Using a standard routine for MD simulations of frictional grains, we simulate over 1000 shear cycles, measuring grain displacements, the local packing density and changes in the contact network. Varying the shear amplitude and the friction coefficient between grains, we map out a phase diagram for the different types of behavior exhibited by these sheared grains. With low friction and high enough shear, the grains can spontaneously order into densely packed crystals. With low shear and increasing friction the packing remains disordered, yet the grains arrange themselves into configurations which exhibit limit cycles where all grains return to the same position after each full shear cycle. At higher shear and friction there is a transition to a diffusive state, where grains continue rearrange and move throughout the shear cell.

A Continuous Time Random Walk Description of Monodisperse, Hard-Sphere Colloids below the Ordering Transition, Jeremy Lechman, Flint Pierce, Sandia National Laboratories — Diffusive transport is a ubiquitous process that is typically understood in terms of a classical random walk of non-interacting particles. Here we present the results for a model of hard-sphere colloids in a Newtonian incompressible solvent at various volume fractions below the ordering transition (~50%). We numerically simulate the colloidal systems via Fast Lubrication Dynamics — a Brownian Dynamics approach with corrected mean-field hydrodynamic interactions. Colloid-colloid interactions are also included so that we effectively solve a system of interacting Langevin equations. The results of the simulations are analyzed in terms of the diffusion coefficient as a function of time with the early and late time diffusion coefficients comparing well with experimental results. An interpretation of the full time dependent behavior of the diffusion coefficient and mean-squared displacement is given in terms of a continuous time random walk. Therefore, the deterministic, continuum diffusion equation which arises from the discrete, interacting random walkers is presented. 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.

Shear failure of granular materials, Eric DeGiuli, Neil Balfmorth, Department of Mathematics, UBC, Jim McElwaine, DAMTP, University of Cambridge, Christian Schoof, Dept. Earth and Ocean Sciences, UBC, Ian Hewitt, Department of Mathematics, UBC — Connecting the macroscopic behavior of granular materials with the microstructure remains a great challenge. Recent work connects these scales with a discrete calculus [1]. In this work we generalize this formalism from monodisperse packings of disks to 2D assemblies of arbitrarily shaped grains. In particular, we derive Airy’s expression for a symmetric, divergence-free stress tensor. Using these tools, we derive, from first-principles and in a mean-field approximation, the entropy of frictional force configurations in the Force Network Ensemble. As a macroscopic consequence of the Coulomb friction condition at contacts, we predict shear failure at a critical shear stress, in accordance with the Mohr-Coulomb failure condition well known in engineering. Results are compared with numerical simulations, and the dependence on the microscopic geometric configuration is discussed.

A simple analytic theory for the statistics of avalanches in sheared granular materials, Karin Dahmen, University of Illinois at Urbana Champaign, Yehuda Ben-Zion, University of Southern California, Los Angeles, Jonathan Uhl, private — Slowly sheared granular materials at high packing fractions deform via slip avalanches with a broad range of sizes. Conventional continuum descriptions are not expected to apply to such highly inhomogeneous, intermittent deformations. Here, we show that it is possible to analytically compute the dynamics using a simple model that is inherently discrete. This model predicts quantities such as the avalanche size distribution, power spectra and temporal avalanche profiles as functions of the grain number fraction and the frictional weakening. A dynamical phase diagram emerges with quasi-static avalanches at high number fractions, and more regular, fluid-like flow at lower number fractions. The predictions agree with experiments and simulations for different granular materials, motivate future experiments and provide a fresh approach to data analysis. The simplicity of the model reveals quantitative connections to plasticity and earthquake statistics. (Reference: K.A. Dahmen, Y. Ben-Zion, J.T. Uhl, Nature Physics 7, 554-557 (2011)).

Simulation of 2D Granular Hopper Flow, Zhusong Li, Mark Shattuck, CUNY Graduate Center and the Benjamin Levich Institute and Physics Department of The City College of New York — Jamming and intermittent granular flow are big problems in industry, and the vertical hopper is a canonical example of these difficulties. We simulate gravity driven flow and jamming of 2D disks in a vertical hopper and compare with identical companion experiments presented in this session. We measure and compare the flow rate and probability for jamming as a function of particle properties and geometry. We evaluate the ability of standard Hertz-Mindlin contact mode to quantitatively predict the experimental flow. The simplicity of the model reveals quantitative connections to plasticity and earthquake statistics. (Reference: K.A. Dahmen, Y. Ben-Zion, J.T. Uhl, Nature Physics 7, 554-557 (2011)).

Forces on intruders in granular media, Ibar Delacruz, Stephan Koehler, WPI — We measure the forces acting on intruders moving in different directions in a granular medium consisting of mono-disperse spherical glass beads. We present the dependence of the drag force on the intruder’s geometry and surface roughness, bead size, dragging speed and immersion depth. We also determine the distribution of the forces on the intruder’s surfaces. We compare our results with lithostatic pressure (p = ρ gz).

2D Granular Impact Dynamics with Photoelastic Particles, Abe Clark, Duke University, LOU KONDIC, New Jersey Institute of Technology, R.P. Behringer, Duke University — What is the response of a granular material to a high speed impact from a foreign object? To answer this question, we use a large 2D granular system which is impacted from above by an intruder. Using photoelastic discs and a high-speed camera (frame rates at 7,000-775,000 fps at varied resolution, typically 40,000 fps at 504x256 pixels), we are able to observe the dynamics in this process in a way which has not been done previously. Data consists of the trajectory of the intruder, as well as either particle positions or interparticle force information. High frame rates allow observation of complex acoustic waves during the impact process. We examine the effects of varying the initial velocity, density, shape, and size of the intruder, with the goal of extracting the grain-scale mechanisms responsible for the dissipation of the intruder’s kinetic energy. In comparing our data to macroscopic frictional models used in past work, we observe good agreement with the low-frequency behavior in our experiments, but we also observe large high-frequency fluctuations in the acceleration which are inherently granular, and not captured by these models. The large fluctuations are well correlated to the emission of localized intermittent stress pulses, seen in the photoelastic response.

This work is supported by DTRA, grant HDTRA1-10-0021
Cooperative rotations of 2d frictional disks under oscillatory shear

Mitchell Mailman, Michelle Girvan, Wolfgang Losert, University of Maryland — We explore the dynamics of the contact network under cyclic shear, with a particular focus on cooperative rolling and sliding contacts, using a molecular dynamics (MD) simulation approach and external fixed pressure. We systematically study the formation and persistence of clusters of cooperatively rolling grains for a range of reversal amplitudes. The propensity for cooperative rotation dictates structural properties of the contact network; loop configurations of even numbers of grains are able to rotate without sliding, while odd numbers of grains must have at least one sliding contact. We report on the statistics of loop structures in the contact network, as well as their relationships to cooperatively rotating grains. Finally, we demonstrate a characteristic scale over which grains can cooperatively rotate as well as the dependence on friction parameters.

High-speed measurement of axial grain motion in a rotating drum

Frank van Bussem, Max Planck Institute for Dynamics and Self-Organization, Zeina Khan, Chemical Engineering, Texas Tech University, Marc Schaber, Ralf Seemann, Experimental Physics, Saarland University, Mario Scheel, Marco Dimchio, European Synchrotron Radiation Facility — Over short timescales granular mixtures separate by size when tumbled in a partially filled horizontal drum. The smaller grains move toward the axis of rotation to form a central core; undulations in this core gradually increase in amplitude until they grow into axial bands. Using non-invasive high-speed synchrotron x-ray particle tracking, we investigate the axial transport properties of tracer particles traveling amongst glass spheres. This new technique allows us to gather data on time scales not previously possible. When the tracers are present in larger proportions the mixtures we used should have different tendencies to segregate axially according to size ratio; one of our findings, however, is that when the tracer concentration is low the single-particle dynamics of these mixtures do not depend on the relative particle sizes in any appreciable way. This implies that the potential for a mixture to axially segregate cannot be inferred from the microscopic dynamics of individual small particles. A second finding is that while the slope of the mean-squared displacement is close to that expected from diffusive transport, as determined from the single-particle dynamics, more detailed analyses indicate anomalous transport.

Supported by an Undergraduate Research Grant from Penn State Erie, The Behrend College.

Ordered and disordered granular sphere packings obtained by epitaxial growth

Andreea Panaitescu, Arshad Kudrolli, Clark University — We study granular packings obtained by depositing spheres on a substrate under the influence of gravity. By exploiting the direct particle tracking enabled by X-ray tomography, the nature of the order and disorder is investigated using statistical measures including density pair correlation function, and the orientational order parameter. We find that by using a low deposition rate, impinging particles with sufficient energy can overcome friction and come to rest in a potential minimum of a periodic substrate, giving rise to ordered face-centered cubic structures. However, impinging particles with large kinetic energy can dislodge particles in the substrate leading to disorder as mobile particles cooperatively form arches while they come to rest. Thus, a wide range of volume fractions and packing structures is accessed by simply controlling the nature of the substrate and deposition rate and energy, along with the shape of the impinging particles. We contrast the ordered and disordered phases observed as a function of packing fraction with our previous study with cyclically sheared packings. We illustrate the nature of this bifurcation using numerical simulations and experiments.

Supported by an Undergraduate Research Grant from Penn State Erie, The Behrend College.

Tunable acoustic switching and rectification in one-dimensional granular crystals

Nicholas Boechler, Massachusetts Institute of Technology, Georgios Theocaris, Chiara Daraio, California Institute of Technology — We study a new mechanism for tunable acoustic switching and rectification, which we experimentally demonstrate in a one-dimensional granular crystal. The granular crystal is composed of an array of statically compressed elastic spherical particles that interact nonlinearly via Hertzian contact. The granular crystal is uniform except for a single light-mass defect placed near one boundary of the crystal. Because of the interplay of the periodicity, nonlinearity, dissipation, and asymmetry of the granular crystal, vibrations applied near the defect position cause the system response to bifurcate from periodic non-transmitting states to periodic transmitting states with broadband frequency content. We illustrate the nature of this bifurcation using numerical simulations and compare these results to experimental observations. Because the bifurcation causes a sharp transition between states, this mechanism can lead to phononic switching and sensing. Furthermore, as switches and rectification devices are fundamental components used for controlling the flow of energy in numerous applications, we envision that this mechanism could more generally enable the design of advanced photonic, thermal, and acoustic materials and devices.

Granular compaction under confinement

Nathan Mueggenburg, Lake Forest College — A granular pack that is vertically vibrated undergoes rearrangements and often progresses to more dense configurations. The experiments presented here study the role of dilation in this granular compaction process. By applying a confining force to the granular pack during vibration, the dilation is inhibited and the compaction process is significantly reduced. In general, systems with different accelerations during vibration will compact differently. However, these systems will compact in the same manner if the confining force is tuned to result in the same amount of dilation. Under large confining forces, there is very little dilation. In this regime, the compaction is significantly slowed and may approach a steady state packing fraction of approximately 0.60, consistent with ideas of a critical packing fraction for the onset of dilation.

Densest columnar structures of hard spheres from sequential deposition

Ho-Kei Chan, Foams & Complex Systems, School of Physics, Trinity College Dublin, Ireland, Aberystwyth University Collaboration — The rich variety of densest columnar structures of identical hard spheres inside a cylinder can surprisingly be constructed from a simple and computationally fast sequential deposition of cylinder-touching spheres, if the cylinder-to-sphere diameter ratio D is within [1.2,7013]. This provides a direction for theoretically deriving all these densest structures and for constructing such densest packings with nano-, micro-, colloidal or charged particles, which all self-assemble like hard spheres [Rapid Communication, Physical Review E (in press)].

Funded by IRCSET
heterogeneities proportional to those for the dynamical heterogeneity, while the correlation volumes for the longitudinal fluctuations remain small and approximately constant.

We perform our test on data obtained in simulations of four postulated time-fluctuation soft modes, and a longitudinal component, which is unrelated to them. We illustrate our results with granular materials. In particular, we show how Newton’s laws for a single grain reproduce their continuum equivalent in the calculus. This allows introduction of a discrete Airy stress function, exactly as in the continuum. As an application of the formalism, we show how these results give the natural mean-field variation of discrete quantities, in agreement with numerical simulations. The discrete calculus thus acts as a bridge between discrete microscale quantities and continuous macroscale quantities.


11:15AM B53.00001 Nanoscale dynamics of binary metallic glass Cu$_2$Hf$_{1−x}$Hf$_x$ films$^1$. JACOB BURGESS, University of Alberta Department of Physics, National Institute for Nanotechnology, CHRIS HOLT, University of Alberta Department of Chemical and Materials Engineering, National Institute for Nanotechnology, DAVID FORTIN, GREG POPÓWICH, University of Alberta Department of Physics, ERIK LUBER, DAVID MITLIN, University of Alberta Department of Chemical and Materials Engineering, National Institute for Nanotechnology, MARK FREEMAN, University of Alberta Department of Physics, National Institute for Nanotechnology — Scanning probe microscopy provides a valuable tool for investigating nanoscale structure of thin films. Less commonly it can be applied to study the low speed dynamical behavior of these systems as well. Presented here are scanning tunneling microscope investigations of sputtered glass Cu$_2$Hf$_{1−x}$Hf$_x$ films which reveal the nanocrystalline structure of the films as well as hopping dynamics of crystal clusters on the surface. A correction for limited bandwidth and a range of activation energies is developed in the context of an Arrhenius process to allow extraction of the average energy barrier for cluster hopping. Concentration of the component metals in the films was varied allowing observation of the change in cluster size as well as the transition to the amorphous state. A second form of dynamics, more diffusive in character, was found for amorphous samples.

$^1$This work was supported by NSERC, CIFAR, NRC, Alberta Innovates, and CRC

11:27AM B53.00002 Isothermal Pressurizations and Glass Transition Dynamics in the Intermediate Glass-Forming Liquid Glycerol$.^1$, WILLIAM OLIVER, University of Arkansas, Department of Physics, TITUS MORRIS, Michigan State University, Department of Physics and Astronomy, TIM RANSOM, University of Arkansas, Department of Physics — Brillouin scattering data along both a 75 °C and 100 °C isotherm to pressures as high 6 GPa are reported for glycerol an intermediate strength glass forming liquid. This represents the highest pressure data of any type reported for glycerol, and enables us to probe directly the alpha relaxation process at these high pressures. Acoustic mode frequencies and linewidths are obtained from fits to the spectra. These frequency shifts and linewidths are fit for each isotherm with an iterative technique in which parameters are adjusted until self consistency is obtained. The Tait equation of state along with a complex expression for the dynamical longitudinal modulus, $M(\omega)$, and quantitative models for other physical quantities such as the adiabatic index are used in our analysis. A Cole-Davidson function is used to model the dynamical modulus, and self-consistent fits indicate that the stretching parameter, $\beta$, is pressure independent with a value of 0.37 consistent with other low pressure acoustic results in the literature. Final values for the pressure dependent dynamical longitudinal modulus and relaxation time are obtained. In contrast to the results of recent pressure-dependent dielectric studies, there does not appear to be a second process that obscures the alpha process.

$^1$We gratefully acknowledge support from the NSF under grant NO.: DMR-0552944

11:39AM B53.00003 Fast Scanning Calorimetry study of non-equilibrium relaxation in 2-Ethyl-1-Hexanol$^1$, VLAD SADTCHENKO, DEEPAK BHATTACHARYA, The George Washington University, Department of Chemistry, CANDACE PAN, The University of Aberdeen — Fast scanning calorimetry (FSC), capable of heating rates in excess of 1000000 K/s, was combined with vapor deposition technique to investigate non-equilibrium relaxation in micrometer thick ultraviscous of 2-Ethyl-1-Hexanol (2E1H) films under high vacuum conditions. Rapid heating of 2E1H samples prepared at temperatures above approximately 145 K (standard glass transition temperature of 2E1H, Tgs), resulted in well manifested dynamic glass transitions at temperatures tens of degrees higher than Tgs. Furthermore, strong and complex dependence of dynamic glass transition temperature on the sample’s initial state, i.e., the starting temperature of FSC scan was also observed. We discuss implications of these results for contemporary models of non-equilibrium relaxation in glasses and supercooled liquids.

$^1$Supported by National Science Foundation grant 1012692.

11:51AM B53.00004 Fluctuating Relaxation Times in Glass-forming Liquids, GCINA A. MAVIMBELA, HORACIO E. CASTILLO, Department of Physics and Astronomy, Ohio University, Athens OH, AZITA PARSAEIAN, Materials Research Center, Northwestern University, Evanston IL — The presence of fluctuating local relaxation times, $\tau(\vec{r}, t)$ has been used for some time as a conceptual tool to describe dynamical heterogeneities $^\text{[?]}$. Here we report on a new method for determining the local phase field, $\phi(\vec{r}, t)$ $\equiv \int \frac{dt}{\tau(\vec{r}, t)}$ from snapshots $\{\vec{r}(t), t\}_{i=1...M}$ of the positions of the particles in a system, and we apply it to extract $\phi(\vec{r}, t)$ from simulations of glass forming models. By studying how the phase field depends on the number of snapshots, we find that it is a well defined quantity. By studying fluctuations of the phase field, we find that they describe heterogeneities well at long distance scales. We also determine how the stretching exponent $\beta$ depends on the coarse graining volume, in order to test the hypothesis that relaxation in small regions is exponential and it only becomes non-exponential when considering large regions of the system.


12:03PM B53.00005 Mapping dynamical heterogeneity in structural glasses to correlated fluctuations of the time variables, KARINA E. AVILA, HORACIO E. CASTILLO, Ohio University, AZITA PARSAEIAN, Northwestern University — Dynamical heterogeneity is believed to play an important role in the dynamical behavior of slowly relaxing disordered materials. In this work, we test one hypothesis for its origin, namely that it emerges from soft (Goldstone) modes associated with a broken continuous symmetry under time reparametrizations. We do this by constructing coarse grained observables and decomposing the fluctuations of these observables into transverse components, which is associated with the postulated time-fluctuation soft modes, and a longitudinal component, which is unrelated to them. We perform our test on data obtained in simulations of four models of structural glasses. We find that as time is lowered and timescales are increased, the time reparametrization fluctuations become increasingly dominant. In particular, the ratio between the strengths of the transverse fluctuations and the longitudinal fluctuations grows as a function of the dynamical susceptibility $\chi_4$, which represents the strength of the dynamical heterogeneity; and the correlation volumes for the transverse fluctuations are approximately proportional to those for the dynamical heterogeneity, while the correlation volumes for the longitudinal fluctuations remain small and approximately constant.
12:15PM B53.00006 High Pressure Brillouin Scattering in the Fragile Glass Former Cumene1.
TIM RANSOM, WILLIAM OLIVER, University of Arkansas — In recent years full-spectrum analysis in light-scattering has been utilized to explore the liquid-glass transition at variable temperature and ambient pressure. In this study we present temperature- and pressure-dependent Brillouin scattering results for the fragile glass-former cumene. Both equal-angle forward scattering and depolarized backscattering geometries are used, and high pressures are attained by the use of a diamond anvil cell mounted in a custom temperature-controlled housing. Opening up the variable pressure regime to full-spectrum analysis will allow more stringent tests of mode-coupling theory as well as greater insight into the behavior of glass-forming systems.

1We gratefully acknowledge support from NSF under grant NO: DMR-0552944

12:27PM B53.00007 Molecular modeling of ultra-stable vapor deposited glasses, SADANAND SINGH, DEVIN AVERETT, CHI-CHENG CHIUI, JUAN J. DE PABLO, University of Wisconsin-Madison — Recent studies have shown that physical vapor deposition can be used to prepare glasses of small organic molecules with remarkably high kinetic stability and low enthalpy, particularly when compared to ordinary glasses prepared by cooling the supercooled liquid. The thermophysical properties of these new ultra-stable glasses are equivalent to those of common glasses after thousands of years of aging. However, experimental studies have so far been limited to relatively few types of molecules. We propose a molecular modeling scheme to prepare stable glasses that mimics the experimental procedure of vapor deposition. For simple disaccharides, such as trehalose, the thermophysical properties of our simulated glasses are consistent with those measured experimentally. We also prepare stable glasses of trehalose and glycero1 mixture, which are of interest for their use in stabilization of biomolecules in the glass state. Results for model binary Lennard-Jones glasses, which have been studied extensively in the literature, are also discussed. We find that the most stable glasses formed by vapor deposition are equivalent to ordinary glasses formed by cooling at a rate approximately 10 orders of magnitude slower than those accessible by ordinary cooling methods.

12:39PM B53.00008 Dynamic heterogeneity above and below the mode-coupling temperature, ELLIJA FLENNER, GRZEGORZ SZAMEL, Chemistry Department, Colorado State University — We study the temperature dependence of the spatial extent of the dynamic heterogeneity in a soft sphere system near the so-called mode-coupling temperature $T_c$. Utilizing a recently introduced procedure to calculate the ensemble independent dynamic susceptibility $\chi(t_{\alpha})$ and the dynamic correlation length $\xi(t_{\alpha})$ at the alpha relaxation time $t_{\alpha}$. Above $T_c$, we find that $\chi(t_{\alpha}) \sim \xi(t_{\alpha})^3$ and $\xi(t_{\alpha}) \sim \ln(t_{\alpha})$, which is the same behavior found in a binary hard-sphere system. We track these relationships below $T_c$ to examine the recently reported non-monotonic temperature dependence of dynamic correlations found in the same system. Finally, we examine the relationship between dynamic susceptibilities that can be determined from experiments and the dynamic correlation length $\xi(t_{\alpha})$.

2W. Kob, S. Roland-Vargas and L. Berthier, Nat. Phys. DOI:10.1038/NPHYS2133

12:51PM B53.00009 Fast Scanning Calorimetry studies of glassy and supercooled water1.
DEEPAK BHATTACHARYA, The George Washington University, CANDACE PAYNE, The University of Aberdeen, VLAD SADTCHENKO, The George Washington University — Despite intense efforts, development of a comprehensive system of relationships between various condensed phases of water remains an illusive goal. The lack of consensus on the nature of supercooled and glassy water is due primarily to the lack of kinetic and thermodynamic data at temperatures from 150 to 235 K. Because supercooled water undergoes rapid crystallization near 235 K, application of standard experimental methods is virtually impossible. With the objective of gaining insights into properties of water, we have developed an experimental approach which relies on rapid (100000 K/s) heating of micro- and mesoscopic aqueous samples prepared by vapor deposition in vacuum at cryogenic temperatures. Due to high heating rates, this Fast Scanning Calorimetry approach, makes it possible to bypass crystallization and to obtain new data on molecular kinetics and thermodynamics in glassy water in previously inaccessible temperature interval. We will report the results of our FSC studies and discuss their impact on fundamental and applied research areas where glassy and supercooled water plays significant role.

1Supported by National Science Foundation Grant 1012692

1:03PM B53.00010 Volume and structural analysis of super-cooled water under high pressure
SOLOMON F. DUKI1, Department of Physics and Astronomy, Rowan University, 201 Mullica Hill Road, Glassboro, NJ 08028-1701, MESFIN TSIGE2, Department of Polymer Science, Goodyear Polymer Center 1021, The University of Akron, Akron, OH 44325-3909 — Motivated by recent experimental study of super-cooled water at high pressure [1], we performed atomistic molecular dynamic simulations study on bulk water molecules at isothermal-isobaric ensemble. These simulations are performed at temperatures that range from 40 K to 380 K using two different cooling rates, 10K/ns and 10K/5ns, and pressure that ranges from 1atm to 10000 atm. Our analysis for the variation of the volume of the bulk sample against temperature indicates a downward concave shape for pressures above certain values, as reported in [1]. The same downward concave behavior is observed at high pressure on the mean-squared-displacements (MSD) of the water molecules when the MSD is plotted against time. To get further insight on the effect of the pressure on the sample we have also performed a structural analysis of the sample.

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1:15PM B53.00011 A field theory approach to the dynamics of classical particles, DAVID MCCOWAN, GENE MAZENKO, University of Chicago — For nearly 30 years, mode-coupling theory (MCT) has been regarded as the de facto theoretical description of dense fluids and the transition from the fluid to glassy state. But MCT is limited by its ad hoc construction and lacks a mechanism to institute corrections. We present a new fundamental theory for the kinetics of systems of classical particles which represents a unification of kinetic theory, Brownian motion and field theory. It is developed from first principles via a self-consistent perturbation in terms of an effective two-body potential, and we use this theory to investigate the existence of ergodic-nonergodic (ENE) transitions near the liquid-glass transition. After a brief introduction of the theory, we will address the development of a kinetic equation of the memory function form. The memory function kernel (or self-energy) determined by the theory shares properties with the MCT form, however our theory provides the crucial advantage of well-defined, perturbative corrections.

1:27PM B53.00012 N.Q.R measurements of low energy Chiral structures in powdered glassy As$_2$Se$_3$, CHRIS NELSON, A.P.S — Experimental and theoretical work on the As-chalcogen glasses have shown that in the glassy state the local cylindrical symmetry associated with the elemental pyramidal unit is preserved. Here we introduce a local paracrystalline model of glassy As$_2$Se$_3$. This model is based on a tight binding calculation of the electric field gradient (EFG) at the core of an As atom located at the apex of the pyramidal structure. This EFG is shown to be hyper sensitive to the bond angles and bond lengths the As atom forms with the chalcogen nearest neighbors, as well as the hybrid angle formed with second neighbor As atoms. A continuous variation of the bonding parameters produces a unique set of these pyramidal units which are shown to fit the NQR data for powdered glassy samples. The best fit to the NQR data indicates that the pyramidal units organize themselves into Chiral structures in the glass. A plot of the electronic energy per molecular site shows that the chiral structures have on average a lower electronic energy than a random configuration.
1:39PM B53.00013 Slow relaxations in glasses: full aging and beyond. YOSEPH IMRY, The Weizmann Institute of Science, ARIEL AMIR, Harvard University, YUVAL OREC, The Weizmann Institute of Science, STEFANO BORINI, INRIM, Torino — Experiments performed in the last years demonstrated slow relaxations and aging in the conductance of a large variety of materials. Here, we present experimental and theoretical results for conductance relaxations and aging for the case-study example of porous silicon. The relaxations are experimentally observed even at room temperature over time scales of hours, and when a strong electric field is applied for a time $t_w$, the ensuing relaxation depends on $t_w$. We derive a theoretical curve and show that experimental data collapse on it with a single time scale as a fitting parameter. This time scale is found to be of the order of thousands of seconds at room temperature. The generic theory suggested is not fine-tuned to porous silicon, and thus we believe the results should be universal, and the presented method should be applicable for many other systems manifesting memory and other glassy effects. Reference: Phys. Rev. Lett. 107, 186407 (2011)

1:51PM B53.00014 Voids and molecular hydrogen in hydrogenated amorphous silicon. RAJENDRA TIMILSINA, PARTHAPRATIM BISWAS, The University of Southern Mississippi — Nuclear magnetic resonance (NMR) and Infrared (IR) spectroscopy experiments show that hydrogen microstructure consists of clustered and diluted hydrogen atoms as well as voids and hydrogen molecules in hydrogenated amorphous silicon. Several theoretical studies have also attempted that whether the microstructure incorporates voids and hydrogen molecules or not, by introducing hydrogen atoms within single-clustered hydrogenated amorphous silicon. However, up until now, has conclusively demonstrated that the voids and molecular hydrogen are built-in features of the microstructure. We generate several realistic models of hydrogenated amorphous silicon at different hydrogen concentrations by developing an information-based inverse method. The models not only satisfy structural and electronic properties but also provide correct NMR line spectra as compare to NMR experiments. The microstructure at high ($>15\%$) hydrogen concentration shows the presence of voids and some hydrogen molecules within the voids. The voids with molecular hydrogen are built-in microstructures because they evolve themselves while relaxing the models via the first-principles density functional method.

2:03PM B53.00015 Structural and microscopic relaxations in glycerol: an IXS study. ALESSANDRO CUNSOLO, Brookhaven National Laboratory — We present an Inelastic X Ray Scattering study of the THz dynamics of room temperature glycerol at pressures spanning the 0.66-3 Kbar range. We propose a comparison with ultrasound absorption results available in literature, which leads to infer the presence of two distinct relaxation phenomena, a slow and a fast one. Although the former relaxation has been thoroughly studied in glycerol by lower frequency spectroscopic techniques, no experimental evidences of the latter were so far reported in literature. A line-shape modeling based upon the memory function formalism allows us to observe that the characteristic timescale of the fast relaxation ranges in the sub-picosecond, tends to decrease with increasing the wave-vector and is rather insensitive to pressure changes. More in general, the observed phenomenology definitely reveals the microscopic, single particle, nature of this addition relaxation process.

Monday, February 27, 2012 11:15AM - 2:15PM — Session B54 GSNP: Focus Session: Complex and co-evolving networks - Modeling Social and Biological Networks 152

11:15AM B54.00001 Human travel and time spent at destination: impact on the epidemic invasion dynamics. CHIARA POLETTI, MICHELE TIZZONI, ISI Foundation, Turin, Italy, VITTORIA COLIZZA, INSERM and Univ Pierre et Marie Curie, UMR-S 707, Paris, France — Human mobility has a strong impact on the spatial spread of infectious diseases. Analyses of metapopulation models, that consider the epidemic spreading on a network of populations, show that topological and traffic fluctuations favor the global epidemic invasion. These studies consider markovian mobility (i.e. the memory of the origin of traveling individuals is lost) or non-markovian mobility with homogeneous timescales (i.e. individuals travel to a destination and come back with a homogenous rate). However, the time spent at destination is found to exhibit wide fluctuations. Such varying length of stay crucially affects the mixing among individuals and hence the disease transmission dynamics. In order to explore this aspect, we present a modeling framework that, by using a time-scale separation technique, allows analyzing the behavior of spreading processes on a complex metapopulation network with non-markovian mobility characterized by heterogeneous distributed timescales. Analytical and numerical results show how the degree of heterogeneity of the length of stay is able, alone, to drive a phase transition between local outbreak and global invasion. This highlights the importance of the interplay between mobility and disease timescales in the propagation of an epidemic.

11:27AM B54.00002 Effect of Spatial-Dependent Utility on Social Group Domination. NATHANIEL RODRIGUEZ, ANDREW MEYERTOLEN, University of Redlands — The mathematical modeling of social group competition has garnered much attention. We consider a model originated by Abrams and Strogatz [Nature 424, 900 (2003)] that predicts the extinction of one of two social groups. This model assigns a utility to each social group, which is constant over the entire society. We find by allowing this utility to vary over a society, through the introduction of a network or spatial dependence, this model may result in the coexistence of the two social groups.

11:39AM B54.00003 Evolution of opinions on social networks in the presence of competing committed groups. SAMEET SREENIVASAN, Dept. of Computer Science, Dept. of Physics, Rensselaer Polytechnic Institute, JIERUI XIE, BOLESŁAW SZYMŃSKI, Dept. of Computer Science, Rensselaer Polytechnic Institute, JEFF EMMENHEISER, MATT KIRBY, GYORGY KORNISZ, Dept. of Physics, Rensselaer Polytechnic Institute — Using a model of pairwise social influence, the binary agreement model (Xie et. al, Phys. Rev. E 84, 011130 (2011)), we study how the presence of two groups committed to competing opinions affect the steady-state opinion of influential individuals on a social network. We assume that two groups committed to distinct opinions $A$ and $B$, and constituting fractions $p_A$, $p_B$ of the total population respectively, are present in the network. We show using mean-field theory that the phase diagram of this system in parameter space $(p_A, p_B)$ consists of two regions, one where two stable steady-states coexist, and the remaining where only a single stable steady-state exists. For finite networks (complete graphs, Erdős-Rényi networks and Barabási-Albert networks), these two regions are separated by three first order transition lines which terminate and meet tangentially at $p_A = p_B \approx 0.1623$, which constitutes a second-order transition point. Firstly, we quantify how the exponentially large switching times between steady states in the coexistence region depend on the distance from the second-order transition point for equal committed fractions.

11:51AM B54.00004 Strategy of Competition between Two Groups based on an Inflexible Contrarian Opinion Model. QIAN LI, Boston University, LIDIA BRAUNSTEIN, Universial Nacional de Mar del Plate-CONICET, SHLOMO HAVLIN, Bar Ilan University, GENE STANLEY, Boston University — We introduce an inflexible contrarian opinion (ICO) model in which a fraction $p$ of inflexible contrarians within a group holds a strong opinion opposite to the opinion held by the rest of the group. At the initial stage, stable clusters of two opinions, A and B exist. Then we introduce inflexible contrarians which hold a strong B opinion into the opinion A group. Through their interactions, the inflexible contrarians are able to decrease the size of the largest A opinion cluster, and even destroy it. We see this kind of method in operation, when companies send free new products to potential customers in order to convince them to adopt their product and influence others to buy it. We study the ICO model, using two different strategies, on both ER and SF networks. In strategy I, the inflexible contrarians are positioned at random. In strategy II, the inflexible contrarians are chosen to be the highest degrees nodes. We find that for both strategies the size of the largest A cluster decreases to zero as $p$ increases as in a phase transition. At a critical threshold value $p_c$, the system undergoes a second-order phase transition that belongs to the same universality class of mean field percolation. We find that even for an ER type model, strategy II is significantly more effective.
12:03PM B54.00005 Consensus in evolving networks of mobile agents, ANDREA BARONCHIELLI, Universitat Politecnica de Catalunya, ALBERT DÍAZ-GUILERA, Universitat de Barcelona — Populations of mobile and communicating agents describe a vast array of technological and natural systems, ranging from sensor networks to animal groups. Here, we investigate how a group-level agreement may emerge in the continuously evolving networks defined by the local interactions of the moving individuals. We adopt a general scheme of motion in two dimensions and we let the individuals interact through the minimal naming game, a prototypical scheme to investigate social consensus. We distinguish different regimes of convergence determined by the emission range of the agents and by their mobility, and we identify the corresponding scaling behaviors of the consensus time. In the same way, we rationalize also the behavior of the maximum memory used during the convergence process, which determines the minimum cognitive/storage capacity needed by the individuals. Overall, we believe that the simple and general model presented in this talk can represent a helpful reference for a better understanding of the behavior of populations of mobile agents.

12:15PM B54.00006 Epidemic and information co-spreading in adaptive social networks, YUNHAN LONG, The College of William and Mary, THILO GROSS COLLABORATION, LEAH B. SHAW TEAM — We model simultaneous evolution of an epidemic and information about the epidemic on an adaptive social network. The classical Susceptible-Infected-Susceptible (SIS) model is extended. Susceptible and infectious nodes are each divided into informed and uninformed types. Informed nodes affect the network structure by rewiring their network connections adaptively to avoid disease exposure. The effects of mass media influence and communication on the disease spreading and network structure are explored, and stochastic simulations are compared with a moment closure approximation. When the rewiring rate is high, the infection and information levels of the population show periodic oscillations for certain ranges of contact rate, and the moment closure approximation predicts similar dynamics. The epidemic threshold in the presence of rewiring and information is considered. Our results indicate that information can play a significant role in minimizing disease spread.

12:27PM B54.00007 Asymptotically inspired moment-closure approximation for adaptive networks, MAXIM SHKARAYEV, LEAH SHAW, College of William and Mary — Adaptive social networks, in which nodes and network structure co-evolve, are often described using a mean-field system of equations for the density of node and link types. These equations constitute an open system due to dependence on higher order topological structures. We propose a moment-closure approximation based on a reduced analytical description of the system in an asymptotic regime. We apply our approach to two examples of adaptive networks: recruitment to a cause model and epidemic spread model. We show a good agreement between the improved mean-field prediction and simulations of the full network system.

12:39PM B54.00008 Epidemics on Interacting Networks, MARK DICKISON, Boston University, SHLOMO HAVLIN, Bar-Ilan University, H.E. STANLEY, Boston University — Epidemic spreading is of great importance in public health, as well as in related fields such as infrastructure. While complex network models have been used with great success to analyze epidemic behavior on single networks, the reality is that our world is made up of a system of interacting networks that do not necessarily share common characteristics. I introduce a model for constructing interacting networks and show that the phase transition depends on the parameters \(\kappa_T, \kappa_{\text{A}},\) \(\kappa_B\), \(\kappa_{\text{A}},\) and \(\kappa_B\) are over the networks considered individually, with no internetwork links. For strongly interacting networks \((\kappa_T > \kappa_{\text{A}} + \kappa_{\text{B}})\), there exists only one phase transition, between a disease-free phase and an epidemic phase across both networks. For weakly interacting networks \((\kappa_T < \kappa_{\text{A}} \text{ or } \kappa_B)\), a third, “mixed,” phase exists, where the disease enters an epidemic on one network alone. The analytic predictions are confirmed by Monte-Carlo simulations.

12:51PM B54.00009 Epidemic spreading on interacting networks with preferred degrees, SHIVAKUMAR JOLAD, R.K.P. ZIA, B. SCHMITTMANN, Virginia Tech — We discuss the SIS contact process on a network of two interacting communities, each with its own preferred degree of connections. Postulating various rules for an individuals to form intra-community and inter-community links, we find novel stationary (active) states, in addition to the absorbed absorbing states. The dynamics of infected individuals in the two communities can be quite different. Using Monte Carlo techniques, we explore the effects on both the network structure and the contact process due to different types of interactions between the communities. We will also present a mean field analysis of contact processes on a generic interacting communities and compare these results with the simulation data.

1 Supported in part by NSF DMR-1005417 and ICTAS- Virginia Tech.

1:03PM B54.00010 Scaling theory of human dynamics and network science, CHAOMING SONG, DASHUN WANG, ALBERT-LASZLO BARABÁSI, Center for Complex Network Research, Northeastern University — The increasing availability of large-scale real data has fueled simultaneous advances in network theory, aiming to characterize the scaling of complex networks, and human dynamics, capturing the temporal characteristics of human activity patterns. Yet, these two areas remain disjoint, with their separate scaling laws and modeling framework. Here we show that the exponents characterizing the degree and link weight distribution of the underlying social network can be expressed in terms of the dynamical exponents characterizing human activity patterns, establishing the first formal link between the two areas.

1:15PM B54.00011 Network model explains why cancer cells use inefficient pathway to produce energy, JOO SANG LEE, Department of Physics and Astronomy, Northwestern University, JOHN MARKO, Department of Molecular Biosciences, Northwestern University, ADILSON MOTTER, Department of Physics and Astronomy, Northwestern University — The Warburg effect—the use of the energetically inefficient fermentative pathway as opposed to (energetically efficient) respiration even in the presence of oxygen—is a common property of cancer metabolism. Here, we propose that the Warburg effect is in fact a consequence of a trade-off between the benefit of rapid growth and the cost for protein synthesis. Using genome-scale metabolic network, we modeled the cellular resources for protein synthesis as a growth defect that increases with enzyme concentration. Based on our model, we demonstrate that the cost of protein production during rapid growth drives the cell to rely on fermentation to produce ATP. We also predict a critical link between extensive fermentation and rapid biosynthesis. Our results emphasize the importance of protein synthesis as a limiting factor on cell proliferation and provide a novel mathematical framework to analyze cancer metabolism.

1:27PM B54.00012 Physiological Networks: towards systems physiology, RONNY P. BARTSCH, Harvard Medical School and Division of Sleep Medicine, Brigham and Womens Hospital, Boston, MA 02115, USA, AMIR BASHAN, Department of Physics, Bar-Ilan University, Ramat-Gan, Israel, JAN W. KANTHELHARDT, Institute of Physics, Martin-Luther-Universitaet Halle-Wittenberg, Halle (Saale), Germany, SHLOMO HAVLIN, Department of Physics, Bar-Ilan University, Ramat-Gan, Israel, PLAMEN CH. IVANOV, Harvard Medical School and Division of Sleep Medicine, Brigham and Womens Hospital, Boston, MA 02115, USA — The human organism is an integrated network where complex physiological systems, each with its own regulatory mechanisms, continuously interact, and where failure of one system can trigger a breakdown of the entire network. Identifying and quantifying dynamical networks of diverse systems with different types of interactions is a challenge. Here, we develop a framework to probe interactions among diverse systems, and we identify a physiological network. We find that each physiological state is characterized by a specific network structure, demonstrating a robust dynamical networks of diverse systems with different types of interactions is a challenge. Here, we develop a framework to probe interactions among diverse systems, and we identify a physiological network. We find that each physiological state is characterized by a specific network structure, demonstrating a robust
1:30PM B54.00013 Detecting and evaluating communities in complex human and biological networks, GREG MORRISON, L. MAHADEVAN, Harvard University School of Engineering and Applied Sciences — We develop a simple method for detecting the community structure in a network by utilizing a measure of closeness between nodes. This approach readily leads to a method of coarse-graining the network, which allows the detection of the natural hierarchy (or hierarchies) of community structure without appealing to an unknown resolution parameter. The closeness measure can also be used to evaluate the robustness of an individual node’s assignment to its community (rather than evaluating only the quality of the global structure). Each of these methods in community detection and evaluation are illustrated using a variety of real world networks of either biological or sociological importance and illustrate the power and flexibility of the approach.

1:51PM B54.00014 Small-world organization of self-similar modules in functional brain networks, MARIANO SIGMAN, Buenos Aires University, LAZAROS GALLOS, HERNAN MAKSE, City College of New York — The modular organization of the brain implies the parallel nature of brain computations. These modules have to remain functionally independent, but at the same time they need to be sufficiently connected to guarantee the unitary nature of brain perception. Small-world architectures have been suggested as probable structures explaining this behavior. However, there is intrinsic tension between shortcuts generating small-worlds and the persistence of modularity. In this talk, we study correlations between the activity in different brain areas. We suggest that the functional brain network formed by the percolation of strong links is highly modular. Contrarily to the common view, modules are self-similar and therefore are very far from being small-world. Incorporating the weak ties to the network converts it into a small-world preserving an underlying backbone of well-defined modules. Weak ties are shown to follow a pattern that maximizes information transfer with minimal wiring costs. This architecture is reminiscent of the concept of weak-ties strength in social networks and provides a natural solution to the puzzle of efficient information flow in the highly modular structure of the brain.

2:03PM B54.00015 Unraveling the rules of evolution in the yeast protein-protein interaction network, YULIANG JIN, HERNAN MAKSE, Levich Institute and Physics Department, the City College of New York; THOMAS WEINMAYER, DMITRIU TURAEV, THOMAS RATTEI, Department of Computational Systems Biology, University of Vienna — A question of fundamental importance is to understand the dynamical principles according to which biological networks have acquired their topological structures and functional modules. Here, we perform an empirical study of the yeast protein-protein interactions (PPI), combined with theoretical modeling of the genomic duplication-divergence processes. Our duplication-divergence model agrees with experimental data, and provides a novel approach to reconstruct ancestral PPI networks. Following the phylogenetic tree, our analysis unravels that the ancient networks evolve into the present day yeast network by a multiplicative growth. The rule of multiplicative growth demonstrates the relationship between the topological exponents and the evolution growth rates of interactions. An important consequence of this evolutorial principal is the emergence of self-similar modular structure, which is confirmed by the analysis of functional modules of proteins.

Monday, February 27, 2012 2:30PM - 5:18PM —
Session D40 DBIO GSNP: Focus Session: Systems Biology and Biochemical Networks I 156A

2:30PM D40.00001 Optimal Information Processing in Biochemical Networks, CHRIS WIGGINS, Columbia University — A variety of experimental results over the past decades provide examples of near-optimal information processing in biological networks, including in biochemical and transcriptional regulatory networks. Computing information-theoretic quantities requires first choosing or computing the joint probability distribution describing multiple nodes in such a network — for example, representing the probability distribution of finding an integer copy number of each of two interacting reactants or gene products while respecting the “intrinsically” small copy number noise constraining information transmission at the scale of the cell. I’ll give an overview of some recent analytic and numerical work facilitating calculation of such joint distributions and the associated information, which in turn makes possible numerical optimization of information flow in models of noisy regulatory and biochemical networks. Illustrating cases include quantification of form-function relations, ideal design of regulatory cascades, and response to oscillatory driving.

3:06PM D40.00002 Adaptation at the output of the chemotaxis signaling pathway, JUNHUA YUAN, RICHARD BRANCH, BASARAB HOSU, HOWARD BERG, Department of Molecular and Cellular Biology, Harvard University — The chemotaxis signaling pathway allows bacterial cells to sense and respond to changes in concentrations of chemical attractants or repellents. In E. coli, the machinery required for bacterial chemotaxis includes two large membrane-embedded multiprotein complexes, one that processes input (receptor clusters) and the other that generates output (flagellar motors). These complexes are coupled by diffusion of a small phosphorylated cytoplasmic protein, CheY-P, which binds to the flagellar motors, increasing the probability that they spin clockwise. Receptor output (the steady-state concentration of CheY-P) varies from cell to cell. However, the motor is ultrasensitive, with a narrow [CheY-P] operating range. How might the receptor output and motor input be matched? By combining various techniques such as FRET, single-motor TIRF, and single-motor bead assay, we showed that the motor shifts its operating range to match the receptor output by changing its composition. The number of FliM subunits in the C-ring increases in response to a decrement in the concentration of CheY-P, increasing motor sensitivity. Such adaptive remodeling is likely to be a common feature in the operation of many molecular machines.

3:18PM D40.00003 The energy cost of accurate adaptation in networks with incoherent type-1 feed-forward loop, GANHUI LAN, YUHAI TU, IBM T. J. Watson Research Center — The incoherent type-1 feed forward loop (I1-FFL) is a common regulatory motif in many biochemical networks, some of which are responsible for accurate sensory adaptation. In this work, we analyze the sensitivity and adaptation function of the I1-FFL type enzymatic reaction networks. We show that detailed balance is broken in I1-FFL and continuous energy dissipation is needed to improve both the sensitivity and the adaptation accuracy of the network. Our study revealed a relation between the performance improvement and the energy dissipation rate. We find that this energy-assisted improvement is bounded (limited) by intrinsic properties of the molecular reaction system. The performance-energy relation in I1-FFL is similar to the recently obtained Energy-Speed-Accuracy relation in networks with negative-feedback-loop, another key motif for accurate sensory adaptation.

3:30PM D40.00004 Noise places constraints on eukaryotic gradient sensing and chemotaxis, BO HU, DANNY FULLER, WILLIAM LOOMIS, University of California - San Diego; WEN CHEN, University of Maryland - College Park; WOUTER-JAN RAPPEL, HERBERT LEVINE, University of California - San Diego — Chemotaxis is characterized by the directional cell movement following external chemical gradients. It plays a crucial role in a variety of biological processes including neuronal development, wound healing and cancer metastasis. Ultimately, the accuracy of gradient sensing is limited by the fluctuations of signaling components, e.g. the stochastic receptor occupancy on cell surface. We use concepts and techniques from statistical physics, estimation theory, and information theory to quantify the stochastic and nonlinear information processing in eukaryotic chemotaxis. We mainly address the following questions: (1) What are the physical limits of eukaryotic signal processing? (2) How to characterize the movements of chemotactic cells? (3) How much gradient information can be reliably gained by a chemotactic cell? By answering those questions, we expect to derive new insights for general biological signal processing systems.

This work was supported by National Institutes of Health Grant AI016478.

This work was supported by NIH Grant No. P01 GM078586 and NSF Grant No. PHY-0822283.
3:42PM D40.00005 Process-driven inference of biological network structure: feasibility, minimality, and multiplicity. CHEN ZENG, Department of Physics, The George Washington University, Washington, DC 20052 — For a given dynamic process, identifying the putative interaction networks to achieve it is the inference problem. In this talk, we address the computational complexity of inference problem in the context of Boolean networks under dominant inhibition condition. The first is a proof that the feasibility problem (is there a network that explains the dynamics?) can be solved in polynomial-time. Second, while the minimality problem (what is the smallest network that explains the dynamics?) is shown to be NP-hard, a simple polynomial-time heuristic is shown to produce near-minimal solutions, as demonstrated by simulation. Third, the theoretical framework also leads to a fast polynomial-time heuristic to estimate the number of network solutions with reasonable accuracy. We will apply these approaches to two simplified Boolean network models for the cell cycle process of budding yeast (Li 2004) and fission yeast (Davidich 2008). Our results demonstrate that each of these networks contains a giant backbone motif spanning all the network nodes that provides the desired main functionality, while the remaining edges in the network form smaller motifs whose role is to confer stability properties rather than provide function. Moreover, we show that the bioprocesses of these two cell cycle models differ considerably from a typically generated process and are intrinsically cascade-like.

1The work is supported by National Science Foundation (NSF) Grant CMMI-0941228

4:18PM D40.00006 Communication channels between membrane bound proteins, JAMES SETHNA, BENJAMIN MACHTA, Department of Physics, Cornell University, SARAH VEATCH, Department of Biophysics, University of Michigan, Ann Arbor — Much of what might be called biological computation takes place on the plasma membrane, a 2D liquid composed of a diverse soup of lipids and embedded proteins. Motivated by the recent discovery that these membranes seem to be tuned close to a 2D liquid-liquid critical point, we set out to understand the different channels through which membrane bound proteins can communicate. Diffusing proteins can carry out reactions like phosphorylation when they come in contact with each other. Near criticality, proteins can also exert long-range critical Casimir forces on one another by coupling to the local composition order parameter. By modulating the growth and breakdown of the rigid cytoskeleton, they can direct forces on even more distant regions. In addition, proteins can control the release and production of second messengers that diffuse either through the bulk, or in the plane of the membrane itself. By making simple models for these processes we bound functional measures for them as communication channels. These include information theoretic measures of bandwidth, as well as physical measures of energetic efficiency and speed. Our results will likely shed light on the functional role of clustering and other collective behaviors often seen in experiments.

4:30PM D40.00007 Maximum entropy principle for predicting response to multi-drug exposure in bacteria and human cancer cells, KEVIN WOOD, SATOSHI NISHIDA, Harvard University, EDUARDO SONTAG, Rutgers University, PHILIPPE CLUZEL, Harvard University — Drugs are commonly used in combinations larger than two for treating infectious disease. However, it is generally impossible to infer the net effect of a multi-drug combination on cell growth directly from the effects of individual drugs. We combined experiments with maximum entropy methods to develop a mechanism-independent framework for calculating the response of both bacteria and human cancer cells to a large variety of drug combinations comprised of anti-microbial or anti-cancer drugs. We experimentally show that the cellular responses to drug pairs are sufficient to infer the effects of larger drug combinations in gram negative bacteria, Escherichia coli, gram positive bacteria, Staphylococcus aureus, and also human breast cancer and melanoma cell lines. Remarkably, the accurate predictions of this framework suggest that the multi-drug response obeys statistical rather than chemical laws for combinations larger than two. Consequently, these findings offer a new strategy for the rational design of therapies using large drug combinations.

4:42PM D40.00008 Robust regulation of oscillatory Min-protein patterns, JACOB HALATEK, ERWIN FREY, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München — Robust spatial patterning was crucial just from the beginning of cellular evolution, and is key to the development of multicellular organisms. In E. Coli, the oscillatory pole-to-pole dynamics of MinCD proteins functionality prevent improper cell divisions apart from midcell. Min-oscillations are characterized by the remarkable robustness with which spatial patterns dynamically adapt to variations of cell geometry. Moreover, adaption, and therefore proper cell division, is independent of temperature. These observations raise fundamental questions about the underlying core mechanisms, and about the role of spatial cues. With a conceptually novel and universal approach to cellular geometries, we introduce a robust model based on experimental data, consistently explaining the mechanisms underlying pole-to-pole, striped and circular patterns, as well as the observed temperature-dependence. Contrary to prior conjectures, the model predicts that MinD and cardiopin domains are not colocalized. The key mechanisms are transient sequestration of MinE, and highly canalized transfer of MinD between polar zones. MinD channeling enhances midcell localization and facilitates stripe formation, revealing the potential optimization process from which robust Min-oscillations originally arose.

1This project has been supported by the German Excellence Initiative via the program “Nanosystems Initiative Munich” (NIM).

4:54PM D40.00009 Mathematical Analysis of Biomolecular Network Reveals Connections Between Diseases, GUANYU WANG, The George Washington University — Connections between cancer and metabolic diseases may consist in the complex network of interactions among a common set of biomolecules. By applying singularity and bifurcation analysis, the phenotypes constrained by the AKT signaling pathway are identified and mapped onto the parameter space, which include cancer and certain metabolic diseases. By considering physiologic properties (sensitivity, robustness and adaptivity) the AKT pathway must possess in order to efficiently sense growth factors and nutrients, the region of normal responses is located. The analysis identifies the parameter space and reveals system-level mechanisms in regulating biological functions (cell growth, survival, proliferation and metabolism) and how their deregulation may lead to the development of diseases. The analytical expressions summarize the synergistic interactions among many molecules, which provides valuable insights into therapeutic interventions.

1This work was supported by an Institutional Research grant (IRG-08-091-01) from the American Cancer Society to The George Washington University Cancer Institute.

5:06PM D40.00010 Modeling the mammalian circadian clock, CRAIG JOLLEY, HIROKIUEDA, RIKEN Center for Developmental Biology, Laboratory for Systems Biology — In biology, important processes often depend on a temporal schedule. The 24-hour periodicity of solar illumination caused by the earth’s rotation has consequences for environmental factors such as temperature and humidity as well as ecological factors such as the presence of food, predators, or potential mates. As a result, many organisms have evolved to develop a circadian clock that allows them to anticipate environmental changes that are likely to occur. The circadian clock is a system of interacting genes and proteins that is able to maintain rhythmic activity patterns over time.

5:42PM D40.00011 Probing the Transcriptional Network of a Hypoxic Microenvironment, JACOB HALATEK, ERWIN FREY, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München — Under hypoxia, cells switch to glycolysis, a metabolic route that allows cells to continue to produce ATP in the absence of oxygen. This rewiring is crucial for the survival of cells in the hypoxic microenvironment, such as those found in tumors. Hypoxia is associated with the development of cancer and other diseases.

6:24PM D40.00012 Reaction network analysis of mammalian cell cycle control, JONATHAN DAVIS, YUETONG ZHENG, Department of Physic, University of Chicago, ROBERT PENG, Department of Medicine, University of Chicago, GEORGE CHURCH, Department of Biochemistry, University of California — The cell cycle is a fundamental biological process that drives cell growth and proliferation. In eukaryotic cells, the cell cycle is controlled by a network of proteins and enzymes that work together to regulate the transition between different phases of the cell cycle. Understanding the dynamics of this network is crucial for understanding the mechanisms that control cell growth and proliferation.

6:42PM D40.00013 Dynamics of a multistable network: models for gene regulatory networks, JONATHAN DAVIS, YUETONG ZHENG, Department of Physic, University of Chicago, ROBERT PENG, Department of Medicine, University of Chicago, GEORGE CHURCH, Department of Biochemistry, University of California — Gene regulatory networks are commonly modeled as multistable systems, where the network can exist in multiple stable states. Understanding the dynamics of these systems is crucial for understanding the mechanisms that control gene expression and have implications for understanding disease.

6:42PM D40.00013 Dynamics of a multistable network: models for gene regulatory networks, JONATHAN DAVIS, YUETONG ZHENG, Department of Physic, University of Chicago, ROBERT PENG, Department of Medicine, University of Chicago, GEORGE CHURCH, Department of Biochemistry, University of California — Gene regulatory networks are commonly modeled as multistable systems, where the network can exist in multiple stable states. Understanding the dynamics of these systems is crucial for understanding the mechanisms that control gene expression and have implications for understanding disease.

6:42PM D40.00013 Dynamics of a multistable network: models for gene regulatory networks, JONATHAN DAVIS, YUETONG ZHENG, Department of Physic, University of Chicago, ROBERT PENG, Department of Medicine, University of Chicago, GEORGE CHURCH, Department of Biochemistry, University of California — Gene regulatory networks are commonly modeled as multistable systems, where the network can exist in multiple stable states. Understanding the dynamics of these systems is crucial for understanding the mechanisms that control gene expression and have implications for understanding disease.
2:30PM D43.00001 Failure of molecules, bones, and the Earth itself. SINAN KETEN, Northwestern University — Materials fail by recurring rupture and shearing of interatomic bonds at microscopic, molecular scales, leading to disintegration of matter at macroscale, and a loss of function. In this talk, the state-of-the-art of investigations on failure mechanisms in materials will be presented, in particular focusing on atomistic origin of deformation and fracture, and the relationships between molecular mechanics and macroscale behavior. Simple examples of fracture phenomena are used to illustrate the significance and impact of material failure on our daily lives. Based on case studies, mechanisms of failure of a wide range of materials are discussed, ranging from tetmonic platoes to rupture of single molecules, and an explanation on how atomistic simulation can be used to complement experimental studies and theory to provide a novel viewpoint in the analysis of complex systems is provided. Biological protein materials are used to illustrate how extraordinary properties are achieved through the utilization of intricate structures where the interplay of weak and strong chemical bonds, size and confinement effects, and hierarchical features play a fundamental role. This leads to a discussion of how even the most robust biological material systems fail, leading to diseases that arise from structural and mechanical alterations at molecular, cellular, and tissue levels. New research directions in the field of materials failure and materials science are discussed and the impact of improving the understanding of materials failure for applications in nanotechnology, biotechnology, medicine as well as the built environment.

3:06PM D43.00002 Fast fracture in slow motion: Dynamic fracture and the effect of near-tip elastic nonlinearities in brittle gels, JAY FINEBERG, The Racah Institute of Physics, The Hebrew University of Jerusalem — We present recent results of fracture experiments in poly-acrylamide gels [1]. These gels are soft polymers in which the characteristic sound speeds are on the order of a few meters/sec - thereby slowing down fracture dynamics by 3 orders of magnitude. We first show that the dynamics of rapid cracks are universal; the fracture of gels exhibits characteristic features that are identical with those seen in "classic" materials such as glass. These include:

• Excellent quantitative agreement with the two different equations of motion for single dynamic cracks predicted by Linear Elastic Fracture Mechanics (LEFM) – each for different classes of loading conditions.
• The same branching instabilities, localized waves confined to the crack front, and the characteristic structure formed on the resulting fracture surface as observed in “standard” amorphous brittle materials, such as soda-lime glass.

We utilize the "slow motion" inherent in the fracture of gels to experimentally and theoretically investigate the structure of the deformation fields that surround the tip of highly dynamic cracks. We find that:

• The singular fields predicted by LEFM change their structure due to nonlinear elastic effects that dominate the near-tip region [3].
• This non-linear elastic region provides a quantitative explanation for the oscillatory instability of cracks [2,4] as their speed approaches the Rayleigh wave speed.

These results provide a quantitative first-principles description of how elastic nonlinearities influence the rapid dynamics of a crack.


3:42PM D43.00003 Shapes formed by interacting cracks, KAREN DANIELS, Dept. of Physics, North Carolina State University — Brittle failure through multiple cracks occurs in a wide variety of contexts, from microscopic failures in dental enamel and cleaved silicon to geological faults and planetary ice crusts. In each of these situations, with complicated stress geometries and different microscopic mechanisms, pairwise interactions between approaching cracks nonetheless produce characteristically curved fracture paths. We investigate the origins of this widely observed “en passant” crack pattern by fracturing a rectangular slab which is notched on each long side and subjected to quasi-static uniaxial strain from the short side. The two cracks propagate along approximately straight paths until they pass each other, after which they curve and release a lens-shaped fragment. We find that, for materials with diverse mechanical properties, each curve has an approximately square-root shape, and that the length of each fragment is twice its width. We are able to explain the origins of this universal shape with a simple geometrical model.

4:18PM D43.00004 Fracture Statistics: Universality vs. Nucleation1, ASHIVNI SHEKHAWAT, Cornell University — We reexamine several common assumptions about fracture strength, utilizing large-scale simulations of a fuse network model and applying both renormalization-group and nucleation theory methods. Statistical distributions of fracture strengths are believed to be universal and material independent. The universal Weibull and Gumbel distributions emerge as a consequence of the “weakest-link hypothesis” and have been studied in the classical theory of extreme value statistics. These distributions are also the fixed points of a renormalization group (RG) flow. However, the engineering community often ignores the Gumbel distribution and uses the Weibull form almost exclusively to fit experimental data. Further, such fits are often extrapolated beyond the available data to estimate the probability of rare events in a variety of applications ranging from structural reliability to insurance pricing. Our recent studies of the random fuse network model raises doubts about most of these practices. We find that materials with diverse mechanical properties, each curve has an approximately square-root shape, and that the length of each fragment is twice its width. We are able to explain the origins of this universal shape with a simple geometrical model.

1This research was partially supported by DOE-BES DE-FG02-07ER-46393

4:54PM D43.00005 Avalanches in crack front propagation1, STEFANO ZAPPERI, National Research Council of Italy CNR — We study avalanches in a model for a planar crack propagating in a disordered medium. Due to long-range interactions, avalanches are formed by a set of spatially disconnected local clusters, the sizes of which are distributed according to a power law. We derive a scaling relation between the local cluster and the spatial extent of the avalanche. Even for small size clusters, the avalanche size is determined by the largest size cluster. We show that our theoretical predictions are in excellent agreement with numerical simulations. In particular, the avalanche size distribution is well described by the Gumbel distribution, which is universal and does not depend on the details of the disorder distribution.

1in collaboration with L. Laursen, S. Santucci and G. Durin
2:30PM D52.00001 Dynamic phase transition in the classical anisotropic XY model on a square lattice[1], WILLIAM BAEZ, The Ohio State University, TRINANJAN DATTA, Augusta State University — Ginzburg-Landau analysis of the anisotropic XY model in a spatially homogeneous oscillating magnetic field on a square lattice suggests the existence of several dynamical phases – Ising symmetry restoring order (Ising SRO), Ising symmetry breaking order (SBO), XY symmetry restoring order (XY SRO), and XY symmetry breaking order (XY SBO). We investigate the presence of these phases and the dynamic phase transition (DPT) between these phases using classical Monte Carlo simulation techniques. We explore the system for a range of values for the external field amplitude, field frequency, and anisotropy parameter. Utilizing the period-averaged magnetization (in both the x- and y-component) as the dynamic order parameter we confirm the presence of multiple DPT transitions in the model. We also construct the probability density histograms of the dynamic order parameter to validate the existence of the four DPT phases.

[1] Cottrell College Science Awards (RCSA Award #20073)

2:42PM D52.00002 Non-universal local critical exponents at a non-equilibrium phase transition[1], MICHEL PLEIMLING, HYUNHANG PARK, Virginia Tech — We study the dynamic phase transition in the two-dimensional semi-infinite kinetic Ising model in an oscillating field. We focus on the critical regime where the competition between the half-period of the oscillating field $t_{1/2}$ and the metastable lifetime ($\tau$) is most pronounced. We focus on layer-dependent quantities, such as the period-averaged magnetization per layer $Q(z)$ and the layer susceptibility $\chi_{Q}(z)$, and determine surface critical exponents through finite-size scaling. We find that the values of these non-equilibrium exponents are non-universal as they depend on the strength of the surface couplings. Results for the three-dimensional model are also briefly discussed and compared to the two-dimensional case.

[1] Supported in part by the US National Science Foundation through Grant DMR-0904999.

2:54PM D52.00003 ABSTRACT WITHDRAWN —

3:06PM D52.00004 Extremal Optimization for p-Spin Models[1], STEFAN FALKNER, STEFAN BOETTCHER, Emory University — It was shown recently that finding ground states in the 3-spin model on a 2d dimensional triangular lattice poses an NP-hard problem [1]. We use the extremal optimization (EO) heuristic [2] to explore ground state energies and finite-size scaling corrections [3]. EO predicts the thermodynamic ground state energy with high accuracy, based on the observation that finite size corrections appear to decay purely with system size. Just as found in 3-spins models on r-regular graphs, there are no noticeable anomalous corrections to these energies. Interestingly, the results are sufficiently accurate to detect alternating patterns in the energies when the lattice size $L$ is divisible by 6. Although ground states seem very prolific and might seem easy to obtain with simple greedy algorithms, our tests show significant improvement in the data with EO.

[1] PRE 83 (2011) 046709,

3:18PM D52.00005 A novel Kinetic Monte Carlo algorithm for Non-Equilibrium Simulations[1], PRATEEK JHA, Northwestern University, VLADIMIR KUZOVKOV, University of Latvia, BARTOSZ GRZYBOWSKI, MONICA OLVERA DE LA CRUZ, Northwestern University — We have developed an off-lattice kinetic Monte Carlo simulation scheme for reaction-diffusion problems in soft matter systems. The definition of transition probabilities in the Monte Carlo scheme are taken identical to the transition rates in a renormalized master equation of the diffusion process and match that of the Glauber dynamics of Ising model. Our scheme provides several advantages over the Brownian dynamics technique for non-equilibrium simulations. Since particle displacements are accepted/rejected in a Monte Carlo fashion as opposed to moving particles following a stochastic equation of motion, nonphysical movements (e.g., violation of a hard core assumption) are not possible (these moves have zero acceptance). Further, the absence of a stochastic “noise” term resolves the computational difficulties associated with generating statistically independent trajectories with definitive mean properties. Finally, since the timestep is independent of the magnitude of the interaction forces, much longer time-steps can be employed than Brownian dynamics. We discuss the applications of this scheme for dynamic self-assembly of photo-switchable nanoparticles and dynamical problems in polymeric systems.

3:30PM D52.00006 How an aggregation process helps us understanding solid fragmentation[1], VLEDOUTS ALEXANDRE, NICOLAS VANDENBERGHE, EMMANUEL VILLERMAUX, IRPHE — We report on an experiment intended to understand the fragmentation of a ring composed of cohesive solid spheres (magnets in dipolar interaction). At initial time, the ring is forced to expand radially and the spheres separate from each other. Because of the dipolar attractive force between the spheres, their uniform angular distribution is unstable and the spheres aggregate with each other to form fragments. We record the full dynamics of the spheres assembly and we show that the final fragment size distribution is the signature of the aggregation process giving birth to it. In particular, we introduce a Weber number $We$, based on the radial velocity of the ring, the density of the spheres and their magnetization. We find that the final mean fragment size scales like $We^{-1/3}$ and that the standard deviation of the fragments distribution is proportional to it. We will also discuss the relation between our findings and the fragmentation of elastic rings studied by Sir N. Mott.

3:42PM D52.00007 Thermodynamic limit, quasi-stationary states and the range of pair interactions[1], ANDREA GABRIELLI, Istituto dei Sistemi Complessi - CNR (Rome, Italy), MICHAEL JOYCE, LPNHE - Université Paris 6 (France), BRUNO MARCOS, Lab. J.A. Dieudonné, UMR 6621, Université de Nice (France) — “Quasi-stationary” states are approximately time-independent out of equilibrium states which have been observed in a variety of systems of particles interacting by long-range interactions. We investigate here the variety of conditions for their occurrence for a generic pair interaction $V(r \to \infty) \sim 1/r^\gamma$ with $\gamma > 0$, in $d > 1$ dimensions. We generalize analytic calculations known for gravity in $d = 3$ to determine the scaling parametric dependencies of their relaxation rates due to two body collisions, and report extensive numerical simulations testing their validity. Our results lead to the conclusion that, for $\gamma < d - 1$, the existence of quasi-stationary states is ensured by the large distance behavior of the interaction alone, while for $\gamma > d - 1$ it is conditioned on the short distance properties of the interaction, requiring the presence of a sufficiently large soft-core in the interaction potential.

3:54PM D52.00008 ABSTRACT WITHDRAWN
We perform a numerical study of Potts models on a rectangular lattice with aperiodic interactions along one spatial direction. The number of states \( q \) is such that the transition is a first-order one for the uniform model. The Wolff algorithm is employed, for many lattice sizes, allowing for a finite-size scaling analyses to be carried out. Three different self-dual aperiodic sequences are employed, such that the exact critical temperature is known: this leads to precise results for the exponents. We analyze models with \( q = 6 \) and 15 and show that the Harris-Luck criterion, originally introduced in the study of continuous transitions, is obeyed also for first-order ones. The new universality class that emerges for relevant aperiodic modulations depends on the number of states of the Potts model, as obtained elsewhere for random disorder, and on the aperiodic sequence. We determine the occurrence of log-periodic behavior, as expected for models with aperiodic modulated interactions.

1. We acknowledge financial support from Brazilian Agencies FAPESC, CNPq, and CAPES.

153B. The dark brushes seen in Schlieren textures of two-dimensional samples of nematics. Manipulations of these surfaces correspond to deformations of the nematic phase. These surfaces turn out to be a generalization to 3 dimensions of construction.

Our results give a qualitative explanation for the success of simple models: most directions in parameter space become fundamentally indistinguishable after coarse-graining. We show that under certain conditions, the metric in the original parameters, taking care to use only information available after coarse-graining, correlates with the force effects on cell or colony size. This is in agreement with recent experiments on keratinocyte colonies adhered to fibronectin coated surfaces. In the presence of active viscoelastic fluids, the coupling to the substrate enters as a boundary condition that relates the cell's deformation field to local stress gradients. In the presence of actomyosin activity, the substrate also enhances the cell polarization, breaking the cell's front-rear symmetry. Maximal polarization is observed when the shear strain matches that of the cell, in agreement with experiments on stem cells.

We present a continuum mechanical model of rigidity sensing by cells. The cell or colony size. This is in agreement with recent experiments on keratinocyte colonies adhered to fibronectin coated surfaces. In the presence of actomyosin activity, the substrate also enhances the cell polarization, breaking the cell's front-rear symmetry. Maximal polarization is observed when the shear strain matches that of the cell, in agreement with experiments on stem cells.

4:42PM D52.00012 Dynamics near shear-jamming for a dense granular system 1, JIE REN, JOSHUA DIJKSMAN, ROBERT BEHRINGER, Duke University — This talk will present several systematic experimental studies of a two-dimensional, frictional dense granular system subjected to simple shear deformation. The first experiment consists of linear shear for densities smaller than the isotropic jamming point, and examines both the evolution of the average stress and the evolution of force network. These measures reveal three distinguishable regimes of the granular system with increasing shear strain: unjammed, fragile, and shear-jammed regimes. The second experiment uses small amplitude cyclic shear to probe the dynamical response of the states from the first experiment. For fragile or jammed regimes, cyclic shear drives the system through transient states that evolve towards relatively stable forces networks and system-averaged stress. The timescale of the transient increases rapidly as the system moves deeper into the fragile, or shear-jammed regimes. These experiments also involve particle tracking (displacements and rotations) to search for and characterize non-affine motion and spatial heterogeneity. There is a clear increase in particle diffusion with increasing density and shear strain amplitude, even when the system is still unjammed and experiences only minimal stress. When the system is fragile or jammed, the heterogeneity of particle displacements reveals subtle correlations with the force network.

4:54PM D52.00013 Elasticity of adherent active cells on a compliant substrate 1, SHILADITYA BANERJEE, Department of Physics, Syracuse University, AARON F. MERTZ, ERIC R. DUFRESNE, Department of Physics, Yale University, M. CRISTINA MARCHETTI, Department of Physics and Syracuse Biomaterials Institute, Syracuse University — We present a continuum mechanical model of rigidity sensing by living cells adhering to a compliant substrate. The cell or cell colony is modeled as an elastic active gel, adapting recently developed continuum theories of active viscoelastic fluids. The coupling to the substrate enters as a boundary condition that relates the cell’s deformation field to local stress gradients. In the presence of actomyosin activity, the substrate also enhances the cell polarization, breaking the cell’s front-rear symmetry. Maximal polarization is observed when the substrate stiffness matches that of the cell, in agreement with experiments on stem cells.

This work was supported by NSF grants: DMR0906908, DMS0835571, NASA grant NNX10AU01G and ARO grant W911NF-11-1-0110.

5:06PM D52.00014 Differential geometry of the space of Ising models 1, BENJAMIN MACHTA, RICKY CHACHRA, Department of Physics, Cornell University, MARK TRANSTRUM, Department of Bioinformatics and Computational Biology at the MD Anderson Cancer Center, JAMES SETHNA, Department of Physics, Cornell University — We use information geometry to understand the emergence of simple effective theories, using an Ising model perturbed with terms coupling non-nearest-neighbor spins as an example. The Fisher information is a natural metric of distinguishability for a parameterized space of probability distributions, applicable to models in statistical physics. Near critical points both the metric components (four-point susceptibilities) and the scalar curvature diverge with corresponding critical exponents. However, connections to Renormalization Group (RG) ideas have remained elusive. Here, rather than looking at RG flows of parameters, we consider the reparameterization-invariant flow of the manifold itself. This is in agreement with recent experiments on keratinocyte colonies adhered to fibronectin coated surfaces. In the presence of actomyosin activity, the substrate also enhances the cell polarization, breaking the cell’s front-rear symmetry. Maximal polarization is observed when the substrate stiffness matches that of the cell, in agreement with experiments on stem cells.

1. We credit this work supported by NSF grants to MCM (DMR-0806511 and DMR-1004789) and ERD (DBI-0619674) and NSF graduate fellowship to AFM.

2. Additional Affiliations: Department of Mechanical Engineering and Materials Science, Department of Chemical and Environmental Engineering, Department of Cell Biology, Yale University.

5:18PM D52.00015 Seeing and Sculpting Nematic Liquid Crystal Textures with the Thom construction 1, BRYAN CHEN, University of Pennsylvania, GARETH ALEXANDER, University of Warwick — Nematic liquid crystals are the foundation for modern display technology and also exhibit topological defects that can readily be seen under a microscope. Recently, experimentalists have been able to create and control several new families of interesting defect textures, including reconfigurably knotted defect lines around colloids (Ljubljana) and the “toron,” a pair of hedgehogs bound together with a ring of double-twist between them (CU Boulder). We apply the Thom construction from algebraic topology to visualize 3 dimensional molecular orientation fields as certain colored surfaces in the sample. These surfaces turn out to be a generalization to 3 dimensions of the dark brushes seen in Schlieren textures of two-dimensional samples of nematics. Manipulations of these surfaces correspond to deformations of the nematic orientation fields, giving a hands-on way to classify liquid crystal textures which is also easily computable from data and robust to noise.

Monday, February 27, 2012 2:30PM - 5:30PM –
Session D53 GSNP DFD: Focus Session: Jamming – Nonlinear Acoustics and Vibrational Response 153B
Beyond certain wave amplitude, the sound-matter interaction becomes irreversible, leaving the medium in a weakened and slightly compacted state. A slow and also allow investigating the irreversible rearrangement of the contact network at large vibration amplitude. In this talk, we describe two distinct types of TEAM — Elastic waves propagating through a dense granular pack provide a unique probe of the elastic properties and internal dissipation of the medium [1], XIAOPING JIA, JEROME LAURENT, Université Paris-Est, SIET WILDENBERG, MARTIN VAN HECKE, Universiteit Leiden, LPMDI TEAM, ONNES LAB packings.

In vibrated granular packings is reminiscent of the low-frequency behavior of the vibrational density of states in fluid systems. We also investigate the effects exhibit an increase in the number of low-frequency modes over that obtained from linear response of the static packing. The form of the density of states those of the unperturbed packing. The vibrational density of states obtained using the displacement matrix and velocity autocorrelation function methods breaking even when the system is under significant compression. Further, vibrated packings possess well-defined equilibrium positions that are different than shown that granular packings composed of frictionless particles with repulsive contact interactions are strongly nonharmonic. When infinitesimally perturbed along linear response eigenmodes of the static packing, energy leaks from the original mode of vibration to a continuum of frequencies due solely to contact breaking even when the system is under significant compression. Further, vibrated packings possess well-defined equilibrium positions that are different than those of the unperturbed packing. The vibrational density of states obtained using the displacement matrix and velocity autocorrelation function methods exhibit an increase in the number of low-frequency modes over that obtained from linear response of the static packing. The form of the density of states in vibrated granular packings is reminiscent of the low-frequency behavior of the vibrational density of states in fluid systems. We also investigate the effects of inter-particle friction, dissipation, particle shape, and degree of positional order on the density of states and thermal transport properties in driven granular packings.

3:06PM D53.00004 Irreversible Incremental Behavior in a Granular Material1. LUIGI LA RAGIONE, Yale University — We have shown that granular packings composed of frictionless particles with repulsive contact interactions are strongly nonharmonic. When infinitesimally perturbed along linear response eigenmodes of the static packing, energy leaks from the original mode of vibration to a continuum of frequencies due solely to contact breaking even when the system is under significant compression. Further, vibrated packings possess well-defined equilibrium positions that are different than those of the unperturbed packing. The vibrational density of states obtained using the displacement matrix and velocity autocorrelation function methods exhibit an increase in the number of low-frequency modes over that obtained from linear response of the static packing. The form of the density of states in vibrated granular packings is reminiscent of the low-frequency behavior of the vibrational density of states in fluid systems. We also investigate the effects of inter-particle friction, dissipation, particle shape, and degree of positional order on the density of states and thermal transport properties in driven granular packings.

4:06PM D53.00007 Nonlinear acoustics of glass bead packings at vanishing static pressures 1. VINCENT TOURNAT, LAUM, CNRS, Université du Maine, Le Mans, France, VITALYI GUSEV, LPEC, CNRS, Universite du Maine, Le Mans, France — We present here a set of recent results obtained in three experimental configurations: linear and nonlinear acoustic probing of a granular slab at different compacities, surface acoustic waves in granular layers submitted to gravity, resonances of a granular layer with an in-depth elasticity gradient. We succeeded to overcome the experimental issues associated to the dramatic increase of acoustic wave attenuation when the confining pressure diminishes. Interpretations reveal that the manifestations of nonlinear effects (self-demodulation, nonlinear resonance, second harmonic or subharmonic generation...) allow to isolate the different types of nonlinearities involved (Hertz, clapping, stick-slip, hysteresis...). Also, some discrepancies are observed for the extracted linear elastic parameters scaling laws as a function of vanishing pressure (lower than 100 Pa typically) between the different developed experimental configurations and the theoretical predictions. Explanations for these discrepancies are given. We show that under some conditions, it is necessary to take into account the coupling of grain motion with that of the saturating air. Application of these results to the probing of granular layers under destabilization will be presented.

1This work is supported by ANR contract “Stabingram” ANR-2010-BLAN-0927-03.
quantities are non self-averaging, namely, they fluctuate from realization to realization even in the thermodynamic limit. We estimate the number of steps until the giant component spans the entire system and the total number of steps until the regular random graph forms. These of nodes at random and connect them with a link if both of their degrees are smaller than \( d \geq 3 \). Also, changes in the density of vibrational modes due to the change in the average crystallite size and perturbation amplitude in partially crystalline granular packings. In particular we determine how the number of contacts (above the isostatic value) affects anharmonic response in granular packings. The convenience of jamming at finite temperature and how jamming impacts the thermodynamics of glasses remain open issues. We address these questions by investigating the dynamics of both the density field and the force network of an horizontally shaken bi-disperse packing of photo-elastic disks. The average number of contact clearly displays an abrupt transition which we interpret as the jamming transition. Besides, dynamical heterogeneities are observed and their amplitude exhibits a maximum, which, in turn, signals a dynamical transition. We discuss in detail the interplay between these two transitions and how they depend on the particle softness and amplitude of the horizontal vibration. 

The Team is in Saclay and Olivier Dauchot has recently move to ESPCI

Acknowledgement: NSF CBET-0967262, CBET-0968013

We show that, in contrast to conventional wisdom, the quasi-localized, strongly anharmonic, normal modes of jammed systems \([2] \) can produce acoustic echoes due to the shift in the mode frequency with increasing amplitude. We observe this both in jammed packings of spherical particles with finite-range, Hertzian repulsions, and in model glasses interacting with a Lennard-Jones potential. In contrast to pulse echoes in two-level systems, a distinguishing feature of these “anharmonic echoes” is the appearance of multiple echoes after two excitation pulses, a feature also observed in experiments \([1] \).


2:42PM D54.00002 Influence of Boundary Conditions on Metastable Lifetimes for The Ising Model on the Hyperbolic Plane

HOWARD L. RICHARDS, Physics, Marshall University, DIPENDRA SHARMA CHAPAGAIN, Physics, Berea College, JAMES MOLCHANOFF, Math, West Virginia Wesleyan University — Some corals grow in shapes that resemble 3D models of the hyperbolic plane, so this allows them to have greater area for a given growth radius. Each polyp could be represented by an Ising site, with “feeding” = “up” and “retracted” = “down”. The mechanisms of metastable decay could be interpreted as how the coral as a whole reacts to changing conditions of food availability or predation. Previous studies have shown that there is a spinodal field for the Ising model on a regular lattice in the hyperbolic plane if it is infinite or has periodic or mean-field boundary conditions. This happens because the size of the boundary grows asymptotically at the same rate as the droplet volume, in clear contrast with droplets in the Euclidean plane. Our simulations show, however, that the spinodal field disappears if more physically relevant open boundary conditions are used instead.

3:06PM D54.00004 Synchronization in Noisy Networks with Multiple Time Delays

DAVID HUNT, GYORGY KORNISS, BOLESLAW SZYMANSKI, Rensselaer Polytechnic Institute — We expand our previous work of uniform time delays in stochastic, linearly-coupled synchronization problem by including descriptions of networks with multiple delays. Non-uniform time delays can arise when there are multiple sources of delay, e.g. the time to transmit and the time to process information. In this particular two-delay case, the primary limitation on the network to synchronize without any centralized direction does not come from restrictions in the transmission of a node’s state to its neighbors; rather it depends on the ability for each node to process and respond to the information about itself in the context of its local environment. Furthermore, given a network’s structure, there are optimal transmission delays for which the network remains synchronizable for longer processing delays. As a result, synchronization is not always improved—and in some cases it can be totally destroyed—by minimizing the transmission delays. For special cases we also study the scaling function that quantifies the synchronization of the system. This shows the limitation of synchronization in a noisy network.

3:18PM D54.00005 Continuous Percolation by Discontinuities

JAN NAGLER, MPI DS, Goettingen — In the very recent article [Science 333, 322 (2011)], O. Riordan and L. Warnke, state that (i) any rule based on picking a fixed number of random vertices gives a continuous transition, and (ii) that therefore explosive percolation is continuous. It is equally true that certain percolation processes based on picking a fixed number of random vertices are discontinuous. Here we resolve this seeming paradox. We exemplify this by studying an extremal case of a process that is continuous in the sense of Riordan and Warnke but still exhibits infinitely many discontinuous jumps in arbitrary vicinity of the onset of the continuous phase transition. Moreover, we demonstrate analytically that continuity at the phase transition and discontinuity of the percolation process are compatible and generic for certain competitive percolation systems.

3:30PM D54.00006 Random Transverse Ising Model on Annealed Complex Networks

GINESTRA BIANCONI, Northeastern University — In order to shed light on critical phenomena on cuprates, here we propose a stylized model capturing the essential characteristics of the superconducting-insulator transition of a highly dynamical, heterogeneous granular material: the Disordered Quantum Transverse Ising Model (DQTIM) on Annealed Complex Network. We show that when the networks encode for high heterogeneity of the expected degrees described by a power law distribution, the critical temperature for the onset of the superconducting phase diverges to infinity as the power-law exponent \( \gamma \) of the expected degree distribution is less than 3, i.e. \( \gamma < 3 \). Moreover we investigate the case in which the critical state of the electronic background is triggered by an external parameter \( g \) that determines an exponential cutoff in the power law expected degree distribution characterized by an exponent \( \gamma \). We find that for \( g = g_c \), the critical temperature for the superconductor-insulator transition has a maximum if \( \gamma > 3 \) and diverges if \( \gamma < 3 \).

3:42PM D54.00007 Dynamical Instability in Boolean Networks as a Percolation Problem

SHANE SQUIRES, MICHELLE GIRVAN, EDWARD OTT, University of Maryland – College Park — Boolean networks, a widely used model of gene regulatory networks, exhibit a phase transition between a stable regime, in which small perturbations die out, and an unstable regime, in which small perturbations grow exponentially. We show that this phase transition can be mapped onto a static percolation problem which predicts the critical point and the long-time Hamming distance between perturbed and unperturbed systems. The results, which apply to Boolean networks with a broad class of topologies and update functions, are confirmed by numerical simulations.

3:54PM D54.00008 Critical Behavior of the Ising Model on Small-world Hanoi Networks

TRENT BRUNSON, STEFAN BOETTCHER, Emory University — The addition of small-world bonds on hierarchical lattices changes a typical Ising model ferromagnetic phase transition to one of infinite order, referred to as the inverted-Berezinski-Kosterlitz-Thouless transition. We study this shift in phase behavior on Hanoi networks, which are one-dimensional Ising chains connected by small-world bonds that are self-similar and hierarchical in structure [1]. The phase behavior of the Ising model near \( T_c \) on Hanoi networks is studied using an exact renormalization group and Monte Carlo techniques. We show that compared to the Migdal-Kadanoff hierarchical lattice, Hanoi networks possess characteristics in their thermodynamic densities that are more physical. These densities are studied in detail and the behavior of their critical exponents near \( T_c \) is described. By introducing a continuous parameter which regulates the strength of small-world bonds in the Hanoi networks, we begin to uncover the essential small-world properties that dictate this change in phase behavior from second- to infinite-order.

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1 This research was conducted as part of Marshall University’s REU in Scientific Computing, supported by NSF grant OCI-1005117. For more information see www.marshall.edu/reu.

2 This research is supported by the Duke Network Analysis Center.

3 This research has been supported in part by DTRA and ONR.


4:06PM D54.00009 Popularity versus similarity in growing networks, DMITRI KRIOUKOV, University of California San Diego, FRAGKISKOS PAPADOPOULOS, Cyprus University of Technology, MAKSIM KITSAK, University of California San Diego, MARIAN-GELES SERRANO, MARIAN BOGUNA, University of Barcelona — Preferential attachment is a powerful mechanism explaining the emergence of scaling in growing networks. If new connections are established preferentially to more popular nodes in a network, then the network is scale-free. Here we show that not only popularity but also similarity is a strong force shaping the network structure and dynamics. We develop a framework where new connections, instead of preferring popular nodes, optimize certain trade-offs between popularity and similarity. The framework admits a geometric interpretation, in which preferential attachment emerges from local optimization processes. As opposed to preferential attachment, the optimization framework accurately describes large-scale evolution of technological (Internet), social (web of trust), and biological (E.coli metabolic) networks, predicting the probability of new links in them with a remarkable precision. The developed framework can thus be used for predicting new links in evolving networks, and provides a different perspective on preferential attachment as an emergent phenomenon.

4:18PM D54.00010 Is it really a small world after all, BARUCH BARZEL, ALBERT-LASZLO BARABASI, Northeastern University, THE CENTER FOR COMPLEX NETWORK RESEARCH TEAM — One of the most intriguing revelations in the study of complex networks is the ubiquitous appearance of small worlds, that is networks exhibiting a small, and sometimes even ultra-small, average path length. This suggests that these networks feature globally connected dynamics, where all nodes are affected by all other nodes, given the short distance between them. Nevertheless, empirical data on the dynamics of such networks shows that practice, such global connectedness is rarely observed. To address this gap between the topology and the observed dynamics of networks we developed the network correlation function method, a framework in which we obtain the patterns of influence between nodes in the network. In simple words we complement the topological description of who is connected to whom, by the dynamical description of who is affected by whom. Strikingly, using this method, we find that small world topology tends to avoid global dynamics, while non-small worlds could potentially support it. We test our results on a set of networks from various fields, ranging from social to biological networks, and discuss the implications on the dynamical stability of these systems.

4:30PM D54.00011 Metric Structure of Bipartite Networks, MAKSIM KITSAK, UCSD, FRAGKISKOS PAPADOPOULOS, Cyprus University of Technology, DMITRI KRIOUKOV, UCSD — Many social, biological and technological systems can be conveniently represented as bipartite networks, consisting of two disjoint sets of elements along with edges connecting only elements from different sets. Many of such systems are characterized by high values of bipartite clustering coefficient. We also find that pairs of elements in these bipartite systems tend to have many common neighbors. We present a natural interpretation of these observations. We suggest that elements of the above bipartite systems exist in underlying metric spaces, such that the observed high clustering is a topological reflection of the triangle inequality, the key property of metric space. We propose a simple stochastic mechanism of formation of bipartite networks embedded in metric spaces. We prove that this mechanism is able to reproduce the observed topological properties of bipartite networks. We also discuss the possibility of constructive embedding of real bipartite systems into metric spaces. In my talk I will overview the concept of hidden metric spaces with respect to both unipartite and bipartite networks. I will also discuss existing methods used to infer hidden metric spaces in real networks and possible applications for bipartite networks.

4:42PM D54.00012 Topological features of a fractal model for complex networks, LIN BO, HERNAN MAKSE, Levich Institute and Physics Departement, the City College of New York — We study the construction and topological features of fractal and non-fractal hierarchical tree-like models generated through an inverse-renormalization growth mechanism with various parameters. These complex networks are characterized by scale-free distribution of connections, clustering coefficient, modular structure, degree correlation and a set of fractal dimensions. We compare the results with analytic expressions and show the dependence of topological properties on growing parameters. Networks with different tendency of hub-hub repulsion are produced and classified in terms of degree correlations. Interloops and intraloops are introduced into growing process to test robustness and stability of networks under attack.

4:54PM D54.00013 Control Centrality and Hierarchical Structure in Complex Networks, YANG-YU LIU, Northeastern University, JEAN-JACQUES SLOTINE, Massachusetts Institute of Technology, ALBERT-LASZLO BARABASI, Northeastern University — We introduce the concept of control centrality ($C_c$) to quantify the ability of a single node to control a directed weighted network. We map the control centrality into a combinatorial optimization problem. We calculate the distribution of control centrality for several real networks and find that it is mainly determined by the network’s degree distribution. We show that the underlying hierarchical structure of a general directed network plays a significant role in determining the distribution of control controllability. We rigorously prove that in directed acyclic graphs, i.e. directed networks without loops, a node’s control centrality is uniquely determined by its topological position in the underlying hierarchical structure of the network. Our finding on the relation between control centrality and the hierarchical structure inspires us to design an effective random attack strategy against the controllability of malicious networks, without requiring the detailed knowledge of the network structure. We test our random attack strategy on several real networks and find it is indeed effective and even comparable to those targeted attacks which rely on the detailed knowledge of the network structure.

5:06PM D54.00014 A community detection approach to image segmentation and its phases, DANDAN HU, PETER RONHOVDE, ZOHAR NUSINOV, Department of Physics, Washington University in St. Louis — In this talk, I will discuss “unsupervised” image segmentation that relies on phase diagram structure of the community detection method. Specifically, we apply a replica-inference-based community detection method. “Community detection” describes the general problem of partitioning a complex system involving many elements into optimally decoupled communities of such elements. In our image segmentation analysis, we invoke a multi-resolution community detection variant to ascertain the overall structure of the image at different resolutions. Information based measures (e.g., the normalized mutual information) are used to determine the significant structures at which “replicas” of the systems are strongly correlated. We report on the “easy”, “hard”, and “unsolvable” phases of the corresponding Potts model at both zero and finite temperatures. The optimal image segmentations are obtained by choosing parameters at the easy phase of the Potts model. The determination of the phase diagram in the analysis of the image segmentation is proved to be highly efficient. We demonstrate in a detailed study of various test cases that our method is fast and accurate and to be especially suited to the detection of camouflaged images.

5:18PM D54.00015 Ordinary Percolation with Discontinuous Transitions1, VIJAY SINGH, STEFAN BOETTCHER, Dept. of Physics, Emory University, Atlanta, GA 30322 USA — We study percolation on hierarchical networks using generating functions and renormalization group techniques. Our exact results show the presence of novel features in these networks including the existence of non-trivial critical points, three distinct regimes in the phase diagram and, most importantly, a discontinuity in the formation of the extensive cluster at a critical point $p_c < 1$. At $p_c$, the order parameter $\phi$, describing the probability of any node to be a part of the largest cluster, jumps instantly to a finite value. We present simple examples of small-world networks with various hierarchies of long range bonds, indicating that the presence of discontinuous transitions is generic.

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1Supported by NSF grant # 0812204.

Tuesday, February 28, 2012 8:00AM - 11:00AM
Session H20 GSNP DFD: Invited Session: Hydrodynamics and Microstructure: From Single Self-Propelled Particles to Active Soft Matter
8:00AM H20.00001 Swimming & Propulsion in Viscoelastic Media. PAULO ARRATIA, University of Pennsylvania — Many microorganisms have evolved within complex fluids, which include soil, intestinal fluid, and mucus. The material properties or rheology of such fluids can strongly affect an organism’s swimming behavior. A major challenge is to understand the mechanism of propulsion in media that exhibit both solid- and fluid-like behavior, such as viscoelastic fluids. In this talk, we present experiments that explore the swimming behavior of biological organisms and artificial particles in viscoelastic media. The organism is the nematode Caenorhabditis elegans, a roundworm widely used for biological research that swims by generating traveling waves along its body. Overall, we find that fluid elasticity hinders self-propulsion compared to Newtonian fluids due to the enhanced resistance to flow near hyperbolic points for viscoelastic fluids. As fluid elasticity increases, the nematode’s propulsion speed decreases. These results are consistent with recent theoretical models for undulating sheets and cylinders. In order to gain further understanding on propulsion in viscoelastic media, we perform experiments with simple reciprocal artificial ‘swimmers’ (magnetic dumbbell particles) in polymeric and micellar solutions. We find that self-propulsion is possible in viscoelastic media even if the motion is reciprocal.

8:36AM H20.00002 Assembly and dynamics of synthetic cilia. TIM SANCHEZ, Brandeis University, Physics Department — From motility of simple protists to determining the handedness of complex vertebrates, highly conserved eukaryotic cilia and flagella are essential for the reproduction and survival of many biological organisms. Despite extensive studies, the exact mechanism by which individual components coordinate to produce ciliary beating patterns remains unknown. We describe a novel approach towards studying ciliary beating. Instead of deconstructing a fully functional organelle from the top-down, we describe a process by which synthetic cilia-like structures are assembled from the bottom-up. We find that simple mixtures of microtubules, kinesin clusters, and a bundling agent produce spontaneous oscillations in MT bundles, suggesting that self-organized beating may be a generic feature of internally driven bundles. Furthermore, bundles in close proximity spontaneously coordinate their beating to generate metachronal traveling waves, reminiscent of the waves seen in ciliary fields. These findings and future refinements of the system can potentially provide insights into general design principles required for engineering synthetic cilia as well as understanding the biological analogues.

9:12AM H20.00003 Polar patterns in active fluids. M. CRISTINA MARCHETTI, Physics Department & Syracuse Biomaterials Institute, Syracuse University. Active fluids are a new class of soft materials composed of interacting units that consume energy and collectively generate motion and mechanical stress. Examples include bacterial suspensions, mixtures of cytoskeletal filaments and motor proteins, and migrating epithelial cell layers. Due to their elongated shape, active particles can exhibit orientational order at high concentration and have been likened to “living liquid crystals”, with either nematic or p - polar symmetry. In this talk I will discuss the spatio-temporal dynamics of continuum models of active fluids in two dimensions, focusing on the case of a system with polar symmetry as relevant to bacterial suspensions. Upon increasing activity, the active fluid displays increasingly complex patterns, including traveling bands, traveling vortices and chaotic behavior. The nonlinear hydrodynamic equations can be mapped onto a diffusion-reaction-convection model, highlighting the connection between the complex dynamics of active system and that of excitable systems.

9:48AM H20.00004 Swimming of Paramecium in confined channels. SUNGHWAN JUNG, Virginia Tech — Many living organisms in nature have developed a few different swimming modes, presumably derived from hydrodynamic advantage. Paramecium is a ciliated protozoan covered by thousands of cilia with a few nanometers in diameter and tens of micro-meters in length and is able to exhibit both ballistic and meandering motions. First, we characterize ballistic swimming behaviors of ciliated microorganisms in glass capillaries of different diameters and explain the trajectories they trace out. We develop a theoretical model of an undulating sheet with a pressure gradient and discuss how it affects the swimming speed. Secondly, investigation into meandering swimming within rectangular PDMS channels of dimension smaller than Paramecium length. We find that Paramecium executes a body-bend (an elastic buckling) using the cilia while it meanders. By considering an elastic beam model, we estimate and show the universal profile of forces it exerts on the walls. Finally, we discuss a few other locomotion of Paramecium in other extreme environments like gel.

10:24AM H20.00005 Helical swimming in viscoelastic and porous media. BIN LIU, School of Engineering, Brown University — Many bacteria swim by rotating helical flagella. These cells often live in polymer suspensions, which are viscoelastic. Recently there have been several theoretical and experimental studies showing that viscoelasticity can either enhance or suppress propulsion, depending on the details of the microswimmer. To help clarify this situation, we study experimentally the motility of the flagellum using a scaled-up model system - a motorized helical coil that rotates along its axial direction. A free-swimming speed is obtained when the net force on the helix is zero. When the helix is immersed in a viscoelastic (Boger) fluid, we find an increase in the force-free swimming speed as compared with the Newtonian case. The enhancement is maximized at a Deborah number of approximately one, and the magnitude depends not only on the elasticity of the fluid but also on the geometry of the helix. In the second part of my talk, I will discuss how spatial confinements, such as a porous medium, affect the flagellated swimming. For clarity, the porous media are modeled as cylindrical cavities with solid walls. A modified boundary element method allows us to investigate a situation that the helical flagella are very close to the wall, with high spatial resolution and relatively low computational cost. To our surprise, at fixed power consumption, a highly coiled flagellum swims faster in narrower confinements, while an elongated flagellum swims faster in a cavity with a wider opening. We try understanding these effects with simple physical pictures.

Tuesday, February 28, 2012 8:00AM - 11:00AM –  
Session H26 DCOMP GSNP: Focus Session: Friction, Fracture and Deformation Across Length Scales - Friction Across Length Scales 257B
8:00AM H26.00001 Rock Friction from the Nanoscale to the San Andreas Fault, DAVID L. GOLDSBY, Brown University — Nucleation of earthquakes (EQs) and the resistance of faults to shearing during EQs are determined by nano-to-micro-scale frictional processes that occur on tectonic-scale faults. A first-order observation from rock-friction studies is that of ageing, i.e., the linear increase in friction with the log of the time of stationary contact, manifest as a positive or negative dependence of friction on sliding rate. A necessary condition for EQ nucleation is a negative rate dependence of friction. In spite of the success of friction ‘laws’ which encapsulate the rate and time dependences of friction in fitting experimental data and reproducing natural phenomena in EQ models, these laws lack a physical basis. Atomic force microscope (AFM) experiments on silica-silica contacts explore the physics of ageing, more specifically increases in adhesion of nanometers-sized contacts with time (Li et al., Nature, 2011). The experiments reveal prominent ageing which increases with humidity, as in rock friction tests, without increases in contact area due to creep (the canonical explanation for ageing in rock-friction tests). Ageing in the AFM tests is in fact much larger than in rock-friction tests, a discrepancy explained with a simple multi-asperity contact model. At EQ slip rates (≥1 m/s) a variety of dynamic fault-weakening mechanisms may decrease the shear resistance of faults, which would have important consequences for the magnitudes of EQ stress drops, strong ground motions and accelerations, for the EQ energy budget, and for the state of stress on faults. Experiment on rock found in the Earth’s crust for slip rates up to ~0.4 m/s over ~40 m of slip, reveals a dramatic 1/3 decrease in frictional strength above a characteristic weakening velocity $V_w$ of ~0.1 m/s (Goldsby and Tullis, Science, 2011). Friction is also revealed to be a nearly pure function of slip rate, i.e., it adjusts to the ambient slip rate over only microns of slip. The observations are explained by ‘flash heating’, whereby microscopic asperity contacts become intensely frictionally heated and weakened above $V_w$. Dramatically lower friction due to flash heating may explain why heat flow along active faults like the San Andreas Fault is much lower than expected. Strong velocity-sensitive friction and the rapid strength recovery with decreasing slip rate from flash heating may explain why EQ ruptures propagate as slip pulses rather than as cracks.

8:36AM H26.00002 Avalanche Distributions and the Effect of Inertia in Strained Amorphous Solids1, K. MICHAEL SALERNO, MARK O. ROBBINS, Johns Hopkins University, CRAIG MALONEY, Carnegie Mellon University — We present results from two- and three-dimensional simulations of a disordered, binary Lennard-Jones solid under quasi-static, steady-state shear. The solid responds to the applied shear strain with bursts of particle movement and plasticity. The energy $E$ of these avalanches spans a wide range and follows a power-law distribution $N(E) \propto E^{-\gamma}$ with three distinct exponents, depending on the importance of inertia. In the limit of overdamped dynamics, or no inertia, we find $\gamma \approx 0.8$, consistent with previous energy minimization simulations. As inertia becomes more important, the system approaches an unstable critical point where $\gamma = 1$. In the underdamped limit, where inertia plays a large role, the distribution of avalanches follows a power-law with exponent $\gamma \approx 1.4$ with an excess of system-spanning events. The three regimes have distinct finite-size-scaling exponents. The regime that consistently exponents are found in two and three dimensions indicates that both may be in the mean-field limit. Spatial correlations in avalanches under different damping regimes will be contrasted.

8:48AM H26.00003 Dynamic Phase Diagram and Jamming for Driven Dislocation Assemblies, CHARLES REICHHARDT, CYNTHIA REICHHARDT, CAIZHI ZHOU, IRENE BEYERLEIN, Los Alamos National Laboratory — By using large scale numerical simulations for driven dislocations in 2D, we show that the resulting dynamic phase diagram has the same features found for driven vortex matter and charge density waves in the presence of random disorder. For low loads the system is pinned or jammed. Just above the onset of motion we observe strong velocity fluctuations with 1/f noise properties and bimodal size distributions associated with rapidly fluctuating structures. At higher loads there is a dynamic reordering into a state of partially ordered domain walls with a pronounced drop in the velocity fluctuations as well as a reduction in the noise power. Experiments on rock found in the Earth’s crust for slip rates up to ~0.4 m/s over ~40 m of slip, reveals a dramatic 1/3 decrease in frictional strength above a characteristic weakening velocity $V_w$ of ~0.1 m/s (Goldsby and Tullis, Science, 2011). Friction is also revealed to be a nearly pure function of slip rate, i.e., it adjusts to the ambient slip rate over only microns of slip. The observations are explained by ‘flash heating’, whereby microscopic asperity contacts become intensely frictionally heated and weakened above $V_w$. Dramatically lower friction due to flash heating may explain why heat flow along active faults like the San Andreas Fault is much lower than expected. Strong velocity-sensitive friction and the rapid strength recovery with decreasing slip rate from flash heating may explain why EQ ruptures propagate as slip pulses rather than as cracks.

9:00AM H26.00004 Scale invariant avalanches: a critical confusion, OSVANNY RAMOS, Laboratoire PMCN, University Lyon 1, 43 bd. du 11 novembre 1918, 69622 Villeurbanne, France — In the last decades considerable efforts have been devoted to understanding single events related to friction, fracture and unjamming transition, commonly denominated avalanches. However, in many different natural scenarios -from subcritical fracture to earthquake dynamics- these events are of all scales, a situation that has often been interpreted within the formalism of critical phenomena, and having as a relevant consequence the inherently unpredictability of scale-invariant avalanches. A revision of this interpretation which departs from standard ideas is presented here, resulting in [1]: (i) critical systems are not necessarily unpredictable; (ii) slowly driven systems evolving through power-law distributed avalanches are not necessarily critical; and (iii) scale-invariant avalanches are not necessarily unpredictable. Simple simulations and granular experiments [2] confirm the findings.

1Supported by NSF DMR-1006805

9:12AM H26.00005 Unjamming of amorphous films probed with a transverse shear ultrasonic oscillator, JULIEN LEOPOLDES, GUILLAUME CONRAD, XIAOPING JIA, Université Paris Est, France, LPMDI TEAM — Friction between solids depends essentially on the response of the interfacial amorphous layer to shear and compressive stresses. Hence, the transition from static to dynamic friction corresponds to the unjamming transition of confined amorphous materials [1]. With a shear ultrasonic oscillator, we study the boundary lubrication due to molecular films confined between a plane and a sphere [2]. We observe a linear viscoelastic behaviour at low oscillation amplitude and a nonlinear frictional microslip regime at high amplitude. In a new set of experiments, the system is brought near the unjamming transition by applying a static force. The interfacial layer softens before unjamming, as indicated by the linear response of the oscillator. We suggest an interpretation based on a stress-induced decrease of the free volume, and propose a corresponding heuristic model. Last, we show how ultrasonic in-plane oscillations of ~ 10 nm amplitude can trigger unjamming, and we discuss the possible related mechanisms.


9:24AM H26.00006 Universality of Deformation Down to the Nanoscale, NIR FRIEDMAN, Department of Physics, University of Illinois at Urbana-Champaign, ANDREW T. JENNINGS, Division of Engineering and Applied Sciences, Caltech, GEORGIOS TSEKENIS, Department of Physics, University of Illinois at Urbana-Champaign, JU-YOUNG KIM, Division of Engineering and Applied Sciences, Caltech, MOLEI TAO, Department of Computing and Mathematical Sciences, Caltech, JONATHAN T. UHL, None, JULIA R. GREER, Division of Engineering and Applied Sciences, Caltech, KARIN A. DAHMEN, Department of Physics, University of Illinois at Urbana-Champaign — Deformation on macroscopic scales is often modeled as a continuous process, which in reality occurs via a sequence of nanometer-sized discrete slips. We report statistical analyses of slip size distributions obtained by uniaxial compression experiments on nano-crystals of different crystal structures and sizes down to 75 nm. We show that a simple mean field theory (MFT) correctly predicts the statistical behavior by collapsing data using the MFT exponents and scaling function. This study demonstrates that a simple model captures the statistics and universality class of discrete deformation events in a variety of metallic nano-crystals down to the smallest experimentally accessed length scales.
9:36AM H26.00007 Boundary lubrication under pressure: could the friction jump down instead of up? ANDREA VANOSSE, SISSA & CNR-IOM DEMOCRITOS, Trieste, Italy, ANDREA BENASSI, CNR-IEI, Milano, Italy, NICOLA VARINI, ICHEC, Dublin, Ireland, ERIO TOSATTI, SISSA & CNR-IOM DEMOCRITOS, ICTP, Trieste, Italy — The sliding friction during pressure squeezeout of a boundary lubricated contact has been shown [1,2] to undergo upward jumps every time a lubricant atomic layer is expelled. Here we ask the question whether the jump could not be downward. Whereas most studies focus on the layered structure which the confined lubricant takes in the normal direction, the element we wish to consider is a possible change of parallel periodicity occurring at the squeezeout transition. Such changes have been reported in simulations [3], but their effect has not been discussed so far. One possible effect could be a transition of the slider-lubricant interface commensurability, producing a switch of the frictional mechanism, from lubricant melting-freezing in a commensurate state, to superlubric in an incommensurate one — in this case with a drop of friction for increasing load. We exemplify this effect by MD simulations, where we replace for convenience the open squeezeout system with a closed system, where the lubricant is sealed between the sliders. As the number of layers under pressure, the planar lubricant structural parameter also drops. This change reflects in a sliding friction jump, which is easily observed to be downwards. The potential observability of load-induced friction drops will be discussed.


9:48AM H26.00008 Plasticity as a Depinning Phase Transition GEORGIOS TSEKENIS, University of Illinois at Urbana-Champaign, PAK YUEN CHAN, None, THOMAS FEHM, Ludwig-Maximilians-Universität Muenchen, JONATHAN T. UHL, None, JONATHAN DANTZIG, NIGEL GOLDENFELD, KARIN DAHMEN, University of Illinois at Urbana-Champaign, Crystaline materials deform in an intermittent way via slip-avalanches, which exhibit a variety of scale-invariant behaviors that have been interpreted as a pinning-depinning transition. We use discrete dislocation dynamics at zero temperature to resolve the temporal profiles of slip-avalanches and extract the finite-size scaling properties of the dislocation system, thus going beyond gross aggregate statistics. We provide a comprehensive set of scaling exponents, which establishes that the dynamics of plasticity, in the absence of hardening, is consistent with the mean field interface depinning universality class, even though there is no quenched disorder. Finally, we show how Phase Field Crystal simulations should act on the effect of temperature on intermittent dislocation dynamics and its critical scaling behavior.

10:00AM H26.00009 Tribo-induced melting and temperature gradients at slidingasperity contacts J. Krim, L. Pan, D.J. Lichtenwalner, North Carolina State University, A.I. Kingon, Brown University — Tribo-induced nanoscale surface melting phenomena have been investigated by means of a combined QCM-STM technique [1] for a range of Au and Au-Ni alloys with varying compositional percentages and phases. The QCM-STM setup allows studies to be performed at sliding speeds of up to m/s, and also reveals valuable information concerning tip-substrate temperature gradients. [3] A transition from solid-solid to solid-“liquid like” contact was observed for each sample at sufficiently high asperity sliding speeds. Pure gold, solid-solution and two-phase Au-Ni (20 at.% Ni) alloys were compared, which are materials of great relevance to MEMS RF switch technology. [2] The transition points agree favorably with theoretical predictions for their surface melting characteristics. We acknowledge NSF and AFOSR support for this research.


10:12AM H26.00010 Formation of Stable Metallic Nanocontacts by mechanical annealing CARLOS SABATER, Dep. of Applied Physics University of Alicante, Spain, CARLOS UNTIEDT, Dep. App. Phys. Univ. Alicante, SP, JUAN JOSE PALACIOS, Dep. of Condensed Matter Physics, Univ. Autonoma de Madrid, SP, MARIA JOSE CATURLA, Dep. App. Phys., Univ. Alicante, Spain, — Metallic nanocontacts (NC) can be fabricated using STM or related techniques. In these experiments the size of the NC can be followed, down to the atomic contact, by measuring its electrical conductance. Such evolution will normally differ for each experimental realization and therefore conductance histograms are used to identify preferential configurations. It can be shown that occasionally there are some atomic configurations that can be repeated during consecutive cycles of mechanical deformation of the contacts. Here we report experiments for gold NC where the same trace of conductance can be observed for hundreds of cycles of formation and rupture. We have studied the process leading to such repetitiveness of the traces and found that this is possible when the two surfaces to a conductance value of approximately 5-6 G_0.

10:24AM H26.00011 Scaling in earthquake models with inhomogeneous damage RACHELE DOMINGUEZ, Randolph-Macon College, KRISTY TIAMPO, University of Western Ontario, C.A. SERINO, W. KLEIN, Boston University — We study the scaling of earthquake models that are variations of Olami-Feder-Christensen and Burridge-Knopoff models, in order to explore the effect of spatial inhomogeneities on earthquake-like systems when interaction ranges are long, but not necessarily longer than the distances associated with the inhomogeneities of the system. For long ranges and without inhomogeneities, such models have been found to produce scaling similar to GR scaling found in real earthquake systems. In the earthquake models discussed here, damage is distributed inhomogeneously throughout and the interaction ranges, while long, are not longer than all of the damage length scales. We find that the scaling depends not only on the amount of damage, but also on the spatial distribution of that damage.

10:36AM H26.00012 Stress Corrosion Fracture of Silicate Glasses: How Far Can Water Penetrate? ELISABETH BOUCHAUD, CEA-Saclay ESPCI ParisTech, CINDY ROU NTREE, FABRICE COUSIN, CEA-Saclay, FREDERIC LECHEAULT, ENS Paris, STEPHANNE CHAPULIOT, AREVA, LAURENT PONSON, I D Alembert Paris, JEAN-PHILIPPE BOUCHAUD, CFM Paris — Although glass can be considered as homogeneous at scales as small as a few tens of nanometers, since it exhibits no density fluctuations beyond, its amorphous structure makes it a disordered material with respect to fracture properties. Fluctuations of the orientations of Si-O bonds with respect to the external stress make it unlikely that bonds closest to the crack tip break first, despite the high stress concentration. As a consequence, glass behaves in a quasi-brittle manner rather than in a purely elastic way. In situ Atomic Force Microscopy experiments tracking the slow progression of a stress corrosion crack seemed to show indeed the opening and growth of nano size flaws ahead of the tip. However, these results are controversial, because of artifacts which may seriously affect the observations. Furthermore, the low diffusion coefficient of water in silica should forbid hydrolysis at a distance from the crack tip, except at the free surface. Nevertheless, our recent neutron reflectivity experiments show that water actually penetrates into the material during stress corrosion fracture. Comparing two experiments performed for different crack velocities shows that the diffusion coefficient is hugely increased under stress, allowing for bond breakings at ~ten nanometers ahead of the main crack tip.
a phase separation of hemi-helical structure, helical structure and hybrid structure which have similarities to coiled polymer molecules and plant tendrils. Helix deforming principally by bending from those where twisting dominates. Changing the prestrain and the ratio between the thickness and the width induce the strip cross-section, the constitutive behavior of the elastomer and the value of the pre-strain. Topologically, the perversions also separate regions of the helical sections of half wavelength in opposite chiralities and separated by perversions. The hemi-helix wavelength and the number of perversions are determined by the strip cross-section, the constitutive behavior of the elastomer and the value of the pre-strain. In particular, we aim to gain predictive understanding of the transition from planar to non-planar solutions as well as the localization of torsion in the non-planar configurations. The experimentally observed behavior of our custom-fabricated naturally curved rods is captured well by simulations and is rationalized through scaling arguments.

SUO, DAVID CLARKE, Harvard University — A variety of three dimensional curls are produced by a simple generic process consisting of pre-straining one, JIANGSHUI HUANG, JIA LIU, BENEDIKT KROLL, KATIA BERTOLDI, ZHIGANG DOMINIC VELLA, EMMANUEL DU PONTAVICE, CAMERON HALL, ALAIN GORIELY, OCCAM, University of Oxford — Spherical neodymium magnets have become a popular toy in recent years. In this talk, we present the results of some experimental and theoretical investigations into the peculiar elastic-like behaviour exhibited by chains of these magnetic spheres. We show how the dipole-dipole interactions between spheres penalise deformation, and we find that the effect is demonstrated in both, the Ising (one spin dimension) and the Heisenberg model (three spin dimensions), irrespective which kind of dynamics (Metropolis spin-flip dynamics or Landau-Lifshitz-Gilbert precessional dynamics) is used. For both models the limiting case of Coulomb friction can be treated analytically. Furthermore we present an empirical expression reflecting the correct Stokes behavior and therefore yielding the correct cross-over velocity and dissipation. arXiv:1111.2494

1Financial support by the German Research Foundation (DFG, via SFB616) and the German Academic Exchange Service (DAAD, PROBRAL programme) is acknowledged.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H52 GSNP DFD: Focus Session: Extreme Mechanics - Rods 153C

8:00AM H52.00001 Dynamiccurling of a naturally curved Elastica1, BASILE AUDOLY, Institut Jean le Rond d'Alembert, University Paris 6 and CNRS — We consider the motion of a naturally curved Elastica that has been flattened onto a hard surface. When it is released from one end, the Elastica lifts off the surface and curls dynamically into a moving spiral. The motion is governed by inertia, bending and geometric nonlinearity. At long times, the dynamics follows a self-similar regime: the size of the spiral grows like the cubic root of time, while the velocity of the front reaches a constant value. The asymptotic velocity is derived analytically, and compared to numerical simulations and to experiments.

1Joint work with Andrew Callan-Jones and Pierre-Thomas Brun

8:36AM H52.00002 The Mechanics of Curly Hair, JAMES MILLER, Massachusetts Institute of Technology, ARNAUD LAZARUS, BREENNA BERRY, MIT, BASILE AUDOLY, Institut d’Alembert (University Paris 6), PEDRO REIS, MIT — We explore the oft-neglected role of intrinsic natural curvature on the mechanics of elastic rods. Our testbed, a hanging hair, is a deceivingly simple system that exhibits complex mechanics and geometrically nonlinear behavior. Through a combination of precision desktop-scale experiments, numerical simulations, and theoretical analysis, we seek physical insight into the nontrivial configurations adopted by a naturally curved elastic rod that is suspended under its own weight. In particular, we aim to gain predictive understanding of the transition from planar to non-planar solutions as well as the localization of torsion in the non-planar configurations. The experimentally observed behavior of our custom-fabricated naturally curved rods is captured well by simulations and is rationalized through scaling arguments.

8:48AM H52.00003 The Shape of a Ponytail and the Statistical Physics of Hair Fiber Bundles, RAYMOND E. GOLDSTEIN, University of Cambridge, PATRICK B. WARREN, Unilever R&D Port Sunlight, ROBIN C. BALL, University of Warwick — From Leonardo to the Brothers Grimm our fascination with hair has endured in art and science. Yet, a quantitative understanding of the shapes of a hair bundles has been lacking. Here we combine experiment and theory to propose an answer to the most basic question: What is the shape of a ponytail? A model for the shape of hair bundles is developed from the perspective of statistical physics, treating individual fibers as elastic filaments with random intrinsic curvatures. The combined effects of bending elasticity, gravity, and bundle compressibility are recast as a differential equation for the envelope of a bundle, in which the compressibility enters through an “equation of state.” From this, we identify the balance of forces in various regions of the ponytail, extract the equation of state from analysis of ponytail shapes, and relate the observed pressure to the measured random curvatures of individual hairs.

9:00AM H52.00004 Following the equilibria of slender elastic rods, ARNAUD LAZARUS, JAMES MILLER, PEDRO REIS, Massachusetts Institute of Technology — We present a novel continuation method to characterize and quantify the equilibria of elastic rods under large geometrically nonlinear displacements and rotations. To describe the kinematics we exploit the synthetic power and computational efficiency of quaternions. The energetics of bending, stretching and torsion are all taken into account to derive the equilibrium equations which we solve using an asymptotic numerical continuation method. This provides access to the full set of analytical equilibrium branches (stable and unstable), a.k.a bifurcation diagrams. This is in contrast with the individual solution points attained by classic energy minimization or predictor-corrector techniques. We challenge our numerics for the specific problem of an extremely twisted naturally curved rod and perform a detailed comparison against a precision desktop-scale experiments. The quantification of the underlying 3D buckling instabilities and the characterization of the resulting complex configurations are in excellent agreement between numerics and experiments.

9:12AM H52.00005 The elasticity of magnetic chains: From self-buckling to self-assembly, DOMINIC VELLA, EMMANUEL DU PONTAVICE, CAMÉRON HALL, ALAIN GORIELY, OCCAM, University of Oxford — Spherical neodymium magnets have become a popular toy in recent years. In this talk, we present the results of some experimental and theoretical investigations into the peculiar elastic-like behaviour exhibited by chains of these magnetic spheres. We show how the dipole-dipole interactions between spheres penalise deformation, and we find that the form of this penalty is different for a long chain compared to a short chain. Finally, we investigate the dynamic self-assembly of these chains into cylindrical structures.

9:24AM H52.00006 Spontaneous and Deterministic Three-dimensional Curling of Pre-strained Elastomeric Strips: From Hemi-helix to Helix, JIASUHUI HUANG, JIA LUI, BENEDIKT KROLL, KATIA BERTOLDI, ZHIGANG SUO, DAVID CLARKE, Harvard University — A variety of three dimensional curls are produced by a simple generic process consisting of pre-straining one elastomeric strip, joining it to another and then releasing the bi-strip. The heli-helix, one kind of three dimensional curls, consists of multiple, alternating helical sections of half wavelength in opposite chiralities and separated by perversions. The hemi-helix wavelength and the number of perversions are determined by the strip cross-section, the constitutive behavior of the elastomer and the value of the pre-strain. Topologically, the perversions also separate regions of the helix deforming principally by bending from those where twisting dominates. Changing the prestrain and the ratio between the thickness and the width induce a phase separation of hemi-helical structure, helical structure and hybrid structure which have similarities to coiled polymer molecules and plant tendrils.
The observed behavior is rationalized through scaling arguments and captured by numerical simulations. We quantify the wavelength and pitch of the periodic patterns through direct digital imaging and record the reaction forces at both ends of the pipe. The buckling and post-buckling behavior is found to be highly dependent on the systems' geometry, in particularly the aspect ratio of the rod to pipe. These experiments are also modeled using a discrete elastic rod simulation that includes frictional effects. A hyper-elastic rod inside a transparent acrylic pipe. These experiments are also modeled using a discrete elastic rod simulation that includes frictional effects.

PABON, Schlumberger-Doll Research, KATIA BERTOLDI, Harvard University, PEDRO REIS, Massachusetts Institute of Technology — We investigate the rectification, and advection of slack. Twist resistance. Local arc length conservation is enforced by the stress, a Lagrange multiplier field screened by curvature. Uniform stress fields are generated by the first five multiples of Ωc/3. The dynamics of the patterns can be described by matching the upper (linear) and the lower (non-linear) portions of the thread. Following this path we propose a toy model that successfully reproduces the observed transitions from the steady dragged configuration to sinusoidal meanders, alternating loops, and the translated coiling pattern as the belt speed is varied.

We acknowledge the funding from FQRNT, NSERC and CFI.

9:36AM H52.00007 Snakes Out of the Plane, ANDREW MCCORMICK, BRUCE A. YOUNG, L. MAHADEVAN, Harvard University — We develop a new computational model of elastic rods, taking into account shear and full rotational dynamics, as well as friction, adhesion, and collision. This model is used to study the movement of snakes in different environments. By applying different muscular activation patterns to the snake, we observe many different patterns of motion, from planar undulation to sudden strikes. Many of the most interesting behaviors involve the snake rising out of the horizontal plane in the vertical direction. Such behaviors include a sand snake sidewinding over the hot desert sand and a cobra rearing up into a defensive striking position. Experimental videos of live snakes are analyzed and compared with computational results. We identify and explain a new form of movement previously unobserved: “collateral locomotion.”

1 We acknowledge support from the NDSEG program.

9:48AM H52.00008 Analysis of the fluid mechanical sewing machine, PIERRE-THOMAS BRUN, Institut Jean le Rond d’Alembert/Lab. FAST, UPMC, Univ Paris-Sud, CNRS, BASILE AUDOLY, Institut Jean le Rond d’Alembert, UPMC, CNRS, NEIL RIBE, Lab FAST, UPMC, Univ Paris-Sud, CNRS — A thin thread of viscous fluid falling onto a moving belt generates a surprising variety of patterns, similar to the stitch patterns produced by a traditional sewing machine. By simulating the dynamics of the viscous thread numerically, we can reproduce these patterns and their bifurcations. The results lead us to propose a new classification of the stitch patterns within a unified framework, based on the Fourier spectra of the motion of the point of contact of the thread with the belt. The frequencies of the longitudinal and transverse components of the contact point motion are locked in most cases to simple ratios of the frequency Ωc of steady coiling on a surface at rest (i.e., the limit of zero belt speed). In particular, the “alternating loops” pattern involves the first five multiples of Ωc/3. The dynamics of the patterns can be described by matching the upper (linear) and the lower (non-linear) portions of the thread. Following this path we propose a toy model that successfully reproduces the observed transitions from the steady dragged configuration to sinusoidal meanders, alternating loops, and the translated coiling pattern as the belt speed is varied.

1 We acknowledge the funding from FQRNT, NSERC and CFI.

10:00AM H52.00009 Microfabrication of a spider-silk analogue through the liquid rope coiling instability, FREDERICK P. GOSSelin, DANIEL THERRAULT, MARTIN LEVESQUE, Ecole Polytechnique de Montreal — Spider capture silk outperforms most synthetic materials in terms of specific toughness. We developed a technique to fabricate tough microstructured fibers inspired by the molecular structure of the spider silk protein. To fabricate microfibers (with diameter ~ 30 µm) with various mechanical properties, we yield the control of their exact geometry to the liquid rope coiling instability. This instability causes a thread of honey to wiggle as it buckles when hitting a surface. Similarly, we flow a filament of viscous polymer solution towards a substrate moving perpendicularly at a slower velocity than the filament flows. The filament buckles repetitively giving rise to periodic meanders and stitch patterns. As the solvent evaporates, the filament solidifies into a fiber with a geometry bestowed by the instability. Microfracture tests performed on fibers show interesting links between the mechanical properties and the instability patterns. Some coiling patterns give rise to high toughness due to the sacrificial bonds created when the viscous filament loops over itself and fuse. The sacrificial bonds in the microstructured fiber play an analogous role to that of the hydrogen bonds present in the molecular structure of the silk protein which give its toughness to spider silk.

10:12AM H52.00010 Buckling Instability and Stress Propagation in Rods with Elastic Support, ZI CHEN, Biomedical Engineering, Washington Univ. in St. Louis, WANLIANG SHAN, Mechanical & Aerospace Engineering, Princeton Univ., ANKITA GUMASTE, Neuroscience & Behavioral Biology, Emory Univ., WINSTON SOBOYEJO, Mechanical & Aerospace Engineering, Princeton Univ., CLIFFORD BRANGWYNE, Chemical & Biological Engineering, Princeton Univ. — The cytoskeleton of living cells is a composite material consisting of a network of biopolymers including f-actin and microtubules (MTs). MTs are able to bear significant compressive loads in cells as a result of reinforced short wavelength buckling, due to the surrounding actin network. However, the length scale of compressive force propagation, even for macroscopic rods, remains poorly understood. Here we propose a minimal theory that incorporates elastic restoring forces from the surrounding network, elucidating the compressive force-dependence of the buckled rod shape. We identify a threshold length as the effective distance stresses can propagate in such network, and show that the decay length is tunable by modifying the longitudinal mechanical coupling coefficients. We test these predictions with experiments in macroscopic rods, and show that the degree of mechanical coupling directly controls the penetration depth of buckling, in agreement with theoretical and numerical predictions. Our results suggest that the length scale over which mechanical signals are transduced in cells may be actively controlled, and could provide design principles for novel types of fiber composite materials based on biomimetic control of the longitudinal coupling coefficients.

10:24AM H52.00011 Undulatory buckling of a rod constrained by an elastic matrix, JIA LIU, TIANXIANG SU, Harvard University, OSCAR LOPEZ-PAMIES, UIUC, PEDRO REIS, MIT, KATIA BERTOLDI, Harvard University — Elastic instabilities of rods constrained by an elastic matrix and subjected to axial compression have long been recognized as essential for structural applications in the context of failure mitigation and, more recently, towards exploitation of functionality. Relevant fields for this class of problems include drilling, biomedical instrumentation and root growth in plants. We explore the two possible scenarios observed when, above a threshold load, compression is applied to a rod constrained by a matrix: i) the rod can develop a planar oscillatory solution (sinusoidal buckling) or ii) it can take the configuration of a helix (helical buckling). We identify the principal parameters of this system, perform a systematic parametric study and rationalize the phase diagram through a hybrid of theoretical and numerical analyses. Particular attention is devoted to the effect of the mechanical properties of the constraining matrix which is found to have a critical influence on this buckling scenario.

10:36AM H52.00012 Slack, stress, and noisy structures in inertial strings, JAMES HANNA, CHRISTIAN SANTANGELO, Department of Physics, University of Massachusetts - Amherst — Strings and chains are inextensible filaments with negligible bending and twist resistance. Local arc length conservation is enforced by the stress, a Lagrange multiplier field screened by curvature. Uniform stress fields are generated by a wide class of inertial motions that includes travelling waves of curvature and torsion, while gradients in stress result in more complicated dynamics. We will discuss a theoretical example inspired by experimental and numerical observations of the growth of an arch in a straightening chain, involving the amplification, rectification, and advection of slack.

10:48AM H52.00013 Sinusoidal to helical buckling of an elastic rod under a cylindrical constraint, TIANXIANG SU, Harvard University, JAMES MILLER, ARNAUD LAZARUS, Massachusetts Institute of Technology, NATHAN WICKS, JAHI PABON, Schlumberger-Doll Research, KATIA BERTOLDI, Harvard University, PEDRO REIS, Massachusetts Institute of Technology — We investigate the buckling and post-buckling behavior of an elastic rod loaded under cylindrical constraint. Our precision desktop-scale experiments comprise of axially compressing a hyper-elastic rod inside a transparent acrylic pipe. These experiments are also modeled using a discrete elastic rod simulation that includes frictional effects. Under imposed displacement, the initially straight rod first buckles into a sinusoidal mode and eventually undergoes a secondary instability into a helical buckling regime. The buckling and post-buckling behavior is found to be highly dependent on the systems’ geometry, in particularly the aspect ratio of the rod to pipe diameter. We measure the wavelength and pitch of the periodic patterns through direct digital imaging and record the reaction forces at both ends of the pipe. The observed behavior is rationalized through scaling arguments and captured by numerical simulations.

Tuesday, February 28, 2012 8:00AM - 11:00AM – Session H53 GSNP: Focus Session: Continuum Descriptions of Discrete Materials
8:00AM H53.00001 Failure of a loose packing of grains, GREG FARRELL, NARAYANAN MENON, UMass-Amherst — One-sided repulsive interactions and history-dependent friction forces can cause the mechanics of real granular systems to deviate significantly from that of cohesive solids. Marked deviations from elastic behavior can be seen in the mechanical response and structure of sedimented loose packings of frictional spheres even for very delicate perturbations. In our experiments, particles’ displacements are observed with 3D fluorescent imaging as a shear plane is displaced through the packing. As anticipated, we find the shear force is approximately linear with the displacement between discrete yielding events. However, even in this apparently linear regime, structural aging continues to occur for the smallest displacements that we can apply. This suggests the inaccessibility of a reversible shear deformation regime in loose packings of granular material. We present a spatial characterization of the particle motion that distinguishes between these continuous instances of irreversibility and the larger discrete failure events.

8:12AM H53.00002 Jamming in Hopper Flows: Analysis of Survival Times1, MICHAL DICHTER, Brandeis University, SHUBHA TEWARI, Western New England University, BULBUL CHAKRABORTY, Brandeis University — Many granular systems experience a transition from a fluid-like state to a solid-like state characterized by a sudden arrest in dynamics, or “jamming.” Recent experiments by the Behringer Group at Duke University suggest a probabilistic model of jamming in hopper flows. We will show the results of numerical simulations of dense, gravity-driven, granular flows in a two-dimensional hopper with a tapered outlet [PRE 79, 011303 (2009)]. We will present results for the statistics of mass flow at the outlet, and the probability of survival without a jam. We will correlate the survival times with velocity and density distributions near the hopper opening.

8:24AM H53.00003 Experimental analysis on how grain properties affect the performance of jammed granular systems for variable stiffness robotic applications1, NADIA CHENG, KARL IAGNEMMA, ANETTE HOSOI, KATY GERÓ, Massachusetts Institute of Technology — Jamming of granular media has become increasingly utilized as a variable stiffness mechanism for industrial and robotic applications. The goal of our work is to better understand how grain properties affect jamming so that granular systems can be designed to fulfill the requirements of a given application. We have primarily focused on experimental studies to analyze how certain grain properties—such as shape, surface roughness, size distribution, and shape distribution—affect the performance of granular systems. Potential applications that utilize jamming would typically require that a contained granular system transition between effective solid states (e.g., when particular shape or strength needs to be maintained) and effective liquid states (e.g., when the system needs to be compliant such that it can be shaped or actuated by its environment). Therefore, we are interested in quantifying 1) the strength of compacted granular systems in their effective solid states and 2) the “ease of flow” and compliance of granular systems in their effective liquid states.

8:36AM H53.00004 Shear-Transformation-Zone Theory of Glassy Diffusion, Stretched Exponentials, and the Stokes-Einstein Relation, JAMES LANGER, University of California, Santa Barbara — The success of the shear-transformation-zone (STZ) theory in accounting for broadly peaked, frequency-dependent, glassy viscoelastic response functions is based on the theory’s first-principles prediction of a wide range of internal STZ transition rates. Here, I propose that the STZ’s are the dynamic heterogeneities frequently invoked to explain Stokes-Einstein violations and stretched-exponential relaxation in glass-forming materials. I find that, to be consistent with observations of Fickian diffusion near \( T_g \), an STZ-based diffusion theory must include cascades of correlated events, but that the temperature dependence of the Stokes-Einstein ratio is determined by an STZ-induced enhancement of the viscosity. Stretched-exponential relaxation of density fluctuations emerges from the same distribution of STZ transition rates that predicts the viscoelastic behavior.

9:12AM H53.00005 A granular flow law based on nonlocal fluidity, KEN KAMRIN, MIT, GEORG KOVAL, INSA Strasbourg — A general, three-dimensional law to predict granular flow in an arbitrary geometry has been an elusive goal for decades. Recently, an elasto-plastic continuum model has shown the ability to approximate steady flow and stress profiles in multiple inhomogeneous flow environments. However, the model does not capture some phenomena observed in the slow, creeping flow regime. As normalized flow-rate decreases, granular stresses are observed to become largely rate-independent and a dominating length-scale emerges in the mechanics. This talk attempts to account for these effects using the notion of nonlocal fluidity, which has proven successful in treating nonlocal effects in emulsions. The idea is to augment the usual granular fluidity law with a diffusive second-order term scaled by the particle size that spreads flowing zones accordingly. Below the yield stress, the local contribution of the fluidity becomes rate-independent, as we require. We implement the modified law in multiple geometries and validate its predictions for velocity, shear-rate, and stress against discrete particle simulations.

9:24AM H53.00006 Rheology of discontinuously shear thickening suspensions beyond simple shear, PAWEL ZIMOCH, GARETH MCKINLEY, ANETTE HOSOI, Massachusetts Institute of Technology — The behavior of discontinuously shear thickening suspensions in flows other than simple shear is not well understood, in part due to unresolved experimental challenges. For example, such suspensions thicken most easily close to rigid boundaries due to the no-slip condition. This makes experiments highly dependent on the shape and size of the container used. We show that by placing a lubricating layer of oil between the suspension and the container we can generate flows where thickening is nearly independent of rigid boundaries. This method is particularly useful in creating quasi one- and two-dimensional flows, which can be easily visualized. We use this method to conduct capillary breakup experiments with thickening suspensions of silica and cornstarch particles, in which we observe the formation of beads-on-a-string morphologies with multiple satellite and sub-satellite bead generations, similar to the morphologies observed in breakup of viscoelastic fluids. Using a one-dimensional continuum model, we show how nonlinear rheology of thickening suspensions results in the creation of these complex morphologies.

9:36AM H53.00007 Activated processes in a stress landscape: a rheological model for dense driven granular materials1, BULBUL CHAKRABORTY, DAPENG BI, Brandeis University — We model (Phil. Trans. R. Soc. A 2009 367) the rheological behavior of granular materials based on a stress-based statistical ensemble and the Soft Glassy Rheology framework (SGR). It takes into account the disordered nature of granular packings and the metastability of jammed states, as well as spatial heterogeneity and intermittency. In this model, mesoscopic subregions of a driven granular material undergo activated processes in a stress landscape with a broad distribution of barrier heights. Due to the athermal nature of granular materials, the activated processes are induced not by the thermodynamic temperature, but by a temperature-like quantity which is a measure of the fluctuation of stresses. Results and predictions of the model have been successfully applied to analyze experiments in a Couette geometry. We will discuss applications of the stress-activated framework in, for example, recent experiments that study non-local rheology in dense flows (PRL 106 108301(2011)).

1This project is funded by NSF.

2This work has been supported by NSF.
networks are discussed in this talk. The scale cannot be determined exclusively based on geometric anisotropy of the randomness induced decay.

In 2D square packed systems simulated with a modified version of the molecular dynamics package LAMMPS, we note that the decay in peak compressive potential energies of the system as a function of time shows the gradual transfer of energy from potential to kinetic with increase in the level of randomness. A power-law decay is shown to occur when the amplitude of the leading pulse reduces below that of the scatter. Investigation into the ensemble kinetic and potential energies of the system as a function of time shows the gradual transfer of energy from potential to kinetic with increase in the level of randomness. The 1D study (motivated by M. Manciu et. al. (2001)) reveals the presence of two distinct regimes of decay in peak compressive force with distance for any level of randomness. The transition between the regimes of exponential and power-law decay is associated with either the mass, Young’s modulus or radius of the spheres. The 1D study demonstrates the presence of naturally-persistent granular mixing patterns (“strange” eigenmodes) for intermediate numbers of revolutions. Unlike fluid mixing, however, strong diffusive effects (due to particle collisions in granular flows) result in fast decay of these transient patterns in monodisperse mixtures. Meanwhile, segregation leads to permanent excitation of eigenmodes in bidisperse mixtures.

3Supported by Schlumberger and by the Swiss SNSF.

10:36AM H53.00012 Effect of randomness on wave propagation in granular systems , MOHITH MANJUNATH, AMNAYA P. AWASTHI, PHILIPPE H. GUEBELLE, Department of Aerospace Engineering, University of Illinois at Urbana-Champaign — Granular systems have been shown to possess energy absorbing and potential wave mitigation characteristics due to the flexibility in tuning the properties of the particles. The present study focuses on the impact of randomness on wave propagation in 1D and 2D lattices of spherical particles where the randomness is associated with either the mass, Young’s modulus or radius of the spheres. The 1D study (motivated by M. Manciu et. al. (2001)) reveals the presence of two distinct regimes of decay in peak compressive force with distance for any level of randomness. The transition between the regimes of exponential and power-law decay is shown to occur when the amplitude of the leading pulse reduces below that of the scatter. Investigation into the ensemble kinetic and potential energies of the system as a function of time shows the gradual transfer of energy from potential to kinetic with increase in the level of randomness. In 2D square packed systems simulated with a modified version of the molecular dynamics package LAMMPS, we note that the decay in peak compressive force is present due to dimensionality as well as randomness. Normalization is then used to quantify the decay due to randomness alone and we investigate the anisotropy of the randomness induced decay.

10:48AM H53.00013 Continuum Representation of the Mechanics of Random Fiber Networks , ALI SHAHSAVARI, CATALIN PICU, Rensselaer Polytechnic Institute — Solving boundary value problems over large domains of random fiber networks is important in the design of fiber-based engineering materials and in the understanding of the biophysics of biological materials. In most of these applications, systems contain a very large number of fibers, which renders nearly impossible solving boundary value problems while resolving every fiber in the problem domain. Therefore, developing a continuum model for the discrete system is desirable. This presentation focuses on conditions under which this mapping can be performed and the minimum size of the problem beyond which the continuum representation is valid. Random fiber networks are highly heterogeneous and exhibit non-affine deformation with correlated fields at different observation length scales. The scale of transition from the discrete to the continuum model must be large enough to capture all the statistically independent subdomains of the network. This scale cannot be determined exclusively based on geometric considerations (e.g. based on fiber density). These considerations, along with a constitutive model for the small deformation of continuum models of fiber networks are discussed in this talk.
8:00AM H54.00001 Robustness and Assortativity for Diffusion-like Processes in Scale-free Networks1, ANTONIO SCALA, CNR-ISC, Uso “La Sapienza”, GREGORIO D’AGOSTINO, ENEA - CR “Casaccia”, VINKO ZLATIC, Theoretical Physics Division, Rudjer Boskovic Institute, GUIDO CALDARELLI, IMT Lucca Institute for Advanced Studies — By analyzing the diffusive dynamics of epidemics and distress in complex networks, we study the effect of the assortativity on the robustness of the networks. We first determine by spectral analysis the thresholds above which epidemics/failures can spread; we then calculate the slowest diffusional times. Our results show that disassorted networks exhibit a higher epidemiological threshold and are therefore easier to immunize, while in assortative networks there is a longer time for intervention before epidemic/failure spreads. Moreover, we study by computer simulations a diffusive model of distress propagation (financial contagion). We show that, while assortative networks are more prone to the propagation of epidemic/failures, degree-targeted immunization policies increases their resilience to systemic risk.

1FET Open Project “FOC” nr. 255987, European project “MOTIA” ILS-2009-CIPS-AG-C1-016

8:12AM H54.00002 Time scales and dynamical processes in activity driven networks, NICOLA PERRA, BRUNO GONCALVES, Northeastern University, ROMUALDO PASTOR-SATORRAS, UPC, ALESSANDRO VESPIGNANI, Northeastern University — Network science has undergone explosive growth in the last ten years. This growth has been driven by the recent availability of huge digital databases, which has facilitated the analysis and construction of large-scale networks from real data and the identification of statistical regularities and structural principles common to many systems. Network modeling has played an essential role in this endeavor; however models are chiefly constructed by considering as relevant ingredients only the connectivity and statistical properties of the networks, while disregarding the actual agents’ behavior. Here we address this challenge by measuring the agents’ interaction activity in real-world networks and defining a minimal model capable of reproducing the intrinsically additive nature of connectivity patterns obtained from time-aggregated network representations. Additionally, we demonstrate that processes such as epidemic and information spreading in highly dynamical networks can be better characterized in terms of agent social activity than by connectivity based approaches.

8:24AM H54.00003 Network growth dynamics of fire ant (Solenopsis invicta) nests, NICK GRAVISH, School of Physics, Georgia Tech, MICHAEL A.D. GOODMAN, School of Biology, Georgia Tech, DANIEL I. GOLDMAN, School of Physics, Georgia Tech — We study the construction dynamics and topology of fire ant (Solenopsis invicta) nests. Fire ants in colonies of hundreds to hundreds of thousands create subterranean tunnel networks through the excavation of soil. We observed the construction of nests in a laboratory experiment. Workers were isolated from focal colony and placed in a quasi 2D, vertically oriented arena with wetted soil. We monitored nest growth using time-lapse photography. We found that nests grew linearly in time through tunnel lengthening and branching. Tunnel path length followed an extended power law distribution, $P(l)\propto l^{-2.17}$, and networks were cyclical. In simulation we model the nest growth as a branching and annihilating levy-flight process. We study this as a function of dimensionality (2D and 3D space considered) and step length distribution function $P(l)$. We find that in two-dimensions path length distribution is exponential, independent of the functional form of $P(l)$ consistent with a poisson spatial process while in three-dimensions $P(l)\propto l^{-1}$.

8:36AM H54.00004 The Impact of Time Delays in Network Synchronization in a Noisy Environment1, G. KORNISS, RPI — Coordinating, distributing, and balancing resources in networks is a complex task and it is very sensitive to time delays. To understand and manage the collective response in these coupled interacting systems, one must understand the interplay of stochastic effects, network connections, and time delays. In synchronizion and coordination problems in coupled interacting systems individual units attempt to adjust their local state variables (e.g., pace, orientation, load) in a decentralized fashion. They interact or communicate only with their local neighbors in the network, often with explicit or implicit intention to improve global performance. Applications of the corresponding models range from physics, biology, computer science to control theory. I will discuss the effects of nonzero time delays in stochastic synchronization problems with linear couplings in an arbitrary network. Further, by constructing the scaling theory of the underlying fluctuations, we establish the absolute limit of synchronization efficiency in a noisy environment with uniform time delays, i.e., the minimum attainable value of the width of the synchronization landscape. These results have also strong implications for optimization and trade-offs in network synchronizion with delays.

1Supported in part by DTRA, ARL, and ONR.

8:48AM H54.00005 Predicting theImpact of Time Delays on Contagion Processes on Complex, Multi-scale Networks, RAFAEL BRUNE, CHRISTIAN THIEMANN, DIRK BROCKMANN, Northwestern University — Contagion phenomena in space often exhibit complex, multiscale spatio-temporal patterns driven by the interaction of non-local dispersal and nonlinear dynamics. A key challenge is the prediction of dynamic patterns based on information on human interactions, mobility and initial conditions. The development of computational models has thus received considerable attention. However, in many realistic situations, a process has already evolved for some period before detection and identifying the spatial origin is difficult. Surprisingly, this “inverse problem” has received little attention in the past. We show in a paradigmatic model for human disease dynamics that despite considerable attention, the process has already evolved for some period before detection and identifying the spatial origin is difficult. However, in many realistic situations, a process has already evolved for some period before detection and identifying the spatial origin is difficult. Surprisingly, this “inverse problem” has received little attention in the past. We show in a paradigmatic model for human disease dynamics that despite considerable attention, the process has already evolved for some period before detection and identifying the spatial origin is difficult. However, in many realistic situations, a process has already evolved for some period before detection and identifying the spatial origin is difficult. Surprisingly, this “inverse problem” has received little attention in the past. We show in a paradigmatic model for human disease dynamics that despite considerable attention, the process has already evolved for some period before detection and identifying the spatial origin is difficult. However, in many realistic situations, a process has already evolved for some period before detection and identifying the spatial origin is difficult. Surprisingly, this “inverse problem” has received little attention in the past. We show in a paradigmatic model for human disease dynamics that despite considerable attention, the process has already evolved for some period before detection and identifying the spatial origin is difficult. However, in many realistic situations, a process has already evolved for some period before detection and identifying the spatial origin is difficult. Surprisingly, this “inverse problem” has received little attention in the past. We show in a paradigmatic model for human disease dynamics that despite considerable attention, the process has already evolved for some period before detection and identifying the spatial origin is diffi...
Altogether, these results provide a new framework for the rescue, control, and reprogramming of complex networks in various domains.

The response of complex networks to perturbations is of critical importance in areas as diverse as ecosystem management, power system design, and cell reprogramming. These systems have the potential to adapt and self-organize in response to external perturbations.

We introduce a method to identify such compensatory perturbations in general complex networks, underpinning the ability to control and reprogram these systems to achieve desired states.

The response of complex networks to perturbations is of critical importance in areas as diverse as ecosystem management, power system design, and cell reprogramming. These systems have the potential to adapt and self-organize in response to external perturbations.

In conclusion, we have presented a new framework for the control and reprogramming of complex networks, which can be applied in various domains ranging from ecosystems to infrastructure systems.

**References**


11:15AM J42.00001 Cyclic competition of four or more species: Results from mean field theory and stochastic simulations1, R.K.P. ZIA, Physics Department, Virginia Tech, Blacksburg, VA 24061 — Population dynamics is a venerable subject, dating back two centuries to Malthus, Verhulst, Lotka, Volterra, and many others. Nonetheless, new and interesting phenomena are continually being discovered. For example, the recent discovery of “Survival of the Weakest” in cyclic competition between 3 species with no spatial structure (Berr, Reichenbach, Schottenloher, and Frey, Phys. Rev. Lett. 102, 048102 (2009)) attracted considerable attention, e.g., http://www.sciencedaily.com/releases/2009/02/090213115127.htm. Considering a similar system with 4 or more species, we find a more intuitively understandable principle which appears to underpin all systems with cyclically competing species. We will present several interesting aspects of the 4 species system—from non-linear dynamical phenomena in a deterministic mean-field approach to remarkable extinction probabilities in the stochastic evolution of a finite system. Some insights into the deterministic dynamics, gained from generalizing this system to one with any number of species with arbitrary pairwise interactions, will also be discussed.

1Supported in part by NSF-DMR-0904999 and 1005417.

11:51AM J42.00002 Varieties of extinction scenarios when four species compete cyclically1, S.O. CASE, C.H. DURNEY, M. PLEIMLING, R.K.P. ZIA, Virginia Tech — We study a stochastic system with N individuals, consisting of four species competing cyclically: A → B → C → D → A. Randomly choosing a pair and letting them react, N is conserved but the fractions of each species evolve non-trivially. At late times, the system ends in a static, absorbing state — typically, coexisting species AC or BD. The master equation is shown and solved exactly for N = 4, providing a little insight into the problem. For large N, we rely on simulations by Monte Carlo techniques (with a faster dynamics where a reaction occurs at every step). Generally, the results are in good agreement with predictions from mean field theory, after appropriate rescaling of Monte Carlo time. The theory fails, however, to describe extinction or predict their probabilities. Nevertheless, it can hint at many remarkable behavior associated with extinction, which we discover when studying systems with extremely disparate rates.

1Supported in part by NSF-DMR-0705152, 0904999, 1005417.

12:03PM J42.00003 The effects of mobility on the one-dimensional four-species cyclic predator-prey model1, DAVID KONRAD, MICHEL PLEIMLING, Virginia Tech — The dynamics of a one-dimensional lattice composed of four species cyclically dominating each other is very much dependent on the rates of mobility in the system. We realize mobility as the exchange of two particles located at two nearest neighbor sites with some species dependent rate s. Allowing for only one particle per site, the different species interact cyclically, with species dependent consumption rate k, such that k+s ≤ 1. When varying the exchange rates, we see vastly different behavior when compared to the three-species model. The patterns of domain growth and decay still show an overall power law behavior, however the fundamental trend of domain growth does not follow the three-species case. We also look at the space-time diagrams to see precisely how the domains form, grow, and decay.

1Supported in part by the US National Science Foundation through Grant DMR-0904999.

12:15PM J42.00004 Boundary conflicts and cluster coarsening: Waves of life and death in the cyclic competition of four species1, AHMED ROMAN, MICHEL PLEIMLING, Virginia Tech — In the cyclic competition among four species on a two-dimensional lattice, the partner particles, which swap positions on the lattice with some probability, produce clusters with a length that grows algebraically as t^4/5 where s is the dynamical exponent. Further investigation of the dynamics at the boundary of the clusters is realized by placing one partner particle pair in the upper half of the system and the other pair in the lower half. Using this technique, results about the fluctuations of the interface are obtained. We also observe wave fronts in the case of non-symmetric reaction rates where extinction of a partner particle pair takes place.

1Supported in part by the US National Science Foundation through Grant DMR-0904999.

12:27PM J42.00005 Discriminating the effects of spatial extent and population size in cyclic competition among species, DAVID LAMOUROUX, STEPHAN EULE, THEO GEISEL, JAN NAGLER, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — Quantifying and understanding the stability and biodiversity of ecosystems is a major task in biological physics as well as in theoretical ecology. From the perspective of game theory, this is highly relevant for questions pertaining to the emergence of cooperation or the coexistence of cyclically competing species. The latter has been recently proposed as a paradigm for biodiversity and it has been shown that the mobility of individuals can support the stability of biodiversity by the formation of spirals. In this contribution, we present a population model for species under cyclic competition that extends earlier lattice models to allow the single cells to accommodate more than one individual by introducing a per cell carrying capacity. We confirm that the emergence of spirals induce a transition from an unstable to a stable regime. This transition however does not appear to be sharp and we find a broad intermediate regime that exhibits an ambiguous behavior. The separation of the two regimes by the usual scaling analysis is thus hampered. The newly introduced carrying capacity offers an alternative way of characterizing the transition. We thus overcome the original limitations by separately analyzing the effect of spatial extent and population size.

12:39PM J42.00006 Stochastic extinction dynamics of HIV-11, IRA SCHWARTZ2, US Naval Research Laboratory, ERIC FORGOSTON3, Montclair State University, LEOR WEINBERGER4, Gladstone Institute of Virology and Immunology and University of California, San Francisco — We consider an HIV-1 within host model in which T cells are infected by the virus. Due to small numbers of molecules, stochastic effects play an important role in the dynamical outcomes in that two states are observed experimentally: a replication state in which the virus is active, or a dormant state leading to latency in which the virus becomes active after a delay. The two states are conjectured to be governed by the Tat gene protein transcription process, which does not possess two stable attractors. Rather, the active state is stable, while the dormant state is unstable. Therefore the dormant state can only be achieved through the dynamics of stochastic fluctuations in which noise organizes a path to dormancy. Here we use optimal path theory applied to a Tat gene stochastic model to show how random fluctuations generate the dormant state by deriving a path which optimizes the probability of achieving the dormant state. We explicitly show how the probability of achieving dormancy scales with the transition rate parameters.

1We acknowledge support from the Office of Naval Research and the National Institutes fo Health

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extinction times scale with epidemiological and social parameters. We quantify the effectiveness of the randomly applied theory, we identify the location of the optimal path to extinction in epidemic models with stochastic vaccine controls. These models not only capture internal noise from random transitions, but also external fluctuations, such as stochastic vaccination scheduling. We suggest to shift the focus to the persistence of an established population. Due to fluctuations, the population will (after a long time) eventually go extinct; persisters act as a life insurance against this. We study a simple stochastic model of these processes. Using a WKV approximation, we find the most likely path to extinction and quantify the extinction risk under both favorable and adverse conditions. Analytical results are obtained both in the biologically relevant regime when the switching is rare compared with the birth and death processes, and in the opposite regime of frequent switching. We explain how persisters strongly reduce the extinction risk and show that rare switches are most beneficial to this end. [I. Lohmar and B. Meerson, Phys. Rev. E 84 051901 (2011)]

This work was supported by the Minerva foundation (IL), by the Israel Science Foundation (Grant No. 408/08), and by the U.S.-Israel Binational Science Foundation (Grant No. 2008075).

1:27PM J42.00010 Vaccine enhanced extinction in stochastic epidemic models1, LORA BILLINGS, Montclair State University, LUIS MIER-Y-TERAN, Johns Hopkins Bloomberg School of Public Health, IRA SCHWARTZ, U.S. Naval Research Laboratory — We address the problem of developing new and improved stochastic control methods that enhance extinction in disease models. In finite populations, extinction occurs when the invader initially propagates with the resident allele, but after excluding the resident, cannot survive on its own. We also found that stable coexistence of the two alleles is possible, but only males can differ; one female phenotype is present. Our results show that the success and Sex Ratio

1Supported by National Institute of General Medical Sciences Award No. R01GM090204.

1:39PM J42.00011 Fast stochastic algorithm for simulating evolutionary population dynamics1, LEV TSIMRING, JEFF HASTY, WILLIAM MATHER, University of California, San Diego — Evolution and co-evolution of ecological communities are stochastic processes often characterized by vastly different rates of reproduction and mutation and a coexistence of very large and very small sub-populations of co-evolving species. This creates serious difficulties for accurate statistical modeling of evolutionary dynamics. In this talk, we introduce a new exact algorithm for fast fully stochastic simulations of birth/death/mutation processes. It produces a significant speedup compared to the direct stochastic simulation algorithm in a typical case when the total population size is large and the mutation rates are much smaller than birth/death rates. We illustrate the performance of the algorithm on several representative examples: evolution on a smooth fitness landscape, NK model, and stochastic predator-prey system.

Supported by NIH

Tuesday, February 28, 2012 11:15AM - 2:15PM

11:15AM J43.00001 Stochastic geometry of turbulence, GREGORY FALKOVICH, Weizmann Institute of Science — Geometric statistics open the window into the most fundamental aspect of turbulence flows, their symmetries, both broken and emerging. On one hand, the study of the stochastic geometry of multi-point configurations reveals the statistical conservation laws which are responsible for the breakdown of scale invariance in direct turbulence cascades. On the other hand, the numerical and experimental studies of inverse cascade reveal that some families of isolines can be mapped to a Brownian walk (i.e. belong to the so-called SLE class) and are thus not only scale invariant but conformally invariant. That means that some aspects of turbulence statistics can be probably described by a conformal field theory. The talk is a review of broken and emerging symmetries in turbulence statistics.
11:51AM J43.00002 Stochastic geometry in disordered systems, applications to quantum Hall transitions. ILYA GRUZBERG, The University of Chicago — A spectacular success in the study of random fractal clusters and their boundaries in statistical mechanics systems at or near criticality using Schramm-Loewner Evolutions (SLE) naturally calls for extensions in various directions. Can this success be repeated for ordered and/or non-equilibrium systems? Naively, when one thinks about disordered systems and their average correlation functions one of the very basic assumptions of SLE, the so called domain Markov property, is lost. Also, in some lattice models of Anderson transitions (the network models) there are no natural clusters to consider. Nevertheless, in this talk I will argue that one can apply the so called conformal restriction, a notion of stochastic conformal geometry closely related to SLE, to study the integer quantum Hall transition and its variants. I will focus on the Chalker-Coddington network model and will demonstrate that its average transport properties can be mapped to a classical problem where the basic objects are geometric shapes (loosely speaking, the current paths) that obey an important restriction property. At the transition point this allows to use the theory of conformal restriction to derive exact expressions for point contact conductances in the presence of various non-trivial boundary conditions.

12:27PM J43.00003 Efficient SLE algorithms and numerical pitfalls of the method1, TOM KENNEDY, Departments of Mathematics and Physics, University of Arizona — We consider a physical experiment or a numerical simulation of a physical phenomena that produces a random family of two-dimensional systems. We would like to know if there is a conformal invariance underlying this stochastic geometry. The Schramm-Loewner evolution (SLE) is a conformally invariant stochastic process which depends on a single parameter \( \kappa \). For different values of \( \kappa \) it is known to describe the scaling limit of many conformally invariant 2d systems, e.g., percolation, the Ising model, self-avoiding walks and many more. So it is a natural candidate for describing the stochastic geometry of other physical systems. The classical Loewner equation provides a correspondence between curves in the plane and “driving functions,” and SLE is obtained by taking the driving function to be a Brownian motion. Given a collection of random curves in the plane one would like to determine if the curves come from an SLE process for some value of \( \kappa \). One method is to compute the driving processes of the curves and test if they are a Brownian motion. We discuss algorithms for doing this efficiently and some of the pitfalls in this approach.

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research supported by NSF grant DMS-0758649

1:03PM J43.00004 Search for Conformal Invariance in Two-dimensional Compressible Turbulence. STEFANUS, University of Pittsburgh — We present a viable way of experimentally testing for conformal invariance at the surface of a turbulent fluid. The theory being tested here is related to the behavior of random curves on a plane and is associated with the work of Loewner, Schramm and others. It is usually referred to as Schramm-Loewner evolution (SLE). The scalar random variables that are put to this test are the vorticity and the divergence of the surface flow. Both of these variables display certain characteristics of Brownian motion, but the divergence field does not exhibit the Gaussian behavior required by SLE.

1:39PM J43.00005 Schramm-Loewner (SLE) analysis of quasi two-dimensional turbulent flows. SIMON THALABARD, SPEC/IRAMI/CEA Saclay — Quasi two-dimensional turbulence can be observed in several cases: for example, in the laboratory using liquid soap films, or as the result of a strong imposed rotation as obtained in three-dimensional large direct numerical simulations. We study and contrast SLE properties of such flows, in the former case in the inverse cascade of energy to large scale, and in the latter in the direct cascade of energy to small scales in the presence of a fully-helical forcing. We thus examine the geometric properties of these quasi 2D regimes in the context of stochastic geometry, as was done for the 2D inverse cascade by Bernard et al. (2006). We show that in both cases the data is compatible with self-similarity and with SLE behaviors, whose different diffusivities can be heuristically determined.

Tuesday, February 28, 2012 11:15AM - 2:15PM
Session J52 GSNP DFD: Focus Session: Extreme Mechanics - Plates 153C

11:15AM J52.00001 Radial stretching of thin sheets: A prototypical model for morphological complexity. BENNY DAVIDOVITCH, UMass Amherst — The complex morphologies of thin sheets consist of wrinkles, crumples, folds, creases, and blisters. These descriptive words may sound lucid – but do they carry any quantitatively distinguishable content? Following the classical approach of pattern formation theory, we seek to impart a universal meaning to these modes of deformation as distinct types of symmetry-breaking instabilities of a flat, featureless sheet. This idea motivates us to consider the general problem of axisymmetric stretching of a sheet. A familiar realization of this problem is the “map maker’s conflict”: projecting a flat sheet onto a foundation of spherical shape. Another representative realization is the Lame’ set-up: exerting a radial tension gradient on a sheet, which may be free-standing or resting on a solid or liquid foundation. I will introduce a set of generic parameters: bendability, confinement, stiffness, adhesiveness, that span a phase space for the morphology of radially stretched sheets. In this phase space, wrinkling, crumpling, folding, creasing and blistering could be identified as primary and secondary symmetry-breaking instabilities.

11:27AM J52.00002 Bending of a surface with spontaneous curvature. CATHERINE QUILLIET, PHILIPPE MARMOTTANT, ALEXANDRE FARUTIN, CHAOUQI MISBAH, LIPhy, Univ. Grenoble, France — We are interested in curvature deformations that can be described by Helfrich’s energy: a quadratic mean curvature term, and a gaussian curvature term. When the surface is not strictly incompressible and presents a nonzero spontaneous mean curvature, we focus on simple cases to show that a priori determination of key features (spontaneous curvature, equilibrium area) may be biased according the expression taken for the energy.

11:39AM J52.00003 Deformations of 2D Random Elastic Networks. HENDRIK FLORIJN, M. VAN DEEN, HENK IMTHORN, MARTIN VAN HECKE, Leiden University, GRANULAR & DISORDERED MEDIA TEAM — We study the linear and nonlinear behavior of random 2D elastic networks at the desktop scale. We demonstrate how to fabricate random networks and characterize them with the lattice coordination number \( Z \). We investigate experimentally if there is a relation between the mechanical response and the lattice coordination number \( Z \) of the network.

11:51AM J52.00004 Packing with a twist: from Wrinkles to Scrolls. ARSHAD KUDROLLI, JULIEN CHOPIN, Department of Physics, Clark University — We discuss an experimental investigation of a thin elastic sheet in the form of a ribbon with clamped boundary conditions at both ends which is then subjected to a twist by rotating the ends through a prescribed angle. We find that a wrinkling instability appears even at a small twist angle which depends on the aspect ratio of the ribbon, its bending modulus and initial tension. Using x-ray tomography, we show that the pattern of this first instability has an impact on the folding at larger twist angles which can result in ordered configurations including Fermat scrolls. Still further twisting results in a highly compressive packing as in wringing a towel without application of direct radial compression. Implications for developing yarns with novel mechanical and transport properties [Lima, et al., Science 331, 51 (2011)] will be discussed.
12:03PM J52.00005 Geometry and Mechanics of Chiral Pod Opening¹, ERAN SHARON, SHAHAF ARMON, The Hebrew University of Jerusalem, EFI EFRATI, University of Chicago, RAZ KUPFERMAN, The Hebrew University of Jerusalem — We study the geometry and mechanics that drive the opening of Bauhinia seeds pods. The pod valve wall consists of two fibrous layers oriented at ±45º with respect to the pod axis. Upon drying, each of the layers shrinks uniaxially, perpendicularly to the fibers orientation. This active deformation turn the valve into an incompatible sheet with reference saddle-like curvature tensor and a flat (Euclidean) reference metric. These two intrinsic properties are incompatible. The shape is, therefore, selected by a stretching-bending competition. Strip cuts from the valve tissue and from synthetic model material adopt various helical configurations. We provide analytical expressions for these configurations in the bending and stretching dominated regimes. Surface measurements show the transition from minimal surfaces (narrow limit) to cylindrical ones (wide limit). Finally, we show how plants use these mechanical principles using different tissue architectures.

¹Supported by ERC “soft Growth” project and by BSF grant #2008432

12:15PM J52.00006 Flat-twisted-helical transition in composed gel sheets and self assembled chiral molecules¹, SHAHAF ARMON, ERAN SHARON, Hebrew University, Jerusalem, EFI EFRATI, University of Chicago, RAZ KUPFERMAN, Hebrew University, Jerusalem — We recently presented a new chirality creating mechanism in elastic strips. in such frustrated bodies, the chiral configuration is determined in a competition between bending and stretching energies, controlled by a dimensionless parameter \( \frac{w}{\sqrt{t/k}} \), in which \( w \) is the strip’s width, \( t \) – its thickness and \( k \) – the spontaneous curvature. I will show the geometrical and mechanical equivalence between such elastic strips and self assembled molecules made of twisted elements. I will also show experiments in responsive gels, showing how a continuous variation in \( \frac{w}{\sqrt{t/k}} \) yields an ordered shape transition from flat to twisted and helical shapes and to tubes. Similar transitions have been observed in self assembled macromolecules.

¹This work was supported by Eshkol scholarship of the Israeli ministry of Science and ERC “SoftGrowth” project.

12:27PM J52.00007 Curvature and defects in soft membranes with orientational order¹, THANH SON NGUYEN, JUN GENG, JONATHAN V. SELINGER, Liquid Crystal Institute, Kent State University — Previous research has demonstrated that soft membranes have a coupling between curvature and in-plane orientational order. Defects in the orientational order can induce curvature, and conversely, curvature leads to an effective geometrical potential acting on defects [1]. Recently, our group has done simulations which show that the interaction between curvature and defects depends on several important issues, including the baseline curvature of the membrane (flat, cylinder, sphere, torus), the phase of the defects (radial or tangential), and the relative contribution of in-plane (intrinsic) vs. out-of-plane (extrinsic) variations of the director [2]. To understand the simulations, we develop a theoretical approach that can address those issues. Using this approach, we calculate the energy of defect structures in curved geometries, and determine how the energy varies as a function of the defect position and separation and the membrane distortions. The interaction energy depends on the relative magnitude of intrinsic vs. extrinsic couplings, and on the mechanical properties of the membrane. This approach provides opportunities to design membranes that will relax into selected shapes. [1] AM Turner et al, Rev Mod Phys 82, 1301 (2010). [2] RLB Selinger et al, J Phys Chem B, in press.

¹This work was supported by NSF DMR-1106014.

12:39PM J52.00008 Capillary induced buckling of floating sheets, MIGUEL PINEIRUA, JOSE BICO, BENOIT ROMAN, PMMH-ESPCI, NARAYANAN MENON, Umass — When a water droplet is deposited over a thin floating sheet, radial wrinkles appear in the vicinity of the droplet as a result of capillary forces exerted at the contact line [1]. However, determining the stress state at the contact line is still challenging and limits the full description of the wrinkling pattern. In order to avoid this contact line ambiguities, we propose the experimental study of the buckling of a macroscopic annulus floating on the surface of water and submitted to a difference in surface tension between its inner and outer edges. This particular configuration allows to generate radial wrinkles on the membrane with well defined border conditions. The topography of the wrinkled patterns are precisely measured using a synthetic Schlieren technique. Based on the standard buckling theory, we develop scaling laws for the buckling threshold of the annulus as well as for the wave length and radial extension of the wrinkles, which are compared to our experimental results and numerical simulations.


12:51PM J52.00009 The wrinkle transition of a sheet on a drop, ROBERT SCHROLL, BENNY DAVIDOVITCH, HUNTER KING, NARAYANAN MENON, Physics Department, University of Massachusetts — A thin sheet subject to confinement will wrinkle in order to relieve compressive stress. We discuss the case of a circular sheet living on the surface of a liquid drop. The pressure of the drop forces the sheet to be non-planar, which may induce confinement along the outer edge of the sheet. We show that, in the limit of very thin, highly bendable sheets, the system is governed by a single confinement parameter. This parameter determines if and where wrinkles appear on the sheet. Comparison to experimental results provides the first detailed confirmation of a new far-from-threshold theory to describe such ultra-thin sheets. According to this model, the transition to the wrinkled state represents the loss of axisymmetry in the height field, while the stress field maintains its symmetry.

1:03PM J52.00010 Transition from Wrinkling to Crumpling in a Sheet Floating on a Drop¹, HUNTER KING, NARAYANAN MENON, ROBERT SCHROLL, BENNY DAVIDOVITCH, University of Massachusetts, Amherst — An ultrathin* circular polystyrene sheet floating on the surface of a water drop stretches radially and compresses along its circumference as the curvature of the drop increases. The compression is at first fully relaxed by a wrinkle pattern extending inward from the edge. When the wrinkles occupy too large a fraction of the area of the sheet, the system sharp, localized, crumpled features continuously emerge. We show that the onset of crumpling is a primary symmetry breaking transition of the stress field. We experimentally characterize this transition from wrinkling to crumpling by studying the distribution of gaussian curvature in the film, measured by optical profilometry. *Typical dimensions are tens of nanometers in thickness and millimeters in lateral size.

¹NSF DMR 0907245

1:15PM J52.00011 Supported conical defects, EFI EFRATI, University of Chicago — In this work we study the elastic equilibrium configurations of a hyperbolic conical defect (a flat disc with a single negative Gaussian curvature condensation), supported on a rigid plane. Originating from the study of strictureplasty, this problem which seems to be a natural extension to the D-cone problem displays a distinct behavior.

1:27PM J52.00012 Stamping and wrinkling of elastic plates, JEREMY HURE, JOSE BICO, BENOIT ROMAN, PMMH - ESPCI ParisTech — In classical Euler buckling a beam is found to buckle with the lowest mode as a compressive strain is applied. Higher modes are however observed if the amplitude of the out-of-plane displacement is bounded by geometrical constraints. What is the limit when the maximum amplitude prescribed is decreased to zero? We show that the wavelength tends towards a finite value dictated by the thickness of the beam. This one-dimensional model is used to describe the compression of a circular elastic plate into an hemispherical mold.
the hole size and the critical hole size. This helps to explain the clogging transition and its relationship to the jamming transition. We study how these quantities depend on the distance to the clogging transition, defined as the difference between positions of grains to sub-pixel accuracy. We then use this information to determine various local and global properties, including strain rate, velocity correlations, and dynamical heterogeneity time scales. We propose that the frictional jamming transition is not mean field and is triggered by the nucleation of unstable regions, which are themselves dynamical objects due to the Coulomb criterion. We create frictional packings using MD simulations and test for the presence and shape in accounting for the transition. We follow the behavior of individual grains in the bulk. Using a quasi-2D hopper and a fast CCD, we can measure the patterns in providing multifunctional performance is illustrated and discussed.

**Tuesday, February 28, 2012 11:15AM - 2:15PM**

**Session J53 GSNP: Disordered Systems: Jamming 153B**

11:15AM J53.00001 The contact percolation transition1. TIANQI SHEN, Physics Department at Yale University, COREY O'HERN, Department of Mechanical Engineering & Materials Science, Yale University, MARK SHATTUCK, Benjamin Levich Institute and Department of Physics, City College of New York of the City University New York — Typical quasi-critical compression algorithms for generating jammed packings of athermal, purely repulsive particles begin with dilute configurations and then apply successive compressions with relaxation of the elastic energy allowed between each compression step. It is well-known that during isotropic compression athermal systems with purely repulsive interactions undergo a jamming transition at packing fraction $\phi_J$ from an unjammed state with zero pressure to a jammed, rigid state with nonzero pressure. Using extensive computer simulations, we show that a novel second-order-like, contact percolation, which signals the formation of a system-spanning cluster of mutually contacting particles, occurs at $\phi_p < \phi_J$, preceding the jamming transition. By measuring the number of non-floppy modes of the dynamical matrix, the displacement field between successive compression steps, and the overlap between the adjacency matrix, which represents the network of contacting grains, at $\phi_p$ and $\phi_J$, we find that the contact percolation transition also heralds the onset of nontrivial response to applied stress. Highly heterogeneous, cooperative, and non-affine particle motion occurs in unjammed systems significantly below the jamming transition for $\phi_p < \phi < \phi_J$.

11:27AM J53.00002 Constraint counting for frictional jamming . D.A. QUINT, University of California Merced, S. HENKES, J.M. SCHWARZ, Syracuse University — While the frictionless jamming transition has been intensely studied in recent years, more realistic frictional packings are less well understood. In frictionless sphere packings, the transition is predicted by a simple mean-field constraint counting argument, the isostaticity argument. For frictional packings, a modified constraint counting argument, which includes slipping contacts at the Coulomb threshold, has had limited success in accounting for the transition. We propose that the frictional jamming transition is not mean field and is triggered by the nucleation of unstable regions, which are themselves dynamical objects due to the Coulomb criterion. We create frictional packings using MD simulations and test for the presence and shape of rigid clusters with the pebble game to identify the partition of the packing into stable and unstable regions. To understand the dynamics of these unstable regions we follow perturbations at contacts crucial to the stability of the “frictional house of cards.”

11:39AM J53.00003 Decoupling of Rotational and Translational Diffusion in a 2D Granular Experiment . NABIHA SAKLAYEN, GARY L. HUNTER, ERIC R. WEEKS, Emory University — We experimentally study the rotation and diffusion of granular clusters in a 2D binary granular system. Our apparatus vibrates a 2D system of densely packed granular bidisperse disks (to avoid crystallization) containing trackable 3-particle clusters. We use this system to mimic hard-sphere fluids and the clusters probe the system’s local translational and rotational dynamics. As the area fraction of the bidisperse disks is increased, diffusion within the sample becomes slower, and above a critical area fraction, the sample behaves as a granular glass. We analyze the rotational and translational motions of the clusters to determine whether they decouple with changing area fraction of the system. As we approach the glass transition, we observe a decoupling between the two motions.

11:51AM J53.00004 Characterizing the clogging transition by individual grain behavior . CHARLES THOMAS, DOUGLAS DURIAN, University of Pennsylvania — Granular media clogs as it flows out of a hopper when the exit hole is appropriately small. However, when the hole enlarged, the grains will never clog: there exists a well-defined transition between these two regimes at a particular critical hole size. To understand the origin of this clogging transition we follow the behavior of individual grains in the bulk. Using a quasi-2D hopper and a fast CCD, we can measure the positions of grains to sub-pixel accuracy. We then use this information to determine various local and global properties, including strain rate, velocity correlations, and dynamical heterogeneity time scales. We study how these quantities depend on the distance to the clogging transition, defined as the difference between the hole size and the critical hole size. This helps to explain the clogging transition and its relationship to the jamming transition.
12:03PM J53.00005 Jamming around fixed obstacles

Networks with the mean field exponent. However, we argue that the mean field arguments fail due to non-local interactions between mass clusters.

Contract W911NF-09-D-0001 from the US Army Research Office.

1Acknowledgement is made to the Donors of the Petroleum Research Fund administered by the American Chemical Society, a Eugene M. Lang Faculty Fellowship and the Division of Natural Sciences of Swarthmore College, and DOE grant DE-FG02-05ER46199.

12:15PM J53.00006 Frictional Jammed Packings: Classification, Protocol Dependence and the Phase Diagram

1STEFANOS PAPANIKOLAOU, COREY O'HERN, Departments of Mechanical Engineering & Materials Science and Physics, Yale University, New Haven, Connecticut 06520, MARK D. SHATTUCK, Benjamin Levich Institute and Physics Department, The City College of the City University of New York, New York, New York 10031 — We probe the nature of the jamming transition in systems of frictional disks, where static friction is modeled geometrically using “bumpy-particles” with uniform circular asperities on the disks’ surface. First, we enumerate and classify the mechanically stable (MS) packings in small systems using exhaustive numerical simulations. We explicitly show that finite friction stabilizes packings that are unstable for frictionless particles, which causes the number of MS packings to increase strongly with the friction coefficient. MS packings for frictional particles are organized into low-dimensional geometric families in configuration space. We then calculate the critical behavior of the structural and mechanical properties near the jamming transition for frictional particles and as a function of protocol and show that friction drastically alters the nature of the transition.

12:27PM J53.00007 Jammed 2D circle packing reconsidered as a jigsaw puzzle

1ERIC CORWIN, Department of Physics, University of Oregon, KENNETH DESMOND, ERIC WEEKS, Department of Physics, Emory University — Athermal random packings are inherently non-equilibrium structures. For a bidisperse jammed packing of N disks the global packing structure can be thought of as composed of N jigsaw pieces, each representing the local structure around a disk. We show that we can assign a unique identifier, termed a jigsaw number, to each local packing structure. We find that as the number of disks grows to infinity the number of different jigsaw numbers present in a packing remains finite. We report on the distribution of jigsaw numbers and find that certain local packing structures are more common than others, demonstrating that the non-equilibrium packing structure is incompatible with a flat measure over all configurations. We further report on the correlations present between jigsaw pieces.

12:39PM J53.00008 An experimental test of equilibration of temperature-like variables in jammed granular materials

1JAMES PUCKETT, Dept. of Physics, North Carolina State University, BRIAN TIGHE, Process & Energy Laboratory, TU Delft, KAREN E. DANIELS, Dept. of Physics, North Carolina State University — Although jammed granular systems are athermal, a number of thermodynamic-like descriptions have been proposed which make predictions about the distributions of volume and stress fluctuations. We perform experiments with an apparatus designed to generate a large number of jammed two-dimensional configurations, which consists of a single layer of photoelastic disks supported by a layer of air driven through a microporous membrane. New configurations are automatically generated by alternately dilating the system (permitting large-scale rearrangements) and compressing it biaxially until a desired volume or pressure is reached. Within each configuration, a bath of $\sim 10^4$ particles surrounds a smaller subsystem of particles with either the same or a different inter-particle friction coefficient than the bath. The use of photoelastic particles permits us to find all particle positions, and to numerically solve for the vector forces at each inter-particle contact. By comparing temperature-like quantities between subsystems, we test whether equilibration is observed under several proposed volume and stress ensembles.

1We acknowledge support from NSF DMR-0644743.

12:51PM J53.00009 Energy decay of freely cooling granular gases in three dimensions

1ZAHERA JABEEN, Department of Physics, University of Michigan, Ann Arbor, MI 48109-1040, SUDHIR N. PATHAK, RAJESH R., Institute of Mathematical Sciences, CIT Campus, Taramani Chennai-600 113, India — Freely cooling granular gases, wherein a dilute system of macroscopic particles with uncorrelated initial velocities lose energy through inelastic collisions, have been extensively studied both as a simple model for granular systems as well as a nonequilibrium system showing nontrivial coarsening at late times. As the system cools, inelasticity induces clustering, making the system inhomogeneous. While the form of energy decay $\langle E(t) \rangle \sim t^{-\theta}$ in the initial homogeneous regime is well established by Haff’s law ($\theta = 2$), the energy decay in the clustered regime is still unresolved in higher dimensions. Within mean field theory, $\theta = 2d/(d+2)$ (where $d$ is the spatial dimension), while a correspondence to Burgers equation implies an exponent $\theta = 2/3(d = 1), d/2(d > 1)$. In one and two dimensions, the two formulae predict the same exponents. By performing extensive event driven molecular dynamics simulations, we show that in three dimensions, the energy decays asymptotically with a power $\sim 1.2$, for coefficients of restitution $r < 1$, consistent with the mean field exponent. However, we argue that the mean field arguments fail due to non-local interactions between mass clusters.

1Supported in part by the David and Lucile Packard Foundation, Public Health Service Grant NS44393, the Institute for Collaborative Biotechnologies through Contract W911NF-08-D-0001 from the US Army Research Office.

1:03PM J53.00010 The Influence of Topology on Signal Propagation in Granular Force Networks

1DANIELLE BASSETT, University of California Santa Barbara, ELI OWENS, KAREN DANIELS, North Carolina State University, MAISON PORTER, Oxford University — Granular materials exhibit numerous rich and complex behaviours, which have been investigated from both continuum and particulate perspectives. In particular, sound propagation through granular materials is both heterogeneous and complicated, and understanding its features is important not only from the perspective of fundamental physics but also for practical applications such as the characterization and non-destructive testing of such materials. Unfortunately, continuum models of sound propagation have been unable to explain the full range of observed behaviours. Here we represent granular materials as spatially-embedded networks composed of nodes (particles) and weighted edges (contact forces between particles) located in Euclidean space, and use network science to provide fundamental insights into how sound propagates. Using photoelastic particles, we quantify and characterize the internal force structure and show that its meso-scale network structure plays a crucial role in sound propagation. These results might help to explain the failure of previous physical models, and illustrate that contact topology alone is insufficient to understand signal propagation in granular materials.

1Supported in part by the David and Lucile Packard Foundation, Public Health Service Grant NS44393, the Institute for Collaborative Biotechnologies through Contract W911NF-08-D-0001 from the US Army Research Office.
phone-call or face-to-face interactions characterizing in this way different types of human social behavior. Indeed, the statistics of duration of phone calls is described by a Weibull distribution and is significantly different from the distribution of network interactions. We propose a simple model for users’ behavior that includes finite priority queuing and time resources that reproduce the observed social behavior.

We acknowledge financial support by NSF grant CBET 1059745.

To be or not to be jammed. SIMON DAGOIS-BOHY, Kamerling Ohnes Laboratory - Leiden University, BRIAN TIGHE, TU Delft - 3me, JOHANNES SIMON, Kamerling Ohnes Laboratory - Leiden University, SILKE HENKES, Syracuse University, MARTIN VAN HECKE, Kamerling Ohnes Laboratory - Leiden University — When are packings of soft athermal spheres jammed? Any experimentally relevant definition must at least require a jammed packing to resist compression and shear. Numerical algorithms usually rely on a global compression monitored by a parameter (like pressure) that signals whether the packing is jammed or not. Here we show that compression is not sufficient to ensure properly jammed packings; some of those packings have positive pressures and bulk moduli, but negative shear moduli, and even for large systems, the number of these “bad apples” diverges as the jamming point is approached. We will discuss how to understand this situation and propose as a remedy the boundary relaxation, that is including the boundary shape parameters as variables in the equilibrium process; finally we will compare the distribution of shear moduli obtained for both methods.

Jamming, Yielding and Rheology of Weakly Vibrated Granular Media. GEERT WORTEL, JOSHUA DIJKSMAN, University of Leiden; OLIVIER DAUCHOT, CÉA-Saclay; MARTIN VAN HECKE, University of Leiden, GRANULAR AND DISORDERED MEDIA TEAM, GROUPE INSTABILITÉS ET TURBULENCE TEAM — We establish that the rheological curve of dry granular media is nonmonotonic, both in the presence and absence of external mechanical agitation. In the absence of vibrations, the nonmonotonic flow curve governs the yielding behavior of granular media. In the presence of weak vibrations, the nonmonotonic flow curves govern a hysteretic transition between slow but steady and fast, inertial flows. For large agitations, the transition becomes non-hysteretic. We probe the fluctuations near the point where the 1st order transition becomes of 2nd order.

Dynamics near shear-jamming for a dense granular system. JIE REN, JOSHUA DIJKSMAN, ROBERT BEHRINGER, Duke University — This talk will present several systematic experimental studies of a two-dimensional, frictional dense granular system subjected to simple shear deformation. The first experiment consists of linear shear for densities smaller than the isotropic jamming point, and examines both the evolution of the average stress and the evolution of force network. These measures reveal three distinguishable regimes of the granular system with increasing shear strain: unjammed, fragile, and shear-jammed regimes. The second experiment uses small amplitude cyclic shear to probe the dynamical response of the states from the first experiment. For fragile or jammed regimes, cyclic shear drives the system through transient states that evolve towards relatively stable forces networks and system-averaged stress. The timescale of the transient increases rapidly as the system moves deeper into the fragile, or shear-jammed regimes. These experiments also involve particle tracking (displacements and rotations) to search for and characterize non-affine motion and spatial heterogeneity. There is a clear increase in particle diffusion with increasing density and shear strain amplitude, even when the system is still unjammed and experiences only minimal stress. When the system is fragile or jammed, the heterogeneity of particle displacements reveals subtle correlations with the force network.

2:03PM J53.00015 Tricriticality in constraint percolation.  L. CAO, J. M. SCHWARZ, Physics Department, Syracuse University — Constraint percolation goes beyond ordinary percolation to include constraints on the occupation of sites/bonds. For instance, k-core site percolation implements a geometric constraint requiring each occupied vertex on a network have at least k occupied neighboring vertices. It turns out that the percolation transition in such a model is essentially equivalent to the study of a dynamical glass transition in the Fredrickson-Andersen model, one of the models underlying the kinetically-constrained approach to the glass transition. We study heterogeneous k-core bond percolation on a random network with f denoting the probability of a k = 2-core vertex and 1 – f the probability of a k = 3-core vertex. This model corresponds to a heterogeneous extension of the Fredrickson-Andersen model. For f = 1, the percolation transition is continuous, while for f = 0, it is discontinuous. Using a master equation approach, we show that there exists a tricritical point at f = 1/2 with a new order parameter exponent of unity. Our results are consistent with other mean field results obtained via a different method. We also look for tricriticality beyond mean field by investigating another constraint percolation model dubbed force-balance percolation.

Tuesday, February 28, 2012 11:15AM - 2:03PM — Session J54 GSNP: Focus Session: Complex and Co-evolving Networks - Empirical Studies of Social Networks 152

Modeling users’ activity on Twitter networks: validation of Dunbar’s number. BRUNO GONCALVES, NICOLA PERRA, ALESSANDRO VESPIGNANI, Northeastern University — Microblogging and mobile devices appear to augment human social capabilities, which raises the question whether they remove cognitive or biological constraints on human communication. In this paper we analyze a dataset of Twitter conversations collected across six months involving 1.7 million individuals and test the theoretical cognitive limit on the number of stable social relationships known as Dunbar’s number. We find that the data are in agreement with Dunbar’s result; users can entertain a maximum of 100-200 stable relationships. Thus, the “economy of attention” is limited in the online world by cognitive and biological constraints as predicted by Dunbar’s theory. We propose a simple model for users’ behavior that includes finite priority queuing and time resources that reproduces the observed social behavior.

Entropy of dynamical social networks. KUN ZHAO, Northeastern University, MARTON KARSAY, Aalto University, FINLAND; GINESTRA BIANCONI, Northeastern University — Dynamical social networks are evolving rapidly and are highly adaptive. Characterizing the information encoded in social networks is essential to gain insight into the structure, evolution, adaptability and dynamics. Recently, entropy measures have been used to quantify the information in email correspondence, static networks and mobility patterns. Nevertheless, we still lack methods to quantify the information encoded in time-varying dynamical social networks. In this talk we present a model to quantify the entropy of dynamical social networks and use this model to analyze the data of phone-call communication. We show evidence that the entropy of the phone-call interaction network changes according to circadian rhythms. Moreover we show that social networks are extremely adaptive and are modified by the use of technologies such as mobile phone communication. Indeed the statistics of duration of phone-call is described by a Weibull distribution and is significantly different from the distribution of duration of face-to-face interactions in a conference. Finally we investigate how much the entropy of dynamical social networks changes in realistic models of phone-call or face-to-face interactions characterizing in this way different type human social behavior.
11:39 AM J54.00003 The nature and perception of fluctuations in human musical rhythms¹, HOLGER HENNIG, Harvard University, and Max Planck Institute for Dynamics and Self-Organization (MPIDS), Goettingen, Germany, RAGNAR FLEISCHMANN, MPIDS, ANNEKE FREDEBOHM, Institute of Psychology, University of Goettingen, YORK HAGMAYER, Kings College, London, UK, JAN NAGLER, ANNETTE WITT, MPIDS, FABIAN THEIS, Institute for Bioinformatics and Systems Biology, Helmholtz Zentrum München, Germany, THEO GEISEL, MPIDS — Although human musical performances represent one of the most valuable achievements of mankind, the best musicians perform imperfections. Musical rhythms are not entirely accurate and thus inevitably deviate from the ideal beat pattern. Nevertheless, computer generated perfect beat patterns are frequently deviated by listeners due to a perceived lack of human touch. Professional audio editing software therefore offers a humanizing feature which artificially generates rhythmic fluctuations. However, the built-in humanizing elements are essentially random number generators producing only simple uncorrelated fluctuations. Here, for the first time, we establish long-range fluctuations as an inevitable natural companion of both simple and complex human rhythmic performances [1]. Moreover, we demonstrate that listeners strongly prefer long-range correlated fluctuations in musical rhythms. Thus, the favorable fluctuation type for humanizing interbeat intervals coincides with the one generally inherent in human musical performances. [1] HH et al., PLoS ONE,6,626457 (2011)

¹We acknowledge financial support by the BCCN, grant no. 01GQ0430 (AW and TG).

11:51 AM J54.00004 Structural and asymptotic aspects of human mobility , JAMES BAGROW, Northwestern University, YU-RU LIN, Northeastern University — Research on human mobility has been revolutionized by cellular phone data, capturing activity patterns across extensive populations. A number of interesting features have been discovered, including the ultra-slow growth of human mobility patterns, which cannot be reproduced by traditional random-walk models. However, the spatiotemporal flows and detailed microstructure of human mobility have not been well studied. Inferring complex mobility networks from country-wide data from mobile phone data, we find that human mobility is dominated by a small group of frequently visited and dynamically close locations, forming a primary “habitat” that captures typical behavior, along with subsidiary habitats representing additional travel. These habitats are both well separated and spatially compact. We find that motion within habitats exhibits distinct temporal scaling and that the time delay to enter subsidiary habitats is a primary factor in the spatiotemporal growth of human travel. Mobility is also coupled with social activity. Interestingly, many phone users possess habitats that occupy single temporal and social contexts and display high temporal and social predictability when occupying subsidiary habitats, revealing new connections between human activity and mobility dynamics.

12:03PM J54.00005 Temporal and spatial regularity of mobile-phone data¹, PHILIPP HOEVEL, TU Berlin, Germany, ALBERT-LASZLO BARABASI, CCNR, Northeastern University — Network science is a vibrant, interdisciplinary research area with strong connections to a plethora of different fields. As the amount of empirically obtained datasets increases more and more, approaches from network sciences continue to enhance our understanding, for instance, of human dynamics. The available data often consist of temporal as well as spatial information. In our case they originate from anonymized mobile-phone traces, which include information about the timing of the connections between two mobile phones and also their positions. Thus, the data contains an additional social component. In this study, we evaluate patterns of human behavior identifying both temporal and spatial regularity. This leads to a detailed mobility analysis on various timescales and contributes to a general theory of synchronization in complex, real-world networks.

¹This work is supported by a postdoctoral fellowship of the Deutsche Akademische Austauschdienst (DAAD).

12:15PM J54.00006 Scale-free correlations in the geographical spreading of obesity , LAZAROS GALLOS, City College of New York, PABLO BARTTFIELD, Buenos Aires University, SHLOMO HAVLIN, Bar-Ilan University, MARIANO SIGMAN, Buenos Aires University, HERNAN MAKSE, City College of New York — Obesity levels have been universally increasing. A crucial problem is to determine the influence of global and local drivers behind the obesity epidemic, to properly guide effective policies. Despite the numerous factors that affect the obesity evolution, we show a remarkable regularity expressed in a predictable pattern of spatial long-range correlations in the geographical spreading of obesity. We study the spatial clustering of obesity and a number of related health and economic indicators, and we use statistical physics methods to characterize the growth of the resulting clusters. The resulting scaling exponents allows us to broadly classify these indicators into two separate universality classes, weakly or strongly correlated. Weak correlations are found in generic human activity such as population distribution and the growth of the whole economy. Strong correlations are recovered, among others, for obesity, diabetes, and the food industry sectors associated with food consumption. Obesity turns out to be a global problem where local details are of little importance. The long-range correlations suggest influence that extends to large scales, hinting that the physical model of obesity clustering can be mapped to a long-range correlated percolation process.

12:27PM J54.00007 Mining networks of human contact with wearable sensors, ALAIN BARRAT, CPT Marseille, CNRS, France & ISI Foundation, Torino, Italy — Due to the development of sensors of various types and the use of digital media and computational devices, we increasingly leave digital traces of our daily activities. The scale at which such data can be gathered and analyzed makes possible a novel, data-driven approach to the investigation of various aspects of human behavior. In this talk, I will focus on the research done within the SocioPatterns project (www.sociopatterns.org), in which we have developed the SocioPatterns sensing platform to obtain longitudinal datasets on face-to-face contact events between individuals in a variety of contexts ranging from scientific conferences to museum, schools or hospitals. The gathered data sets consists in dynamic networks of human contacts, and their analysis reveal interesting similarities and differences of human interaction patterns across contexts. I will also consider the impact of the temporal resolution, which allows to take into account causality constraints, on dynamical processes occurring on networks, such as spreading processes.

1:03PM J54.00008 Are we in our travel decisions self-determined?, CHRISTIAN SCHNEIDER, MIT, THOMAS COURONNE, ZBIGNIEW SMOREDA, Orange Labs, MARTA GONZALEZ, MIT — Mobile phone data, as saved by every phone provider worldwide, allows us to extract information about human mobility. It can be mainly used to study the locations and routes of each mobile phone user during entire months. In order to gain deeper understanding of the inherent travel decisions of the daily trips measured by phone data, we compare them statically with those extracted from 10,000 trajectories reported in a travel diary survey. We identify and compare from both data sets the underlying trip decisions networks or motifs. Interestingly, although millions of different motifs are possible, in both data sets we found similar motif distributions. Hence, we develop a simple model, which could reproduce not only the size distribution of the motifs, but the motifs themselves and answer the opening question.

1:15PM J54.00009 A cross-section test of Cobb-Douglas production function between market capitalization and GDP , ADAM AVAKIAN, Boston University, Boston, MA 02215, USA, BORIS PODOBNIK, Faculty of Civil Engineering, University of Rijeka, 51000 Rijeka, Croatia, H. EUGENE STANLEY, Boston University, Boston, MA 02215, USA — Most classical economic theories imply that both (a) economies with lower output (GDP) per person tend to grow faster in per capita terms and (b) economies with lower capital per person tend to grow faster in per capita terms. It is well-known that the former was found to be wrong. Taking market capitalization as a proxy for physical capital, we analyze a cohort of countries over a 17-year period (1994-2010) and we find the latter statement in agreement with empirical data implying a contradictive result that while capital data worldwide tend to converge, GDP data tend to diverge. However, for the countries analyzed, for which we have both market capitalization and GDP data, we find that even economies with lower output (GDP) per person tend to grow faster in per capita terms. The result that for all countries one obtains divergence while for a group of countries having both market capitalization and GDP data we have convergence is in contrast with the refutation of (a) but our results only apply to countries that have an exchange market, and are thus participating in globalization, indicating the convergent effect of globalization.
and lower friction. 

controlled plasticity. In alloys, however, differing lattice constants suppress the reorientation of grains at the contact point, which leads to grain boundary sliding 
in pure metals, cold welding and microstructural reorientation lead to the formation of a commensurate sliding interface and high friction resulting from dislocation 

In the middle and are stags, and compare with published data. We study the formation of second-level administrative divisions, e.g. French arrondissements. We study the actual distribution of arrondissements and the Voronoi tessellation associated with the chief town in each. While generally applicable, there are subtleties in some cases. Lastly, we consider the pattern formed by Paris Métro stations and show that near the central area, the associated Voronoi construction has this sort of distribution.

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Tuesday, February 28, 2012 2:30PM - 5:18PM —
Session L26 DCOMP GSNP: Focus Session: Friction, Fracture and Deformation Across Length Scales - Dislocations and Fracture 257B

2:30PM L26.00001 How dislocations and grain boundaries control wear at the nanoscale, IZABELA SZLUFARSKA, University of Wisconsin — Ceramics show outstanding mechanical properties such as high strength and high hardness over a wide range of temperatures and are stable in harsh environments. However, the low fracture toughness of ceramics limits their practical utility for instance as wear-resistance coatings. There have been several reports of improving wear resistance of ceramics by reducing the grain sizes and/or the dimension of the cutting tools to the nanometer regime. Using SiC as a model covalent ceramic, we performed molecular dynamics (MD) simulations of wear for both single crystal and nanocrystalline material. We determined the role of dislocations and grain boundary sliding in improving wear resistance of SiC and we have quantified contributions from these mechanisms to friction and wear. We have discovered instabilities that control sliding of the amorphous-like highly disordered grain boundaries in SiC, in analogy to instabilities and deformation mechanisms that occur in bulk amorphous materials. In this talk we will also present our newly developed analytical model for plowing friction in nanoscale contacts, which model has been validated for both ceramics and metals. In order to isolate the contribution from grain boundary sliding to deformation of nanocrystalline materials, we have performed MD simulations of nanoindentation and uniaxial testing on ultranano crystalline diamond (UNCD). We have shown that in the absence of dislocation plasticity, hardness and yield strength of nanocrystalline materials scale linearly with the grain boundary shear strength, where the latter property can be controlled by grain boundary doping. Our findings explain the experimental observations that hardness and elastic properties of UNCD decrease with an increasing H content.

3:06PM L26.00002 Plastic flow and failure in metallic glass/nanocrystal composites, MICHAEL FALK, PENGFEI GUAN, Johns Hopkins University — The exploitation of metallic glasses’ high strength in structural applications is limited by their lack of any hardening subsequent to yield. This lack of hardening leads to plastic localization as evidenced by the spontaneous formation of shear bands. One proposed method of forestalling such instabilities is to introduce nanocrystal inclusions to disrupt shear band nucleation and propagation. We have undertaken a series of molecular dynamics simulations of glasses with different morphologies of nanocrystaliteites. We report the resulting plastic response, and we use various simulations of these types to test the applicability of the shear transformation zone (STZ) constitutive relation for modeling such complex nano-composite materials.

Funded by NSF under grant DMR0808704

3:18PM L26.00003 Atomic Origins of Friction Reduction in Metal Alloys, MICHAEL CHANDROSS, SHENGFENG CHENG, Sandia National Laboratories — Gold is a desirable material for use in high performance electrical contacts because it offers low contact resistance, does not corrode or oxidize, and can be easily made into thin sheets. However, gold contacts generally suffer from high adhesion and friction. The tribological issues are mitigated in nanocrystalline gold alloys (with, for example, Ni or Co), which can exhibit both low friction and low contact resistance. The atomic scale mechanisms responsible for the change in frictional response are poorly understood. We will present the results of large scale molecular dynamics simulations which study the tribological response of nanocrystalline films of pure gold and alloys under a variety of sliding conditions. Our results indicate that in pure metals, cold welding and microstructural reorientation lead to the formation of a commensurate sliding interface and high friction resulting from dislocation controlled plasticity. In alloys, however, differing lattice constants suppress the reorientation of grains at the contact point, which leads to grain boundary sliding and lower friction.
3:30PM L26.00004 Deformation Initiation by Non-planar \{10-12\} Twinning Nucleation in Magnesium Crystal, SUNGHO KIM, HAITHAM KADIRI, MARK HORSTMeyer, Mississippi State University — The nucleation mechanism of experimentally most commonly observed twinning in Mg crystal initiates deformation process are studied using molecular dynamic simulation. We observed nucleation of radially growing \{10-12\} twinning under tensile loading in Mg rectangular wire system without artificial creation of an twinning. The twinning nucleation mechanism is very different from the conventional twinning mechanism in that the twin nucleates from a point source rather than the fault plane following the partial dislocation line in FCC crystal. The wire axis is normal to basal plane of Mg crystal. The tensile deformation in c-axis nucleates \{10-12\} twinning starting at the corner of square of cross section of the wire. The twin boundary is spherical at the beginning and become linear boundaries in \{10-12\} planes as time goes by.

3:42PM L26.00005 Softening of nanocrystalline materials at small grain size, GEORGIOS KOPIDAKIS, NIKOS GALANIS, IOANNIS REMEDIAKIS, Dept. of Materials Science and Technology, University of Crete — We examine the dependence of the mechanical properties of nanocrystalline materials on grain size. Our extensive atomistic simulations for seven nanocrystalline solids show a universal softening at grain sizes of less than a few nanometers. The elastic constants decrease as the average grain size becomes smaller, in analogy with the reverse Hall-Petch effect for nanocrystalline metals. This behavior is explained by the increase of the fraction of grain boundary atoms as grain size decreases. We derive simple scaling laws for various mechanical properties as a function of the grain size by decomposing the energy into contributions from atoms in the bulk of grains and from atoms at the interfaces. Our theoretical predictions fit very well our results from atomistic simulations of different nanocrystalline materials, from nanocrystalline metals to ultrananocrystalline diamond. It is therefore argued, and quantitatively explained, that softening at small grain size is a general nanoscale effect.

3:54PM L26.00006 Large scale NEMD simulations of polycrystalline Al sliding interfaces, JACQUELINE MILHANS, J.E. HAMMERBERG, R. RAVELO, T.C. GERMANN, B.L. HOLIAN, Los Alamos National Laboratory — We present the results of NonEquilibrium Molecular Dynamics (NEMD) simulations for the frictional force between polycrystalline Al samples. Polycrystalline Al samples of order 26M atoms with grain sizes from 10 - 20 nm at compressions of 15 GPa are considered as a function of sliding velocity. Typical sample dimensions are 58nm in the sliding and transverse directions and 116nm in the direction normal to the sliding interface. A constant temperature (300K) and constant tangential velocity boundary condition is imposed at the boundaries in the direction normal to the sliding plane. We discuss the modes of plastic deformation and polycrystalline deformation which determine the steady state frictional force and compare these results with results for defect free Al single crystals and highly defective Al single crystal samples.

1This work was performed under the auspices of the U.S. Dept. of Energy under contract DE-AC52-06NA25396.

4:06PM L26.00007 Fracture In Disordered Media: Nucleated, Critical or Percollative?, ASHVIVI SHEKHAWAT, Cornell University, STEFANO ZAPPERRI, CNR - Consiglio Nazionale delle Ricerche, JAMES SETHNA, Cornell University — Fracture is often considered to be an abrupt transition and is modeled by nucleation theory. However, the precursor events leading to macroscopic failure display scaling behavior and are understood in terms of critical phenomena. Further, the universal roughness properties of fracture surfaces have been explained by modeling fracture as a percolative process. We attempt to unify these disparate descriptions of fracture in one comprehensive theory. We study the random fuse network as a typical model of disordered brittle media. We show that in this model fracture can be nucleated, critical or percolative depending on the behavior of the tail of the distribution of fuse strengths. We explore the phase diagram by using numerical simulations as well as theoretical arguments.

1This research was supported by DOE-BES DE-FG02-07ER46393.

4:18PM L26.00008 Homogeneous Dislocation Nucleation, ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — We perform atomistic computer simulations to study the mechanism of homogeneous dislocation nucleation (HDN) in a 2D hexagonal crystalline film under circular indentation. The nucleation process is governed by vanishing of energy associated with a single normal mode. For fixed film thickness, \(L\), the spatial extent, \(\xi\), of the critical mode grows with indenter radius, \(R\). For fixed \(R/L\), \(\xi\) scales roughly as \(\xi \sim D^5\). We perform a mesoscale analysis to determine the lowest energy normal mode for regions of varying radius, \(r_{\text{meso}}\), centered on the critical mode's core. The energy of the lowest normal mode \(\Delta U_{\text{meso}}\) rapidly, as \(r_{\text{meso}} \rightarrow 0\) as \(r_{\text{meso}} \rightarrow \xi\). The lowest mode shows a spatial extent, \(\xi_{\text{meso}}\), which increases sublinearly for \(r_{\text{meso}} \leq \xi\) and saturates at \(r_{\text{meso}} \approx 1.5\,\xi\). We demonstrate that the \(\xi_{\text{meso}}/\xi\) versus \(r_{\text{meso}}/\xi\) curve is universal (independent of \(L\) or \(R\)). Hence small regions, \(r_{\text{meso}} \ll \xi\), can reveal the presence of incipient instability but give excellent estimates for the critical mode's energy and spatial extent only for \(r_{\text{meso}} \geq 1.5\,\xi\). Thus HDN is a quasi-local phenomenon.

4:30PM L26.00009 Fracture Energy Issues of Brittle, Microcrack Brittleness, and Dislocation Ductile Materials, RAY B. STOUT, RhoBetaSigma Aff, 954 Venus Way, Livermore CA 94550-6346, RHOBETASIGMA AFF COLLABORATION — Somigliana elasticity models[1915] for dislocation-microcrack defect discontinuities in a material form an analog basis to relate dislocation density evolution to microcrack density evolution near an existing idealized crack-tip. Thus, a recent idealized field solution derived for stochastic dislocation density evolution near a crack-tip in a ductile material is also an analog applicable field solution for stochastic microcrack density evolution in a brittle material near a crack-tip. A non-equilibrium thermodynamic functional is derived and integrated to evaluate rates of dislocation and microcrack internal energy evolution due to the singularity terms of these crack-tip solutions in an arbitrary spatial crack-tip neighborhood and during an arbitrary fracture toughness load-up time interval of \([0, t^{*}]\). At some time greater than \(t^{*}\), the available inter-atomic lattice(analog recoverable elastic) internal energy at a crack-tip becomes probabilistically sufficient, in an energy transfer-stability sense of Gibbs[1906], Griffith[1920], and Eschelby[Phil Trans Roy Soc, 1951], to be configurationally transported from locally recoverable internal energy at a crack-tip to non-recoverable crack-tip surface energy as a crack-tip propagates.

3N/A

4:42PM L26.00010 Role of interactions and damage in a cohesive fracture model, JOSEPH GRAN, JOHN RUNDLE, DONALD TURCOTTE, University of California, Davis, WILLIAM KLEIN, Boston University — We study the influences of local and long range interactions in a numerical model of tensile fracture. Our model simulates fracture events on a 2D square lattice plane with a Metropolis algorithm. We chose a Hamiltonian that is written as a function of the crack separation (offset field) and includes contributions from an external field, interactions, as well as a cohesive energy across the crack surfaces. Included in our study is both a ferromagnetic-type (attractive) and antiferromagnetic-type (repulsive) interactions. We test both of these interactions individually as well as a hybrid interaction in which over a short range the interaction is antiferromagnetic and in the long range the interaction becomes ferromagnetic. This dual interaction approximates a Lennard-Jones potential. We also propose a characterization of damage range the interaction becomes ferromagnetic. This dual interaction approximates a Lennard-Jones potential. We also propose a characterization of damage to interactions with neighboring sites and cannot hold any load. We compare our damage model to previous studies of fiber-bundle models.
Experiment and simulation are in accord with the theoretical prediction, and demonstrate that swimming in sand can be viewed as movement in a localized field and constraint curvature function visualizations of the system dynamics. From these we predict optimal gaits for forward, lateral and rotational motion during reversals of body segments. Despite the inaccuracy of the steady-state assumption, we use the force laws and a recently developed geometric mechanics forces resemble those in viscous fluids while the ratio of thrust to drag forces is always larger in the granular media than in viscous fluids. Using the force laws on a small cylinder oriented at different angles relative to the displacement direction. Unlike in Newtonian fluids, resistive forces are independent of speed. Drag these models to discuss principles of swimming within these granular "frictional fluids". The empirical drag force laws are measured as the steady-state forces of limbs. To model the locomotion of the sandfish, we previously developed an empirical resistive force theory (RFT), a numerical sandfish model coupled to an of Technology — X-ray imaging reveals that the sandfish lizard swims within granular media (sand) using axial body undulations to propel itself without the use of limbs. To model the locomotion of the sandfish, we previously developed an empirical resistive force theory (RFT), a numerical sandfish model coupled to an. Indentation of Graphene Membranes: Non-Linear Response, Nano-Fracture, and Crack Propagation. ROMAIN PERRIOT, YOU LIN, VASILY ZHAKHOVSKY, Department of Physics, University of South Florida, XIANG GU, Department of Applied Physics, Aalto University, IVAN OLEYNIK, Department of Physics, University of South Florida — Recent indentation experiments on graphene have revealed its exceptional strength, making it an excellent candidate for the design of nano- and micro-electromechanical systems. Therefore, it is critical to understand the mechanical properties of graphene, and its response to a wide range of loading pressures beyond the elastic regime. In this work molecular dynamics (MD) simulations of indentation of circular graphene membranes were performed with a newly developed interatomic potential, specifically designed to study graphene under extreme tensile stress. The indentation curves confirmed the experimental observation of a non-linear response at large loads, as well as the brittle failure of the membranes via the generation of nano-cracks. Our MD simulations showed that the fracture process consists of two consecutive stages: an initial bond-breaking event followed by the formation and propagation of cracks. The kinetic theory of bond breaking was applied to determine the breaking strength of graphene and its dependence on the indenter radius, as well as the waiting time for failure. MD simulations were used to provide an atomic-scale description of fracture dynamics.

5:06PM L26.00012 Investigation of Nonlinear Elastic Behavior of Two-Dimensional Molybdenum Disulfide, RYAN COOPER, Columbia University, CHANGGU LEE, Sung Kyun Kwan University, CHRISTOPHER MARIANETTI, JAMES HONE, JEFFREY KYSAR, Columbia University — The present study investigates the nonlinear elastic properties of a single-layer molybdenum disulfide crystal through experiment, finite element modeling, and density functional theory. Suspended single-layer molybdenum disulfide crystals are suspended over circular holes that were etched on a silicon oxide surface. Crystals are loaded at the center with an atomic force microscope until fracture occurs. The load-displacement curve is used to determine the pretension and linear-elastic response of the crystal. The force at which fracture occurs gives insight into the intrinsic strength and higher order elastic constants of the crystal. These experiments provide a platform to validate first-principles derivation of fifth-order elastic constants for in-plane stiffness using density functional theory. The derived higher order elastic constants are used in a finite element model to predict the breaking strength of two-dimensional molybdenum disulfide. The study bridges the gap between density functional theory and finite element analysis with experimental evidence.

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L33 GSNP DFD: Invited Session: Frontiers of Granular Physics

2:30PM L33.00001 Packing Nonspherical Particles: All Shapes Are Not Created Equal, SALVATORE TORQUATO, Departments of Chemistry and Physics, and Princeton Center for Theoretical Science, Princeton University, Princeton, NJ 08544 — Over the past decade there has been increasing interest in the effects of particle shape on the characteristics of dense particle packings, since deviations from sphericity can lead to more realistic models of granular media, nanostructured materials, and tissue architecture. It is clear that the broken rotational symmetry of a nonspherical particle is a crucial aspect in determining its resulting packing characteristics, but given the infinite variety of possible shapes (ellipsoids, superballs, regular and irregular polyhedra, etc.) it is desirable to formulate packing organizing principles based the particle shape. Such principles are beginning to be elucidated; see Refs. 1 and 2 and references therein. Depending upon whether the particle has central symmetry, inequivalent principle axes, and smooth or flat surfaces, we can describe the nature of its densest packing (which is typically periodic) as well as its disordered jammed states (which may or may not be isostatic). Changing the shape of a particle can dramatically alter its packing attributes. This tunability capability via particle shape could be used to tailor many-particle systems (e.g., colloids and granular media) to have designed crystal, liquid and glassy states.

3:06PM L33.00002 Network Analysis of Granular Flows, MICHELLE GIRVAN, University of Maryland — The flow of granular materials is important to many natural and industrial processes, yet connecting microscale materials properties of grains to bulk flow behavior has remained a challenging task. Our work leverages tools from complex network theory to study granular flow at multiple scales. By characterizing the statistical properties of time-evolving contact networks using metrics like average path length, giant component size, and modularity, we are able to identify how macroscale system features like the loss of reversibility are connected to micro- and meso-scale rearrangements in the contact network. In addition, we employ a network-based approach to explore the role of rotations in facilitating cooperative rearrangements. For both the reversibility and rotation studies, we apply network analysis to time-dependent contact network data obtained from both experiments and simulations and show that this approach can provide new insights on how bulk system properties are connected to particle-scale motion.

3:42PM L33.00003 Swimming in a granular frictional fluid, DANIEL GOLDMAN, School of Physics, Georgia Institute of Technology — X-ray imaging reveals that the sandfish lizard swims within granular media (sand) using axial body undulations to propel itself without the use of limbs. To model the locomotion of the sandfish, we previously developed an empirical resistive force theory (RFT), a numerical sandfish model coupled to an experimentally validated Discrete Element Method (DEM) model of the granular medium, and a physical robot model. The models reveal that only grains close to the swimmer are fluidized, and that the thrust and drag forces are dominated by frictional interactions among grains and the intruder. In this talk I will use these models to discuss principles of swimming within these granular "frictional fluids". The empirical drag force laws are measured as the steady-state forces on a small cylinder oriented at different angles relative to the displacement direction. Unlike in Newtonian fluids, resistive forces are independent of speed. Drag forces resemble those in viscous fluids while the ratio of thrust to drag forces is always larger in the granular media than in viscous fluids. Using the force laws as inputs, the RFT overestimates swimming speed by approximately 20%. The simulation reveals that this is related to the non-instantaneous increase in force during reversals of body segments. Despite the inaccuracy of the steady-state assumption, we use the force laws and a recently developed geometric mechanics theory to predict optimal gaits for a model system that has been well-studied in Newtonian fluids, the three-link swimmer. The combination of the geometric theory and the force laws allows us to generate a kinematic relationship between the swimmer’s shape and position velocities and to construct connection vector field and constraint curvature function visualizations of the system dynamics. From these we predict optimal gaits for forward, lateral and rotational motion. Experiment and simulation are in accord with the theoretical prediction, and demonstrate that swimming in sand can be viewed as movement in a localized frictional fluid.

This work was supported by NSF Physics of Living Systems.
4:18PM L33.00004 Geometrically Cohesive Granular Materials\textsuperscript{1}, SCOTT FRANKLIN, Rochester Institute of Technology — Geometrically cohesive granular materials (GCCM) are collections of particles whose individual shape leads to entanglements that resist extension forces, resulting in a non-zero Young's modulus. Examples include long, thin (anisometric) rods, arcs of varying length, and U-shaped staples. I will report on experimental and computational work that investigates the peculiar rigidity of GCCM. These include canonical stress-strain and vibration-induced melting experiments on U-shaped staples that have revealed a non-monotonic dependence of collective rigidity on particle shape. For concave particles, rigidity appears proportional to an “entanglement number” — the number of neighbors that pass through the area partially bounded by the particle. Computational and analytic work on arcs and staples confirm the non-monotonic behavior of the entanglement number, and simulations that match the experimental conditions are underway to confirm entanglement as the basic mechanism of GCCM’s rigidity.

\textsuperscript{1}This work funded in part by the National Science Foundation and Donors from the Petroleum Research Fund.

4:54PM L33.00005 Strain-stiffening in random packings of entangled granular chains\textsuperscript{1}, ERIC BROWN, University of California, Merced — Random packings of granular chains are presented as a model polymer system to investigate the consequences of entanglements in the absence of Brownian motion. The packings are compressed uniaxially and the structure is characterized by x-ray tomography. For short chain lengths, these packings yield when the shear stress exceeds the scale of the confining pressure, similar to packings of spherical particles. In contrast, packings of chains which are long enough to bind into closed loops exhibit strain-stiffening, in which the effective stiffness of the material increases with strain, similar to many polymer materials. The latter packings can sustain stresses orders-of-magnitude greater than the confining pressure, and do not yield until the chain links break. These strain-stiffening packings are found to contain system-spanning clusters of entangled chains.

\textsuperscript{1}This work was done with Alice Nasto, Athanasios G. Athanassiadis, and Heinrich M. Jaeger at The University of Chicago

Tuesday, February 28, 2012 2:30PM - 5:18PM – Session L40 DBIO GSNP: Focus Session: Systems Biology and Biochemical Networks II 156A

2:30PM L40.00001 Microbial interaction networks in soil and in silico, KALIN VETSIGIAN, University of Wisconsin-Madison — Soil harbors a huge number of microbial species interacting through secretion of antibiotics and other chemicals. What patterns of species interactions allow for this astonishing biodiversity to be sustained, and how do these interactions evolve? I used a combined experimental-theoretical approach to tackle these questions. Focusing on bacteria from the genus Steptomyces, known for their diverse secondary metabolism, I isolated 64 natural strains from several individual grains of soil and systematically measured all pairwise interactions among them. Quantitative measurements on such scale were enabled by a novel experimental platform based on robotic handling, a custom scanner array and automatic image analysis. This unique platform allowed the simultaneous capturing of \textasciitilde15,000 time-lapse movies of growing colonies of each isolate on media conditioned by each of the other isolates. The data revealed a rich network of strong negative (inhibitory) and positive (stimulating) interactions. Analysis of this network and the phylogeny of the isolates, together with mathematical modeling of microbial communities, revealed that: 1) The network of interactions has three special properties: “balance”, “bi- modality” and “reciprocity”; 2) The interaction network is fast evolving; 3) Mathematical modeling explains how rapid evolution can give rise to the three special properties through an interplay between ecology and evolution. These properties are not a result of stable co-existence, but rather of continuous evolutionary turnover of strains with different production and resistance capabilities.

3:06PM L40.00002 ABSTRACT WITHDRAWN

3:18PM L40.00003 Regulatory schemes to achieve optimal flux partitioning in bacterial metabolism\textsuperscript{1}, LEI-HAN TANG, Department of Physics, Hong Kong Baptist University and Beijing Computational Science Research Center, ZHU YANG, Department of Physics, Hong Kong Baptist University, SHENG HUI, Department of Physics, UCSD, PAN-JUN KIM, APCTP, Korea, XUE-FEI LI, Department of Physics, Hong Kong Baptist University, TERENCE HWA, Department of Physics, UCSD — The flux balance analysis (FBA) offers a way to compute the optimal performance of a given metabolic network when the maximum incoming flux of nutrient molecules and other essential ingredients for biosynthesis are specified. Here we report a theoretical and computational analysis of the network structure and regulatory interactions in an E. coli cell. An automated scheme is devised to simplify the network topology and to enumerate the independent flux degrees of freedom. The network organization revealed by the scheme enables a detailed interpretation of the three layers of metabolic regulation known in the literature: i) independent transcriptional regulation of biosynthesis and salvage pathways to render the network tree-like under a given nutrient condition; ii) allosteric end-product inhibition of enzyme activity at entry points of synthesis pathways for metabolic flux partitioning according to consumption; iii) homeostasis of currency and carrier compounds to maintain sufficient supply of global commodities. Using the amino-acid synthesis pathways as an example, we show that the FBA result can be reproduced with suitable implementation of the three classes of regulatory interactions with literature evidence.

\textsuperscript{1}Work supported in part by the RGC of the HKSAR under grant 201910.

3:30PM L40.00004 A Realtime Active Feedback Control System For Coupled Nonlinear Chemical Oscillators, NATHAN TOMPKINS, SETH FRADEN, Brandeis University — We study the manipulation and control of oscillatory networks. As a model system we use an emulsion of Belousov-Zhabotinsky (BZ) oscillators packed on a hexagonal lattice. Each drop is observed and perturbed by a Programmable Illumination Microscope (PIM). The PIM allows us to track individual BZ oscillators, calculate the phase and order parameters of every drop, and selectively perturb specific drops with photo illumination, all in realtime. To date we have determined the native attractor patterns for drops in 1D arrays and grammable Illumination Microscope (PIM). The PIM allows us to track individual BZ oscillators, calculate the phase and order parameters of every drop, and a model system we use an emulsion of Belousov-Zhabotinsky (BZ) oscillators packed on a hexagonal lattice. Each drop is observed and perturbed by a Pro-

4:22PM L40.00005 Stochastic gene expression with bursting and positive feedback, THIERRY PLATINI, Virginia Bioinformatics Institute, HODJAT PENDAR, RAHUL KULKARNI, Department of Physics, Virginia Tech — Stochastic (or noise) in the process of gene expression can play a critical role in cellular circuits that control switching between probabilistic cell-fate decisions in diverse organisms. Such circuits often include positive feedback loops as critical elements. In some cases (e.g. HIV-1 viral infections), switching between different cell fates occurs even in the absence of bistability in the underlying deterministic model. To characterize the role of noise in such systems, we analyze a simple gene expression circuit that includes contributions from both transcriptional and translational bursting and positive feedback effects. Using a combination of analytical approaches and stochastic simulations, we explore how the underlying parameters control the corresponding mean and variance in protein distributions.

3:42PM L40.00005 Stochastic gene expression with bursting and positive feedback, THIERRY PLATINI, Virginia Bioinformatics Institute, HODJAT PENDAR, RAHUL KULKARNI, Department of Physics, Virginia Tech — Stochastic (or noise) in the process of gene expression can play a critical role in cellular circuits that control switching between probabilistic cell-fate decisions in diverse organisms. Such circuits often include positive feedback loops as critical elements. In some cases (e.g. HIV-1 viral infections), switching between different cell fates occurs even in the absence of bistability in the underlying deterministic model. To characterize the role of noise in such systems, we analyze a simple gene expression circuit that includes contributions from both transcriptional and translational bursting and positive feedback effects. Using a combination of analytical approaches and stochastic simulations, we explore how the underlying parameters control the corresponding mean and variance in protein distributions.
3:54PM L40.00006 mRNA Noise Reveals that Activators Induce a Biphasic Response in the Promoter Kinetics of Highly Regulated Genes, KATIE QUINN, Massachusetts Institute of Technology, TSZ-LEUNG TO, University of California, San Francisco, NARENDRA MAHESHWARI, Massachusetts Institute of Technology — A dominant source of fluctuations in gene expression is thought to be the process of transcription. The statistics of these fluctuations arise from the kinetics of transcription. Multiple studies suggest the bulk of fluctuations can be understood by a simple process where genes are inactive for exponentially distributed times punctuated by geometric bursts of mRNA. Yet it’s largely unknown how cis and trans factors affect the two lumped kinetic parameters, burst size and burst frequency, that describe this process. Importantly, how these parameters are regulated in a single gene can qualitatively affect the dynamical behavior of the network it is embedded within. Here, we ask whether transcriptional activators increase gene expression by increasing the burst size or burst frequency. We do so by deducing these parameters from steady-state mRNA distributions measured in individual yeast cells using single molecule mRNA FISH. We find that for both a synthetic and natural promoter, activators appear to first increase burst size, then burst frequency. We suggest this biphasic response may be common to all highly regulated genes and was previously unappreciated because of measurement techniques. Furthermore, its origins appear to relate to cis events at the promoter, and may arise from combinations of basal and activator-dependent bursts. Our measurements shed new light on transcriptional mechanisms and should assist in building synthetic promoters with tunable statistics.

4:06PM L40.00007 Determining the stability of genetic switches: Explicitly accounting for mRNA noise, MICHAEL ASSAF, ELIJAH ROBERTS, ZAN LUTHEY-SCHULTEN, University of Illinois at Urbana-Champaign — Cells use genetic switches to shift between alternate gene expression states, e.g. to adapt to new environments or to follow a developmental pathway. Here, we study the dynamics of switching in a generic-feedback on/off switch. Unlike protein-only models, we explicitly account for stochastic fluctuations of mRNA, which have a dramatic impact on the genetic switch dynamics. Employing a semi-classical theory to treat the underlying chemical master equations, we obtain accurate results for the quasi-stationary distributions of mRNA and protein copy numbers and for the mean switching time, starting from either state. Our analytical results agree well with extensive Monte Carlo simulations. Importantly, one can use the approach to study the effect of varying biological parameters, and of extrinsic noise, on the switch stability.

4:18PM L40.00008 Quantitative Model of microRNA-mRNA interaction, JAVAD NOORBakhsh, ALEX LANG, PANKAJ MEHTA, Boston University — MicroRNAs are short RNA sequences that regulate gene expression and protein translation by binding to mRNA. Experimental data reveals the existence of a threshold linear output of protein based on the expression level of microRNA. To understand this behavior, we propose a mathematical model of the chemical kinetics of the interaction between mRNA and microRNA. Using this model we have been able to quantify the threshold linear behavior. Furthermore, we have studied the effect of internal noise, showing the existence of an intermediary regime where the expression level of mRNA and microRNA has the same order of magnitude. In this crossover regime the mRNA translation becomes sensitive to small changes in the level of microRNA, resulting in large fluctuations in protein levels. Our work shows that chemical kinetics parameters can be quantified by studying protein fluctuations. In the future, studying protein levels and their fluctuations can provide a powerful tool to study the competing endogenous RNA hypothesis (ceRNA), in which mRNA crosstalk occurs due to competition over a limited pool of microRNAs.

4:30PM L40.00009 On the control of gene expression in small RNA post-transcriptional regulation pathway: role of conserved weak targets, DANIEL JOST, ANDRZEJ NOWOJEWSKI, EREL LEVINE, Department of Physics and FAS Center for Systems Biology - Harvard University — Small RNA molecules play critical regulatory roles in organisms across all kingdoms of life. Many small RNA families achieve target-specificity via base-pairing of a very short (6-8 nucleotides) “seed” region with the targeted mRNA, and consequently many genes carry a matching seed in their sequence. Evidence in bacteria and animals suggest that a single small RNA may regulate the gene expression of many different targets, although most of them very weakly. On the other hand, in all cases we are aware of where the functionality of a small RNA has been carefully studied, only a small number of target genes were identified as being phenotypically relevant. Here, we present a Langevin formalism which describes the dynamics of the different interacting entities (small RNA and targets), including the stochasticity of the underlying biochemical reactions and the effect of mRNA crosstalk occurs due to competition over a limited pool of microRNAs.

4:42PM L40.00010 Approaches to Chemical and Biochemical Information and Signal Processing, VLADIMIR PRIVMAN, Clarkson University — We outline models and approaches for error control required to prevent buildup of noise when “gates” and other “network elements” based on (bio)chemical reaction processes are utilized to realize stable, scalable networks for information and signal processing. We also survey challenges and possible future research.

1 Control of Noise in Chemical and Biochemical Information Processing, V. Privman, Israel J. Chem. 51, 118-131 (2010).

4:54PM L40.00011 Organizing biochemical reactions: Lessons from cyanobacteria, NIALL MANGAN, Harvard University Systems Biology PhD Program, MICHAEL BRENNER, Harvard School of Engineering and Applied Sciences — Cyanobacteria are model organisms for photosynthesis and are of interest for bio-fuel production and carbon dioxide sequestration. I present a mathematical model of the carbon concentrating mechanism (CCM) in cyanobacteria. The CCM is a combination of transporters and enzymes distinctively organized in the cell, which increase the internal concentration of carbon dioxide, and improve the efficiency of converting carbon dioxide to sugar. I find that the internal carbon concentration can be completely described by solutions in two parameter regimes of the model. These solutions correspond to varying transporter and enzymatic activity, which can be directly connected to experimental measurements. I also find a dependence of the carbon concentration on the spatial organization of the reactions within the cell. Understanding the CCM in cyanobacteria gives us insight into design principles for the cellular organization of biological reactions.

1 NSF Graduate Fellowship

5:06PM L40.00012 ABSTRACT WITHDRAWN —
2:30PM L52.00001 Extreme Folding, ERIK DEMAINE, Massachusetts Institute of Technology — Our understanding of the mathematics and algorithms behind paper folding, and geometric folding in general, has increased dramatically over the past several years. These developments have found a surprisingly broad range of applications. In the art of origami, it has helped spur the technical origami revolution. In engineering and science, it has helped solve problems in areas such as manufacturing, robotics, graphics, and protein folding. On the recreational side, it has led to new kinds of folding puzzles and magic. I will give an overview of the mathematics and algorithms of folding, with a focus on new mathematics and sculpture.

3:06PM L52.00002 Geometry in the mechanics of origami, MARCELO A. DIAS, CHRISTIAN D. SANTANGELO, University of Massachusetts Amherst — We present a mechanical model for curved fold origami in which the bending energies of developable regions are balanced with a phenomenological energy for the crease. The latter energy comes into play as a source of geometric frustration, allowing us to study shape formation by prescribing crease patterns. For a single fold annular configuration, we show how geometry forces a symmetry breaking of the ground state by increasing the width of the ribbon. We extend our model to study multiple fold structures, where we derive geometrical constraints that can be written as recursive relations to build the surface from valley to mountain, and so on. We also suggest a mechanical model for single vertex folds, mapping this problem to an elastica on the sphere.

3:18PM L52.00003 Photo-Origami — Using Light to Bend, Fold, and Buckle, JENNIE RYU, University of Colorado, MATTEO D'AMATO, University of Trento, KEVIN LONG, Sandia National Laboratories, XIAODONG CUI, H. JERRY QI, MARTIN DUNN, University of Colorado — We describe photo-origami, a method to program spatially- and temporally-variable mechanical, chemical, and optical fields into a polymer that enable controllable, sequenced, macroscopic bending and folding to create three-dimensional structures. We combine mechanical and optical stimuli to locally rearrange the polymer's network topology which allows us to program a residual stress state into the film; upon release of mechanical constraints, we realize a wide variety of desired shapes. We demonstrate, through a combination of theory, simulation-based design, synthesis, and experiment, the operable phenomena and capabilities of photo-origami. We demonstrate architectures that rely on bending, folding, instabilities, and post-buckling behavior to achieve their three-dimensional form, starting from a flat sheet. We also describe a theory that couples the hereditary nature of photoelectrics, chemistry, and large-deformation mechanics and enables simulations of the fabricated structures that are in good agreement with the experiments.

1 AFOSR, National Science Foundation, Sandia National Laboratories

3:30PM L52.00004 Pleated and Creased Structures, LEVI DUDTE, ZHIYAN WEI, L. MAHADEVAN, Harvard University — The strategic placement of curved folds on a paper annulus produces saddle-shaped origami. These exotic geometries resulting from simple design processes motivate our development of a computational tool to simulate the stretching, bending and folding of thin sheets of material. We seek to understand the shape of the curved origami figure by applying the computational tool to simulate a thin annulus with single or multiple folds. We aim to quantify the static geometry of the simple models and develop a framework of methodologies for actuation. We develop a formulation that will enable us to simulate the equilibrated state of a pleated structure defined in terms of 2 angles and 2 lengths. The unit cell embodies the basic element in all non-trivial pleated structures - the mountain or valley folds, wherein four folds come together at a single vertex. The ability of this structure to pack and unpack with a few degrees of freedom leads to their use in deployable structures such as solar sails and maps, just as this feature is useful in insect wings, plant leaves and flowers. We probe the qualitative and quantitative aspects of the mechanical behavior of these structures with a view to optimizing material performance.

1 Grant Acknowledgement: Harvard NSF MRSEC, DARPA, Kavli Institute, Wyss Institute

3:42PM L52.00005 Hierarchical Stress Focusing in Elastic Ridge, LEE WALSH, BENNY DAVIDOVITCH, University of Massachusetts — A crumpled or confined elastic sheet contains many stress-focusing structures and singularities, primarily ridges and vertices, which may contain much of the strain. We seek to determine the degree and quality of stress focusing within the geometry of a single ridge. Previous work on the ridge assumes the asymptotic limit of infinitely sharp vertices. However, in a physically realistic sheet any vertex or intersection of ridges will naturally have a finite radius of curvature greater than the sheet's thickness. We simulate these more physically realistic boundary conditions in a ridge using Surface Evolver.

3:54PM L52.00006 Stress focusing and collapse of a thin film under constant pressure, EUGENIO HAMM, NICOLAS CABEZAS, Universidad de Santiago de Chile — Thin elastic sheets and shells are prone to focus stress when forced, due to their near-inextensibility. Singular structures such as ridges, vertices, and folds arising from wrinkles, are characteristic of the deformation of such systems. Usually the forcing is exerted at the boundaries or at specific points of the surface, in displacement controlled experiments. On the other hand, much of the phenomenology of stress focusing can be found at micro and nanoscales, in physics and biology, making it universal. We will consider the post-buckling regime of a thin elastic sheet that is subjected to a constant normal distributed force. Specifically, we will present experiments made on thin elastoplastic sheets that collapse under atmospheric pressure. For instance, in vacuum-sealing technology, when a flat plastic bag is forced to wrap a solid volume, a series of self-contacts and folds develop. These are similar in appearance to the folds found on the surface of a pizza, and by the exact way it sticks to its surface, by friction. Inspired by this everyday example we study the geometry of folds that result from collapsing a hermetic bag on regular rigid bodies.

1 Fondecyt 1110584 and Anillo ACT95

4:06PM L52.00007 Creasy modeling of a compressed elastic surface, TUOMAS TALLINEN, L. MAHADEVAN, Harvard University — Compression of an elastic layer attached to a rigid substrate leads to nucleation and growth of creases. We explore crease formation by a numerical model allowing control of compressive strain, anisotropy and bulk modulus. We address questions on arrangement and geometry of creases and model also the stabilizing effect of surface tension at small scales.

4:18PM L52.00008 Creasing instability of elastomers under uniaxial compression, DAYONG CHEN, RYAN HAYWARD, Polymer Science and Engineering Department at UMass-Amherst — Soft polymers placed under compressive stress can undergo an elastic creasing instability in which sharp folds spontaneously form on the free surfaces. This process may play an important role in contexts as diverse as brain morphogenesis, failure of tires, and electrical breakdown of soft polymer actuators, but our understanding of this instability is still quite limited. We describe a simple experimental system to study creasing of thin elastomer films under uniaxial compression. The equilibrium depths, spacings and shapes of creases are characterized and found to show excellent agreements with numerical results. Further, we use this system to explore the important roles played by surface energy and adhesion in the onset and hysteretic behavior of creases.

4:30PM L52.00009 Sulcus formation in a compressed elastic half space, JOHN BIGGINS, L. MAHADEVAN, Harvard University — When a block of rubber, biological tissue or other soft material is subject to substantial compression, its surfaces undergo a folding instability. Rather than having a smooth profile, these folds contain cusps and hence have been called creases or sulci rather than wrinkles. The stability of a compressed surface was first investigated by Biot (1965), assuming the strains associated with the instability were small. However, the compression threshold predicted with this approach is substantially too high. I will introduce a family of analytic area preserving maps that contain cusps (and hence points of infinite strain) that save energy before the linear stability threshold even at vanishing amplitude. This establishes that there is a region before the linear stability threshold is reached where the system is unstable to infinitesimal perturbations, but that this instability is quintessentially non-linear and cannot be found with linear strain elasticity.
4:42PM L52.00010 Compression induced folding of a sheet: An integrable system. HAIM DIAMANT, Tel Aviv University, THOMAS A. WITTEN, University of Chicago — The apparently intractable shape of a fold in a compressed elastic film lying on a fluid substrate is found to have an exact solution. Such systems buckle at a nonzero wave vector set by the bending stiffness of the film and the weight of the substrate fluid. Our solution describes the entire progression from a weakly displaced sinusoidal buckling to a single large fold that contacts itself. The pressure decrease is exactly quadratic in the lateral displacement. We demonstrate a subtle connection to the sine-Gordon problem, which reveals a new symmetry in the folding phenomenon.

4:54PM L52.00011 Wrinkles or creases in a bi-layer structure. LIHU JIN, School of Engineering and Applied Sciences, Kavli Institute, Harvard University, ANESIA BURNS, RYAN HAYWARD, Department of Polymer Science & Engineering, University of Massachusetts, ZHIGANG SUO, School of Engineering and Applied Sciences, Kavli Institute, Harvard University — Wrinkles and creases are different modes of instability. In this work, we try to answer for a bi-layer structure with different modulus ratios and thickness ratios of the film and substrate whether wrinkles or creases form first when the bi-layer is under uniform compression. The onset of wrinkles corresponds to a bifurcation point, and we use the linear perturbation method to analyze the critical strain for the onset of wrinkles. Since the initiation of creases is autonomous, we directly apply the critical condition for crease initiation in a half space calculated by the finite element method in the literature to the situation of a bi-layer structure with finite thickness. By comparing the critical strains for the formation of wrinkles and creases under different modulus and thickness ratios, a phase diagram of the formation of wrinkles or creases is obtained. Although the critical strains for both wrinkle and crease initiation depend on the state of strain, remarkably the phase diagram is independent of the state of strain. As a result, creases tend to set in for more compliant and thicker films, while wrinkles tend to set in for stiffer and thinner films. Especially, when the modulus ratio of the film and substrate is smaller than 1.67, creases always form earlier than wrinkles, no matter what the thickness ratio is. We further verify the result experimentally by compressing a bi-layer of polymers with different modulus and thickness ratios.

5:06PM L52.00012 Wrinkles and Folds in Ultra-Thin Polymer Films. YURI EBATA, University of Massachusetts, Amherst, ANDREW B. CROLL, North Dakota State University, ALFRED J. CROSBY, University of Massachusetts, Amherst — Wrinkles and folds are observed in many biological systems during morphogenesis processes. However, the mechanics of how these wrinkles and folds form are not completely understood. Studying the mechanics of wrinkles and folds will not only provide us with fundamental insights of nonlinear deformation processes but also allow for the fabrication of unique patterned surfaces that can be controlled reversibly. In this study, we examine wrinkles and folds of polystyrene films of thickness ranging from 5 nm to 180 nm attached to uniaxially-strained polydimethylsiloxane substrates. The strain is released incrementally to apply increasing compressive strain to the attached film. The wavelength and the amplitude of local out-of-plane deformation are measured as global compression is increased to distinguish between different buckling modes. The transition from wrinkling to folding is observed by tracking the statistics of amplitude distribution sampled across a large lateral area, and a critical strain map is constructed to observe how film thickness affect the resulting buckling modes.

5:18PM L52.00013 Relaxation mechanisms in the unfolding of thin sheets. BENJAMIN THIRIA, PMMH-ESPCI, MOKHTAR ADDA-BEDIA, LPS-ENS — When a thin sheet is crumpled, creases form in which plastic deformations are localized. Here we study experimentally the relaxation process of a single fold in a thin sheet subjected to an external strain. The unfolding process is described by a quick opening at first, and then a progressive slow relaxation of the crease. In the latter regime, the necessary force needed to open the folded sheet at a given displacement is found to decrease logarithmically in time, allowing its description through an Arrhenius activation process. We accurately determine the parameters of this law and show its general character by performing experiments on both Mylar and paper sheets.

Tuesday, February 28, 2012 2:30PM - 5:30PM
Session L53 GSNP DCMP: Frontiers of Statistical Physics

2:30PM L53.00001 Lars Onsager Prize Lecture: A Random Walk Through Theoretical Physics. IAN AFFLECK, University of British Columbia — A historical account will be given of my efforts to apply conformal field theory techniques to experimentally relevant models of condensed matter. This began with a so far unsuccessful attempt to find the exact critical exponents for the localization transition in the integer quantum Hall effect, using techniques developed by field/string theorists. It was followed by a program to classify critical behavior of Heisenberg antiferromagnetic spin chains of arbitrary spin magnitude. It eventually led to a general theory of the low energy behavior of quantum impurity models including exact solutions for non-Fermi liquid critical points.

3:06PM L53.00002 Dannie Heineman Prize for Mathematical Physics Lecture: Understanding Nonequilibrium via Rare Fluctuations. GIOVANNI JONA-LASINIO, Dipartimento di Fisica, Università di Roma “La Sapienza” and INFN, Roma, Italy — Irreversible processes are a hot subject in statistical mechanics. During the last decade through the effort of several people, including the recipient of the prize and his collaborators, a progress in understanding stationary nonequilibrium states has been achieved. The key has been the study of rare fluctuations. The talk will review some basic ideas, results and perspectives.

3:42PM L53.00003 Experimental confirmation of Landauer’s principle. JOHN BECHHOEFER, YONGGUN JUN2, Simon Fraser University — Landauer’s principle, formulated in 1961, postulates that irreversible logical or computational operation such as memory erase must dissipate heat, no matter how slowly they are performed. For example, to “reset to one” a memory that can be in state 0 or 1 requires at least kT ln2 of work, which is dissipated as heat. In 1982, Bennett pointed out a link to Maxwell’s Demon: Were Landauer’s principle to fail, it would be possible to repeatedly extract work from a heat bath. We report the first confirmation of Landauer’s principle in an experimental system, where a virtual double-well potential is created via a feedback loop. We observe the position of a charged, fluorescent, colloidal particle in water and calculate and then apply a force = -grad U(x,t) via an electric field. In a first experiment, the probability of “erasure” (resetting to one) is unity, and at long cycle times, we observe that the work tend to zero.

1Supported by NSERC, Canada
2Present address: Department of Developmental and Cell Biology, School of Biological Sciences, Univ. of Calif., Irvine
We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature. We study radiation amorphization in a simple molecular dynamics model and show that one can describe the amorphous steady-state using a structural effective temperature.
8:00AM P2.00001 Characterizing Order in Glassy Systems, DOV LEVINE, Technion - IIT — Crystals and quasicrystals can be characterized by an order that is a purely geometric property of an instantaneous configuration, independent of particle dynamics or interactions. Glasses, on the other hand, are ostensibly amorphous arrangements of particles. A natural and long-standing question has been whether they too have, albeit in a hidden way, some form of geometric order. I will examine a recent proposal for a coherence length that applies to systems which are typically characterized as amorphous, as well as to those that are conventionally ordered. The question of whether exotic order can arise in physical systems will be addressed.

8:36AM P2.00002 Drift, diffusion and barrier crossing of small objects on a surface assisted by an external noise: roles of non-linear friction, MANOJ CHAUDHURY, Lehigh University — We study experimentally the behaviors of several driven diffusive systems that involve the sliding and rolling of small solid objects or liquid drops on a surface with an external noise and an external field. The displacement statistics here are non-Gaussian at short observation time, but they tend towards a Gaussian behavior at long time scale. Furthermore, in each of these cases, the drift velocity increases sub-linearly, but the diffusivity increases super-linearly with the strength of the noise. These observations reflect the underlying non-linear friction control of their stochastic dynamics. Specific experiments have also been designed to study the hopping of a small object over a physical barrier assisted by an external noise. These results mimic the classical Arrhenius behavior from which an effective temperature may be deduced. However, the regimes controlled by a Coulombic like friction and a linear kinematic friction need to be treated somewhat differently. All the drifted diffusive systems studied here exhibit substantial negative fluctuations of displacement at a short observation time that diminishes at longer time scale. Using the integrated fluctuation theorem, we characterize the persistence time of negative fluctuations in terms of the diffusivity and the drift velocity that can be measured experimentally.

9:12AM P2.00003 Noise induced stabilization in population dynamics1, ALEX KAMENEV, University of Minnesota — We investigate a model where strong noise in a sub-population creates a metastable state in an otherwise unstable two-population system. The induced metastable state is vortex-like, and its persistence time grows exponentially with the noise strength. A variety of distinct scaling relations are observed depending on the relative strength of the sub-population noises.

9:48AM P2.00004 Speeding up spontaneous disease extinction, MICHAEL KHASIN2, University of Michigan — The dynamics of epidemic in a susceptible population is affected both by the random character of interactions between the individuals and by environmental variations. As a consequence, the sizes of the population groups (infected, susceptible, etc.) fluctuate in the course of evolution of the epidemic. In a small community a rare large fluctuation in the number of infected can result in extinction of the disease. We suggest a novel paradigm of controlling the epidemic, where the control field, such as vaccination, is designed to maximize the rate of spontaneous disease extinction. We show that, for a limited-scope vaccination, the optimal vaccination protocol and its impact on the epidemics have universal features: (i) the vaccine must be applied in pulses, (ii) the spontaneous disease extinction is synchronized with the vaccination. We trace this universality to general properties of the response of large fluctuations to external perturbations.

10:24AM P2.00005 Cooperativity-Driven Singularities in Cooperative Asymmetric Exclusion1, SIDNEY REDNER, Boston University — We investigate the effect of cooperative interactions on the asymmetric exclusion process. In the simplest case a particle can hop to its vacant right neighbor only if its left neighbor is occupied. We show that an initial density downstep develops into a rarefaction wave that can have a jump discontinuity at the leading edge, while an upstep results in a shock wave. We also investigate a more general model in which the particle velocity can be an increasing function of the density. Within a hydrodynamic theory, initial density upsteps and downsteps can evolve into: (a) shock waves, (b) continuous compression or rarefaction waves, or (c) a mixture of shocks and continuous waves. These unusual phenomena arise because the current versus density relation has an inflection point, so that the group velocity can either be an increasing or a decreasing function of the density on either side of the inflection point.

1Supported by NSF grant DMR-0804266

1in collaboration with Mark Dykman, Michigan State University, and Baruch Meerson, Hebrew University of Jerusalem

10:48AM P2.00006 Cooperative Asymmetric Exclusion: Molecular Dynamics Simulations, TRISTAN A. SHARP, MARK O. ROBBINS, Johns Hopkins University — We study microscopic roughness on real surfaces by a method that is motivated by the fact that surfaces differ only at the atomic level can show different relationships between load, stiffness, and friction. Here we use molecular dynamics simulations to study contact properties of self-affine rough surfaces that are identical at continuum scales, but differ at the atomic scale. We compare surfaces that have atomic positions displaced to a self affine surface to “stepped” surfaces that have been cut from a lattice. The stepped surfaces exhibit more plasticity, contributing to a larger contacting area at a given load. A unified framework captures the relation between roughness, system size, surface separation, stiffness, and contact area.
8:12AM P26.00002 Breakdown of Amontons’ Law of Friction in Sheared-Elastomer with Local Amontons’ Friction, HIROSHI MATSUKAWA, Department of Physics and Mathematics, Aoyama Gakuin University, 5-10-1 Fuchinobe, Sagamihara 252-5258, MICHIKO OTSUHI, Retired — It is well known that Amontons’ law of friction i.e. the frictional force against the sliding motion of solid object is proportional to the loading force and not dependent on the contact area, holds well for various systems. Here we show, however, the breakdown of the Amontons’ law for the elastic object which have local friction obeying Amontons’ law and is under uniform pressure by FEM calculation. The external shearing force applied to the trailing edge of the sample induces local slip. The range of the slip increases with the increasing external force adiabatically at first. When the range reaches the critical magnitude, the slips moves rapidly and reaches the leading edge of the sample then the whole system slides. These behaviors are consistent with the experiment by Rubinstein et.al. (Phys. Rev. Lett. 98, 226103). The static frictional coefficient, the ratio between the static frictional force for the whole system and the loading force, decreases with the increasing pressure. This means the breakdown of Amontons’ law. The pressure dependence of the frictional coefficient is caused by the change of the critical length of the local slip. The behaviors of the local slip and the frictional coefficient are well explained by the 1 dimensional model analytically.

8:42AM P26.00003 Geometry and elasticity for detachment fronts in friction, ALESSANDRO TALONI, ANDREA BENASSI, STEFANO ZAPPERI, CNR-İENİ istituto per l'energetica e le interfasi — Meso-scale friction bridges nanoscale contact mechanics to the macroscopic Amontons laws and is relevant for several mechanical problems including seismicity. Recent experiments on polymeric blocks show that the onset of friction occurs by nucleation of detachment fronts and that frictional properties vary along the sample surface. The earthquake-like dynamics found at the millimeter scale is in contrast with the usual assumption of uniform detachment without a coherent pattern in the front formation. Simulating the quasi-equilibrium dynamics of an elastic sample sliding on a rough surface under a shear force, we show that the dynamics of detachment fronts depends on the sample geometry. In particular, we study the effect of the sample aspect ratio by computing the elastic Green function for a finite three-dimensional slider. Our model allows to study the onset of friction in different geometries, from the thin slabs used in the aforementioned experiments to more general samples shapes.

8:36AM P26.00004 Local friction at a rubber/glass multicontact interface, ANTOINE CHATEAUMINOIS, DANH TOAN NGUYEN, CHRISTIAN FRETIGNY, ESPCI - PPM Laboratory, YOHAN LE CHENADEC, MAUTE PORTIGLIATTI, Manufacture Française des Pneumatiques Michelin — When rubber is squeezed against a hard, rough surface contact only occurs at localized spots between surface asperities. Friction thus involves the shearing of a myriad of micro-contacts which are distributed over length scales ranging from micrometers down to nanometers. In order to get more insights into this widely debated problem, spatially resolved measurements of frictional stresses are much needed. We recently proposed a method to measure local friction of rubbers by means of a contact imaging approach. Silicon rubber substrates marked on their surface are prepared in order to measure the displacement field induced by the steady state friction of a glass lens. Then, the deconvolution of this displacement field provides a spatially resolved measurement of the actual shear stress and contact pressure distributions within the contact interface. As a result, the local friction law, i.e. the relationship between the actual shear stress and normal pressure, is obtained. The effect of roughness are analyzed from experiments using statistically rough surfaces differing in their roughness power density spectrum. Experimental results are discussed in the light of theoretical contact models for the friction of multi-contact interfaces.

8:48AM P26.00005 Adhesive contact of randomly rough surfaces, LARS PASTEWKA, MARK ROBBINS, Johns Hopkins University — The contact area, stiffness and adhesion between rigid, randomly rough surfaces and elastic substrates is studied using molecular statics and continuum simulations. The surfaces are self-affine with Hurst exponent 0.3 to 0.8 and different short $\lambda_s$ and long $\lambda_L$ wavelength cutoffs. The rms surface slope and the range and strength of the adhesive potential are also varied. For parameters typical of most solids, the effect of adhesion decreases as the ratio $\lambda_s/\lambda_L$ increases. In particular, the pull-off force decreases to zero and the area of contact $A$ becomes linear in the applied load $L$. A simple scaling argument is developed that describes the increase in the ratio $A_s/L$ with increasing adhesion and a corresponding increase in the contact stiffness [1]. The argument also predicts a crossover to finite contact area at zero load when surfaces are exceptionally smooth or the ratio of surface tension to bulk modulus is unusually large, as for elastomers. Results that test this prediction will be presented and related to the Maugis-Dugdale [2] theories for individual asperities and the more recent scaling theory of Persson [3]. [1] Akarapu, Sharp, Robbins, Phys. Rev. Lett. 106, 204301 (2011) [2] Maugis, J. Colloid Interface Sci. 150, 243 (1992) [3] Persson, Phys. Rev. Lett. 74, 75420 (2006)

9:00AM P26.00006 The Effect of Surface Topography on Interface Stresses During Peeling, YE XU, ERIC DUFRESNE, Yale University — Surface topography can have a large impact on the adhesive strength of soft interfaces. While previous experiments have revealed some of the underlying mechanisms, there has been no direct measurement of interface stresses during adhesive failure. We use traction force microscopy to measure the microscopic distribution of interface stresses during peeling. We focus on the relationship between local stresses and topography near the peeling front.

9:12AM P26.00007 Direction dependence of static friction for commensurate and moderately incommensurate surfaces, MICHAEL WOLLOCH, Vienna University of Technology / Austrian Center of Competence for Tribology, PETER MOHN, JOSEF REDINGER, Vienna University of Technology, ANDRAS VERNES, Austrian Center of Competence for Tribology — We present results from our calculations of quasi-static sliding of two atomically flat surfaces in dry, wearless contact using the Density Functional Theory package VASP. The main focus of our work was to determine to which extent commensurability of the surfaces and the sliding direction effects the friction force. The examined systems include commensurable fcc (111) Aluminium slabs and moderately incommensurate surfaces like bcc (110) Titanium on hcp (001) Titanium. A model consistent with stick-slip friction was devised to calculate the friction forces along sliding paths of up to 1 $\mu$m on a quantum mechanical basis. To map all forces and energies for rigid and relaxed atomic positions the top slab was scanned over the bottom one on a properly fine grid, which covers the entire unit cell. In this manner, it is shown that the mean friction force depends on the sliding direction and that due to relaxations incommensurate paths may result, counter-intuitively, in higher friction then commensurate ones.

9:24AM P26.00008 Laser induced projectile impact test (LIPIT): A micron-scale ballistic test for high-strain rate mechanical study of nano-structures, JAE-HWANG LEE, Department of Mechanical Engineering and Materials Science, Rice University, DAVID VEYSSET, KEITH NELSON, Department of Chemistry, MIT, EDWIN THOMAS, Department of Mechanical Engineering and Materials Science, Rice University — We present a method to apply a locally deformed localization at a high-strain-rate for the study of mechanical characteristics of micro- and nano-structures. In the technique, Laser Induced Projectile Impact Test (LIPIT), micro-projectiles (solid silica spheres of 3.7 $\mu$m diameter) are accelerated to a supersonic speed (up to 4 km/s) in air by a micro-explosion created by laser ablation of polystyrene and impact a sample target. The velocity information of the micro- projectiles is explicitly determined by two consecutive high-speed images during the flight of the projectiles. For demonstration, a glassy-rubber micro-projectile consisting of a periodic self-assembled stack of 20 nm thick layers of polystyrene and polydimethylsiloxane blocks (PS-b-PDMS) is tested by LIPIT at extremely high-strain rate of $10^7$ s$^{-1}$. The polymer nanocomposite demonstrates new orientation dependent deformation and failure mechanisms including a surprising disorder to order transition fluidization, and the energy absorbing ability of a layered nanocomposite through plastic deformation leading to a melting of the layered structure.
9:36AM P26.00009 Probing the sliding interactions between bundled actin filaments, ANDY WARD, ZVONIMIR DOGIC, Brandeis University — Assemblies of filamentous biopolymers are hierarchical materials in which the properties of the overall assemblage are determined by structure and interactions between constituent particles at all hierarchical levels. For example, the overall bending rigidity of a two bundled filaments greatly depends on the bending rigidity of, and the adhesion strength between individual filaments. However, another property of importance is the ability for the filaments to slide freely against one another. Everyday experience indicates that it is much easier to bend a stack of papers in which individual sheets freely slide past each other than the same stack of papers in which all the sheets are irreversibly glued together. Similarly, in filamentous structures the ability for local re-arrangement is of the utmost importance in determining the properties of the structures observed. We have developed a method to directly measure the frictional interactions between a pair of aligned filaments in a well-defined and controllable configuration. This enables us to systematically investigate the role of adhesion strength, filament orientation, length, and surface structure.

9:48AM P26.00010 Harnessing polymer gels to regulate friction between sliding surfaces1, HASSAN MASOUD, ALEXANDER ALEXEEV, Georgia Institute of Technology, George W. Woodruff School of Mechanical Engineering — We examine the microscale tribological behavior of a pair of gel coated surfaces separated by a thin layer of lubricant. The soft, elastic gel is modeled using a bond-bending lattice spring model that captures the micromechanics of a random network of interconnected filaments. We couple this model with the dissipative particle dynamics that explicitly models the hydrodynamics of a viscous fluid. We probe how elasticity and internal structure of compliant gels affect the tribological behavior and examine how gel elasticity can be harnessed to regulate friction between sliding surfaces. We also study the effect of lubricant composition and the inclusion of nanoscopic particles of different shapes on the friction forces between wet compliant surfaces. Our findings could be useful for developing new methods for regulating friction and reducing wear of lubricated surfaces and also for understanding the micro-mechanics of friction in biological systems.

1Financial support from the Donors of the Petroleum Research Fund, administered by the ACS, is gratefully acknowledged.

10:00AM P26.00011 On the Equilibrium of an Heavy Elastic Cylinder on Horizontal Non-deformable Plane, LAURENT SHEKYAN, SERGEY VERLINSKI, Dr. — The plane static contact problem of the equilibrium of a homogeneous heavy elastic cylinder on fixed non-deformable horizontal plane is discussed. In the vicinity of the initial contact between these bodies, there is some contact area, which covers the central angle and which are unknown contact stresses. The elastic equilibrium of a cylinder under the influence of its gravity and some unknown contact stress is discussed. To determine the distribution of contact stress, the size of the contact area of the cylinder and immersion in the horizontal plane is required.

10:12AM P26.00012 Internal friction peak in silicon revealed by moderate temperature annealing1, THOMAS METCALF, XIAO LIU, JEREMY ROBINSON, Naval Research Laboratory — In order to maximize the quality factor of a mechanical resonator, one must minimize energy loss mechanisms. We have identified a new internal friction (IF) peak that is present in as-fabricated ultra-high Q silicon resonators known as Double Paddle Oscillators. The IF peak can be removed (and thus its presence revealed) by annealing at moderate (300 °C) temperatures in both inert (Argon) and reactive (H2) atmospheres, and does not re-appear after aging for 107 s. The success of a relatively low temperature operation in eliminating this mechanism indicates that the phenomenon is surface-, as opposed to bulk- related. We compare this loss mechanism to other known loss mechanisms in silicon.

1Work supported by the Office of Naval Research

10:24AM P26.00013 ABSTRACT WITHDRAWN —

10:36AM P26.00014 Investigation of stability for an electrostatically actuated flexible electrode, CORY HINTON, MATTHEW MCFARLAND, THOMAS WARD, North Carolina State University — An argument for employing dimensional analysis to explore stability in an electrostatically actuated flexible electrode is presented theoretically and experimentally. The electrode is configured as a cantilever beam, as many applications in MEMs, medical devices, and sensing devices have been studied for years. This study investigates a macro scale beam (length = 100mm - 150mm), for applications in cooling fan and flapping micro air vehicle devices. The influence of scale is validated, voltage potential and frequency contributions are quantitatively measured, and a comparison of input signal (analog versus digital) is discussed using dynamical systems analysis. Based on experimental data and numerical models, characteristics of stability are presented that could influence design considerations for various micro- and macro-scale devices.

Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P42 DBIO GSNP: Focus Session: Evolutionary Systems Biology II - From molecules to cells 156C

8:00AM P42.00001 Statistical Physics Approaches to RNA Editing1, RALF BUNDSCHUH, Ohio State University — The central dogma of molecular Biology states that DNA is transcribed base by base into RNA which is in turn translated into proteins. However, some organisms edit their RNA before translation by inserting, deleting, or substituting individual or short stretches of bases. In many instances the mechanisms by which an organism recognizes the positions at which to edit or by which it performs the actual editing are unknown. One model system that stands out by its very high rate of on average one out of 25 bases being edited are the slime molds. In this talk we will show how the computational methods and concepts from statistical Physics can be used to analyze DNA and protein sequence data to predict editing sites in these slime molds and to guide experiments that identified previously unknown types of editing as well as the complete set of editing events in the slime mold Physarum polycephalum.

1This presentation is based on work supported by the National Science Foundation under grant number DMR-0706002.

8:36AM P42.00002 Biophysical Models of Evolution: Application to Transcription Factor Binding Sites in Yeast, MICHAEL MANHART, ALLAN HALDANE, ALEXANDRE MOROZOV, Rutgers University — There has been growing interest in understanding the physical driving forces of evolution at the molecular scale, in particular how biophysics determines the fitness landscapes that shape the evolution of DNA and proteins. To that end we study a model of molecular evolution that explicitly incorporates the underlying biophysics. Using population genetics, we derive a steady-state distribution of monomorphic populations evolving on an arbitrary fitness landscape. Compared to previous studies, we find this result is universal for a large class of population models and fully incorporates both stochastic effects and strong natural selection. This distribution can then be used to infer the underlying fitness landscape from genomic data. This model can be applied to a variety of systems, but we focus on transcription factor binding sites, which play a crucial role in gene regulatory networks. Since these sites must be bound for successful gene regulation, we consider a simple thermodynamic model of fitness as a function of the free energy for binding a transcription factor at the site. Using empirical energy matrices and genome-wide sets of binding sites from the yeast Saccharomyces cerevisiae, we use this model to infer the role of DNA-protein interaction physics in evolution.
8:48AM P42.00003 The Fitness of Genomic Order\textsuperscript{1}.
QUICEN ZHANG, SAURABH VYAWAHARE, ROBERT AUSTIN,
Department of Physics, Princeton University — Most bacteria have a single circular chromosome that can range in size from 160,000 to 12,200,000 base pairs. Considering the typical gene density, i.e. 1 gene per 1,000 base pairs, both the number of genes and the ways to arrange are huge. Intuitively, the arrangement of genes on the circle is not important if all of them can be replicated. However, there is typically one origin of replication, and when bacteria is attacked by genotoxic stress during replication, the whole replication process can not be finished. As a result, which gene is replicated first, which is second, ..., becomes very important. Experimentally, we found a broad increase of DNA copy number near the origin of replication (OriC) of bacteria E.coli (~3200 genes) under genotoxic stress. Since the genes near OriC are mostly efflux pump genes, we propose that there is fitness advantage for those rapid stress response genes got replicated first, because they can facilitate the replication of the rest of genome. Similar to bacterial evolution to present genomic order, in the somatic evolution of cancer, genomic shuffling was also frequently observed, especially under genotoxic chemotherapy. Such re-arrangement of genome can be viewed as a journey to optimal point in the rugged fitness landscape of genomic order.

\textsuperscript{1}The research described was supported by Award Number U54CA143803 from the National Cancer Institute.

9:00AM P42.00004 Plasticity of metabolic networks and the evolution of C4 photosynthesis.
ELI BOGART, CHRIS MYERS, Cornell University — Over 50 groups of plants have independently developed a common mechanism (C4 photosynthesis) for increasing the efficiency of photosynthetic carbon dioxide assimilation. Understanding the high degree of evolvability of the C4 system could offer useful guidance for attempts to introduce it artificially to other plants. Previously, the nonlinear relationship between carbon dioxide levels and rates of carbon assimilation and photorespiration has prevented the application of genome-scale metabolic models to the problem of the evolution of the pathway. We apply a nonlinear optimization method to find feasible flux distributions in a plant metabolic model, allowing us to explore the plasticity of the metabolic network and characterize the fitness landscape of the transition from C3 to C4 photosynthesis.

9:12AM P42.00005 Uncovering principles of cellular decision-making.
GUROL SUEL. UT Southwestern — Cells can cope with unpredictable environmental conditions by differentiating into appropriate states. In this talk, I will present our recent attempts to understand the role of genetic circuits in regulating the underlying process of cellular decision-making. Specifically, we are interested in how interactions within and across genetic circuits enable cells to choose among alternative fates. To address this question my laboratory is employing systems and synthetic biology approaches. Our ultimate goal is to uncover possible evolutionary pressures that may have selected for specific gene circuit architectures, dynamics and noise properties.

9:48AM P42.00006 Role of Multisite Phosphorylation in Timing of a Yeast Cell Cycle Event\textsuperscript{1}.
VOLKAN SEVIM, University of California, San Francisco, XIAOJING YANG, University of California, San Francisco; Peking University, KAI-YEUNG LAU, University of California, San Francisco, CHAO TANG, University of California, San Francisco; Peking University — We study the biochemical network that triggers the S phase in yeast cell cycle. Key components of this network are three proteins: two kinases and an inhibitor. First kinase, Cln1/2-Cdk, acts as an input signal, phosphorylating the inhibitor, Sic1. The second kinase, Clb5/6-Cdk, is sequestered into an inactive complex by Sic1. Clb5/6-Cdk is the output signal of the circuit. Sic1 has nine phosphorylation sites, and phosphorylation of six or more of them causes it to degrade rapidly, leading to a sharp rise of free Clb5/6-Cdk. Our experiments indicate that multisite phosphorylation (MSP) is responsible for the timing robustness of this sharp transition. We study the role of MSP in timing using computer simulations. Preliminary results indicate that, MSP does not bring timing robustness when each kinase can phosphorylate each site with identical specificity. We employ in silico evolution to find the specificity configuration for the phosphorylation sites that leads to most robust timing under extrinsic noise.

\textsuperscript{1}This research was supported in part by Lui Fellowship, Li Foundation, Sandler Family Supporting Foundation, NSF, NIH (P50 GM081879), Ministry of Sci. and Tech. of China (2009CB918500) and Natl. Natural Sci. Foundation of China.

10:00AM P42.00007 Precision of sensing, memory and fluctuating environments.
GERARDO AQUINO, ROBERT ENDRES, Division of Molecular Biosciences & Centre for Integrated Systems Biology at Imperial College, Imperial College London — Multiple cell types were recently shown to sense their chemical environment with astonishing accuracy, crucial for nutrient scavenging, mating, immune response, and development. It is currently unknown if this sensing near the single-molecule detection limit is due to highly precise single measurements, or due to learning over time. In this work, we analyze if cell memory allows cells to sense beyond the current estimates of the fundamental physical limit. By merging Bayesian inference with information theoretic concepts, we derive analytical formulas which show that memory improves sensing in correlated fluctuating environments, but not in strongly uncorrelated environments. Despite many analogies with problem solving strategies in engineering, our theory shows fundamental differences in interpreting noisy stimuli in the microscopic and macroscopic world.

10:12AM P42.00008 Rapidly evolving microorganisms with high biofuel tolerance\textsuperscript{1}.
SAURABH VYAWAHARE, QUICEN ZHANG, WENDY LANG, ROBERT AUSTIN, Department of Physics, Princeton University, Princeton NJ 08544 — Replacing non-renewable energy sources is one of the biggest and most exciting challenges of our generation. Algae and bacteria are poised to become major renewable biofuels if strains can be developed that provide a high, consistent and robust yield of oil. One major stumbling block towards this goal is the lack of tolerance to high concentrations of biofuels like isobutanol. Using traditional bioengineering techniques to remedy this face the hurdle of identifying the correct pathway or gene to modify. But the multiplicity of interactions inside a cell makes it very hard to determine what to modify a priori. Instead, we propose a technology that does not require prior knowledge of the genes or pathways to modify. In our approach that marries microfabrication and ecology, spatial heterogeneity is used as a knob to speed up evolution in the desired direction. Recently, we have successfully used this approach to demonstrate the rapid emergence of bacterial antibiotic resistance in as little as ten hours. Here, we describe our experimental results in developing new strains of micro-organisms with high oil tolerance. Besides biofuel production, our work is also relevant to oil spill clean-ups.

\textsuperscript{1}Supported by Award Number U54CA143803 from the National Cancer Institute.

10:24AM P42.00009 A Cahn-Hilliard model of vascularized tumor growth in a complex evolving confinement using a diffuse domain approach\textsuperscript{1}.
YAO-LI CHUANG, University of New Mexico, Dept. Pathology, VITTORIO CRISTINI, University of New Mexico, Dept. Pathology and Dept. Chemical Engineering, YING CHEN, XIAORONG LI, University of California, Irvine, Dept. Math, HERMANN FRIEBOES, University of Louisville, Dept. Bioengineering, JOHN LOWENGRUB, University of California, Irvine, Dept. Math — Understanding the spatiotemporal evolution of tumor growth is essential for developing effective strategies to treat cancers. Various studies have suggested that spatial heterogeneity during tumors growth is a key factor associated with subsequent tumor invasion and the effectiveness of chemotherapy. Spatial heterogeneity may arise due to morphological instability of the tumors and the complex tissue structure surrounding the tumors. In previous works, we have used a Cahn-Hilliard tumor growth model to study the morphological instability for tumors in non-resisting tissues. However, most tumors are surrounded by complex tissue structures and confined in the capsules of some organs or between certain basement membranes. The capsules and basement membranes may be disturbed by interacting with the evolving tumors, affecting the morphological instability. Here we adopt a novel diffuse domain approach to adapt our previous Cahn-Hilliard model for tumor growth in such complex evolving environments. As an example, we apply the model to simulate the evolution of lymphoma in a lymph node, incorporating also the tumor-induced angiogenesis.

\textsuperscript{1}supported by NIH-PSOC grant 1U54CA143907-01
10:36AM P42.00010 Emergence of Information Transmission in a prebiotic RNA Reactor. BENEDIKT OBERMAYER, Harvard University, HUBERT KRAMMER, DIETER BRAUN, ULRICH GERLAND, LMU Muenchen — A poorly understood step in the transition from a chemical to a biological world is the emergence of self-replicating molecular systems. We study how a precursor for such a replicator might arise in a hydrothermal RNA reactor, which accumulates longer sequences from unbiased monomer influx and random ligation. In the reactor, intra- and intermolecular base pairing locally protects from random cleavage. Analyzing stochastic simulations, we observe a strong bias towards long sequences with complex secondary structures, which would facilitate the emergence of ribozymes. Further, we find temporal sequence correlations that constitute a signature of information transmission, weaker but of the same form as in a true replicator.

10:48AM P42.00011 Towards molecular evolution with thermal traps. CHRISTOF MAST, Systems Biophysics, SEVERIN SCHINK, Arnold-Sommerfeld-Center, HUBERT KRAMMER, Systems Biophysics, BENEDIKT OBERMAYER, Arnold-Sommerfeld-Center, ULRICH GERLAND, Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, LMU Munich, DIETER BRAUN, Systems Biophysics and Center for Nanoscience, LMU Munich — Live evolves by replication and selection of nucleotide polymers. Our experiments aim to drive molecular replication and selection with physical nonequilibrium boundary conditions. We discuss three approaches. Replication Trap. Molecules are exponentially accumulated by a combination of thermostoresis and convection, driven both by the same thermal gradient [1]. We have shown last year that with the help of a polyamerses protein, concurrent replication and accumulation is possible [2]. Convection is melting and annealing the DNA in an oscillatory pattern, doubling the DNA in each cycle. Trapped polymerization. The chemical equilibrium of polymerization is expected to shift in the thermal trap. As the trap accumulates the monomers, polymerization yields longer polymers. However, since the trap is exponentially length selective, distributions beyond exponential tails are predicted. Replication by selective degradation. Replication typically is discussed as template directed polymerization. We showed that selective degradation and a thermal trap leads to replication-like behavior using only non templated polymerization [3]. The progression of information is given by the faster degradation of single stranded over double stranded RNA. [1] PNAS 104, 9346 (2007) [2] PRL 104, 188102 (2010) [3] PRL 107, 018101 (2011)

Wednesday, February 29, 2012 8:00AM - 11:00AM —
Session P52 GSNP DFD: Focus Session: Extreme Mechanics - Structures for Form and Function 153C

8:00AM P52.00001 Soft Robots: Manipulation, Mobility, and Fast Actuation. ROBERT SHEPHERD, FILIP ILIEVSKI, WONJAE CHOI, ADAM STOKES, STEPHEN MORIN, AARON MAZZEO, REBECCA KRAMER, Harvard, CARME MAJIDI, Carnegie Mellon, ROB WOOD, GEORGE WHITESIDES, Harvard — Material innovation will be a key feature in the next generation of robots. A simple, pneumatically powered actuator composed of only soft-elastomers can perform the function of a complex arrangement of mechanical components and electric motors. This talk will focus on soft-lithography as a simple method to fabricate robots—composed of exclusively soft materials (elastomeric polymers). These robots have sophisticated capabilities: a gripper (with no electrical sensors) can manipulate delicate and irregularly shaped objects and a quadrupedal robot can walk to an obstacle (a gap smaller than its waking height) then shrink its body and squeeze through the gap using an undulatory gait. This talk will also introduce a new method of rapidly actuating soft robots. Using this new method, a robot can be caused to jump more than 30 times its height in under 200 milliseconds.

8:12AM P52.00002 Low-Dimensional Generalized Coordinate Models of Large-Deformation Elastic Joints1. LAEL ODHNER, AARON DOLLAR, Department of Mechanical Engineering, Yale University — In the field of robotics, it is increasingly common to use elastic elements such as rods, beams or sheets to allow motion between the rigid links of a robot, rather than conventional sliding mechanisms such as pin joints. Although these elastic joints are simpler to manufacture, especially at meso- and micro-scales, representational simplicity is sacrificed. It is far easier to compute the Lagrangian of a robot using joint angles as generalized coordinates, rather than by considering the large-deformation continuum behavior of elastic joints. In this talk, we will discuss our work toward finding accurate, low-dimensional discretizations of elastic joint mechanics, suitable for use in generalized coordinate models of robot kinematics and dynamics. We use modally parameterized backbone curves to describe the kinematic configuration of the elastic joints, and compute the energy associated with deformation using rod and shell theory. In the plane, only three smooth deformation modes are sufficient to describe Euler-Bernoulli bending of 90 degrees to within 1 percent. Parametric models for the three-dimensional motion of sheet hinges are more complex, but can be simplified significantly using boundary conditions and constraints imposed by ruled surface assumptions.

1This work is supported by National Science Foundation grant IIS-0952856.

8:24AM P52.00003 Liquid-Embedded Elastomer Electronics. REBECCA KRAMER, Harvard University, CARME MAJIDI, Carnegie Mellon University, YONG-LAE PARK, JAMIE PAIK, ROBERT WOOD, Harvard University — Hyperelastic sensors are fabricated by embedding a silicone rubber film with microchannels of conductive liquid. In the case of soft tactile sensors, pressing the surface of the elastomer will deform the cross-section of underlying channels and change their electrical resistance. Soft pressure sensors may be employed in a variety of applications. For example, a network of pressure sensors can serve as artificial skin by yielding detailed information about contact pressures. This concept was demonstrated in a hyperelastic keypad, where perpendicular conductive channels form a quasi-planar network within an elastomeric matrix that registers the location, intensity and duration of applied pressure. In a second demonstration, soft curvature sensors were used for joint angle proprioception. Because the sensors are soft and stretchable, they conform to the host without interfering with the natural mechanics of motion. This marked the first use of liquid-embedded elastomer electronics to monitor human or robotic motion. Finally, liquid-embedded elastomers may be implemented as conductors in applications that call for flexible or stretchable circuitry, such as robotic origami.

8:36AM P52.00004 Extreme Mechanics in Soft Pneumatic Robots and Soft Microfluidic Electronics and Sensors. CARME MAJIDI, Carnegie Mellon University — In the near future, machines and robots will be completely soft, stretchable, impact resistance, and capable of adapting their shape and functionality to changes in mission and environment. Similar to biological tissue and soft-body organs- tres, these next-generation technologies will contain no rigid parts and instead be composed entirely of soft elastomers, gels, fluids, and other non-rigid matter. Using a combination of rapid prototyping tools, microfabrication methods, and emerging techniques in so-called “soft lithography,” scientists and engineers are currently introducing exciting new families of soft pneumatic robots, soft microfluidic sensors, and hyperelastic electronics that can be stretched to as much as 10x their natural length. Progress has been guided by an interdisciplinary collection of insights from chemistry, life sciences, robotics, microelectronics, and solid mechanics. In virtually every technology and application domain, mechanics and elasticity have a central role in governing functionality and design. Moreover, in contrast to conventional machines and electronics, soft pneumatic systems and microfluidics typically operate in the finite deformation regime, with materials stretching to several times their natural length. In this talk, I will review emerging paradigms in soft pneumatic robotics and soft microfluidic electronics and highlight design and modeling challenges that arise from the extreme mechanics of inflation, locomotion, sensor operation, and human interaction. I will also discuss perceived challenges and opportunities in a broad range of potential application, from medicine to wearable computing.
9:12AM P52.00005 Macrocomposite mechanical design, modeling and behavior of physical models of bioinspired fish armor, ASHLEY BROWNING, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, CHRISTINE ORTIZ, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, MARY C. BOYCE, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 — The macrocomposite design of flexible biological exoskeletons, consisting of overlapping mineralized armor units embedded in a compliant tissue, is a key determinant of their mechanical function (e.g. penetration resistance and biomechanical flexibility). Here, we investigate the role of macrocomposite structure, composition, geometric orientation, and spatial distribution in a flexible model natural armor system present in the majority of teleost fish species. Physical multi-material composite models are fabricated using a combination of 3-D printing and molding methods. Mechanical experiments using digital image correlation enable measurement of both the macroscopic response and underlying deformation mechanisms during various loading scenarios. Finite element-based mechanical models yield detailed insights into the roles and the tradeoffs of the composite structure providing constraint, shear, and bending mechanisms to impart protection and flexibility.

9:24AM P52.00006 Periodic Structural Solids: Mechanics and Multifunctional Applications, LIFENG WANG, Clarkson University — Triply periodic minimal surfaces have been of great interest to mathematicians, physical scientists, material scientists, and biologists. Close physical approximations to triply periodic minimal surfaces arise in a few material systems, such as block copolymers, nanocomposites, and biological exoskeletons. Here, we demonstrate the potential to design and fabricate two-component periodically ordered structures which correspond to the level set structures associated with triply periodic minimal surfaces. These structures are shown to have a unique combination of stiffness, strength, and energy absorption, as well as damage tolerance. The results provide guidelines for engineering and tailoring the nonlinear mechanical behavior and energy absorption of cocontinuous composites for a wide range of applications and further creating multifunctional materials. For example, polymeric materials which can change shape and material properties in response to external stimuli (temperature or electric field) can provide additional functionality when used as one of the phases, such as 3D shape memory. The periodic and multiphase nature of the structures also enables mechanically tunable band gap (phononic or photonic) materials, and tunable sensors in tissue engineering.

9:36AM P52.00007 Honeycombs with hierarchical organization, AMIN AJDARI, BABAK HAGHPANAH JAHROMI, JIM PAPADOPULOS, ASHKAN VAZIRI, Northeastern University — We investigated the mechanical behavior of two-dimensional hierarchical honeycomb structures using analytical, numerical and experimental methods. Hierarchical honeycombs were constructed by replacing every three-edge vertex of a regular hexagonal lattice with a smaller hexagon. Repeating this process builds a fractal-appearing structure. The resulting isotropic in-plane elastic properties (effective elastic modulus and Poisson’s ratio) of this structure are controlled by the dimension ratios for different hierarchical orders. Hierarchical honeycombs of first and second order can be up to 2.0 and 3.5 times stiffer than regular honeycomb at the same mass (i.e., same overall average density). The Poisson’s ratio varies from nearly 1.0 (when planar “bulk” modulus is considerably greater than Young’s modulus, so the structure acts “incompressible” for most loadings) to 0.28, depending on the dimension ratios. The work provides insight into the role of structural organization in regulating the mechanical behavior of materials, and new opportunities for developing low-weight cellular structures with tailorable properties.

9:48AM P52.00008 Buckling-induced Tunable Chirality in Rationally-Designed Surface-Attached Cellular Structures, SICONG SHAN, SUNG HOON KANG, WIM NOORDUIN, School of Engineering and Applied Sciences, Harvard University, MUGHEES KHAN, WYSS Institute for Biologically Inspired Engineering, KATIA BERTOLDI, JOANNA AIZENBERG, School of Engineering and Applied Sciences, Harvard University — Chirality is crucial in understanding and controlling the behavior of living and non-living systems since the presence or absence of chirality in the structures plays important roles in their interactions with molecules, enzymes, light, and mechanical stress. Processes that induce chirality have been extensively studied at the molecular and macroscopic scales, but are relatively unexplored at the mesoscale. By rational design based on modeling, we experimentally demonstrate the controlled reversible switching between achiral and chiral configurations using swelling/de-swelling of surface-attached cellular structures. Importantly, the buckling patterns and the associated symmetry reduction of the initially achiral centrosymmetric structures could be tuned, simply by changing the dimensions of either mixed (racemic) or chiral phases. In the case of chiral transformations, spontaneous symmetry breaking resulted in the formation of large uniform areas of structures of single handedness. The latter is of particular...
Porous Structures

circular voids

two-dimensional phononic crystals with periodic materials consisting of different constituents with the capability to control the propagation of elastic waves. In this study, the dispersion relations of two-dimensional phononic crystals with circular voids are investigated using Bloch-wave analysis. Porous patterns are derived from the Laves tilings, which are duals of the eleven convex uniform tilings of the Euclidean plane. Numerical simulations are performed on the microstructures using finite element method. Frequency band-gaps are calculated and compared among different geometric configurations, void-volume fractions, and material properties, providing valuable insight into the behavior of phononic crystals. The predictive technique procedure developed here offers opportunities for the design of mechanical wave filters that have many potential applications such as noise-cancelling devices, acoustic wave guides and vibration isolators.

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10:36AM P52.00112 Guiding of High Amplitude Stress Waves Through Stress-Induced Domain Switching in Multiphase Materials, JULIAN RIMOLI, LUCA GUIDONI, BRETT REICHARD, MASSIMO RUZZENE, Georgia Institute of Technology — Periodic and graded Multiphase Materials (MMs) are of great interest to scientists and engineers because of their unique static and dynamic mechanical properties, and the design flexibility they provide. In the linear range operation, MMs can be designed to attenuate vibrations over wide frequency bands and in specified directions, as defined by topology, geometry and material of the unit cell. Similarly, unit cell design and topology can be selected to obtain a desired anisotropy in the material, which can be exploited to alter the path of propagation of elastic and high amplitude stress waves. Specifically, steering of waves in preferential directions can be achieved through the proper arrangement of periodic hard inclusions within a matrix. Such a capability is extremely important for the design of materials capable of guiding stress waves to propagate along specified paths. In the present work, we explore the use of periodic metamaterials for wave management in force protection applications. We define topologies which adapt to high amplitude mechanical inputs, and study through numerical simulations and experiments local and global instabilities which lead to adaptive mechanical behavior through topological and structural modifications.

10:48AM P52.00113 Soft Modes and Deformations of Three-Dimensional Isostatic Periodic Lattices, ANTON SOUSLOV, Georgia Institute of Technology, T.C. LUBENSKY, University of Pennsylvania — Each particle in a three-dimensional isostatic lattice is connected by springs on average to six nearest neighbors, a condition obtained by J.C. Maxwell for marginal stability. The cubic and pyrochlore lattices satisfy this condition. By calculating the dispersion relations and the density of states for phonons in these lattices, we expand on previous studies of isostatic periodic structures [1], which have largely been focused on the simpler two-dimensional cases. The low energy phonon spectrum of these lattices exhibits features common to isostatic systems in any dimension, such as the presence of floppy modes and the scaling of a divergent length and a vanishing critical frequency. However, the allowed symmetries of an elasticity theory and the number of floppy modes depend on dimension and play a crucial role in the structure of the low-frequency response. We relate these findings to the isostatic transition in systems of close-packed athermal spheres and look at an analogy with three-dimensional crystals with zeolite structure.


Wednesday, February 29, 2012 8:00AM - 11:00AM –
Session P53 GSNP: Disordered Systems: Packing 153B

8:00AM P53.00001 Analytical Construction of A Dense Packing of Truncated Tetrahedra and Its Melting Properties, YANG JIAO, SALVATORE TORQUATO, Princeton University — Dense polyhedron packings are useful models of a variety of condensed matter and biological systems and have intrigued scientists and mathematicians for centuries. Here, we analytically construct the densest known packing of truncated tetrahedra with a remarkably high packing fraction 0.995 192, which is amazingly close to unity and strongly implies its optimality. This construction is based on a generalized organizing principle for polyhedra that lack central symmetry that we introduce here. The packing characterizes and equilibrium melting properties of the putative optimal packing as the system undergoes decomposition are discussed.

8:12AM P53.00002 Packing fraction of dimers and anisotropic objects, TAI SHAN ZHU, YULIANG JIN, HERMAN A MAKSE, Levich Institute and Physics Department, the City College of New York, New York, NY 10031, USA, MAXIMILIAN DANISCH, ENS, Cachan, ADRIAN BAULE, School of Mathematical Sciences Queen Mary, University of London — We present a statistical theory and computer simulations for the calculation of the average volume in jammed assemblies of dimer shaped objects and other anisotropic particles like spherocylinders. The theory predicts the volume fraction as a function of the coordination number of the particles.

8:24AM P53.00003 Statistical Mechanics of Athermal Packings: Incorporating Basin Volumes, ASHWIN S. S., Departments of Mechanical Engineering & Materials Science and Physics, Yale University, JERZY BLAWZDZIEWICZ, Mechanical Engineering, Texas Tech University, COREY S. O’HERN, Departments of Mechanical Engineering & Materials Science and Physics, Yale University, MARK D. SHATTUCK, Benjamin Levich Institute and Physics Department, The City College of the New York — We present a first principles formalism for the statistical mechanics of athermal packings subject to driving beyond the weak limit. Edwards hypothesized a statistical mechanics of flat measure associated with packings explored at this weak limit. This ensemble has been found to work well in the limit of very weak (but non-zero) driving. Beyond the weak driving limit, the probability measures associated with jammed states become proportional to the volume of basins of attraction associated with the packings on the density landscape. We propose here, a statistical mechanics which takes into consideration the volume of basins of attraction under certain approximations. Further, the statistical mechanics takes into account the protocol by writing the partition function in terms of an integral over protocol dependent generalized coordinates. This will allow an extremum principle to determine states, in these out of equilibrium systems.

8:36AM P53.00004 Polydisperse sphere packing in high dimensions, a search for an upper critical dimension, PETER MORSSE, Department of Physics: University of Oregon, MAXIME CLUSEL, Laboratoire Charles Coulomb UMR 5221, CNRS and Universite Montpellier 2, F-34095, Montpellier, France, ERIC CORWIN, Department of Physics: University of Oregon — The recently introduced granocentric model for polydisperse sphere packings has been shown to be in good agreement with experimental and simulational data in two and three dimensions. This model relies on two effective parameters that have to be estimated from experimental/simulational results. The non-trivial values obtained allow the model to take into account the essential effects of correlations in the packing. Once these parameters are set, the model provides a full statistical description of a sphere packing for a given polydispersity. We investigate the evolution of these effective parameters with the spatial dimension to see if, in analogy with the upper critical dimension in critical phenomena, there exists a dimension above which correlations become irrelevant and the model parameters can be fixed a priori as a function of polydispersity. This would turn the model into a proper theory of polydisperse sphere packings at that upper critical dimension. We perform infinite temperature quench simulations of frictionless polydisperse sphere packings in dimensions 2–8 using a parallel algorithm implemented on a GPGPU. We analyze the resulting packings by implementing an algorithm to calculate the additively weighted Voronoi diagram in arbitrary dimension.
as the frequency and orientation of density-one solutions as \( N \) goes to infinity. We assess the entropy of some of these configurations, as well as a family of “gapped bricklayer” Bravais lattice solutions with density \( N/(N+1) \), and some surprising non-Bravais lattice configurations – including lattices of 

We study the densest packings of \( N \) unit squares in a torus (i.e., using periodic, square boundary conditions in 2D) using both analytical and simulation methods. We find a rich array of dense packing solutions: density-one packings when \( N \) is the sum of two square integers, a family of “gapped bricklayer” Bravais lattice solutions with density \( N/(N+1) \), and some surprising non-Bravais lattice configurations – including lattices of holes, as well as a configuration for \( N=23 \) in which not all squares share the same orientation. Hence, we propose a model that combines both approaches into a single Hamiltonian imposing force balance constraints and minimization of the volume of the system. The formalism can be put into the framework of constraint optimization problems as recently proposed. The cavity method then solves the problem of force balance providing a prediction of the coordination number of the jammed packing. The model can be applied to spherical frictionless and frictional particles as well as non-spherical particles providing a prediction of the coordination number as a function of the aspect ratio of the particles.

We describe a novel computational method for calculating the MS packing probabilities by directly measuring the random close packing density, which provides new insights into the mathematical problem of packing spheres in large dimension.

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1 NSF Support No. DMR-1055586

2 NSF Support No. DMR-0907235 and DMR-0846582, as well as the NSF-funded Center for Hierarchical Manufacturing, CMMI-1025020

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9:24AM P53.00008 Packing Squares in a Torus

Donald Blair, Christian Santangelo, Jon Mchta, University of Massachusetts Amherst — We study the densest packings of \( N \) unit squares in a torus (i.e., using periodic, square boundary conditions in 2D) using both analytical methods and simulated annealing. We find a rich array of dense packing solutions: density-one packings when \( N \) is the sum of two square integers, a family of “gapped bricklayer” Bravais lattice solutions with density \( N/(N+1) \), and some surprising non-Bravais lattice configurations – including lattices of holes, as well as a configuration for \( N=23 \) in which not all squares share the same orientation. We assess the entropy of some of these configurations, as well as the frequency and orientation of density-one solutions as \( N \) goes to infinity.

1 With support from NSF grants DMR-0907235 and DMR-0846582, as well as the NSF-funded Center for Hierarchical Manufacturing, CMMI-1025020

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9:36AM P53.00009 Characterization of Basin Volumes in Mechanically Stable Packings

Mark D. Shattuck, Benjamin Levine Institute and Physics Department of The City College of New York, S.S. Ashwin, Departments of Mechanical Engineering & Material Science and Physics, Yale University, Jerzy Blawdziewicz, Department of Mechanical Engineering, Texas Tech University, Corey S. O'Hern, Departments of Mechanical Engineering & Material Science and Physics, Yale University — There are a finite number of distinct mechanically stable (MS) packings in granular systems composed of frictionless particles. For typical packing-generation protocols employed in experimental and numerical studies, the probabilities with which the MS packings occur are highly nonuniform and depend strongly on preparation protocol. Despite intense work, it is extremely difficult to predict a priori the MS packing probabilities. We describe a novel computational method for calculating the MS packing probabilities by directly measuring the volume of the MS packing ‘basin of attraction’, which we define as the collection of initial points in configuration space at zero packing fraction that map to a given MS packing by following a particular dynamics in the density landscape. We show that there is a small core region with size \( l \), surrounding each MS packing in configuration space in which all initial conditions map to a given MS packing. However, we find that the MS packing probabilities are not strongly correlated with \( l \), and thus they are determined by complex geometric features of the landscape that are distant from the MS packing.

1 Supported by NSF CBET-0968013, CBET-0967262, NSF PREM DMR-0934206

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9:48AM P53.00010 ABSTRACT WITHDRAWN

10:00AM P53.00011 Hierarchical freezing in a lattice model with a nonperiodic ground state

Joshua E.S. Socollar, Travis Byington, Duke University — A recent result in tiling theory provides a two-dimensional lattice model with nearest and next-nearest neighbor interactions that has a limit-periodic ground state. During a slow quench from the high temperature, disordered phase, the ground state emerges through an infinite sequence of phase transitions, all related by renormalizations of the temperature scale with the sequence of critical temperatures approaching zero. As the temperature is decreased, sublattices with increasingly large lattice constants become ordered. Quenching at any finite rate eventually results in glass-like state due to kinetic barriers created by simultaneous freezing on sublattices with different lattice constants.

1 Supported by NSF's Research Triangle MRSEC (DMR-1121107)

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10:12AM P53.00012 Degenerate Quasicrystal of Hard Triangular Bipyramids Stabilized by Entropic Forces

Amir Haji-Akbari, Michael Engels, Sharon Glotzter, University of Michigan — The assembly of hard polyhedra into novel ordered structures has recently received much attention. Here we focus on triangular bipyramids (TBPs) — i.e. dimers of hard tetrahedra — which pack densely in a simple triclinic crystal with two particles per unit cell [1]. This packing is referred to as the TBP crystal. We show that hard TBPs do not form this densest packing in simulation. Instead, they assemble into a different, far more complicated structure, a dodecagonal quasicrystal, which, in the level of monomers, is identical to the quasicrystal recently discovered in the hard tetrahedron system [2], but the way that tetrahedra pair into TBPs in the nearest neighbor network is random, making it the first degenerate quasicrystal reported in the literature [3]. This notion of degeneracy is in the level of decorating individual tiles and is different from the degeneracy of a quasi-periodic random tiling arising from phason flips [4]. The \((3.4^2\cdot4)\) approximant of the quasicrystal is shown to be more stable than the TBP crystal at densities below 79.7%.

10:24AM P53.00013 A Novel Decomposition of the Structure of Jammed Packings1, MARK KANNER, MARK SHATTUCK, CUNY Graduate Center and the Benjamin Levich Institute and Physics Department of the City College of New York, CORY O’HERN, Departments of Mechanical Engineering and Physics, Yale University — We use novel methods for classifying structural subunits of a packing, using the structures to calculate relevant physical quantities. The classification scheme is based on a 20 type decomposition of the Delaunay triangles extracted from the centers of the particles in the packing. We find that the distribution of each type has a universal form, independent of total number of particles N in the packing for N=8-10,000, and that the parameters describing this form saturate as N is increased beyond N=20. We measure the distribution of the particle connections, the area distributions of the different structures, and nearest neighbor distributions. We explore the extent to which the nearest-neighbor distributions can predict the properties of the entire packing.

1Supported by NSF (CBET-0968013)

10:36AM P53.00014 8x8 and 10x10 Hyperspace Representations of SU(3) and 10-fold Point-Symmetry Group of Quasicrystals1, ALEXANDER ANIMALU2, Emeritus Professor of Physics — In order to further elucidate the unexpected 10-fold point-symmetry group structure of quasi-crystals for which the 2011 Nobel Prize in chemistry was awarded to Daniel Shechtman, we explore a correspondence principle between the number of (projective) geometric elements [points[vertices] + lines[edges] + planes[faces]] of primitive cells of periodic or quasi-periodic arrangement of hard or deformable spheres in 3-dimensional space of crystallography and elements of quantum field theory of particle physics [points (particles), lines (particles, lines, currents) and hence construct 8x8 =64 = 28+36 = 26 + 38, and 10x10 =100= 64 + 36 = 74 + 26 hyperspace representations of the SU(3) symmetry of elementary particle physics and quasicrystals of condensed matter (solid state) physics respectively. As a result, we predict the Cabibbo-like angles in leptonic decay of hadrons in elementary-particle physics and the observed 10-fold symmetric diffraction pattern of quasi-crystals.

1Supported by International Centre for Basic Research, Abuja, Nigeria.
2Dept. of Physics & Astronomy, University of Nigeria, Nsukka, Nigeria

10:48AM P53.00015 Competition of Bergman-type approximants with other packing motifs in the Cu-Zr system, FENG ZHANG, MIN JIN, X.W. WANG, CAI-ZHUANG WANG, M.J. KRAMER, M.I. MENDELEV, KAI-MING HO, Ames Laboratory, US DOE, and Iowa State University — Knowledge about the topological and chemical ordering in metallic liquids and glasses is essential in predicting phase selection and understanding glass formation dynamics. Taking the Cu-Zr system as an example, previous studies have established Bergman-type medium-range ordering (MRO) from a structural analysis with cluster alignment methods [1]. In this study, we examine the thermodynamic stability of a crystalline approximant of Bergman-type quasicrystals [2] against packing geometries existing in other intermetallic compounds for a wide range of Cu compositions. The most stable structures for each structural motif at each Cu composition are obtained using an efficient genetic-algorithm search. Our results show that the Bergman-type approximant structure is thermodynamically favored over other packing geometries at the glass-forming region with Cu compositions around 65%, reaffirming the Bergman-type MRO is the lowest energy in Cu-Zr glasses.


Wednesday, February 29, 2012 11:15AM - 2:15PM — Session Q40 DBIO GSNP: Focus Session: Systems Biology and Biochemical Networks III 156A

11:15AM Q40.00001 TBD, TING LU, —

11:51AM Q40.00002 Fold-change detection and scalar symmetry of sensory input fields, OREN SHOVAL, Weizmann Institute of Science, LEA GOENTO R, California Institute of Technology, YUVAL HART, AVI MAYO, Weizmann Institute of Science, EDUARDO SONTAG, Rutgers University, URI ALON, Weizmann Institute of Science — Recent studies suggest that certain cellular sensory systems display fold-change detection (FCD): a response whose entire shape, including amplitude and duration, depends only on fold-changes in input, and not on absolute changes. We show that FCD is necessary and sufficient for sensory search to depend only on the spatial profile of the input, and not on its amplitude. Such amplitude scalar symmetry occurs in a wide range of sensory inputs, such as source strength multiplying diffusing chemical fields sensed in chemotaxis, ambient light multiplying the contrast field in vision, and protein concentrations multiplying the output in cellular signaling systems. We present a wide class of mechanisms that have FCD, including certain nonlinear feedback and feedforward loops. In addition, we find that bacterial chemotaxis displays feedback within the present class, and has indeed recently been shown to exhibit FCD. This can explain experiments in which chemotaxis searches are insensitive to attractant source levels. This study thus suggests a connection between properties of biological sensory systems and scalar symmetry stemming from physical properties of their input fields.

12:03PM Q40.00003 Network architectural conditions for prominent and robust stochastic oscillations, JAEWOOK JOO, JINMYUNG CHOI, University of Tennessee — Understanding relationship between noisy dynamics and biological network architecture is a fundamentally important question, particularly in elucidate how cells encode and process information. We analytically and numerically investigate general network architectural conditions that are necessary to generate stochastic amplified and coherent oscillations. We enumerate all possible topologies of coupled negative feedbacks in the underlying biochemical networks with three components, negative feedback loops, and mass action kinetics. Using the linear noise approximation to analytically obtain the time-dependent solution of the master equation and derive the algebraic expression of power spectra, we find that (a) all networks with coupled negative feedbacks are capable of generating stochastic amplified and coherent oscillations; (b) networks with a single negative feedback are better stochastic amplified and coherent oscillators than those with multiple coupled negative feedbacks; (c) multiple timescale difference among the kinetic rate constants is required for stochastic amplified and coherent oscillations.

12:15PM Q40.00004 Properties of gene expression including the non-functional binding of transcription factors to DNA, ANAT BURGER, University of California San Diego, ALEKSANDRA WALCZAK, Ecole Normale Superieure, PETER WOLYNES, Rice University — Many eukaryotic transcription factors bind to DNA sequences with a remarkable lack of specificity. This suggests that non-functional binding between transcription factors and DNA might not have the detrimental effect on regulation one would naively assume results from competition for binding. In fact, if binding to DNA protects transcription factors from degradation, the number and binding affinity of these ‘decoy’ binding sites should have no influence on the copy number of transcription factors available for regulation. We calculate the influence of adding decoy binding sites on several important aspects of gene expression including the noise, the time to reach steady state, and bimodal switch rates. Analyzing these effects could shed some light on how a gene functions in the ‘dressed’ environment of a genomic background.
12:27PM Q40.00005 Single promoters as regulatory network motifs . CHRISTOPHER ZOPF, NARENDRA MAHESHTHI, Massachusetts Institute of Technology — At eukaryotic promoters, chromatin can influence the relationship between a gene’s expression and transcription factor (TF) activity. This additional complexity might allow single promoters to exhibit dynamical behavior commonly attributed to regulatory motifs involving multiple genes. We investigate the role of promoter chromatin architecture in the kinetics of gene activation using a previously described set of promoter variants based on the phosphate-regulated PHOS promoter in S. cerevisiae. Accurate quantitative measurement of transcription activation kinetics is facilitated by a controllable, and observable TF input to promoter of interest leading to an observable expression output in single cells. We find the particular architecture of these promoters can result in a significant delay in activation, filtering of noisy TF signals, and a memory of previous activation – dynamical behaviors reminiscent of a feed-forward loop but only requiring a single promoter. We suggest this is a consequence of chromatin transactions at the promoter, likely passing through a long-lived “primed” state between its inactive and competent states. Finally, we show our experimental setup can be generalized as a “gene oscilloscope” to probe the kinetics of heterologous promoter architectures.

12:39PM Q40.00006 Towards a principled way of making kinetic models from data1 , STEVE PRESSE, UCSF — Kinetic model extraction from noisy data is the basic route to mechanistic insight in biology. I will show how the tools of Maximum Caliber (the dynamical analog of Maximum Entropy) can be used to infer -and not fit- models in a way which is driven by the structure and limitations of the data. For instance, the typical output of an experiment in systems biology is the stochastic expression of one reporter gene. Master equations used to model the regulatory process underlying the stochastic gene expression require knowledge of a circuit topology and rates. However rates and topology are often fit as these are rarely all independently determinable from the limited data. Our goal is to build a kinetic model from the data available with no adjustable parameter using the tools of Maximum Caliber. We apply our method to infer the statistics of rare stochastic switching events in the genetic toggle switch from fluctuations on shorter measurable timescales. In addition, we discuss how these tools can be used to infer kinetic models from real single molecule data drawn from anomalous folding kinetics of phosphoglycerate kinase and RNA hairpin zipping-unzipping time traces.

1:03PM Q40.00008 Inference of Mechanical Network Parameters in Epithelial Tissue Development , KEVIN CHIOU, Department of Physics, UCSB, LARS HUFNAGEL, EMBL Heidelberg, BORIS SHRAIMAN, KITP, UCSB — Mechanical stress in cells has been linked to biochemical networks that influence cell structure and function. Yet direct in vivo measurements of mechanical forces in epithelial tissues remain a serious experimental challenge. I will present an alternative approach based on a computational analysis of high resolution images of epithelial tissues. Assuming that epithelial cell layers are close to mechanical equilibrium, we use the observed geometry of the two dimensional cell array to infer interfacial tensions and intracellular pressures. I will present applications of this mechanical parameter inference algorithm in the context of several developmental processes involving epithelial cell layers.

1:15PM Q40.00009 Regulatory dynamics and stability in discrete and continuous models1 . FAKHTEH GHANBARNJEAD, KONSTANTIN KLEMM, Bioinformatics Group, Institute for Computer Science, University of Leipzig — Biological processes such as cell division, cell differentiation and so on are regulated dynamics. These dynamics are often described by continuous rate equations for continuously varying chemical concentrations. Binary discretization of state space and time leads to another class of models. Boolean dynamics, which are dealing with larger systems, higher complexity and less computational details. Here we study the reaction of discrete and continuous dynamics to perturbations. When asking if a gene-regulatory system reproduces a prescribed trajectory despite noise, large perturbations are to be considered in the case of low copy numbers of regulatory molecules and bursty stochastic response. Small perturbations, however, are more appropriate when modelling systems with large copy numbers and an integrative response to filter out bursts. In Boolean networks, the dynamics has been called unstable if flip perturbations lead to damage spreading. We find that this stability classification strongly differs from the stability properties of the original continuous dynamics under small perturbations of the state vector. In particular, random networks of nodes with large sensitivity yield stable dynamics under small perturbations and chaotic regime disappears.

1Physical Review Letters 107, 188701 (2011)

1:27PM Q40.00010 Polarization and molecular information transmission in the cell , ADRIANO VALDEZ-GOMEZ, GUILLERMO RAMIREZ-SANTIAGO, Instituto de Física, Universidad Nacional Autonoma de Mexico — During chemotaxis, pseudopodia are extended at the leading edge and retracted at the back of the cell. Efficient chemotaxis is the result of a refined interplay between signaling modules to transmit and integrate spatial information such as Ptdlns(3,4,5)P3. The localization of Ptdlns(3,4,5)P3 is expected to depend on the distributions or activities of PI3Ks, PTEN, and 5-phosphatases. The spatial signals spread relatively slowly so that high local concentrations of PIP3 in the plasma membrane appear in patches. These gradients induce localization of PIP3 and PTEN to the front and back of the cell, respectively. To simulate this polarization process that involves the action of seven reaction-channels inside the cell we carried out extensive stochastic simulations using Gillespie algorithm. The simulations were done on a square cell with ten thousand sites (100 x 100) emulating a square cell with side 10 mm long. We found that there are localized patches of PIP3 at the active receptors and segregation of PTEN on the opposite side of the cell. When we block the reaction-channel, PTEN+→PIP3 that involves the production of PIP2 we obtained a five-fold increase in the concentration of PIP3. This finding appears to be consistent with the

1:39PM Q40.00011 Energy Flow in Neuronal Systems , ZRINKA GREGURIC FERENCEK, JOHN ROBERT CRESSMAN, ZAID OBAIDA, George Mason University — We present results from a computational model designed to investigate the physical underpinnings of neuronal systems. Most neuronal models assume that the ion flow across neuronal membranes is to small to effect the ionomic composition inside and outside of cells. However neurons exhibiting high levels of activity can produce ionic redistributions large enough to cause significant changes to cellular excitability. Furthermore, physically-accurate neuronal models must obey conservation of mass and energy. Energy is injected into these cells through the consumption of atp, stored in electrochemical gradients, and dissipated through ionic flow down these gradients. Our model incorporates essential biological mechanisms required to reproduce this energy flow and storage. We will discuss the advantages and limitations of this dynamic system in the context of neuronal function.
1:51PM Q40.00012 Rhythm-Induced Spike-Timing Patterns Characterized by 1D Firing Map, JAN ENGELBRECHT, RENNIE MIROLLO, Boston College — A basic problem in neuroscience is to understand how the dynamic mechanisms that govern the responses of nerve cells to stimuli, which are both non-linear and noisy, still produce reliable collective activity. We study patterning in the responses of neurons subjected to periodic rhythms. These patterns are governed by simple, low-dimensional mathematical structures independent of modeling detail. We show both theoretically and in whole-cell recordings that the 1D map generated from successive spike times is such a construct. As expected, the stable periodic points of this 1D map cause a neuron’s entrainment or phase-locking to a periodic rhythm. But our work has also revealed a complementary and unexpected patterning in the spike-timing of un-entrained neurons in the form of repeated sequences of reliable spike-phase advances, which cannot be characterized simply as a noisy perturbation near the stable periodic points of the noise-free return map. This new patterning appears to require both noise and a sufficiently steep return map.

2:03PM Q40.00013 The Effects of Intrinsic Noise on an Inhomogeneous Lattice of Chemical Oscillators, MICHAEL GIVER, Brandeis University; ZAHERA JABEEN, University of Michigan; BULBUL CHAKRABORTY, Brandeis University — Intrinsic or demographic noise has been shown to play an important role in the dynamics of a variety of systems including biochemical reactions within cells, predator-prey populations, and oscillatory chemical reaction systems, and is known to give rise to oscillations and pattern formation well outside the parameter range predicted by standard mean-field analysis. Motivated by an experimental model of cells and tissues where the cells are represented by chemical reagents isolated in emission droplets, we study the stochastic Brusselator, a simple activator-inhibitor chemical reaction model. Our work extends the results of recent studies on the zero and one dimensional system to the case of a non-uniform one dimensional lattice using a combination of analytical techniques and Monte Carlo simulations.

This work was supported by the NSF MRSEC DMR-0820492.

Wednesday, February 29, 2012 11:15AM - 2:03PM – Session Q42 DBIO GSNP: Focus Session: Stochastic Population Dynamics II - Games and Spatial Dynamics 156C

11:15AM Q40.00001 Bacterial Games, ERWIN FREY, Ludwig-Maximilians-Universitaet Muenchen — Microbial laboratory communities have become model systems for studying the complex interplay between evolutionary selection forces, stochastic fluctuations, and spatial organization. Two fundamental questions that challenge our understanding of evolution and ecology are the origin of cooperation and biodiversity. Both are ubiquitous phenomena yet conspicuously difficult to explain since the fitness of an individual or the whole community depends in an intricate way on a plethora of factors, such as spatial distribution and mobility of individuals, secretion and detection of signaling molecules, toxin secretion leading to inter-strain competition and changes in environmental conditions. We discuss two possible solutions to these questions employing concepts from evolutionary game theory, nonlinear dynamics, and the theory of stochastic processes. Our work provides insights into some minimal requirements for the evolution of cooperation and biodiversity in simple microbial communities. It further makes predictions to be tested by new microbial experiments.

11:51AM Q40.00002 Evolutionary dynamics of range expansions with curved fronts and inflationary directed percolation, MAXIM LAURENTOVICH, Harvard University; KIRILL KOROLEV, Massachusetts Institute of Technology; DAVID NELSON, Harvard University — We compare the evolutionary dynamics of populations expanding into a new territory with flat and curved fronts. When actively reproducing individuals confined to a thin, uniform population front experience deleterious mutations, the evolutionary dynamics fall into the directed percolation (DP) universality class. At the DP phase transition, the selective advantage of the fit individuals balances the deleterious mutation rate. Curvature in the front changes the dynamics: Sectors of the population become causally disconnected after a time $t_c = R_0/v$, where $R_0$ is the initial radius of the population and $v$ is the radial front propagation speed. The reproducing population size increases, creating an inflationary effect that prevents the loss of fit individuals due to sector boundary diffusion and sector interactions. We develop a generalization of the Domany-Kinzel model on amorphous, isotropic lattices to simulate radial expansions. We find scaling functions characterizing the effects of inflation at criticality. We also discuss analytic results for two-point correlation functions and survival probabilities in the two limiting cases of no mutations (compact DP) and no selection.

12:03PM Q40.00003 Competition and cooperation in one-dimensional stepping stone models, KIRILL KOROLEV, Massachusetts Institute of Technology; DAVID NELSON, Harvard University — Mutualism and cooperation are major biological forces sustaining ecosystems and enabling complex evolutionary adaptations. Although spatial degrees of freedom and number fluctuations often significantly affect evolutionary dynamics, their effects on mutualism are not fully understood. We show that, even when mutualism confers a distinct selective advantage, it persists only in populations with high density and frequent migrations. When these parameters are reduced, number fluctuations lead to the local extinctions of one of the species, segregating the species in space and decreasing the size of regions where cooperation occurs. The segregated and mutualistic states are separated by a second order nonequilibrium phase transition. Generically, this transition is in the universality class of directed percolation (DP), but the phase diagram is strongly influenced by an exceptional symmetric directed percolation (DP2) transition. This influence is manifested in a strong increase in the resilience to number fluctuations of symmetric mutualism, when organisms benefit equally from interacting.

12:15PM Q42.00004 Range expansion of mutualists, MELANIE J.I. MULLER, Harvard University; KIRILL S. KOROLEV, Massachusetts Institute of Technology; ANDREW W. MURRAY, DAVID R. NELSON, Harvard University — The expansion of a species into new territory is often strongly influenced by the presence of other species. This effect is particularly striking for the case of mutualistic species that enhance each other’s proliferation. Examples range from major events in evolutionary history, such as the spread and diversification of flowering plants due to their mutualism with pollen-dispersing insects, to modern examples like the surface colonisation of multi-species microbial biofilms. Here, we investigate the spread of cross-feeding strains of the budding yeast Saccharomyces cerevisiae on an agar surface as a model system for expanding mutualists. Depending on the degree of mutualism, the two strains form distinctive spatial patterns during their range expansion. This change in spatial patterns can be understood as a phase transition within a stepping stone model generalised to two mutualistic species.

12:27PM Q40.00005 Cooperation, cheating, and collapse in microbial populations, JEFF GORE, Massachusetts Institute of Technology — Natural populations can suffer catastrophic collapse in response to small changes in environmental conditions, and recovery after such a collapse can be exceedingly difficult. We have used laboratory yeast populations to study proposed early warning signals of impending extinction. Yeast cooperatively breakdown the sugar sucrose, meaning that there is a minimum number of cells required to sustain the population. We have demonstrated experimentally that the fluctuations in the population size increase in magnitude and become slower as the population approaches collapse. The cooperative nature of yeast growth on sucrose suggests that the population may be susceptible to cheater cells, which do not contribute to the public good and instead merely take advantage of the cooperative cells. We have confirmed this possibility experimentally by using a cheater yeast strain that lacks the gene encoding the cooperative behavior [1]. However, recent results in the lab demonstrate that the presence of a bacterial competitor may drive cooperation within the yeast population.

12:00PM Q33.00008 The growth and survival of bacterial mats

Johannes Knebel, Jonas Cremer, Anna Melbinger, Erwin Frey, Ludwig-Maximilians University of Munich — Cooperative behavior is essential for microbial biofilms. The structure and composition of a biofilm change over time and thereby influence the evolution of cooperation within the system. In turn, the level of cooperation affects the growth dynamics of the biofilm. Here, we investigate this coupling for an experimentally well-defined situation in which mutants of the Pseudomonas fluorescens strain form a mat at the liquid-air interface by the production of an extracellular matrix [1]. We model the occurrence of cooperation in this bacterial population by taking into account the formation of the mat. The presence of cooperators enhances the growth of the mat, but at the same time cheaters can infiltrate the population and put the viability of the mat at risk. We find that the survival time of the mat crucially depends on its initial dynamics which is subject to demographic fluctuations [2]. More generally, our work provides conceptual insights into the requirements and mechanisms for the evolution of cooperation.


12:15PM Q33.00009 Evolution of cooperation in microbial biofilms - A stochastic model for the growth and survival of bacterial mats

Johannes Knebel, Jonas Cremer, Anna Melbinger, Erwin Frey, Ludwig-Maximilians University of Munich — Cooperative behavior is essential for microbial biofilms. The structure and composition of a biofilm change over time and thereby influence the evolution of cooperation within the system. In turn, the level of cooperation affects the growth dynamics of the biofilm. Here, we investigate this coupling for an experimentally well-defined situation in which mutants of the Pseudomonas fluorescens strain form a mat at the liquid-air interface by the production of an extracellular matrix [1]. We model the occurrence of cooperation in this bacterial population by taking into account the formation of the mat. The presence of cooperators enhances the growth of the mat, but at the same time cheaters can infiltrate the population and put the viability of the mat at risk. We find that the survival time of the mat crucially depends on its initial dynamics which is subject to demographic fluctuations [2]. More generally, our work provides conceptual insights into the requirements and mechanisms for the evolution of cooperation.


Hence, it is promising to design smart bio-mimetic materials and devices with snapping mechanisms as sensors, actuators, artificial muscles and biomedical

Based on the principles learnt from the Venus flytrap, we are also able to manufacture a preliminary “flytrap robot”. Hence, it is promising to design smart bio-mimetic materials and devices with snapping mechanisms as sensors, actuators, artificial muscles and biomedical devices.

Biomedical Engineering, Washington University in St. Louis, HUANG ZHENG, Fujian Radio and Television University, Fuzhou, China, WENZHE CHEN, Fujisho University, FuJian University of Technology, Fuzhou, China — Plants are not well known for fast motions, yet some plants such as the Venus flytrap can move in a fraction of a second to capture insects, even though they do not have nerves or muscles. This type of rapid motion has intrigued scientists for centuries. Darwin did a first systematic study on the trap closure mechanism, and considered the plant as “one of the most wonderful in the world”. Thereafter, several physical mechanisms have been proposed, such as the rapid loss of turgor pressure, an irreversible acid-induced wall loosening mechanism, and the snap-through model by mechanical instability, but with no unanimous agreement among researchers. Here we propose a coupled mechanical bistable mechanism that explains the rapid closure of the Venus flytrap in a comprehensive manner, consistent with a series of experimental observations. Such bistable behaviors are theoretically modeled and validated with table-top experiments. Based on the principles learnt from the Venus flytrap, we are also able to manufacture a preliminary “flytrap robot”.

1The authors acknowledge National Science Foundation of China (Grant No. 11102040) and Sigma Xi GIAR program.

12:03PM Q52.00005 Materials with Tunable Behavior due to Constrained Instabilities: Performance and Stability Analysis . DENNIS KOCHMANN, California Institute of Technology, WALTER J. DRUGAN, University of Wisconsin-Madison — Combining several materials into a composite permits the creation of new materials with overall properties tunable via a careful choice of the constituent materials with favorable specifics. The probably simplest example is a particle-matrix system, in which particles of one material enhance the mechanical behavior of the matrix material. Recent advances have confirmed that the overall performance of such a composite (e.g., its viscoelastic properties) can be dramatically altered, and stiffness and damping can be tuned to an extreme if one allows for temporarily negative elastic moduli in the inclusion. Such incremental negative moduli imply instability: e.g. a free-standing body of negative stiffness is thermodynamically unstable. However, through its geometric constraint a matrix phase can stabilize the otherwise unstable state of the inclusion phase, thus rendering the overall composite stable. In this contribution, we show, based on dynamic stability analyses, that the matrix constraint does indeed allow for the existence and use of negative moduli, and that this effect can be utilized to design novel composites of superior performance. Approaches to stabilize the negative-stiffness effect will be discussed as well as the performance of such composites.

12:15PM Q52.00006 Snap-Through of Graphene: An Elasto-Capillary Perspective , TILL WAGNER, DAMTP, University of Cambridge, DOMINIC VELLA, OCCAM, University of Oxford — Understanding the interaction between graphene flakes and various substrates is of crucial importance for nanoelectromechanical systems (NEMS) applications, among others. The ‘snap-through’ instability of graphene flakes placed onto corrugated substrates has recently received much attention as a potential assay for the study of this interaction. A sharp transition has been found in the morphology of the graphene between a) closely adhering to the corrugations of the substrate and b) lying almost completely flat on top. Which of these morphologies is observed depends on the geometry of the substrate and the mechanical properties of the flake. In this talk we shall focus on understanding the nature of this transition and, in particular, the ‘sharpness’ of the transition. We investigate how the location of snap through and its sharpness might be used to yield estimates of adhesion strength and friction with the substrate.

12:27PM Q52.00007 Electromechanical phase transition in dielectric elastomers under uniaxial tension and electrical voltage , RUI HUANG, University of Texas at Austin, ZHIGANG SUO, Harvard University — Subject to forces and voltage, a dielectric elastomer may undergo electromechanical phase transition. A phase diagram is constructed for an ideal dielectric elastomer membrane under uniaxial force and voltage, reminiscent of the phase diagram for liquid-vapor transition of a pure substance. We identify a critical point for the electromechanical phase transition. Two states of deformation (thick and thin) may coexist during the phase transition, with the mismatch in lateral stretch accommodated by wrinkling of the membrane in the thin state. The processes of electromechanical phase transition under various conditions are discussed. A reversible cycle is suggested for electromechanical energy conversion using the dielectric elastomer membrane, analogous to the classical Carnot cycle for a heat engine. The amount of energy conversion, however, is limited by failure of the dielectric elastomer due to electrical breakdown. With a particular combination of material properties, the electromechanical energy conversion can be significantly extended by taking advantage of the phase transition without electrical breakdown.


12:51PM Q52.00009 Modeling of dielectric elastomeric materials: theory, finite element simulation, and applications . DAVID HENANN, KATIA BERGOLDI, School of Engineering and Applied Science, Harvard University — Elastic materials that undergo large deformations in response to an electric field have garnered attention in recent years. Applications of these dielectric elastomeric materials include actuators capable of converting electrical energy to mechanical work and energy harvesting devices that convert mechanical energy into electrical energy. Furthermore, dielectric elastomers exhibit interesting instabilities, especially under constrained geometries, opening the door for possible applications in active tissue engineering, artificial muscles and other applications. In this talk, the mechanics community concerning the formulation of a finite-deformation constitutive theory for an electro-mechanically-coupled material. While the details of the formulation of such a theory are beginning to come into focus in the literature, numerical techniques for solving these equations are in their infancy. In this work, we have developed a finite-element-based numerical simulation capability for dielectric elastomers. This talk will highlight the application of our numerical simulation capability to dielectric elastomeric actuators, energy harvesting devices, as well bistable behaviors of small dielectric elastomeric structures on a constraining substrate.
More generally, my model of QS divergence suggests a form of kin recognition where different kin types coexist in unstructured populations. This is facilitated by facultative cheating between the competing strains. My results suggest a role for complex social strategies in the long-term evolution of QS systems. We focus on receptor mutations and "cheating immunity" signaling mutations. The maintenance of diversity and the evolution of cross-inhibition between strains are facilitated by the production of extracellular enzymes — "public goods". Diversification can readily evolve. Coevolution is positively selected by cycles of alternating "cheating" and "sneaking". For VHB material, the linear strain of actuation can be 300%. The actuator shows advantages compared to the classic designs (say, tube and circular actuators), and can be used as artificial muscles in soft robots.

1:15PM Q52.00011 Geometry-induced rigidity in pressurized elastic shells, PEDRO REIS, Massachusetts Institute of Technology, BASTIAAN FLORIJN, MIT and Leiden University, ARNAUD LAZARUS, MIT — We study the indenteration of pressurized thin elastic shells, with positive Gaussian curvature. In our precision desktop-scale experiments, the geometry of the shells and their material properties are custom-controlled using rapid prototyping and digital fabrication techniques. The mechanical response is quantified through load-displacement compression tests and the differential pressure is set by a syringe-pump system under feedback control. Focus is given to the linear regime of the response towards quantifying the geometry-induced rigidity of pressurized shells with different shapes. We find that this effective stiffness is proportional to the local mean curvature in the neighborhood of the locus of indentation. Combining classic theory of shells with recent developments by D. Vella et al. (2011), we rationalize the dependence of the geometry-induced rigidity on: i) the mean curvature at the point of indentation, ii) the material properties of the shell and iii) the in-out differential pressure. The proposed predictive framework is in excellent agreement with our experiments, over a wide range of control parameters. The prominence of geometry in this class of problems points to the relevance and applicability of our results over a wide range of length-scales.

1:27PM Q52.00012 S-cones in thin shells under indentation, ALICE NASTO, Massachusetts Institute of Technology, AMIN AJDARI, Northeastern University, ARNAUD LAZARUS, MIT, ASHKAN VAZIRI, Northeastern University, PEDRO REIS, MIT — We perform a hybrid experimental and numerical investigation of the localization of deformation in indented thin spherical elastic shells. Past the initial linear response, an inverted cap develops as a Pogorelov circular ridge. For further indentation, this ridge looses axis-symmetry and sharp points of localized curvature form. We refer to these localized objects as s-cones (for shell-cones), in contrast with their developable cousins in plates (d-cones). We quantify the effect of systematically varying the indenter’s radius of curvature (from point to plate load) on the formation and evolution of s-cones. In our precision desktop-scale experiments we use rapid prototyped elastomeric shells and rigid indenters of various shape. The mechanical response is measured through load-displacement compression tests and the deformation process is further characterized through digital imaging. In parallel, the experimental results are contrasted against nonlinear Finite Element simulations. Merging these two complementary approaches allows us to gain further physical insight towards rationalizing this geometrically nonlinear process.

1:39PM Q52.00013 Folding and buckling pathways in spherical shells with soft spots, JAYSON PAULOSE, Harvard School of Engineering and Applied Sciences, Cambridge, MA 02138, DAVID NELSON, Department of Physics, Harvard University, Cambridge, Past 02138 — Thin elastic spherical shells subject to an external pressure undergo a buckling transition when the pressure reaches a critical value. Past the buckling instability, the shell typically takes on a shape with one or more inversions that focus the elastic deformation energy within narrow circular regions on the sphere. These inversions are associated with large volume changes and hysteresis, and their location is highly sensitive to very slight imperfections in the sphere. Recently, it has been demonstrated [1] that natural pollen grains have evolved soft sectors in their hard outer walls which guide them toward particular folding pathways when their internal volume is reduced due to dessication, thus avoiding sudden and uncontrolled changes in shape. Motivated by these results, we study the effect of circular soft spots on the buckling of otherwise uniform spherical shells. Through a combination of scaling arguments and numerical simulations, we demonstrate that the shell can be tuned to follow distinct buckling pathways by varying the size and stiffness of the soft spot. [1] E. Kathori et al, Proc. Natl. Acad. Sci. USA 107, 7635 (2010)

1:51PM Q52.00014 Buckling-Induced Pattern Transformation of Structured Elastic Shells, KATIA BERTOLDI, JONGMIN SHIM, SEAS, Harvard Univ, CLAUDE J. PERDIGOU, MIT, ELIZABETH R. CHEN, University of Michigan at Ann Arbor, PEDRO M. REIS, MIT — We present a class of continuum shell structures, the buckliball, which, undergo a structural transformation induced by buckling under pressure loading. The geometry of the buckliball comprises a spherical shell patterned with a regular array of circular voids. Moreover, we show that the buckling-induced pattern transformation is possible only with five specific hole arrangements. These voids are covered with a thin membrane, thereby making these localized objects as s-cones (for shell-cones), in contrast with their developable cousins in plates (d-cones). In our precision desktop-scale experiments and finite element simulations, we use rapid prototyped elastomeric shells and rigid indenters of various shape. The mechanical response is measured through load-displacement compression tests and the deformation process is further characterized through digital imaging. In parallel, the experimental results are contrasted against nonlinear Finite Element simulations. Merging these two complementary approaches allows us to gain further physical insight towards rationalizing this geometrically nonlinear process.

2:03PM Q52.00015 Wrinkling of a collapsing viscous bubble, JAMES BIRD, Boston University, HOWARD STONE, Princeton University, JOHN BUSH, Massachusetts Institute of Technology — Thin-sheets of sufficiently viscous liquid can behave similar to elastic sheets and buckle under certain external forces. A classic example is the "parachute instability" for which a ruptured viscous bubble wrinkles as it relaxes, with the explanation for the wrinkles being based on the liquid film falling under its own weight. In this talk we revisit the viscous bubble-bursting experiments and demonstrate that gravity is responsible for neither the collapse nor the resulting wrinkling instability. Using a combination of experiments and theory, we highlight the importance of capillary forces and elucidate their role in the wrinkling instability.

Wednesday, February 29, 2012 2:30PM - 5:06PM
Session T42 DBIO GSNP: Focus Session: Evolutionary Systems Biology III - Evolutionary Games 156C

2:30PM T42.00001 Bacterial tower of Babel —How cheating and lying diversify bacterial communication, AVIGDOR ELDAR, Tel-Aviv University, Department of molecular microbiology and biotechnology — In microbial “quorum sensing” (QS) communication systems, microbes produce and respond to a signaling molecule, enabling a cooperative response at high cell densities. Many species of bacteria show fast, intraspecific, evolutionary divergence of their QS pathway specificity—signaling molecules activate cognate receptors in the same strain but fail to activate, and sometimes inhibit, those of other strains. Despite many molecular studies, it has remained unclear how a signaling molecule and receptor can coevolve, what maintains diversity, and what drives the evolution of cross-inhibition. Here, I use mathematical analysis to show that when QS controls the production of extracellular enzymes — "public goods" — diversification can readily evolve. Coevolution is positively selected by cycles of alternating "cheating" receptor mutations and "cheating immunity" signaling mutations. The maintenance of diversity and the evolution of cross-inhibition between strains are facilitated by facultative cheating between the competing strains. My results suggest a role for complex social strategies in the long-term evolution of QS systems. More generally, my model of QS divergence suggests a form of kin recognition where different kin types coexist in unstructured populations.
3:06PM T42.00002 Coupling between evolutionary and population dynamics in experimental microbial populations. ALVARO SANCHEZ, JEFF GORE, Department of Physics, Massachusetts Institute of Technology — It has been often assumed that population dynamics and evolutionary dynamics occur at such different timescales that they are effectively de-coupled. This view has been challenged recently, due to observations of evolutionary changes occurring in short timescales. This has led to a growing interest in understanding eco-evolutionary dynamics of populations. In this context, recent theoretical models have predicted that coupling between population dynamics and evolutionary dynamics can have important effects for the evolution and stability of cooperation, and lead to extremely rich and varied dynamics. Here, we report our investigation of the eco-evolutionary dynamics of a cooperative social behavior, sucrose metabolism, in experimental yeast populations. We have devised an experimental strategy to visualize trajectories in the phase space formed by the population size (N) and the fraction of cooperator cells in the population (f). Our measurements confirm a strong coupling between evolutionary and population dynamics, and allowed us to characterize the bifurcation plots. We used this approach to investigate how sudden environmental changes affect the stability and recovery of populations, and therefore the stability of cooperation.

3:18PM T42.00003 Competition between species can drive public goods cooperation within a species. HASAN CELIKER, EECS department, MIT, JEFF GORE, Physics department, MIT — Costly cooperative strategies are vulnerable to exploitation by cheats. Microbial studies have suggested that cooperation can be maintained in nature by mechanisms such as reciprocity, spatial structure and multi-level selection. So far, however, almost all laboratory experiments aimed at understanding cooperation have relied on studying a single species in isolation. In contrast, species in the wild live within complex communities where they interact with other species. Little effort has focused on understanding the effect of interspecies competition on the evolution of cooperation within a species. We test this relationship by using sucrose metabolism of budding yeast as a model cooperative system. We find that when co-evolved with a bacterial competitor, yeast populations become more cooperative compared to isolated populations. We show that this increase in cooperation within yeast is mainly driven by resource competition imposed by the bacterial competitor. A similar increase in cooperation is observed in a pure yeast culture when essential nutrients in the media are limited experimentally.

3:30PM T42.00004 The emergence of cooperation from a single cooperative mutant. JONAS CREMER, University of California, San Diego, ANNA MELBINGER, ERWIN FREY, Ludwig-Maximilians University Munich, Germany — Population structure is one central condition which promotes the stability of cooperation: If cooperators more likely interact with other cooperators (positive assortment), they keep most of their benefit for themselves and are less exploited by non-cooperators. However, positive assortment can only act successfully if cooperation is already well established in the population such that cooperative individuals can successfully assort. But how can cooperation emerge when starting with a single cooperative mutant? Here we study this issue for a generic situation of microbial systems where microbes regularly form new colonies and show strong population growth. We show how and when the dynamical interplay between colony formation, population growth and evolution within colonies can provoke the emergence of cooperation. In particular, the probability for a single cooperative mutant to succeed is robustly large when colony-formation is fast or comparable to the time-scale of growth within colonies; growth supports cooperation.

3:42PM T42.00005 Coping with stress in a synthetic world. LINGCHONG YOU, Duke University — A major focus of synthetic biology is the engineering of gene circuits to perform user-defined functions. In addition to generating systems of practical applications, such efforts have led to the identification and evaluation of design strategies that enable robust control of dynamics in single cells and in cell populations. On the other hand, there is an increasing emphasis on using engineered systems programmed by simple circuits to explore fundamental biological questions of broad significance. In this talk, I will discuss our efforts along this line of research, whereby we have used engineered gene circuits to examine the evolutionary dynamics of two common bacterial survival strategies in stress response: programmed death and cell-cell communication.

4:18PM T42.00006 Bacterial cheating limits antibiotic resistance. HUI XIAO CHAO, EUGENE YURTSEV, Gore Lab, Department of Physics, Massachusetts Institute of Technology, MANOISHI DATTA, Computational Systems Biology, Massachusetts Institute of Technology, TANYA ARTEMOVA, JEFF GORE. Gore Lab, Department of Physics, Massachusetts Institute of Technology — The widespread use of antibiotics has led to the evolution of resistance in bacteria. Bacteria can gain resistance to the antibiotic ampicillin by acquiring a plasmid carrying the gene beta-lactamase, which inactivates the antibiotic. This inactivation may represent a cooperative behavior, as the entire bacterial population benefits from removing the antibiotic. The cooperative nature of this growth suggests that a cheater strain—which does not contribute to breaking down the antibiotic—may be able to take advantage of cells cooperatively inactivating the antibiotic. Here we find experimentally that a "sensitive" bacterial strain lacking the plasmid conferring resistance can invade a population of resistant bacteria, even in antibiotic concentrations that should kill the sensitive strain. We observe stable coexistence between the two strains and find that a simple model successfully explains the behavior as a function of antibiotic concentration and cell density. We anticipate that our results will provide insight into the evolutionary origin of phenotypic diversity and cooperative behaviors.

4:30PM T42.00007 Bacterial Transformation and Competition Under Antibiotic Stress. JONAS PEDERSON, Danish Technical University, ANDREW BERGMAN, None, CHRIS CLEVELAND, Princeton University, TOLGA CAGAYT, UT Southwestern, ROBERT AUSTIN, Princeton University, GABOR BALASZI, M.D. Anderson Medical Center — Transformation, the process by which bacteria uptake DNA directly from their environment and incorporate it as their own genetic material, is a form of Horizontal Gene Transfer that occurs throughout nature as an important mechanism for spurring on bacterial evolution. We examine the capacity of bacteria to undergo transformation and will discuss work that has been done by the Austin group using Micro-Habitat Patches (MHPs) to examine the emergence of phenotypes due to horizontal gene transfer.

4:42PM T42.00008 Rapid Antibiotic Resistance Evolution of GASP Mutants. QIUCEN ZHANG, Princeton University, HYUNSUNG KIM, NADER POURMAND, UC Santa Cruz, ROBERT AUSTIN, Princeton University — The GASP phenotype in bacteria is due to a mutation which enables the bacteria to grow under high stress conditions where other bacteria stop growing. We probe using our Death Galaxy microenvironment how rapidly the GASP mutant can evolve resistance to mutagenic antibiotics compared to wild-type bacteria, and explore the genomic landscape changes due to the evolution of resistance.

4:54PM T42.00009 Spatial vs. individual variability with inheritance in a stochastic Lotka-Volterra system. ULRICH DOBRAMSKI, UWE C. TAUBER, Department of Physics, Virginia Tech — We investigate a stochastic spatial Lotka-Volterra predator-prey model with randomized interaction rates that are either affinity to the lattice sites they are located, and / or specific to individuals in either population. In the latter situation, we include rate inheritance with mutations from the particles' progenitors. Thus we arrive at a simple model for competitive evolution with environmental variability and selection pressure. We employ Monte Carlo simulations in zero and two dimensions to study the time evolution of both species' densities and their interaction rate distributions. The predator and prey concentrations in the ensuing steady states depend crucially on the environmental variability, whereas the temporal evolution of the individualized rate distributions leads to largely neutral optimization. Contrary to e.g., linear gene expression models, this system does not experience fixation at extreme values. An approximate description of the resulting data is achieved by means of an effective master equation approach for the interaction rate distribution.
2:30PM T52.00001 Transient and steady state behavior of full counting statistics in thermal transport , BIJAY AGARWALLA, BAOWEN LI, JIAN-SHENG WANG, National University of Singapore — We study the statistics of heat transferred in a given time interval \( t_M \), through a finite harmonic system, which is connected with two heat baths, maintained at two different temperatures. We calculate the cumulant generating function \( (CGF) \) for heat transfer using non-equilibrium Green’s function method. The CGF can be concisely expressed in terms of Green’s functions of the system and the self-energy of the lead with shifted arguments, \( \Sigma^A (\tau, \tau') = \Sigma_p (\tau + h \tau (\tau', \tau') + h \tau (\tau')) - \Sigma_p (\tau, \tau') \), where \( \Sigma_p (\tau, \tau') \) is the contour-ordered self-energy of the left lead. The expression of CGF is valid in both transient and steady state regimes. We present a transient result of the first four cumulants of a graphene junction. It is found that measurement causes the energy to flow into the leads. In the steady state we show that the CGF obey “steady state fluctuation theorem”. We also study the CGF for the joint probability distribution of left and right lead heat flux \( P (Q_L, Q_R) \), which is important to calculate the correlations between \( Q_L \) and \( Q_R \). We also discuss the CGF for the total entropy production for two lead system without the center part.

2:42PM T52.00002 Langevin dynamics beyond the weak coupling limit , ALEXANDER PLYUKHIN, Saint Anselm College — Many popular results of non-equilibrium statistical mechanics hold only in leading order in a small parameter \( \lambda \) which controls the strength of the system-environment coupling. In this approximation the equations for the first two moments \( \langle hX \rangle \) for the tagged particle mobility, \( \langle v^2 \rangle \), and the temperature equal to the effective temperature obtained from the violation of the Einstein relation between the self-diffusion and tagged particle mobility. We thus prove the usefulness of this effective temperature for the description of the tagged particle behavior beyond the realm of linear response.

3:06PM T52.00004 Thermodynamic reversibility in feedback processes¹, JORDAN HOROWITZ, JUAN PARRONDO, Universidad Complutense de Madrid — The information acquired during a thermodynamic process with feedback can be converted into useful work. However, the second law of feedback restricts the amount of useful work that can be obtained from this information. In this presentation, I will discuss optimal thermodynamic processes with feedback, where all the information is converted into work. Utilizing the detailed fluctuation theorem for feedback, I will demonstrate that such processes are feedback-reversible: they are indistinguishable from their time-reversal, thereby extending the notion of thermodynamic reversibility to feedback processes.

1Financial support for this project came from MOSAICO (Spanish Government) and MODELICO (Comunidad de Madrid)

3:18PM T52.00005 Entropy production in non-equilibrium steady states¹, DANIEL BEN-AVRAHAM, Clarkson University, SVEN DOROSZ, University of Luxembourg, MICHEL PLEIMLING, Virginia Tech — We discuss entropy production in non-equilibrium steady states by focusing on paths obtained by sampling at regular (small) intervals, instead of sampling on each change of the system’s state. This allows us to directly study entropy production in systems with microscopic irreversibility. The two sampling methods are equivalent otherwise, and the fluctuation theorem also holds for the three-state loop, as a canonical model of microscopic irreversibility, finding its entropy distribution, rate of entropy production, and large deviation function in closed analytical form, and showing that the observed kink in the large deviation function arises solely from microscopic irreversibility [1].

¹Supported in part by the US National Science Foundation through Grant DMR-0904999.

3:30PM T52.00006 Information, entropy, and heat far from equilibrium¹, SEBASTIAN DEFFNER, University of Maryland — For equilibrium states, the Shannon entropy, \( H = - \int d\sigma p(\sigma) \ln p(\sigma) \), coincides with the thermodynamic entropy. It has lately been recognized that for systems in nonequilibrium steady states a thermodynamic description based on \( H \) becomes feasible, as well. In the present work we derive various generalizations of the second law for nonequilibrium processes with additional information supplied from an external or an internal memory. We will show that the irreversible entropy production is bounded from below by the information transferred from the memory to the system.

³This work was funded by the DAAD.

3:42PM T52.00007 Effective temperature determines density distribution in a slowly varying external potential beyond linear response , GRZEGORZ SZAMEL, MIN ZHANG, Department of Chemistry, Colorado State University — We consider a sheared colloidal suspension under the influence of an external potential that varies slowly in space in the plane perpendicular to the flow and acts on one selected (tagged) particle of the suspension. Using a Chapman-Enskog type expansion we derive a steady state equation for the tagged particle density distribution. We show that for potentials varying along one direction only, the tagged particle distribution is the same as the equilibrium distribution with the temperature equal to the effective temperature obtained from the violation of the Einstein relation between the self-diffusion and tagged particle mobility coefficients. We thus prove the usefulness of this effective temperature for the description of the tagged particle behavior beyond the realm of linear response. We illustrate our theoretical predictions with Brownian dynamics computer simulations.
Dynamic phase transitions in large work diffusion systems, HYUNGGYU PARK, Korea Institute for Advanced Study, CHULAN KWON, Myongji University, JAE DONG NOH, University of Seoul — We present the theoretical study on non-equilibrium (NEQ) fluctuations for diffusion dynamics in high dimensions driven by a linear drift force. We find the time-dependent probability distribution function exactly as well as the NEQ work production distribution $P(W)$ in terms of solutions of nonlinear differential equations. In two dimensions, we find analytically a sequence of dynamic phase transitions in the exponential tail shape of $P(W)$. Their implications and origins are discussed.

Driven Langevin dynamics: heat, work and pseudo-work, DAVID SIVAK, Lawrence Berkeley National Laboratory, JOHN CHODERA, University of California, Berkeley, GAVIN CROOKS, Lawrence Berkeley National Laboratory — Common algorithms for simulating Langevin dynamics are neither microscopically reversible, nor do they preserve the equilibrium distribution. Instead, even with a time-independent Hamiltonian, finite time step Langevin integrators model a driven, nonequilibrium dynamics that breaks time-reversal symmetry. Herein, we demonstrate that these problems can be resolved with a Langevin integrator that splits the dynamics into separate deterministic and stochastic substeps. This allows the total energy change of a driven system to be divided into heat, work, and pseudo-work — the work induced by the finite time step. The extent of time-symmetry breaking due to the finite time step can be measured and true equilibrium properties recovered. This interpretation of discrete time step Langevin dynamics as a driven process provides new insights into the practical use of stochastic integrators for molecular simulation.

Statistical interpretation of heat and work and the adiabatic theorem in irreversible processes, PURU GUJRATI, University of Akron — By generalizing the traditional concept [1] of heat and work to include their irreversible components allows us to express them in statistical terms so that $dW$ is the isentropic energy change; this generalizes the equilibrium adiabatic theorem. Then $dQ$ is then nothing but the energy change solely due to the change in the microstate probability. Accordingly $dQ=TDs$ [2] so that all powerful aspects of the equilibrium formulation are preserved, a quite remarkable but unexpected result. The traditional formulation of the first law of thermodynamics, which uses the fields (temperature, pressure, etc.) of the medium can be equivalently written as $dE=TDW$ using the fields of the system. This makes the two descriptions using the fields of the medium or the system equivalent and settles the long existing dispute in the literature regarding the proper choice of the fields. Moreover, the use of system fields (including affinities) allows us to analyze non-equilibrium processes such as free expansion between non-equilibrium states, which cannot be analyzed in the traditional approach.

Application of the generalized fluctuation-dissipation theorem on a sheared suspension, EMMANUELA FILIPPIDI, ALEXANDRE FRANCESCHINI, DAVID PINE, Center for Soft Matter Research, New York University — We explore the validity of the generalized fluctuation-dissipation theorem for steady-state systems (proposed by Prost, Joanny and Parrondo, PRL 103, 090601 2009) in an experimental system: a suspension of non-colloidal spheres under slow periodic strain. The system is out-of-equilibrium and typically undergoes a phase transition from an active fluctuating to an absorbing state as the strain amplitude is decreased. It is a good candidate for applying the proposed theory since it has Markovian dynamics and fluctuating steady states. The control parameters are the applied strain amplitude and its volume fraction and fluctuations of proper observables such as the individual particle locations can be readily measured. Perturbations of the control parameter of strain can lead in new steady states after a transient response, which in turn can be correlated with the fluctuating observable, thus providing a way of verifying the validity of the proposed version of the generalized fluctuation-dissipation theorem.

Entropy rate of non-equilibrium growing networks, ARDA HALU, KUN ZHAO, Northeastern University, SIMONE SEVERINI, University College London, GINESTRA BIANCONI, Northeastern University — In order to quantify the complexity of networks, new entropy measures have recently been introduced. Most of these entropy measures pertain to static networks or to dynamical processes defined on static complex networks. In this talk, we will discuss the entropy rate of growing network models, which quantifies how many labeled networks are typically generated by those growing network models. We will present an analytical evaluation of the difference between the entropy rate of growing tree network models and the entropy of tree networks that have the same asymptotic degree distribution. We will outline our finding that growing networks with linear preferential attachment generated by dynamical models are exponentially less in number than the static networks with the same degree distribution for a large variety of proper observables such as the individual particle locations can be readily measured. Perturbations of the control parameter of strain can lead in new steady states after a transient response, which in turn can be correlated with the fluctuating observable, thus providing a way of verifying the validity of the proposed version of the generalized fluctuation-dissipation theorem.
2:30PM T53.00001 Fluctuations in Intensity in disordered media as a New Sub-wavelength Microscopy Tool 1, GABRIEL CWILICH, Department of Physics, Yeshiva University, JUAN JOSE SAENZ, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid — The intensity-intensity correlations of waves that propagate coherently through a disordered system are discussed, in the mesoscopic scale. Since many of the properties of those correlations are independent of the transport regime (ballistic, diffusive or localized) they can be discussed using the macroscopic approach of random matrix theory [1]. In that framework we have considered the problem of multiple sources emitting simultaneously in a disordered medium, and we will show that the correlations and even the intensity fluctuations at a fixed point outside the turbid system can provide useful information about both the relative position of the sources and their coherence. Moreover, the information obtained is relevant at subwavelength lengths, opening the possibility of new applications to fluorescence studies, communications and image processing in turbid environments, complementary to traditional techniques.


2:42PM T53.00002 Photon localization in a nematic liquid crystal 2, JIM MCCLYMER, MATT LUDDEN, University of Maine, Dept. of Physics and Astronomy, JESSE WERTHEIM, None — The nematic liquid crystal MBBA, due to director fluctuations, is a highly scattering material with low transparency. We experimentally reported that the transmission coefficient for laser light at 830 nm decays exponentially with a decay length of approximately 0.8 mm while the absorption length is over 30 times larger which we interpret as evidence for photon localization. The data does not fit a model of diffusion or diffusion with absorption. We have extended this work by measuring the decay coefficient for incoherent light from 475 to 825 nm. We find that the absorption remains low over this range, with absorption lengths ranging from 8 mm at the blue end of the spectrum to 12 mm in the near IR. The transmission coefficient shows an exponential decrease with decay constants an order of magnitude smaller than the absorption length, 0.4 mm, in the blue end while increasing to 3 mm in the near IR. The data indicates that photon localization is observed throughout the visible region into the near IR.

3:06PM T53.00004 New perspectives on waves in random media: Speckle, modes, transmission eigenchannels, and focusing 3, AZRIEL GENACK, Queens College of the City University of New York — The understanding of electron localization and conductance fluctuations has been advanced by utilizing notions of speckle, modes, and transmission eigenchannels. These concepts cannot be probed directly for electronic systems but can be explored for classical waves utilizing spectra of field transmission coefficients between arrays of points on the incident and output surfaces of ensembles of random samples. This is illustrated in microwave measurements of transmission through random waveguides in the Anderson localization transition. These experiments supply the link between the statistics of intensity and conductance and show that transmitted wave can be decomposed simultaneously into the underlying quasi-normal modes and transmission eigenchannels of the sample. The power of each of these approaches and the richness of the links between them will be illustrated by examples that reveal new aspects of wave propagation. The delayed onset of transmission following pulse excitation is shown to be the result of destructive interference between highly correlated speckle patterns of neighboring modes, while the falling decay rate at later times reflects the incoherent decay of increasingly prominent long-lived modes. We determine the individual eigenvalues \( \tau_n \) of the transmission matrix and achieve nearly complete transmission in opaque diffusive samples. We demonstrate that when reflection at the sample interface is taken into account, the spacing between average values of \( \ln \tau_n \) is equal to the inverse of the bare conductance, in accord with predictions by Dorokhov [1]. We find that the distribution of total transmission relative to the conductance is determined by the effective number of transmission eigenvalues, \( \xi_{eff} = \left( \sum_{n=1}^{N} \tau_n \right)^2 / \sum_{n=1}^{N} \tau_n^2 \), which provides the link between the statistics of intensity and conductance. For diffusive waves, \( \xi_{eff} \) is the inverse of the degree of intensity correlation. The contrast between the peak and background of maximally focused radiation in the transmitted wave, achieved when the incident is phase conjugated relative to the selected focal point, is equal to \( (1 + \xi_{eff}) \).


3:42PM T53.00005 Experimental Observation of Brachistochrone Wave Dynamics in PT Symmetric Structures 1, JOSEPH SCHINDLER, SAMUEL KALISH, ANG LI, MEI ZHENG, TSAMPIKOS KOTTOS, FRED ELLIS, Wesleyan University, Middletown, CT — Mutually coupled modes of a pair of active LRC circuits, one with amplification and another with an equivalent amount of attenuation, provide an experimental realization of a wide class of systems where gain and loss mechanisms break the Hermiticity while preserving parity-time (PT) symmetry. For a value \( \gamma_{PT} \) of the gain and loss strength parameter the eigenfrequencies undergo a spontaneous phase transition from real to complex values, while the normal modes coalesce, achieving a definite chirality. A dramatic manifestation of PT symmetry is observed in the brachistochrone wave dynamics. Experimental findings support the theoretical prediction of arbitrarily small energy transfer times between the LRC elements of the circuit. We envision that realization of such design strategies can have applications in telecommunications and metamaterial structures.

Wesleyan Project Grant, AFOSR No. FA 9550-10-1-0433

3:54PM T53.00006 Experimental studies of PT-scattering in arrays of active LRC elements 2, ZIN LIN, JOSEPH SCHINDLER, HAMID RAMEZANI, FRED ELLIS, TSAMPIKOS KOTTOS, Wesleyan University, WAVE TRANSPORT IN COMPLEX SYSTEMS TEAM — One of the fundamental tasks in antenna theory is getting an antenna to radiate by removing mismatch losses between the loaded antenna and the transmission line that delivers the power. We will present experimental data suggesting that PT-symmetric antenna structures, where active elements associated with the real part of impedance \( (z_R) \) are involved, can lead to a broadband, reflectionless behavior. The suggested optimal matching strategy can potentially be superior to traditional one where \( z_R \) is purely imaginary in order to balance the reactance. Along these lines, we also envision antenna arrangements with unidirectional ultrafast communication capabilities, where the signal will transfer faster (or slower) between the active elements of the PT-structure depending on the entrance point of the incident wave.

We acknowledge AFOSR No. FA 9550-10-1-0433 grant and a NSF ECCS-1128571 grant.
4:06PM T53.00007 Measurement of the Probability Distribution of Optical Transmittance on the Crossover to Anderson localization, ZHOU SHI, JING WANG, AZRIEL GENACK, Department of Physics, Queens College of the City University of New York — We report measurements of spectra of the field transmission matrix $t$ for microwave radiation propagating through waveguide filled with randomly positioned dielectric scattering spheres in the Anderson localization transition. Diagonalizing the matrix product $t^n$ gives the transmission eigenvalues $\tau_n$, which yields the optical transmittance, $T = \sum_{n=0}^{N} |\alpha_n|^2 = \sum_{n=1}^{N} \tau_n$. The ensemble average of the transmittance is equal to the dimensionless conductance, $g = \langle T \rangle$. We show the probability distribution of transmittance $P(T)$ changes from Gaussian to log-normal as the value of $g$ decreases. The distribution $P(T)$ is analyzed in terms of the underlying transmission eigenvalues $\tau_n$. For random samples with $g \sim 3.9$, we found $P(T)$ follows a Gaussian distribution. For $g \sim 0.37$, we observe a highly asymmetric distribution for $-\ln T$. The sharp drop for high values of $T$ is attributed to the restriction that $\tau_n < 1$ and the repulsion between transmission eigenvalues even for localized samples. For $g \sim 0.04$, the distribution of transmittance is nearly log-normal. The variance of $-\ln T$, $\sigma^2$, scales linearly with $-\langle \ln T \rangle$ as predicted by single parameter scaling even for weakly localized waves.

4:18PM T53.00008 Mode Statistics in Random Media1, JING WANG, AZRIEL GENACK, Department of Physics, Queens College, The City University of New York — The nature of transport through a material is determined by the spectrum of modes or energy levels. We have analyzed the frequency variation of the transmitted microwave field speckle pattern for quasi one-dimensional random samples to obtain the central frequencies, linewidths and speckle patterns of the modes for an ensemble of samples at lengths of two and three times the localization length. The number of modes can be determined unambiguously from the spectrum of the goodness of fit. From these results we obtain the statistics of mode spacings and widths. The distribution of spacings between adjacent modes is close to the Wigner surmise predicted for diffusive waves exhibiting strong level repulsion. However, deviations from the Wigner surmise can be seen in the distribution of spacings beyond nearest modes. A weakening in the rigidity of the modal spectrum is observed as the sample length increases because of reduced level repulsion for more strongly localized waves. In contrast to residual diffusive behavior for level spacing statistics, the distribution of level widths are log-normal as predicted for localized waves.

1The research was supported by the NSF under Grant No. DMR-0907285 and a PSC-CUNY grant.

4:30PM T53.00009 A Random Matrix Approach to Understanding Wave Statistics from Wireless Communications to Quantum Dots1, JEN-HAO YEH, EDWARD OTT, THOMAS ANTONSEN, STEVEN ANLAGE, University of Maryland — Complexity of a wave propagation environment is advantageous from the perspective of wave chaos theory because, in the semiclassical limit, the corresponding ray trajectories of the wave propagate chaotic dynamical behavior, and a statistical description is most appropriate. Random matrix theory (RMT) successfully describes universal properties of the system. We combine RMT with our random coupling model that includes non-universal effects, such as the radiation impedance of the ports and the effect of short ray trajectories in the system, and we establish a first-principles model for wave statistical properties such as the fading amplitude in wireless communications, the scattering matrix, the impedance matrix, and the thermopower of quantum dots. We also report experimental tests on two ray-chaotic microwave cavities with different degrees of loss. In the high loss regime the results demonstrate that our RMT model agrees with traditional fading models (Rayleigh fading and Rice fading) and provides a more general understanding of the models and a detailed physical basis for their parameters. Moreover, in the low loss regime the RMT approach describes the data better.

1This work is funded by the ONR/ Maryland AppEl Center Task A2 (contract No. N000140911190), the AFOSR under grant FA95500710049, and Center for Nanophysics and Advanced Materials (CNAM).

4:42PM T53.00010 Quantifying Volume Changing Perturbations to a Wave Chaotic System1, BIINYAM TADDESE, Department of Electrical & Computer Engineering, University of Maryland, College Park, MD 20742-3285, USA, GABRIELE GRADONI, Department of Physics, University of Maryland, College Park, MD 20742-4111, USA, FRANCO MOGLIE, Dip. di Ingegneria dell’Informazione, Università Politecnica delle Marche, Ancona, Italy, THOMAS ANTONSEN, EDWARD OTT, STEVEN ANLAGE, Department of Physics, University of Maryland, College Park, MD 20742-4111, USA — The Loschmidt Echo and Fidelity decay are used to measure perturbations on a quantum wave chaotic system. We extended these concepts to classical waves to detect perturbations. [1]. In this work, we show that volume changing perturbations to a classical wave chaotic cavity can be quantified with a sub-wavelength sensitivity. This is demonstrated both numerically and experimentally. A wave chaotic quasi-1D star graph model [2], was initially used to show the results. The quantification of electrical-volume changing perturbations to a one cubic meter aluminum box will be demonstrated experimentally; the experimental results are also supported by a finite difference time domain simulation of the box. Finally, the approach to quantify these perturbations will be shown to apply to a generic wave chaotic system by using a time domain version of our Random Coupling Model.

1Work funded by ONR MURI grant N000140710734, AFOSR grant FA95501010106, and the Maryland CNAM.

4:54PM T53.00011 Nonlinear Time-Reversal in a Wave Chaotic System1, MATTHEW CRAZIER, BIINYAM TADDESE, EDWARD OTT, THOMAS ANTONSEN, STEVEN ANLAGE, University of Maryland — Time reversal mirrors are particularly simple to implement in wave chaotic systems and form the basis for a new class of sensors [1-3]. These sensors work by applying the quantum mechanical concepts of Loschmidt echo and fidelity decay to classical waves. We use the method of time-reversal invariance and spatial reciprocity in a wave chaotic system to remotely measure the presence of small perturbations to the system. The underlying ray chaos increases the sensitivity to small perturbations throughout the volume explored by the waves. We extend our time-reversal mirror to include a discrete element with a non-linear dynamical response. The initially injected pulse interacts with the non-linear element, generating new frequency components originating at the element. By selectively filtering for and applying the time-reversal mirror to the new frequency components, we focus a pulse only onto the element, without knowledge of its location. Furthermore, we demonstrate transmission of arbitrary patterns of pulses to the element, creating a targeted communication channel to the exclusion of ‘eavesdroppers’ at other locations in the system. [1] Appl. Phys. Lett. 95, 114103 (2009) [2] J. Appl. Phys. 108, 1 (2010) [3] Acta Physica Polonica A 112, 569 (2007)

1Work funded by the Intelligence Community Postdoctoral Research Fellowship Program and the Center for Nanophysics and Advanced Materials.

5:06PM T53.00012 Low-Diffracting Modes in Surface Plasmon Metamaterials, SANDEEP INAMPUDI, Department of Physics and Applied Physics, University of Massachusetts Lowell, IGOR SMOLYONOV, Department of Electrical and Computer Engineering, University of Maryland, VIKTOR PODOLSKY, Department of Physics and Applied Physics, University of Massachusetts Lowell — Plasmonic structures, with periodic arrays of thin PMMA ridges on metal substrates have been shown experimentally to overcome the diffraction limit. Here we present a theoretical description of this phenomenon. We use microwave matching technique to analyze the dynamics of the electromagnetic waves in the periodic systems, taking into account the extended 3D geometry and the finite thickness of the PMMA ridges. Specifically, we focus on the behavior of plasmonic mode and its non-trivial coupling to the free space waves and to the other guided modes of the system. The eigen states of the periodic system dominated by the surface waves are identified and their dispersion is analyzed via generalization of mode-matching formalism and Bloch-periodic approach. An analytical approximation, adequately describing the behavior of the system is derived and is used to explain the suppression of diffraction in the system.
5:18PM T53.00013 Nonsymmetric Phononic Metamaterials: shaping waves over multiple length scales\textsuperscript{1}, CHEONGYANG KOH, DSO National Laboratories, S118230, Singapore, EDWIN THOMAS, School of Engineering, Rice University, P.O. Box 1892, Houston, Texas 77251, USA — The vector nature of the phonon makes rational design of phononic metamaterials challenging, despite potential in unique wave propagation behavior, such as negative refraction and hyper-lensing. While most designs to date focus on the “meta-atom” (building block) design, their “spatial arrangement” (non-locality) is equally instrumental in dispersion engineering. Here, we present a generalized design framework (DF) for PMM design, utilizing both “global” and “local” symmetry concepts. We demonstrate, utilizing specific properties of nonsymmetric plane groups, PMMs possessing i) a low-frequency in-plane complete spectral gap (ICSG) of 102% (CSG of 88%), ii) a set of polychromatic ICSGs totaling over 100% in normalized gap size. Within the same DF, we further integrate broken symmetry states (BSS) (edge states, waveguides, etc) with designed polarization, (de)localization and group velocities. In particular, we demonstrate how these BSS may be utilized to elucidate signatures of complex polarization fields through phonon-structure interactions, leading to interesting applications in elastic-wave imaging, as well as information retrieval by probing polarization states of scattering bodies over multiple scales.

\textsuperscript{1}We gratefully acknowledge funding from NSF, DSO-Singapore.

\textbf{Thursday, March 1, 2012 8:00AM - 11:00AM}  
\textit{Session V52 GSNP DFD: Focus Session: Extreme Mechanics - Biological Systems and Structures 153C}

8:00AM V52.00001 Micro-actuation through swelling and tissue engineering, NICHOLAS FANG, MIT — No abstract available.

8:36AM V52.00002 Plant tendrils: Nature’s hygroscopic springs, SHARON GERBODE, Harvey Mudd College, JOSHUA PUZEY, ANDREW MCCORMICK, L. MAHADEVAN, Harvard University — Plant tendrils are specialized climbing organs that have fascinated biologists and physicists alike for centuries. Initially straight tendrils attach to the tip of an elevated rigid support and then winch the plant upward by coiling into a helical morphology characterized by two helices of opposite handedness connected by a helical perversion. In his renowned treatise on twining and tendril-bearing plants, Charles Darwin surmised that coiled tendrils serve as soft, springy attachments for the climbing plant. Yet, the true effect of the perverted helical shape of a coiled plant tendril has not been fully revealed. Using a combination of experiments on Cucurbitaceae tendrils, physical models constructed from strained rubber sheets, and numerical models of helical perversions, we have uncovered that tendril coiling occurs via anisotropic shrinkage of a strip of specialized cells in the interior of the tendril. Furthermore, variations in the mechanical behavior of tendrils as they become drier and “woodier” adds a new twist to the story of tendril coiling.

8:48AM V52.00003 Radial force development during root growth measured by photoelasticity, EVELYNE KOLB, PMMH-UMR 7636 ESPCI, 10 rue Vauquelin, 75231 Paris Cedex 5, France; Université Pierre et Marie Curie - Paris 6, 75230 Paris cedex 05, France, CHRISTIAN HARTMANN, IRD-UMR 211 “BIOEMCO,” 46 rue d’Ulm, 75230 Paris cedex 05, France, PATRICIA GENET, CNRS-UMR 7618, 46 rue d’Ulm, 75230 Paris cedex 05, France; Université Paris Diderot - Paris 7, 75205 Paris cedex 13, France — The mechanical and topological properties of a soil like the global porosity and the distribution of void sizes greatly affect the development of a plant root, in which it is driven by shoot growth. In particular, plant roots growing in heterogeneous medium like sandy soils or cracked substrates have to adapt their morphology and exert radial forces depending on the pore size in which they penetrate. We propose a model experiment in which a pivot root (chick-pea seeds) of millimetric diameter has to grow in a size-controlled gap (\( \delta \)) ranging 0.5-2.3 mm between two photoelastic grains. By time-lapse imaging, we continuously monitored the root growth and the development of optical fringes in the photoelastic neighbouring grains when the root enters the gap. Thus we measured simultaneously and in situ the root morphological changes (length and diameter growth rates, circumnutation) as well as the radial forces the root exerts. Radial forces were increasing in relation with gap constriction and experiment duration but a levelling of the force was not observed, even after 5 days and for narrow gaps. The inferred mechanical stress was consistent with the turgor pressure of compressed cells. Therefore our set-up could be a basis for testing mechanical models of cellular growth.

9:00AM V52.00004 Digging Like Plants: Flexible Intruders in Granular Materials, DAWN WENDELL, KATHARINE LUGINBUHL, MIT; DIEGO SOLANO, Northeastern University, PEKO HOSOI, MIT — Inspired by plant root growth in granular media, we report on the effects of flexibility on the mechanical work required to dig through granular systems. In the case where the digger is significantly thinner than the grain diameter, increased flexibility in one-dimension leads to savings of nearly 50%. A simple numerical model based solely on the variability of forces in the granular substrate and the flexibility of the digger gives similar results to those observed in experiments.

9:12AM V52.00005 Helical Buckling of Plant Roots: Mechanics and Morphology, JESSE SILVERBERG, Department of Physics, Cornell University, ROSLYN NOAR, Department of Plant Pathology, North Carolina State University, MICHAEL PACKER, Department of Physics, Cornell University, MARIA HARRISON, Boyce Thompson Institute, Cornell University, CHRIS HENLEY, ITAI COHEN, Department of Physics, Cornell University, SHARON GERBODE, School of Engineering and Applied Sciences, Harvard University — How do plant roots respond to heterogeneities in their environment as they grow? Using a simple model system consisting of a layered hydrogel, we present a controlled mechanical barrier to the roots allowing us to perturb their growth. Interestingly, we find a localized helical root morphology that forms prior to the root passing through the gel layer interface. We interpret this geometry as a combination of a purely mechanical buckling caused by continued root elongation modified by the growth medium and an additional twisting near the root tip. We study the morphology of the helical deformation as the modulus of the gel is varied by continued root elongation modified by the growth medium and a simultaneous twisting near the root tip. We study the morphology of the helical buckling as the modulus of the gel is varied by using 3D time-lapse imaging and demonstrate that its shape scales with gel stiffness as expected by a simple model based on the theory of buckled rods. Our results demonstrate that mechanics is sufficient to account for the shape and its variations. In addition, we hypothesize that the twisted growth near the root tip arises from a touch-activated growth response that we call rhizomotorism.

9:24AM V52.00006 Dislocations and Grain Boundaries in Optimally-Packaged, Twisted Filament Bundles, AMIR AZADI, Department of Physics, University of Massachusetts, Amherst, GREGORY GRASON, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — From the collagen fiber to the parallel-actin bundle, twisted and rope-like assemblies of filamentous molecules are common and vital structural elements in cells and tissue of living organisms. We study the intrinsic frustration occurring in these materials between the two-dimensional organization of filaments in cross-section and out-of-plane filament twist in bundles based on the non-linear continuum elasticity theory of columnar materials. We find that interfilament twist generates in-plane stresses that couple favorably to the presence of topological defects, edge dislocations, in the cross-sectional packing, thereby restructuring the ground state filament packing of twisted bundles. The stability of dislocations increases with increases in both the degree of twist and lateral bundle size. We show that in ground states of large bundles, multiple dislocations pile up into linear arrays, radial grain boundaries, whose number and length grows with bundle twist. Remarkably, the “polycrystalline” texture of these optimal packings of twisted bundles show a striking similarity to models of the “almost crystalline” cross-section of collagen fibers.
Mechanical Behavior of Bio-inspired Model Suture Joints, YANING LI, Department of Mechanical Engineering, ERICA LIN, CHRISTINE ORTIZ, Department of Materials Science and Engineering, MARY BOYCE, Department of Mechanical Engineering, BOYCE GROUP/MIT COLLABORATION, ORTIZ GROUP/MIT COLLABORATION — Suture joints of varying degrees of geometric complexity are prevalent throughout nature as a means of joining structural elements while providing locally tailored mechanical performance. Here, micromechanical models of general trapezoidal waveforms of varying hierarchy are formulated to reveal the role of geometric complexity in governing stiffness, strength, toughness and corresponding deformation mechanisms and failure mechanisms. Physical consequences of the results are evident in the development of novel bio-inspired materials with topological defects [1]. [1] G. Vernizzi, R. Sknepnek, M. Olvera de la Cruz, Proc. Natl. Acad. Sci. USA 108, 4292 (2011).

Morphogenesis of protrusions from confined lipids vesicles, RASTKO SKNEPNEK, MONICA OLVERA DE LA CRUZ, Northwestern University — We use a discretized version of a thin elastic shell model to show that a two-component elastic vesicle can lower its energy by facing into a wide variety of polyhedral shapes. The elastic shell model allows us to completely remove effects of the topological defect and internal forces in order to focus on the competition between bending and stretching energies leading to facets. Present work extends our recent study of the faceting of a two-component shell in the presence of topological defects [1]. [1] G. Vernizzi, R. Sknepek, M. Olivera de la Cruz, Proc. Natl. Acad. Sci. USA 108, 4292 (2011).

10:24AM V52.00011 Denaturation of Circular DNA: Supercoils, overtwist and condensation1, ALKAN KABAKCIOGLU, Koc University, AMIR BAR, DAVID MUKAMEL, Weizmann Institute of Science — The statistical mechanics of DNA denaturation under fixed linking number is qualitatively different from that of the unconstrained DNA. Past work suggests that the nature of this constrained melting transition is sensitive to the mechanism that relaxes the torsional stress induced on the bound portions by the loops. Quantitatively different melting scenarios are reached from two alternative assumptions, namely, that the denatured loops are formed in expense of 1) overtwist, 2) supercoils. Recent work has shown that the supercoiling mechanism results in a BEC-like picture where a macroscopic loop appears at $T_c$, and grows steadily with temperature while no such phenomenon has been reported for the overtwisting case. By extending an earlier result, we show here that a macroscopic loop appears in the overwisting scenario as well. We calculate its size as a function of temperature and show that the fraction of the total sum of microscopic loops decreases above $T_c$, with a cusp at the critical point.

1Supported by TUBITAK through the grant TBAG-11OT618

10:36AM V52.00012 Mechanics of short rod-like molecules in tension, PRASHANT PUROHIT, University of Pennsylvania — Rod like macromolecules such as actin, DNA etc., are most commonly stretched using optical tweezers or fluid flow. In this presentation we will describe the mechanics of short rod like molecules in tension. The mechanics is dominated by the competition between tensile forces (exerted by fluid flow, or by a device, such as, optical tweezers) and the thermal fluctuations of the molecule. For molecules whose contour length is comparable to the persistence length we show that the boundary conditions play major role in determining the mechanical behavior. We use the equipartition theorem of statistical mechanics to obtain expressions for the amplitude of the transverse fluctuations of the molecule and its force-extension relation for various boundary conditions. We then apply our theory to an experiment on short fluctuating actin filaments trapped by a function of position along the filament.

10:48AM V52.00013 Turning by buckling: a cheap evolutionary strategy for turning among marine bacteria, KWANGMIN SON, JEFFREY GUASTO, ROMAN STOCKER, MIT — Marine bacteria have long been known to swim forward and backward (‘run and reverse’) by controlling the rotational direction of a 20 nm helical flagellum. Recent detailed observations have shown that these bacteria can also make sharp, ~90° turns, an astounding feat for a micro-scale organism with just one degree of freedom under its control. We demonstrate that a buckling instability originating from the flexible linkage (‘hook’) between the body and the flagellum is responsible for the reorientation. Using high-magnification (400×100X) observations based on high-speed video microscopy (420×1000 fps), we captured the extreme deformation of the flagellum and the hook involved in the process of turning. Our results reveal that the mechanical properties of the bacterial flagellum, including its flexibility and the amount of hydrodynamic load imposed by the cell, the hook becomes the primary force in generating changes in the bacterial swimming, only when the compressive load during the onset of forward swimming exceeds the threshold for Euler buckling. Combining the data with a model of buckling of thin structures, we show that bacteria take advantage of the flexibility of the flagellum and the hook to generate a turn, which may represent the evolutionarily cheapest bacterial strategy to actively change direction.
When poured into a container, cohesive granular materials form low-density, open granular aggregates. If put under compression, these aggregates densify by particle rearrangement. We seek experimental evidence that particle rearrangement occurs in the form of a phase transition between two configurational phases of the aggregate (G. Gioia, A. M. Cuitiño, S. Zheng, and T. Uribe, PRL 88, 204302, 2002). We use a simple model to show that when an open granular aggregate with two configurational phases is penetrated by a punch that lacks a characteristic length scale, the functional relation between the punching force and the penetration of the punch depends solely on the dimensionality of the punch: for a two-dimensional, wedge-shaped punch the force–penetration curve is linear whereas for a three-dimensional, conical punch the force–penetration curve is quadratic. To test these predictions we carry out experiments with open granular aggregates of a fine powder. The experimental measurements are in accord with the theoretical predictions.

ALEXEI PERELET, TAPAN SABUWALA, GUSTAVO GIOIA, Department of Mechanical Science and Engineering - University of Illinois, Urbana-Champaign — When poured into a container, cohesive granular materials form low-density, open granular aggregates. If put under compression, these aggregates densify by particle rearrangement. We seek experimental evidence that particle rearrangement occurs in the form of a phase transition between two configurational phases of the aggregate (G. Gioia, A. M. Cuitiño, S. Zheng, and T. Uribe, PRL 88, 204302, 2002). We use a simple model to show that when an open granular aggregate with two configurational phases is penetrated by a punch that lacks a characteristic length scale, the functional relation between the punching force and the penetration of the punch depends solely on the dimensionality of the punch: for a two-dimensional, wedge-shaped punch the force–penetration curve is linear whereas for a three-dimensional, conical punch the force–penetration curve is quadratic. To test these predictions we carry out experiments with open granular aggregates of a fine powder. The experimental measurements are in accord with the theoretical predictions.
9:24AM V53.00008 Discrete Particle Dynamics Simulations of Adhesive Systems with Thermostatting

FLINT PIERCE, JEREMY LECHMAN, JOHN HEWSON, Sandia National Laboratories — Aggregation/coagulation/flocculation processes are ubiquitous in modern industry from fields as diverse as waste water treatment, the food industry, algae biofuel production, and materials processing where control of the size and morphology of aggregates is paramount to the application of interest. Population balance models have historically been used with success in predicting aggregation kinetics and size distributions for these processes. However, even the most robust population balance schemes can lack an exact description of the underlying physical processes governing attractive or adhesive particulate matter suspended in a background medium, including finite aggregate structured systems that are subject to hydrodynamic forces (1). Our approach is to develop and use a JKR type model for simulating adhesive particulate matter in a background medium varying from dilute gas to liquid. We evaluate the time and length scales for restructuring/fragmentation that result from this model as a function of aggregate size and fractal dimension. We additionally introduce a method for pairwise thermostating of the adhesive potential and discuss the applicability of this model to various adhesive systems. 

1Supported by LDRD program at Sandia National Laboratories.

9:36AM V53.00009 Normal Mode Spectrum of Finite Sized Granular Systems: The Effects of Fluid Viscosity at the Grain Contacts

JOHN VALENZA, DAVID JOHNSON, Schlumberger-Doll Research — We investigate the effects of adsorbed films on the attenuative properties of loose granular media occupying a finite sized rigid container, which is open on the top. We measure the effective mass, \( M(\omega) \), of loose tungsten particles prepared under two different sets of conditions: 1) We lightly coat tungsten grains with a fixed volume fraction of silicone oil (PDMS), where the liquid viscosity is varied for individual realizations. 2) In the other set of experiments we vary the humidity. On a theoretical level we are able to decompose the effective mass into a sum over the contributions from each of the normal modes of the granular medium. Our results indicate that increasing either the PDMS viscosity or the humidity, as the case may be, does markedly increase the damping rate of each normal mode relevant to our measurements. However, there is appreciable damping even in the absence of any macroscopic film. With a notable exception in the case of the highest humidity in the humidity controlled experiments, all the relevant modes are weakly damped in the sense of a microscopic theory based on damped contact forces between rigid particles.

9:48AM V53.00010 Influence of liquid bridges on the macroscopic properties of granular assemblies

GEOFFROY LUMAY, University of Liege, JORGE FISCINA, Universitat de Sarlandes, FRANCOIS LUDWIG, NICOLAOS VANDEWALLE, University of Liege — We present the results of two experimental studies concerning the compaction dynamics of cohesive granular materials. In the first study, we focus on the effects of liquid bridges on the compaction behaviour of sands and sands mixed with liquids. The second study concerns initially dry granular materials surrounded by a well controlled air humidity. Then, the cohesion inside the packing is controlled through the relative humidity which influence both triboelectric and capillary effects. For both cases, the evolution of the parameters extracted from the compaction curves (the compaction characteristic time \( \tau \), the initial and final packing fractions) have been analyzed as a function of the cohesiveness. A model, based on free volume kinetic equations and the presence of a capillary energy barrier, is able to reproduce quantitatively the experimental results (Phys. Rev. Lett. 105, 048001 (2010)).

10:00AM V53.00011 Wetting and packing effects on evaporation out of a porous medium

CESARE MIKHAIL CEJAS, BERTRAND SELVA, RAPHAEL BEAUFRET, LARRY HOUGH, CNRS UMI 3254 Complex Assemblies of Soft Matter COMPASS, CHRISTIAN FRETTIGNY, CNRS UMR7615 Physico-chimie des Polymères et des Milieux Dispersés (PPMD) - ESPCI Paris, REMI DREYFUS, CNRS UMI 3254 Complex Assemblies of Soft Matter COMPASS, COMPASS TEAM — Evaporation through granular media involves complex fluid transport and exhibits two regimes: (1) a capillary-supported regime maintaining hydraulic continuity to the surface and vapor exchange with the atmosphere followed by (2) a diffusion-limited regime through the medium. A well-defined intermediate partially saturated zone (PSZ) has already been observed in the past. It is evidently seen from our experimental investigations using a 2D model soil of glass beads. The PSZ is the region identified above the interface formed by the drying front, which separates the PSZ from the fully-saturated wet region. This intermediate zone is filled with a dynamic mixture of vapor and liquid. The existence of this zone is of significant importance as it sets the kinetics of the evaporation process. Here we will present how wetting and packing effects influence the size of this partially saturated zone and we will show how a simple model based on geometrical considerations can explain our observations.

10:12AM V53.00012 A coupled deformation-diffusion theory for fluid-saturated porous solids

DAVID HENANN, KEN KAMRIN, LALLIT ANAND, Department of Mechanical Engineering, MIT — Fluid-saturated porous materials are important in several familiar applications, such as the response of soils in geomechanics, food processing, pharmaceuticals, and the biomechanics of living bone tissue. An appropriate constitutive theory describing the coupling of the mechanical behavior of the porous solid with the transport of the fluid is a crucial ingredient towards understanding the behavior of these systems in practical contexts. We present a large-deformation theory for coupled deformation-diffusion in isotropic, fluid-saturated porous solids. The theory synthesizes the classical Biot theory of linear poroelasticity and the more-recent Coussy theory of poroplasticity in a large deformation framework. In this talk, we highlight several salient features of our theory and discuss representative examples of the application of our numerical simulation capability to problems of consolidation as well as deformation localization in granular materials.

10:24AM V53.00013 Water Retention of Sandy Soil with Hydrogel Particle Additives under Steady Rain

YULI WEI, 1. Department of Physics and Astronomy, University of Pennsylvania ; 2. Complex Assemblies of Soft Matter, CNRS-Rhodia-Upenn UMI 3254, DOUGLAS DURIAN, Department of Physics and Astronomy, University of Pennsylvania — We probe the water retention behavior of a dry model sandy soil with hydrogel particle additives under a steady rain using a self-built raindrop impingement set-up. The 0.4mm dry hydrogel particles are sent into a dry model sandy soil, 1mm glass beads, in different methods and a steady rain is created to irrigate the soil packing. The mass of the retained water in the packing is measured as a function of rain time. The influences of packing height, gel concentration, and gel location are examined respectively. For the model sandy soil alone, the packing height has little effect on the results. Rain water wets a shallow top region and flows out through a narrow path in the packing. With hydrogel particles uniformly mixed into the top region of a model sandy soil packing, the retained water increases as the gel number ratio increases or when the hydrogel particles are concentrated into the wet top region. A better way is to place hydrogel particles in a layer at certain depths under the packing. With hydrogel particles uniformly mixed into the top region of a model sandy soil packing, the retained water increases as the gel number ratio increases or when the hydrogel particles are concentrated into the wet top region. A better way is to place hydrogel particles in a layer at certain depths under the packing. With hydrogel particles uniformly mixed into the top region of a model sandy soil packing, the retained water increases as the gel number ratio increases or when the hydrogel particles are concentrated into the wet top region. A better way is to place hydrogel particles in a layer at certain depths under the packing.

10:36AM V53.00014 Period tripling causes rotating spirals in agitated wet granular matter

KAI HUANG, INGO REHBERG, Experimentalphysik V, Universitaet Bayreuth, 95440 Bayreuth, Germany — Pattern formation of a thin layer of vertically agitated granular wet granular matter is investigated experimentally. Due to the strong cohesion arising from the capillary bridges formed between adjacent particles, agitated wet granular matter exhibits a different scenario as its dry counterpart. Rotating spirals with three arms, which correspond to the kinks between regions with different colliding phases, are the dominating pattern. This preferred number of arms corresponds to period tripling of the agitated granular layer, unlike predominantly subharmonic Faraday crispations in dry granular matter. The chirality of the spatiotemporal pattern corresponds to the rotation direction of the spirals. Understanding this well traceable instability could pave a way for testifying elaborate theories on dense flow of wet granular matter.

Supported by LDRD program at Sandia National Laboratories.
Within seconds, a spectacular roll-up motion follows. We explain the observed shapes and curling dynamics. Contact with the liquid surface, water diffuses into the hygroscopic material from below and induces differential swelling, resulting in the curling of the paper.

We controlled the fluid flow rate by coupling the elastic deformation of the arch to the gap within the microchannel, and matched these experimental results with perturbation of lubrication theory and computational simulations. These results illustrate an experimental design paradigm for the preparation of portable microchannels for chemical mixing, self-healing, and in situ diagnostics.

A flexible arch prepared by buckling a thin elastic film. The deflection of the arch can be predicted and controlled using the classical theory of Euler buckling.

Motion of a rigid sphere through an elastic tube. The transport of soft objects through small rigid channels is a common problem in the biological world: red blood cells are deformed when passing through small capillaries and polymer coils can make their way through minute pores. We study the opposite model problem of a rigid sphere moving in a narrower elastic tube. Geometry, mechanical properties of the tube and friction or lubrication conditions determine the dynamics of the entrapped sphere. We present experimental results on this problem, together with scaling law analysis.

We report experimental work on capillary rise of a liquid in a cell formed by parallel plates, one of which is flexible. We show that above a critical width, the cell collapses under the negative capillary pressure in the liquid. This collapse allows the liquid to rise virtually without limit between the plates. The height of the rising front is found to increase with time as $t^{1/3}$, a characteristic of capillary imbibition in a wedge.

As many soft materials, paper is mechanically sensitive to humidity. Owing to its hygroscopic cellulose-based structure, it is known to wrinkle when subject to humidity fluctuations. Here, we present experimental results on the more extreme deformations observed when a sheet of tracing paper is put on a bath of water. After contact with the liquid surface, water diffuses into the hygroscopic material from below and induces differential swelling, resulting in the curling of the paper. Within seconds, a spectacular roll-up motion follows. We explain the observed shapes and curling dynamics.

This work is supported by ANR grant ANR-09-JCJC-0022-01 and “La Ville de Paris - Programme Emergence.”

1:03PM W52.00010 Mechanic instabilities of swelling gels , MARTINE BEN AMAR, JULIEN DERVAUX, Ecole Normale Supérieure — While the study of gels takes undoubtedly its roots within the field of physico-chemistry, the interest for gels has flourished and they progressively became an important object in the study of the mechanics of polymeric materials and volumetric growth, rising some fascinating problems, some of them remaining unsolved. Because gels are multiphase objects, their study represents an important step in the understanding of the mechanics of complex soft matter as well as for the process of shape generation in biological bodies. I will present here experiments and models of swelling gels mainly in the cylindrical geometry which mimic various growth instabilities from tumors up to the morphogenesis of tubular organs.

1:15PM W52.00011 Patterns formed by swelling-induced folding of films1 , SACHIN VELANKAR, VICTORIA LAI, University of Pittsburgh, RICHARD VAIA, Wright Patterson Air Force Base — The solvent swelling of a thin polymer film attached to a rigid substrate is known to induce a creasing pattern on the free surface of the film. Here we show that if the film is weakly attached to the substrate, the swelling-induced compressive stress nucleates buckle delamination of the film from the substrate. Surprisingly, the buckles do not have a sinuosoidal profile, instead, the film near the delamination buckles slides towards the buckles causing growth of sharp folds of high aspect ratio. The folds persist even after the solvent evaporates. Such fold formation depends on the size of the region of the film exposed to solvent. A very small region of exposure (realized by placing a small drop of solvent on the film) does not induce delamination. Remarkably, with moderate sized drops, the delamination and folding occurs around the perimeter of the drop, thus culminating in a corral with tall walls. We quantify the parameters (drop volume, film thickness) which demarcate the transitions between no fold formation, corral formation, and multiple fold formation.

1 Funding support from AFOSR Grant number FA9550-10-1-0329 is acknowledged.

1:27PM W52.00012 Swelling-Driven Shaping of Thermally Responsive Photo-Patterned Gel Sheets , MYUNGHWAN BYUN, JUNWOO KIM, RYAN HAYWARD, Polymer Science and Engineering Department, University of Massachusetts Amherst; JAMES HANNA, CHRISTIAN SANTANGELO, Physics Department, University of Massachusetts Amherst — Swelling-mediated shaping of patterned non-Euclidean plates offers a powerful route to design and engineer complex 3-D structures, with possible applications in biomedicine, robotics, and tunable micro-optics. We have studied the behavior of poly(N-isopropyl acrylamide) (PNIPAm) copolymers containing pendant benzophenone units that allow the degree of crosslinking to be tuned by varying the dosage of ultraviolet light. A halftone (gray) gel lithography approach, wherein two photomasks enable patterning of highly-crosslinked domains within a lightly-crosslinked matrix, is shown to provide effectively continuous variations in swelling in truly two-dimensional patterns. We show how this technique can be harnessed to form complex, reversibly actuating, 3-D structures through patterned growth.

1:39PM W52.00013 Dynamical Actuation and Pattern Formation with Local Swelling in Microgels1 , HOWON LEE, KIN HUNG FUNG, NICHOLAS FANG, MIT — In this invited talk, we present a set of study on swelling-induced actuation and pattern formation in hydrogels of three dimensional microstructures. For example, rapid actuation of a micro hydrogel device is observed by exploiting swelling-induced snap-buckling. Utilizing its fast actuation speed, the device can even jump by itself upon wetting. It is demonstrated that elastic energy is effectively stored and quickly released from the device by incorporating elastic instability. In our experiment, the micro device could generate a snapping motion within 12 milliseconds, releasing power at a rate of 34 mW/g. We also captured the evolution circumferential buckling of tubular shaped microgels. Inhomogeneous stress develops as gel swells under mechanical constraints, which gives rise to buckling instability. A simple analytical model is developed using elastic energy to predict stability and post-buckling patterns upon swelling. Our experiment demonstrates that circumferential buckling of desired mode can be created in a prescribed manner. Our study on the mechanics of three-dimensionally microstructured gels might provide new insights for in morphogenesis in tissue engineering, and provide new gateways in many emerging fields such as soft robotics and tunable metamaterials.

1 partially supported by NSF and LLNL LDRD

1:51PM W52.00014 Separating Viscoelasticity and Poroelasticity of Gels with Different Length and Time Scales , ANIRUDDH MOHAN, XUANHE ZHAO, Soft Active Materials Laboratory, Duke University, SOFT ACTIVE MATERIALS LABORATORY, DUKE UNIVERSITY TEAM — Viscoelasticity and poroelasticity commonly coexist in polymer gels. We propose a method capable of separating the viscoelasticity and poroelasticity of gels in various mechanical tests. The viscoelastic characteristic times and the poroelastic diffusivities of a gel can define intrinsic material length scales of the gel. The experimental setup can give sample length scales, over which the solvent migrates in the gel. By setting the sample lengths to be much larger or smaller than the material lengths, the viscoelasticity and poroelasticity of the gel will manifest at different time scales in a test. Therefore, the viscoelastic and poroelastic properties of the gel can be probed separately at different time scales of the test.

2:03PM W52.00015 A constitutive theory for visco-hyperelastic gels , SHAWN CHESTER, Lawrence Livermore National Laboratory — Many gels operate in chemically saturated environments in a variety of applications. Most constitutive theories for gels are formulated using large deformation hyperelasticity coupled with fluid transport. However, in most cases the mechanical response of such gels show hysteresis and other dissipative effects which are not accounted for in present constitutive theories. We have recently developed a three dimensional continuum level theory to describe the coupled fluid permeation and large deformation response of visco-hyperelastic materials. In this work, we apply our theory and numerical simulation capability to study the indentation response among others of visco-hyperelastic gels.
viscous flow and elastic deformation via a critical creep regime. We give scaling arguments for the critical exponents and confirm our predictions with numerics.

... or absence of floppy motions in the long time limit. We show that nearly isostatic networks display dynamical critical scaling, and that this scaling connects universality on the macroscopic level of rheological observables as well as on the microscopic level of single particle trajectories and collective particle motion.

We analyse the dependence of the shear bands on system size, shear rate and restructuring time. Further we rationalise the scenario within a mean field version of the model, that explains the instability of the homogeneous flow below a critical shear rate. Our study therefore strongly supports the idea that the characteristic time scales involved in the local dynamics are at the physical origin of permanent shear bands.

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... current predictions to be the dominant mechanism determining particle distribution in suspension flows, and this work lends support to that idea.
We acknowledge support by the Spanish Ministry of Science and Innovation (MICINN) through project “Ramón y Cajal” and by MICINN and Comunidad de Madrid through project “I3.”
2:03PM W53.00013 Jamming and Unjamming of the Rigid Amorphous Fraction. PEGGY CEBE, QIAN MA, Tufts University, GEORGII GEORGIEV, Assumption College — Semicrystalline polymers obey a three-phase model comprising crystalline, mobile amorphous (MAF), and rigid amorphous fractions (RAF) as an interphase. Using quasi-isothermal temperature modulated differential scanning calorimetry (QI-TMDC), we investigate the formation behavior of these fractions in poly(trimethylene terephthalate). PTT. PTT was quasi-isothermally cooled step-wise from the melt which causes its crystalline fraction to be fixed below 451K, and RAF is determined as a function of temperature. For PTT, most of the RAF vitrifies between 451K and Tg step-by-step during QI cooling. With lamellar crystals acting as topological constrains, a model is proposed in which the vitrification and devitrification of RAF are interpreted using the concepts of “jamming” and “unjamming.” Constraints of the crystal surfaces reduce the mobility of the highly entangled polymer chains attached to the lamellae, and the layers which constitute RAF are formed one after another in the manner of successive jamming. In this way, several features of the RAF temperature dependence are explained for the first time, with implications in other research areas, such as topological constraints exerted on the polymer melt through effects of inclusions in polymer-based nanocomposites.

For support of this research, the authors thank the NSF, Polymers Program of the Division of Materials Research through DMR-0602473, and the MRI Program under DMR-0520655 for thermal analysis instrumentation. A portion of this work was conducted at the BNL, National Synchrotron Light Source, supported by the DoE. G. Georgiev thanks Assumption College for continuous research support.

Thursday, March 1, 2012 2:30PM - 5:18PM — Session X52 GSIP DFD: Focus Session: Extreme Mechanics - Fracture, Friction, and Frequencies 193C

2:30PM X52.00001 Geometry of Tearing: crack propagation in brittle sheets1. BENITO ROMAN, JOSE BICO, PMMH CNRS/ESPCI/UPMC/Paris7 - Paris France, ENRIQUE CERDA, EUGENIO HAMM, FRANCISCO MELO, VICTOR ROMERO, Departamento de Fisica, Universidad de Santiago de Chile — We experiment the fracture of thin object everyday when trying to open a packaging. From a physics point of view, the propagation of cracks in thin brittle elastic sheets appears to be remarkably reproducible, with very regular crack path. We will present some examples where the crack path can be predicted using classical arguments in fracture and geometrical tools: this is another example where geometry plays a central role in the mechanics of thin sheets.

1We thank ANR MecaWet

2:42PM X52.00002 Spiral and croissant crack in drying thin films. JOEL MARTHELOT, BENITO ROMAN, JOSE BICO, PMMH ESPCI ParisTech, ETIENNE BARTHEL, JEREMIE TEISSEIRE, DAVY DALMAS, SVI CNRS Saint Gobain, FRANCISCO MELO. USACH — Drying mud or crazing in ceramics glaze leads to familiar hierarchical cracks network where a new crack connects perpendicularly to older ones. We report unusual spirals and croissant cracks patterns in methysiloxane drying thin films moderately adhering on a substrate. Such cracks are also observed in a very different situation when magnetron sputtering multilayers are under external tension. The amplitude and wavelength of the pattern are robusts and are orders of magnitude larger than the thickness of the layer. The propagation of the spiral and croissant cracks occurs in a narrow range of adhesion energy between the film and the substrate and strain in the film. We will show how the propagation is driven by a cooperation between fracture and adhesion.

2:54PM X52.00003 Rupture of a highly stretchable acrylic dielectric elastomer. GEORGE PHARR, Harvard University, JEONG-YUN SUN, Seoul National University and Harvard University, ZHIGANG SUO, Harvard University — Dielectric elastomers have found widespread application as energy harvesters, actuators, and sensors. In practice these elastomers are subject to large tensile stretches, which potentially can lead to mechanical fracture. In this study, we have examined fracture properties of the commercial acrylic elastomer VHB 4905. We have found that inserting a pre-cut into the material drastically reduces the stretch at rupture from $\lambda_{rup} = 9.43 \pm 1.05$ for pristine samples down to only $\lambda_{rup} = 3.63 \pm 0.45$ for the samples with a pre-cut. Furthermore, using “pure-shear” test specimens with a pre-crack, we have measured the fracture energy and stretch at rupture as a function of the sample geometry. The stretch at rupture was found to decrease with sample height, which agrees with an analytical prediction. Additionally, we have measured the fracture energy as a function of stretch-rate. The apparent fracture energy was found to increase with stretch-rate from $E = 1500$ J/m$^2$ to $E = 5000$ J/m$^2$ for the investigated rates of deformation. This phenomenon is due to viscoelastic properties of VHB 4905, which result in an apparent stiffening for sufficiently large stretch-rates.

3:06PM X52.00004 How does adhesion impact the formation of telephone cord buckles? ETIENNE BARTHEL, JEAN-YVON FAOU, SERGEY GRACHEV, CNRS / Saint-Gobain, GUILLAUME PARRY, SIMAP — Compressively stressed thin films with low adhesion frequently buckle into telephone cords. Although telephone cord buckles have been studied for decades, no complete understanding of their origin and propagation has so far been presented. Here, using Finite Element Analysis, we have coupled non-linear plate deformation with a cohesive zone model to simulate the kinematics of a propagating telephone cord buckle. On the experimental side, we have developed model thin films with a precise adjustment of both adhesion and residual stresses. From the comparison of the simulations with some experimental observations, we propose a generic mechanism for the formation of telephone cord buckles. Proper inclusion of the dependence of interfacial toughness upon mode mixity proved to be central to the success of the approach so that this clarification of the mechanism of telephone cord formation promises better understanding of interfacial toughness through the analysis of buckle morphology.

3:18PM X52.00005 Nonlinear modal interactions in a microcantilever1. HIDDE WESTRA, HERRE VAN DER ZANT, WARNER VENSTRA, Kavli Institute of Nanoscience, Delft University of Technology — We study the nonlinear interactions between vibrational modes in a microcantilever. The flexural-flexural, torsional-torsional and torsional-flexural modal interactions are investigated theoretically and experimentally. In a cantilever, the nonlinearity arising from geometrical and inertial effects couples the different modes. The motion of one mode influences the resonance frequency of the other modes. We show that depending on the amplitude of one mode, both frequency stiffening and weakening of the other mode occurs. The modal interactions in clamped-clamped beam resonators is recently studied, and several applications have been proposed. Microcantilevers are frequently used in instrumentation, and the modal interactions presented here enable such schemes, including Q-factor tuning and self-detection.

1The authors acknowledge financial support from the Dutch funding organization FOM (Physics for Technology)
3:30PM X52.00006 Effects of Roughness of Predecessors on Precursors to Frictional Sliding. MARK O. ROBBINS, K. MICHAEL SALERNO, Johns Hopkins University. Experiments show that when a PMMA block on a surface is normally loaded and driven by an external shear force, contact at the interface is modified in discrete precursor slips prior to steady state sliding. Our simulations use an atomistic model of a rough two-dimensional block in contact with a flat surface to investigate the evolution of stress and displacement along the contact surfaces. The talk will show how local and global stress conditions govern the initiation of interfacial cracks as well as the spatial extension of the cracked region. Inertia also plays an important role in determining the distribution of stresses at the interface. Finally, the geometry of surface asperities also influences the interfacial evolution and the total friction force. The relationship between the interfacial stress state and rupture velocity will also be discussed. [1] S.M. Rubinstein, G. Cohen and J. Fineberg, PRL 98, 226103 (2007)

3:42PM X52.00007 Novel method for simulation of structural post buckling. RACHMADIAN WULANDANA, Dept. of Mechanical Engineering and Materials Science, University of Pittsburgh, Pittsburgh, PA; SACHIN VELANKAR, Dept. of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA — A new FEM-based method for simulating the onset of buckling instabilities and the post-buckling evolution is developed. The method consists of creating a random spatial perturbation of the elastic modulus and applying a step-by-step loading to approach the critical state and beyond. Prior to buckling, the non-uniform modulus triggers micro bending and lateral deformation. As the compressive load grows, the micro displacement grows non-linearly causing the system to be biased toward the mode that minimizes energy. The system buckles in that mode and the post-buckling deformation can be examined. The technique has been applied to several buckling cases. The results show quantitative agreement with theory and experiments. For problems with continuously-distributed buckling modes and critical values that are close from one to another, the method is able to automatically select the correct critical configuration. Unlike other perturbation methods that are inspired by either Eigen vectors or experimental data, the current method does not need a priori knowledge of the expected buckling mode. This is especially useful in complex problems (e.g. wrinkling of stretched films) for which linear eigenvalue analysis cannot predict the critical conditions.

3:54PM X52.00008 Sliding on a Nanotube: Interplay of Friction, Deformations and Defects. HSIANG-CHIH CHIU, SUENNE KIM, School of Physics, Georgia Institute of Technology; ERIO TOSATTI, International School for Advanced Studies (SISSA), and CNR-ION Democritos, CHRISTIAN KLINKE, Institute of Physical Chemistry, University of Hamburg; ELISA RIEDO, School of Physics, Georgia Institute of Technology — Carbon nanotubes (CNT) have applications as composite material reinforcements and components in nanodevices due to their exceptional physical properties. However, CNTs have structural defects that can change their mechanical properties. For applications, CNTs have to be in contact with other surfaces, thus it is important to understand how defects change their frictional properties. Here, we show that defects can impact the frictional properties of supported Arc Discharge (AD) and Chemical Vapor Deposition (CVD) grown CNTs by sliding an AFM tip along (longitudinal) and across (transverse) the CNT axis. Larger friction coefficient is found during transverse sliding due to a lateral CNT deformation (called hindered rolling) that causes extra friction dissipation which is absent during longitudinal sliding. A friction anisotropy, defined as the ratio of shear strength measured during both sliding directions, can be as high as 13.7 for AD CNTs but less than 6 for CVD CNTs. Extra defects in CVD CNTs couple both sliding motions, resulting in more energy dissipation and higher longitudinal friction. A simple analytical model is developed to explain the observed experimental behavior. Our finding provides a better understanding of tribological properties of individual CNT at the nanoscale. [1] M. Lucas et al., Nature Mater. 8, 876 (2009)

4:06PM X52.00009 Graphene Morphology on Nano-Patterned Electronic Substrates. GUANGXU LI, CIHAN YILMAZ, XIAOHONG AN, SIVASUBRAMANIAN SOMU, SWASTIK KAR, AHMED BUSNAINA, KAI-TAK WAN, Northeastern University, DEPARTMENT OF MECHANICAL AND INDUSTRIAL ENGINEERING COLLABORATION, DEPARTMENT OF PHYSICS COLLABORATION — In order to get high quality of graphene for the application in electronic devices, good transfer of graphene by mechanical exfoliation or chemical vapor deposition is always required and substrate with flat surface is preferred to avoid the crack and destruction of the thin sheets. Here, we studied the graphene morphology on nano-patterned electronic substrates by transferring graphene grown from chemical vapor deposition onto the gold nano pillar patterns on silicon substrate. The adhesion between the graphene and the gold surface makes the flexible thin membrane conform to the substrate geometry and form a series of blisters. By measuring the blister radius and height, the adhesion energy of graphene and gold substrate can be deduced. In the meantime, the morphology of graphene on the pillar patterns was found to strongly relate to the adhesion energy, the height and separation of pillars. By changing these parameters, the blisters may decrease size or expand to coalesce. The critical separation between pillars and the critical height of pillars were predicted to avoid the coalescence of the blisters when the adhesion energy was fixed. The results obtained here can be useful to increase the performance and the durability of the graphene based device.

4:18PM X52.00010 Graphene Blister Adhesion Mechanics. NARASIMHA BODETTI, STEVEN KOENIG, JIAN-LIANG XIAO, SCOTT BUNCH, MARTIN DÜNN, University of Colorado — We describe graphene blister configurations to study the elasticity of mono- and multi-layer graphene as well as the adhesion of the blister to an SiO2 substrate. We create blisters by depositing graphene on a chip containing etched cavities of a prescribed volume. The chip is placed in a high-pressure chamber where the cavities are charged to a prescribed pressure. When the chip is removed from the chamber the pressure difference across the membrane causes it to bulge, while the number of gas molecules in the chamber remains constant. As the pressure is increased the membrane continues to bulge and at a critical pressure can delaminate (in a stable or unstable manner) permitting extraction of the adhesion energy from a combination of theory and measurements of the deformed blister configuration. We describe these experiments and develop a thermodynamic model of the system that identifies interesting nonlinear effects as the membranes deform including instabilities, delamination, and adhesion hysteresis, depending on the configurational parameters. We use the theory and experiments together to determine for the first time the adhesion energy between graphene and SiO2, as well as explore the interesting mechanics that occur.

4:30PM X52.00011 Novel method for simulation of structural post buckling. RACHMADIAN WULANDANA, Dept. of Mechanical Engineering and Materials Science, University of Pittsburgh, Pittsburgh, PA; SACHIN VELANKAR, Dept. of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA. A new FEM-based method for simulating the onset of buckling instabilities and the post-buckling evolution is developed. The method consists of creating a random spatial perturbation of the elastic modulus and applying a step-by-step loading to approach the critical state and beyond. Prior to buckling, the non-uniform modulus triggers micro bending and lateral deformation. As the compressive load grows, the micro displacement grows non-linearly causing the system to be biased toward the mode that minimizes energy. The system buckles in that mode and the post-buckling deformation can be examined. The technique has been applied to several buckling cases. The results show quantitative agreement with theory and experiments. For problems with continuously-distributed buckling modes and critical values that are close from one to another, the method is able to automatically select the correct critical configuration. Unlike other perturbation methods that are inspired by either Eigen vectors or experimental data, the current method does not need a priori knowledge of the expected buckling mode. This is especially useful in complex problems (e.g. wrinkling of stretched films) for which linear eigenvalue analysis cannot predict the critical conditions.
4:42PM X52.00012 Buckling morphologies of crystalline shells with frozen defects, EE HOU YONG, Harvard University, PROF L. MAHADEVAN (HARVARD UNI.) COLLABORATION — The crumpling of spherical crystalline lattices where the topological defects are frozen is studied. The geometry of the crumpled membrane is found to depend on the set of topological defects and more exotic defect sets can result in crumpled shapes resembling that of the Platonic and Archimedean solids. The phase diagram of spherical crystalline lattices where the topological defects are frozen is studied. The geometry of the crumpled membrane is found to depend on the set of topological defects and more exotic defect sets can result in crumpled shapes resembling that of the Platonic and Archimedean solids. The phase diagram...
Disks Approaching the Athermal Jamming Transition

We compare our predictions for the effect of different elastic and geometric ingredients and a power balance that depends on the local viscous law, we predict that the global rheology of disordered media depends.

We generalize our scaling model for the rheology of soft, frictionless repulsive spheres to include general Pennsylvania, MARTIN VAN HECKE, Universiteit Leiden — We generalize our scaling model for the rheology of soft, frictionless repulsive spheres to include general

BRIAN TIGHE, Universiteit Leiden, KERSTIN NORDSTROM, DOUG DURIAN, Haverford College, JERRY GOLLUB, Haverford College, University of Pennsylvania.

Concentrated suspensions of particles are commonly used in the pharmaceutical, cosmetic and food industries. Manufacture of these products often involves flow geometries that are substantially different from those studied by conventional shear rheology. Using a capillary break-up extensional rheometer we stretch fluids of different volume fraction at strain rates just below, at and above the critical rate required to induce jamming. We show that the jamming of a stretched colloidal column is closely related to that observed during shear rheology. However, fascinations with an additional effect due to the geometry are also observed. High speed photography of the filament shows evidence of dilatancy and granulation, leading finally to fracture at a critical strain rate. We also investigate an intriguing aspect of thin fluid filaments of the colloidal suspension, when stretched below the critical strain rate required to produce jamming. These filaments are observed to thin to a critical diameter before rupturing and displaying visco-elastic recoil. Finally, using fluorescent particles we visualise the flow fields inside these filaments to understand the dynamics.

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This work is funded by IFPRI and the grant NSF-CBET-1010008.

3:18PM X53.00005 Effect of Inertial Mass on Velocity Correlations of Shear Driven Soft-Core Disks Approaching the Athermal Jamming Transition

This work has been supported by NSF.

3:30PM X53.00006 Stretching dense colloidal suspensions: from flow to fracture

This work is funded by IFPRI and the grant NSF-CBET-1010008.

3:42PM X53.00007 Fluctuations for Hopper Flow with Circular and Elliptical Particles

3:54PM X53.00008 Rheology and Jamming in Soft Colloidal System

4:06PM X53.00009 Local interactions and global rheology in disordered media

4:18PM X53.00010 Jammed by shear: a new perspective of the jamming transition in frictional granular materials

3:30PM X53.00006 Stretching dense colloidal suspensions: from flow to fracture

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4:06PM X53.00009 Local interactions and global rheology in disordered media

4:18PM X53.00010 Jammed by shear: a new perspective of the jamming transition in frictional granular materials
4:30 PM X53.00011 Deformation of inherent structures to detect short- and long-range correlations in supercooled liquids, EMANUELA DEL GADO, MAJID MOSAYEBI, PATRICK ILG, HANS CHRISTIAN OETTINGER, ETH Zurich, MICROSTRUCTURE AND RHEOLOGY, ETH ZURICH TEAM; POLYMER PHYSICS, ETH ZURICH TEAM — We use deformation of inherent structures as a tool for detecting structural changes and the onset of cooperativity in supercooled liquids. The non-affine displacement (NAD) field resulting from the applied deformation shows characteristic differences between the high temperature liquid and supercooled state, that are typically observed in dynamic quantities and correlated to normal mode structure. The average magnitude of the NAD is very sensitive to temperature changes in the supercooled regime and is found to be strongly correlated with the inherent structure energy. We can rationalize such changes in terms of a crossover from a viscous liquid to a regime dominated by elastic effects. In addition, the NAD field is characterized by a correlation length that increases upon lowering the temperature towards the supercooled regime. By analysing different measures of correlations in the direction of the NAD field, we discuss their analogies with observations in the cooperative dynamics.

4:42 PM X53.00012 Experiments on ordering transitions in mechanically stable structures of granular rods, VIKRANT YADAV, Clark University, JEAN-YONNEL CHASTAING, Ecole Normale Supérieure de Lyon, ARSHAD KUDROLLI, Clark University — We investigated the evolution of granular rods from mechanically stable disordered to crystalline states in response to vibrations. We obtained positions and orientations of the rods in three dimensions using micro-focus X-ray Computed Tomography. Above a critical aspect ratio, we find that rods align vertically within layers with hexagonal order within a layer, independent of the nature of interactions. We also quantitatively study the evolution of local and global ordering using density pair correlation function g(r) and orientational order parameter q_6 as a function of aspect ratio. As the system compacts, local structures emerge and grow, their size and orientation being dependent on volume fraction. Although the initial nucleation of order occurs along the boundaries, we show that the geometry of boundaries have little overall effect on the observed ordering transition. Finally we show that configuration entropy arguments do not play a significant role in the observed ordering, and the system evolves towards increasing stability under small perturbations.

4:54 PM X53.00013 Elasticity of floppy amorphous systems, GUSTAVO DURING, EDAN LERNER, MATTIEU WYART, New York University — Simple amorphous solids made of repulsive particles display curious properties when they are barely mechanically stable, in particular near the unjamming transition where pressure vanishes. Here we focus on another class of materials, including granular flows, covalent glasses or gels of semi-flexible polymers. In such materials the coordination with the dominant interaction is too weak to guarantee mechanical stability. This fact implies the presence of floppy modes, collective motions of particles that have no or very little restoring force, and that strongly affect the properties of these materials. We use analytical methods to derive the response of these systems, their length scale and frequency dependence, and test these numerically. If time permits our results will be compared with numerical observations in simplified suspension flows.

5:06 PM X53.00014 Granular Matter, Foams, and Beyond: Applications of the Granocentric Model, KATHERINE NEWHALL, Courant Institute NYU — We present a local stochastic model that predicts the statistical fluctuations in jammed packings of monodisperse and polydisperse spheres revealed by confocal microscopy. Moreover, we find that this model can account for the properties of looser and denser random packings that result from depletion attraction between the particles or compression by an applied load, respectively. Finally, we extend the model to space-filling packings of cells in tissues and biliquid foams by testing analytic predictions for the dependence of the number of neighbors of a given cell on its volume. Interestingly, the model distinguishes between scenarios in which size or positional disorder in the packing dominate, in good agreement with experimental data. This versatile model can be put into the statistical mechanics framework proposed by Edwards in order to compute the entropy and compactivity of each packing.

5:18 PM X53.00015 Force landscape for particulate systems, LOU KONDIC, New Jersey Institute of Technology, MIROSLAV KRAMAR, Rutgers University, ARNAUD GOULLET, New Jersey Institute of Technology, KONSTANTIN MISCHAIKOV, Rutgers University — We discuss the properties of force landscape for isotropically compressed particulate systems characterized by a wide range of packing fractions. The computational methods used are based on persistence diagrams which allow for clear identification of mathematical properties of force landscapes and help their physical interpretation. We find that using this technique which previously has not been applied to particulate matter, a significant new information can be extracted, going much beyond separation into ‘strong’ and ‘weak’ force networks. One result of this analysis is clear indication that for small packing fractions, polydispersity is a crucial parameter that defines the landscape, while for large packing fractions, friction, if present, becomes dominant. Preliminary results for dynamical features of force networks obtained from time-dependent analysis of force landscapes will be presented as well.

Friday, March 2, 2012 8:00AM - 11:00AM – Session Y20 DCMP GSNP: Invited Session: New Anisotropy-Driven Phenomena in Colloidal Suspensions: 253C

8:00 AM Y20.00001 Entropically patchy particles: Shape-driven self-assembly of hard colloids, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI — Although the structural diversity of colloidal fluids and crystals has grown substantially in recent years, it still aspires to that of atomic and molecular systems. Ionic colloidal crystals and binary nanoparticle superlattices, by exploiting electrostatic interactions in mixtures of particles of opposite charge, have substantially broadened the diversity of structures beyond those obtainable in traditional hard sphere systems, but rely on energetic interactions as well as entropy for their stability. Likewise, “traditional” patchy particles with sticky interactions exploit explicit attractive interactions for assembly. Here we explore the role of shape and entropy in phase transitions of hard particle fluids, in the absence of all other interactions. Using computer simulations, we show that particle shape alone can suffice to produce a rich diversity of colloidal crystals, quasicrystals, glasses and mesophases through thermodynamic self-assembly whose complexity rivals that of atomic analogues. We compare self-assembled phases of hard polyhedra with their dense packings obtained from small unit cell compressions, and show the packings tend to be less structurally complex than the analogues. Based on our findings, we present design rules for anisotropic hard, faceted colloids as “entropically patchy particles” for self assembly.

SCG acknowledges financial support from the U.S. Department of Defense, the National Science Foundation, the Department of Energy Office of Science, and the J.S. McDonnell Foundation.
8:36AM Y20.00002 Lock-and-Key Colloids 1, DAVID PINE, New York University — We have developed a new kind of colloidal particle that is spherical but with one or more spherical dimples in the particle surface. These dimples serve as docking points for colloidal spheres whose radius matches the radius of dimples. The attractive docking force is provided by the depletion interaction and can be controlled by changing the depletant concentration or, in some cases, the temperature. The docking is completely reversible and mimics the classic lock-and-key interaction often used to describe protein binding. The lock-and-key binding is size specific and can be used to assemble a number of interesting colloidal superstructures, including flexible jointed chains, dumbbells, trimers, tetramers, and other assemblies. A new synthetic method for making the dimpled particles can be generalized to make a number of other new structured colloidal particles, with different functionalities analogous to block copolymers.

1This work is supported by the National Science Foundation, Award number DMR-1105455 and was performed in collaboration with S. Sacanna, W. T. M. Irvine, P. M. Chaikin, and G.R. Yi.

9:12AM Y20.00003 Glass transitions in quasi-two-dimensional suspensions of colloidal ellipsoids, YILONG HAN, Hong Kong University of Science and Technology — Colloidal glasses constitute of anisotropic particles were mainly studied by simulations in three dimensions with incomplete phase diagrams. Here we report the experiment about glass transitions in a colloidal suspension of micro-ellipsoids at the single-particle level. Video microscopy revealed a two-step glass transition corresponding to inter-domain freezing and inner-domain freezing respectively. The glass transition in the rotational degree of freedom was at a lower density than that in the translational degree of freedom. Between the two transitions, ellipsoids formed an “orientational glass” in the area fraction range 0.72 < φ < 0.79 for aspect ratio p = 6 ellipsoids and 0.60 < φ < 0.72 for p = 9. Such orientational glass is expected to be replaced by the rotator phase at small aspect ratios and the nematic phase at large aspect ratios. The observed decoupling between diffusion and relaxation for both of translational and rotational motions reflects the dynamic heterogeneity. Approaching the respective glass transitions, the rotational and translational fastest-moving particles in the supercooled liquid moved cooperatively and formed clusters with power-law size distributions. The mean cluster sizes diverge in power law as approaching the glass transitions. The translational and rotational fastest- and slowest-moving ellipsoids are all spatially anticorrelated: most translational fast-moving ellipsoids and rotational slow-moving ellipsoids formed at different areas within pseudonematic domains, while most rotational fast-moving ellipsoids and translational slow-moving ellipsoids formed at different areas around the domain boundaries.

9:48AM Y20.00004 Suppression of the coffee-ring effect by shape-dependent capillary interactions, PETER YUNKER, Univ of Pennsylvania — No abstract available.

10:24AM Y20.00005 Glassy dislocation dynamics in colloidal dimer crystals, SHARON GERBODE, Harvey Mudd College — Dislocation mobility is central to both the mechanical response and the relaxation mechanisms of crystalline materials. Recent experiments have explored the role of novel particle anisotropies in affecting the rules of defect motion in crystals. “Peanut-shaped” colloidal dimer particles consisting of two connected spherical lobes form densely packed crystals in 2D. In these “degenerate crystals,” the particle lobes occupy triangular lattice sites while the particle axes are randomly oriented among the three crystalline directions. One consequence of the random orientations of the dimers is that dislocation glide is severely limited by certain particle arrangements in the degenerate crystals. Using optical tweezers to manipulate single lobe-sized spherical intruder particles, we locally deform the crystal, creating defects. During subsequent relaxation, the dislocations formed during the deformation leave the crystal grain, either via annihilation with other dislocations or by moving to a grain boundary. Interestingly, in large crystalline grains this dislocation relaxation occurs through a two-stage process reminiscent of slow relaxations in glassy systems, suggesting the novel concept that glassy phenomena may be introduced to certain kinds of colloidal crystals via simple anisotropic constituents.

Friday, March 2, 2012 8:00AM - 11:00AM — Session Y52 GSNP: Focus Session: Spin Glasses: Advances, Algorithms, and Applications 153C

8:00AM Y52.00001 How the Edwards-Anderson Model reaches its Mean-Field Limit; Simulations in d=3,...,7, STEFAN BOETTCHER, STEFAN FALKNER, Physics Department, Emory University — Extensive computations of ground state energies of the Edwards-Anderson spin glass on bond-diluted, hypercubic lattices are conducted in dimensions d = 3, ..., 7. Results are presented for bond-densities exactly at the percolation threshold, p = p_c, and deep within the glassy regime, p > p_c, where finding ground-states becomes a hard combinatorial problem. The “stiffness” exponent γ that controls the formation of domain wall excitations at low temperatures is determined in all dimensions. Finite-size corrections of the form 1/N^ω are shown to be consistent throughout with the prediction ω = 1 − y/d. At p = p_c, an extrapolation for d → ∞ appears to match our mean-field results for these corrections. In the glassy phase, ω does not approach the value of 2/3 for large d predicted from simulations of the Sherrington-Kirkpatrick spin glass. However, the value of ω reached at the upper critical dimension does match certain mean-field spin glass models on sparse random networks of regular degree called Beta lattices.


8:12AM Y52.00002 Ensemble Inequivalence in Spin Glasses, ZSOLT BERTALAN, HIDETOSHI NISHIMORI, KAZUTAKA TAKAHASHI, Tokyo Institute of Technology — We report on the ensemble inequivalence in many-body spin-glass models with Ising and integer spins. In the Ising case, for many-body interactions the transition between the ferromagnetic and paramagnetic phases is of first order, and the microcanonical and canonical ensembles give different results. The spin-glass transition is of first order for certain values of the crystal field strength in the integer-spin model and is dependent whether it was derived in the microcanonical or the canonical ensemble. We also discuss the ensemble inequivalence of random models, corresponding to the limit infinitely many-body interactions. This is the first systematic treatment of spin glasses with long-range interactions in the microcanonical ensemble using the replica approach, which shows how the two ensembles give different results.

8:24AM Y52.00003 Algorithms and long-range order in the two-dimensional +/-J spin glass, A. ALAN MIDDLETON, Syracuse University, CREIGHTON K. THOMAS, Northwestern University, DAVID A. HUSE, Princeton University — Numerical methods and results of their application to the two-dimensional Ising spin glasses will be described. For a random mix of ferromagnetic and antiferromagnetic bonds of equal strength, long range correlations at zero-temperature are derived from scaling relations between computed exponents and are confirmed in numerical simulations. This long range order is stabilized by large entropy differences, as large domain walls often have zero energy cost. The order resembles that in higher-dimensional models at finite temperature. A publicly distributed implementation of the algorithms has been developed for computing partition functions and exactly sampling configurations according to their Boltzmann weight for the general spin-glass and related two-dimensional models.

1NSF DMR-1106731, DMR-0818960
8:36 AM Y52.00004 Replica theory of partition-function zeros in spin-glass systems, KAZUTAKA TAKAHASHI, Tokyo Institute of Technology, TOMOYUKI ÔUCHI, Osaka University — We study the phase transitions in spin-glass systems by analysing the partition-function zeros (Lee-Yang zeros) with respect to the complex temperature/field. For several models as the random energy and spherical models with many-body interactions, we extend the replica method and the procedure of the replica symmetry breaking ansatz to be applicable in the complex-parameter case. We derive the phase diagrams in the complex plane and calculate the density of zeros in each phase. We find that there is a replica symmetric phase having a large density near the imaginary axis away from the origin. In the spin-glass phase, the density is finite only when the chaos effect is present. This result indicates that the density of zeros is more closely connected to the chaos effect than the replica symmetry breaking. We also investigate the relevance of our result to the finite-dimensional systems by studying the renormalization group flow in the complex plane.

8:48 AM Y52.00005 Aging behavior in disordered and frustrated spin systems¹, HYUNHANG PARK, MICHEL PLEIMLING, Virginia Tech — Using Monte Carlo simulations we investigate aging in three-dimensional Ising spin glasses as well as in two-dimensional Ising models with disorder quenched to low temperatures. The time-dependent dynamical correlation length $L(t)$ is determined numerically and the scaling behavior of various two-time quantities as a function of $L(t)/L(s)$ is discussed. For disordered Ising models deviations of $L(t)$ from the algebraic growth law show up. The generalized scaling forms as a function of $L(t)/L(s)$ reveal a generic simple aging scenario for Ising spin glasses as well as for disordered Ising ferromagnets.

¹This work was supported by the US Department of Energy through grant DE-FG02-09ER46613.

9:00 AM Y52.00006 Critical behavior of the 1D Lévy lattice spin-glass: from mean-field threshold to the effective lower critical dimension, LUCA LEUZZI, IPCF-CNR, Italy, GIORGIO PARISI, FEDERICO RICCI-TERSENGLI, Dept. Physics, Sapienza University of Rome, Italy, JUAN-JOSE RUIZ-LORENZO, Dept. Physics, University of Extremadura, Badajoz, Spain — By means of Monte Carlo numerical simulations we analyze the critical behavior of a one dimensional spin-glass model with diluted interactions decaying, in probability, as an inverse power of the distance: the Lévy lattice spin-glass. Varying the power $p$, corresponds to change the effective dimension from mean-field-like (small power $p < 4/3$) to finite dimensional-like short-range models ($< 1.3/3 < 2$) and, eventually, to 1D short-range models ($p > 2$), where no phase transition occurs. The bond diluteness drastically reduces the computational time and large sizes can be approached. The one dimensionality allows for studying long systems, e.g., long correlation lengths in the critical region. The spin-glass critical behavior can, therefore, be studied in and out of the range of validity of the mean-field approximation. After reviewing the main results in the Lévy lattice model about the spin-glass transition and the nature of the spin-glass phase for different values of the effective dimension, we will present new results on the critical behavior at $p = 2$, corresponding to the lower critical dimension, and compare them with old and recent renormalization group approaches in this limit.

9:12 AM Y52.00007 Spin glasses: Still frustrating after all these years?, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich — Spin glasses are archetypical model systems to study the effects of frustration and disorder. Despite ongoing research spanning several decades, there remain many fundamental open questions, such as the existence of a spin-glass state in a field or the low-temperature structure of phase space for short-range systems. Novel applications across disciplines, as well as progress in algorithms and the advent of fast and cost-effective computers, have recently revived interest in the study of spin glasses. First, an overview of spin glasses will be given, followed by recent novel applications to fields as diverse as structural glasses and quantum computing.

9:48 AM Y52.00008 The de Almeida-Thouless line of the four-dimensional Ising spin glass, VICTOR MARTIN-MAYOR, Universidad Complutense de Madrid, JANUS COLLABORATION — We present the results of a large scale numerical simulation of the four dimensional Edwards-Anderson model in an external field. Using the Janus computer, as well as standard CPU clusters, we simulate lattices of size up to $L=16$ at several values of the external field. Our analysis method departs from the standard one. In fact, it has been previously noticed that the spin-glass susceptibility (i.e. the spin-glass propagator at zero external momentum) behaves anomalously. Instead, one should focus on the propagator at small but non-vanishing wave-vector. Starting from this observation, we obtain a simple and powerful finite-size scaling method. Clear evidence for a de Almeida-Thouless line is found. We compute critical exponents, widely differing from the zero field case, with an accuracy of five percent. The shape of the de Almeida-Thouless line in the $(T,h)$ plane follows the Fisher-Sompolinsky scaling. Discrepancies with previous work are explained in terms of very strong scaling corrections.

10:00 AM Y52.00009 Reentrance and ultrametricity in three-dimensional Ising spin glasses, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich, CREIGHTON K. THOMAS, Department of Materials Science and Engineering, Northwestern University, ALEXANDER K. HARTMANN, Department of Physics, Oldenburg University, Germany — We study the three-dimensional Edwards-Anderson Ising spin glass with bimodal disorder with a fraction of 22.8% antiferromagnetic bonds. Parallel tempering Monte Carlo simulations down to very low temperatures show that for this fraction of antiferromagnetic bonds the phase diagram of the system is reentrant, in agreement with previous results. Furthermore, using a clustering analysis, we analyze the ultrametric properties of phase space for this model.

10:12 AM Y52.00010 Replica exchange simulations of the three-dimensional Ising spin glass: static and dynamic properties, BURCU YUCESOY, JONATHAN MACHTA, Department of Physics, University of Massachusetts Amherst, HELMUT G. KATZGRABER, Department of Physics, Texas A&M University & ETH Zurich — We present the results of a large-scale numerical study of the equilibrium three-dimensional Ising spin glass with Gaussian disorder. Using replica exchange (parallel tempering) Monte Carlo, we measure various static, as well as dynamical quantities, such as the autocorrelation times and round-trip times for the replica exchange Monte Carlo method. The correlation between static and dynamic observables for 5000 disorder realizations ($N \leq 10^3$ spins) down to very low temperatures ($T \leq 0.2T_c$) is examined. Our results show that autocorrelation times are directly correlated with the roughness of the free energy landscape. We also discuss the size dependence of several static quantities.

¹Supported in part by NSF DMR-0907235

10:24 AM Y52.00011 Monte Carlo Simulations of Random Frustrated Systems on Graphics Processing Units, SHENG FENG, YE FANG, SEAN HALL, Louisiana State University, ARIANE PAPKE, University of Gottingen, CADE THOMASON, KA-MING TAM, JUANA MORENO, MARK JARRELL, Louisiana State University — We study the implementation of classical Monte Carlo simulation for random frustrated models using the multithreaded computing environment provided by the the Compute Unified Device Architecture (CUDA) on modern Graphics Processing Units (GPU) with hundreds of cores and high memory bandwidth. The key for optimizing the performance of the GPU computing is in the proper handling of the data structure. Utilizing the multi-spin coding, we obtain an efficient GPU implementation of the parallel tempering Monte Carlo simulation for the Edwards-Anderson spin glass model. In the typical simulations, we find over two thousand times of speed-up over the single threaded CPU implementation.
10:36AM Y52.00012 Monte Carlo simulations of the LiHo$_x$Y$_{1-x}$F$_4$ diluted dipolar magnet. JUAN CARLOS ANDRESEN, Department of Physics, ETH Zurich, MOSHE SCHECHTER, Department of Physics, Ben Gurion University, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich. — Recent intriguing experimental results on LiHo$_x$Y$_{1-x}$F$_4$, a diluted dipolar magnet, along with new analytical insights, suggest that neither a mean-field treatment nor simulations using simplified versions of the underlying Hamiltonian adequately describe these materials. Not only does this imply that novel disordering mechanisms might be present, it requires a detailed numerical analysis that incorporates all terms in the Hamiltonian. We present large-scale Monte Carlo simulations of the diluted dipolar magnet with competing interactions on a LiHo lattice with the inclusion of a random field term. For low concentrations of Ho atoms we reproduce the peculiar linear dependence of the transition temperature as a function of the random-field strength found in recent experimental results by Silevich et al. [Nature 448, 567 (2007)]. We then find a zero-temperature phase transition between the ferromagnetic and quasi-spin-glass phases, suggesting that it is the underlying spin-glass phase that dictates the above linear dependence of $T_c$ on the random field. For large concentrations we recover the quadratic dependence of the critical temperature as a function of the random field strength.

10:48AM Y52.00013 Novel disordering mechanisms in dipolar spin glasses and ferromagnets. MOSHE SCHECHTER, Physics Department, Ben Gurion University of the Negev. JUAN CARLOS ANDRESEN, Department of Physics, ETH Zurich, HELMUT KATZGRABER, Department of Physics and Astronomy, Texas A&M University and ETH Zurich. — At and below the critical dimension the disordering of an ordered phase by a random field occurs via a collective effect of large domains at infinitesimal random field [Imry & Ma, Phys. Rev. Lett. 35, 1399 (1975)]. At larger space dimensions the disordering requires a large random field, of the order of the interaction energy. In a random field, the lower critical dimension is 2 for Ising ferromagnets, whereas it is infinity for spin glasses. We have generalized the Imry-Ma argument for ferromagnets with competing interactions and for an underlying spin-glass phase, for dilute dipolar spin glasses. For dilute dipolar spin glasses we have found [EPL 88, 66002 (2009)] that the broad distribution of random fields dictates more efficient disordering of the glass phase, and domain sizes which depend explicitly on the concentration, i.e., do not obey simple scaling. Here we show that as a result of a competing spin-glass phase, the disordering of the ferromagnet occurs at a finite random field, which is yet much smaller than the interactions. Our results are verified numerically, explain the recently-observed peculiar linear dependence of $T_c$ on the random field strength [Nature 448, 567 (2007)], and predict a zero-temperature random-field driven transition between a ferromagnetic and a quasi spin glass phase.
9:00AM Y53.00006 Cooperation-induced temporal complexity in networks of pulse-coupled units, ELVIS GENESTON, La Sierra University, PAULO GRIGOLINI, University of North Texas — We study a network of stochastic pulse-coupled units generating bursts with the same size distribution as the neuronal avalanches in mature cultured neurons, recently revealed by the experimental observation. We prove that in addition to this form of complexity this model yields a form of phase transition generating also temporal complexity. This means that the distance from two consecutive bursts fits the prescription of a Mittag-Leffler (ML) function renewal theory. There exists a critical value of the cooperation parameter at which this description applies to the whole time regime. By increasing the cooperation parameter the ML theory breaks down and the sequence of bursts tend to become periodic with the same intensity. We make the conjecture that the analysis of this model may shed light into the theoretical foundation of neuronal burst leaders and that the recently discovered principle of complexity management may be conveniently applied to the neuro-physiological processes that are properly described by this model.

9:12AM Y53.00007 Time dependence of reprecipitation rates in heterogeneous media, DANIEL REEVES, DANIEL ROTHMAN, MIT — The analysis of spatial and temporal variations of the chemical and isotopic compositions of minerals in sedimentary systems provides a powerful tool for calculating dissolution and reprecipitation rates, and has previously been applied to find time-dependent rates in marine sediments. Dissolution and precipitation processes tend to shift the composition of the pore fluids toward that of the solid phase, and vice-versa. Current theory treats both the fluid and solid phases as well-mixed reservoirs, relying on mean-field theory that is inconsistent with the physical structure of the solid, as dissolution and precipitation occur only on the reactive surface of the solid. We present a model that accounts for the heterogeneity of the solid phase by adding and removing material only at the reactive surface. We therefore model the location of the surface with a 1-D random walk, in which the buried bulk of the solid phase can only be modified through repeated dissolution events. We approximate this physical scenario with a three-reservoir kinetic model and more detailed numerical simulations. We develop an understanding of two power-law scaling regimes, the second of which demonstrates t/1 time aging in the rate constant, similar to those observed in marine sediment studies.

9:24AM Y53.00008 Properties of compacton-anticompacton collisions, BOGDAN MIHAILA, Los Alamos National Laboratory, ANDRES CARDENAS, New York University, FRED COOPER, ANDRES SAXENA, Los Alamos National Laboratory — We study the properties of compacton-anticompacton collision processes. We compare and contrast results for the case of compacton-anticompacton solutions of the K(p,q) Rosenau-Hyman (RH) equation for p=q=2, with compacton-anticompacton solutions of the L(l,p) Cooper-Shepard-Sodano (CSS) equation for p=1 and l=3. This study is performed using a Padé discretization of the RH and CSS equations. We find a non-monotone dependence in the behavior of compacton-anticompacton scattering. For the CSS equation, the scattering can be interpreted as “annihilation” as the wave left behind dissolves over time. In the RH equation, the numerical evidence is that multiple shocks form after the collision, which eventually lead to “blowup” of the resulting wave form.

9:36AM Y53.00009 Cardiac arrhythmias and degradation into chaotic behavior prevention using feedback control1, ILLIA UZELAC, VENIAMIN SIDOROV, Vanderbilt University, Nashville TN, USA, MARC HOLCOMB, Hampden-Sydney College, Hampden-Sydney, VA, USA, JOHN WIKSWO, Vanderbilt University, Nashville TN, USA, RICHARD GRAY, Food and Drug Administration, MD, USA — During normal heart rhythm, cardiac cells behave as a set of oscillators with a distribution of phases but with the same frequency. The heart as a dynamical system in a phase space representation can be modeled as a set of oscillators that have closed overlapping orbits with the same period. These orbits are not stable and in case of the chaotic rhythm, such as due to premature beats, the system will have a tendency to leave its periodic orbit unstable. As the chaotic orbit becomes attracted to a phase singularity, their disruption may lead to chaotic behavior, which appears as a life-threatening ventricular fibrillation. Feedback control of fibrillation should any disruption lead to a return to the normal rhythm or modify the system to maintain its orbits. The delay through the feedback network coincides with the period of normal heart beats. To implement this approach we developed a 1 kW arbitrary waveform voltage-to-current converter with a 1 kHz bandwidth driven by a photodiode system that records an optical electrocardiogram and provides a feedback signal in real time. Our goal is to determine whether our novel method to defibrillate the heart will require much lower energies than are currently utilized in single shock defibrillators.

9:48AM Y53.00010 Experiments on oscillator ensemble with global nonlinear coupling, MICHAEL ROSENBLUM, Potsdam University, AMIRKHAN TEMIRBAYEV, ZEINULLA ZHANABAEG, STANISLAV TARASOV, Kazakh National University, VLADIMIR PONOMARENKO, Institute of RadioEngineering and Electronics of Russian Academy of Sciences, Saratov Department — We experimentally analyze collective dynamics of a population of 20 electronic Wien-bridge limit-cycle oscillators with a linear or nonlinear phase-shifting unit in the global feedback loop. With linear unit we observe, with increase of the coupling strength, a standard Kuramoto-like transition to a fully synchronous state; the threshold of the transition depends on the phase shift. In case of nonlinear global coupling we first observe a transition to a state when approximately half of the population forms a synchronous cluster. With further increase of the coupling strength we observe destruction of this cluster and formation of a self-organized quasiperiodic state, predicted in [M. Rosenblum and A. Pikovsky, PRL, 98, 064101 (2007)]. In this state, frequencies of all oscillators are smaller than the frequency of the main field, so that the oscillators are not locked to the mean field they create and their dynamics is quasiperiodic. The transition is characterized by a non-monotonic dependence of the order parameter on the coupling strength. We demonstrate a good correspondence between theory and experiment.

1 Supported in part by NIH R01 HL58241-11 through ARRA 2009

10:00AM Y53.00011 Dynamics of Confident Voting, DANIEL VOLOVIK, SIDNEY REDNER, Boston University — In the classical voter model, a voter has no intrinsic confidence in its current opinion. We introduce the confident voter model in which each voter can be in one of two opinions, and can additionally have two levels of commitment to an opinion — confident and vacillating. Upon interacting with an agent of a different opinion, a confident voter becomes less committed, or vacillating, but does not immediately change opinion. However, a vacillating agent changes opinion upon interacting with an agent of a different opinion. In the mean-field limit, a population of size N is quickly driven to a mixed state before consensus is eventually achieved in a time of order ln N. In two dimensions, the distribution of consensus times is characterized by two distinct times — one that scales linearly with N and another that scales as N^{1/2}. The longer time arises from configurations that fall into long-lived stripe states, which are caused by an effective surface tension between domains of different opinion states, before consensus is finally reached.

10:12AM Y53.00012 Nonuniversal Effects in Mixing Correlation-Growth Processes with Randomness, ALICE KOLAKOWSKA, Valdosta State University, GA — In mixed-growth dynamical process P = Y ∪ X there are two dynamical processes: Y (in one universality class) and X (in another universality class). They alternate with each other: “exclusively either Y is active with probability q) or X is active with probability 1−q).” P models surface growth via deposition/desorption/adsorption with X building universal correlations and Y representing randomness (“e.g., thermal effects), in order to correctly construct a continuum growth equation for P a distinction must be made within a single universality class of X between processes that do and do not create voids in the bulk of deposited material. Then, model-dependent prefactors in universal scaling of the surface roughness can be linked with the bulk morphology and determined from the bulk structures. This connection is essential to finding correct dynamical scaling and to interpretation of scaling laws for mixed-growth dynamical processes.
10:24AM Y53.00013 Non-equilibrium modulated phases in a system with local energy input¹
, LINJUN LI, MICHEL PLEIMLING, Virginia Tech — The equilibrium phase diagram of the two-dimensional Ising model in contact with a single heat bath is well understood. We here study the properties of the two-dimensional Ising model with conserved dynamics where the two halves of the system are in contact with different heat baths. Using Monte Carlo simulations, we identify three different phases for this non-equilibrium system, as a function of the aspect ratio of the lattice and of the temperatures. The first phase is characterized by the complete disorder of the particles, while the second phase is characterized by the complete order of the particles. The third phase is the most interesting one as it displays stripes with widths that depend on the system parameters. The full phase diagram of our non-equilibrium system is determined through the study of the structure factor.

¹Supported in part by the US National Science Foundation through Grant DMR-0904999.

10:36AM Y53.00014 Nonequilibrium relaxation and critical aging for driven Ising lattice gases¹
, GEORGE DAQUILA, UWE C. TAUBER, Department of Physics, Virginia Tech — We employ Monte Carlo simulations to study the non-equilibrium relaxation of driven Ising lattice gases in two dimensions. Whereas the temporal scaling of the density auto-correlation function in the non-equilibrium steady state does not allow a precise measurement of the critical exponents, these can be accurately determined from the aging scaling of the two-time auto-correlations and the order parameter evolution following a quench to the critical point. We obtain excellent agreement with renormalization group predictions based on the standard Langevin representation of driven Ising lattice gases, valid to all orders in the dimensional expansion.

¹Research supported by DOE-BES, Grant No. DE-FG02-09ER46613.

Friday, March 2, 2012 11:15AM - 1:51PM — Session Z41 DBIO GSNP: Focus Session: Non-Covalent Protein Interactions 156B

11:15AM Z41.00001 Novel Aspects of Hydrogen Bonding in Protein Function: Active Site Ionic Hydrogen Bonds , WOUTER D. HOFF, Oklahoma State University — We use photoactive yellow protein (PYP), a bacterial photoreceptor, to explore novel aspects of hydrogen bonding in protein function. PYP exhibits photochemical activity based on its ionized p-coumaric acid (pCA) chromophore, which is hydrogen bonded to Tyr42 and G1u46. We report that these active site ionic hydrogen bonding interactions cause unexpected molecular and functional properties of PYP. First, we describe a novel spectroscopic isotope effect (SIE) in which dissolving PYP in D2O causes a red-shift in its electronic absorbance spectrum. We assign this SIE to the ionic hydrogen bond between pCA and G1u46, which—in contrast to standard hydrogen bonds—is weakened upon H/D exchange. These findings extend the effects of H/D exchange from kinetic isotope effects to include shifts in absorbance spectrum, and illustrate the biological relevance of ionic hydrogen bonding to protein active sites. Secondly, we examine how the protein environment achieves the unusual strong preference of the pCA to remain ionized in the protein interior. We arrive at the conclusion that the recombination of the Y42F mutant of PYP by incorporation of a trans-locked analog of pCA to dissect the contributions of active site hydrogen bonding to the large down-shift in the pKa of the pCA. Together, the Tyr42 and G1u46 hydrogen bonds to the pCA account for ~80% of this shift, which can be quantitatively explained by the loss of ionic hydrogen bonding upon pCA protonation from the solvent. Since ionic hydrogen bonds occur in many proteins, this mechanism of pKa tuning is likely to be of general relevance.

11:51AM Z41.00002 Computational design of protein interactions: designing proteins that neutralize influenza by inhibiting its hemagglutinin surface protein , SAREL FLEISHMAN, Weizmann Institute of Science — Molecular recognition underlies all life processes. Design of interactions not seen in nature is a test of our understanding of molecular recognition and could unlock the vast potential of subtle control over molecular interaction networks, allowing the design of novel diagnostics and therapeutics for basic and applied research. We developed the first general method for designing protein interactions. The method starts by computing a region of high affinity interactions between dismembered amino acid residues and the target surface and then identifying proteins that can harbor these residues. Designs are tested experimentally for binding the target surface and successful ones are affinity matured using yeast cell surface display. Applied to the conserved stem region of influenza hemagglutinin we designed two unrelated proteins that, following affinity maturation, bound hemagglutinin at subnanomolar dissociation constants. We discuss the combination of modeling and high-throughput characterization of design variants which has been key to the success of this approach, as well as how we have used the data obtained in this project to enhance our understanding of molecular recognition. References: Science 332:816 JMB, in press Protein Sci 20:753

12:27PM Z41.00003 The power of simple hard-sphere models in protein structure prediction¹
, LYNN REGAN, Yale University — There are several force-fields that are currently used to describe the potential energy of biological macromolecules such as proteins. These typically include many parameters, derived from a combination of statistical, experimental sources. These work on average to describe a protein, but the large number of parameters moves this description further away from a true physical understanding than is desirable. Our approach is to investigate to what extent simple hard sphere models can be used to model and predict the behavior of different aspects of protein structure. We present the results of specific calculations. The distributions of the side-chain dihedral angle ch1 of Val and Thr in proteins of known structure show distinctive features: Val side chains predominantly adopt dihedral angle, ch1, of 180°, whereas Thr side chains typically adopt a dihedral angle, ch1, of 60 or 300°. Several hypotheses have been proposed to explain these differences, including inter-residue steric clashes and hydrogen-bonding interactions. In contrast, we show that the observed side-chain dihedral angle distributions for both Val and Thr can be explained using only local steric interactions in a dipeptide mimetic. Our results emphasize the power of a simple physics-based approaches and their importance for future advances in protein engineering and design.

¹In collaboration with Alice Zhou and Corey O’Hern, Yale University.

1:03PM Z41.00004 Acetylation of LYS-16 of H4 Histone Tail May Sequester the Tail and Inhibit its Interactions with Neighboring Nucleosomes , DAVID POTOTOYAN, GAREGIN PAPAOIAN, University of Maryland — Histone tails are highly flexible N terminal protrusions of histone proteins, which help to fold DNA into dense superstructures known as chromatin. On a molecular scale histone tails are poly-electrolytes with high degree of conformational disorder, allowing them to function as bio-molecular “switches,” regulating various genetic regulatory processes via diverse types of covalent modifications. Because of being intrinsically disordered, the structural and dynamical aspects of histone tails are still poorly understood. Using multiple explicit solvent and coarse-grained MD simulations we have investigated the impact of the acetylation of LYS-16 residue on the conformational and binding properties of the tail. The potential of mean force computed as a function of distance between a model DNA and histone tail center of mass showed a dramatic enhancement of binding affinity upon mono-acetylation of the H4 tail. The estimated binding free energy gain for the wild type is 2kT, while for the acetylated it reaches 4-5 kT. Additionally our structural analysis shows that acetylation is driving the chain into collapsed states, which get enriched in secondary structural elements upon binding to the DNA. We suggest a non-electrostatic mechanism that explains the enhanced binding affinity of the acetylated H4 tail. At last our findings lead us to propose a hypothesis that can potentially account for the celebrated chromatin “fiber loosening effects” observed in many experiments.
1:15PM Z41.00005 Exploring copper chelation in Alzheimer’s disease protein. FRISCO ROSE, MIROSLAV HODAK, JERRY BERNHOLC, CHIPS /NCSU — Alzheimer’s disease (AD) is a neurodegenerative disorder affecting millions of aging people in the U.S. alone. Clinical studies have indicated that metal chelation is a promising new approach in alleviating the symptoms of AD. Our study explores the as yet undetermined mechanism of copper chelation in amyloid-β, a protein implicated in AD. The structure of amyloid-β is derived from experimental results and incorporates a planar copper-ion-binding structure in a semi-solvated state. We investigate the chelation process using the nudged elastic band method implemented in our ab initio real-space multisite code. We find that an optimal sequence of unbonding and rebonding events as well as proton transfers are required for a viable chelation process. These findings provide fundamental insight into the process of chelation that may lead to more effective AD therapies.

1:27PM Z41.00006 Transition-metal prion protein attachment: Competition with copper. MIROSLAV HODAK, JERRY BERNHOLC, North Carolina State University — Prion protein, PrP, is a protein capable of binding copper ions in multiple modes depending on their concentration. Misfolded PrP is implicated in a group of neurodegenerative diseases, which include “mad cow disease” and its human form, variant Creutzfeld-Jacob disease. An increasing amount of evidence suggests that attachment of non-copper metal ions to PrP triggers transformations to abnormal forms similar to those observed in prion diseases. In this work, we use hybrid Kohn-Sham/orbital-free density functional theory simulations to investigate copper replacement by other transition metals that bind to PrP, including zinc, iron and manganese. We consider all known copper binding modes in the N-terminal domain of PrP. Our calculations identify modes most susceptible to copper replacement and reveal metals that can successfully compete with copper for attachment to PrP.

1:39PM Z41.00007 Steric clashes determine differences in side chain dihedral angle distributions: A study of Thr versus Val. ALICE ZHOU, COREY O’HERN, LYNNE REGAN, Yale University — With the long-term goal to improve the design of protein-protein interactions, we develop a simple hard sphere model for dipeptides that can predict the side-chain dihedral angle distributions of Val and Thr in both the α-helix and β-sheet backbone conformations. We find that it is essential to include the non-polar hydrogens in the model; indeed interatomic clashes involving the non-polar hydrogens largely determine the form of side-chain dihedral angle distributions. Further, we are able to explain key differences in the side-chain dihedral angle distributions for Val and Thr from intra-residue steric clashes rather than inter-residue steric clashes or hydrogen bonding. These results are the crucial first step in developing computational models that can predict the side chain conformations of residues at protein-peptide interfaces.


11:15AM Z43.00001 Robotics using sand. HEINRICH JAEGGER, Univ of Chicago — No abstract available.

11:51AM Z43.00002 Shocks in fragile matter. VINCENZO VITELLI, Instituut Lorentz for Theoretical Physics — Non-linear sound is an extreme phenomenon typically observed in solids after violent explosions. But granular media are different. Right when they unjam, these fragile and disordered solids exhibit vanishing elastic moduli and sound speed, so that even tiny mechanical perturbations form supersonic shocks. Here, we perform simulations in which two-dimensional jammed granular packings are continuously compressed, and demonstrate that the resulting excitations are strongly nonlinear shocks, rather than linear waves. We capture the full dependence of the shock speed on pressure and compression speed by a surprisingly simple analytical model. We also treat shear shocks within a simplified viscoelastic model of nearly-isostatic random networks comprised of harmonic springs. In this case, anharmonicity does not originate locally from nonlinear interactions between particles, as in granular media; instead, it emerges from the global architecture of the network. As a result, the diverging width of the shear shocks bears a nonlinear signature of the diverging isostatic length associated with the loss of rigidity in these floppy networks.

12:27PM Z43.00003 Controlling the jamming transition of sheared hard spheres. THOMAS HAXTON, Lawrence Berkeley National Laboratory — Many applications require understanding how disordered materials flow under an external load such as a shear stress. Since external loads drive systems out of equilibrium, their behavior cannot be described solely in terms of equilibrium parameters like temperature and pressure. However, simulations and experiments show that sheared spherical particles possess an effective temperature that relates low-frequency fluctuations of various observable quantities to their associated response functions. Here, we show that the mobility of a mixture of sheared hard spheres is largely controlled by the dimensionless ratio of effective temperature to pressure, $T_{eff}/\sigma^3$, where $\sigma$ is the sphere diameter. We define the effective temperature as the consistent value that relates the amplitudes of low-frequency shear stress and density fluctuations to their associated response functions. We find that the relaxation time $\tau$ characterizing the mobility depends on $T_{eff}/\sigma^3$ according to two distinct mechanisms in two distinct regimes. In the solid response regime, the behavior at fixed packing fraction $\phi$ satisfies $\tau \propto \frac{1}{V} \exp(-c\phi^3/T_{eff})$, where $c$ is the strain rate and $V$ depends weakly on $\phi$, suggesting that the effective temperature controls the average local yield strain. In the fluid response regime, $\tau$ depends on $T_{eff}/\sigma^3$ as it depends on $T_{eff}$ in equilibrium. This regime comprises a large part of the hard-sphere jamming phase diagram including both near-equilibrium conditions where $T_{eff}$ is similar to the kinetic temperature $T_{kin}$ and far-from-equilibrium conditions where $T_{eff} \neq T_{Kin}$. In particular, the dynamic jamming transition is largely controlled by the fluid-response mechanism; like equilibrium hard spheres, sheared hard spheres can flow only if low-frequency fluctuations are large enough compared to the pressure. By presenting our results in terms of the dimensionless jamming phase diagram, we show how these mechanisms likely apply to systems with soft repulsive interactions.

1:03PM Z43.00004 Density-Temperature-Softness Scaling of the Dynamics of Glass-forming Soft-sphere Liquids. MAGDALENO MEDINA-NOYOLA, Instituto de Física, Universidad Autónoma de San Luis Potosí — We employ the principle of dynamic equivalence between soft-sphere and hard-sphere fluids [Phys. Rev. E 68, 011405 (2003); Phys. Rev. Lett. 107, 155701 (2011)] to describe the interplay of the effects of varying the density $n$, the temperature $T$, and the softness (characterized by a softness parameter $\nu^{-1}$) on the dynamics of glass-forming soft-sphere liquids in terms of simple scaling rules. The main prediction is the existence of a dynamic universality class associated with the hard sphere fluid, constituted by the soft-sphere systems whose dynamic parameters, such as the $\alpha$-relaxation time and the long-time self-diffusion coefficient, depend on $n$, $T$, and $\nu$ only through the reduced density $n^{*} \equiv n^{*} (n, T, \nu)$, where the effective hard-sphere diameter $a_{HS}(n, T, \nu)$ is determined by the Andersen-Weeks-Chandler condition for soft-sphere-hard-sphere structural equilibrium. A number of scaling properties observed in recent experiments and simulations involving glass-forming fluids with repulsive short-range interactions are found to be a direct manifestation of this general dynamic equivalence principle. The self-consistent generalized Langevin equation (SCGLE) theory of colloid dynamics [Phys. Rev. E 76, 041504, 062502 (2007)] is shown to accurately capture these scaling rules. The non-equilibrium extension of this theory [Phys. Rev. E 82, 061503, 061504 (2010)] is employed to describe the manifestation of this scaling on the aging of instantaneously-quenched soft-sphere liquids.

1Work supported by the Consejo Nacional de Ciencia y Tecnología (CONACYT, México), through Grants No. 84076 and 132540, and through the Red Temática de Materia Condensada Blanda.
What determines the mechanical properties of dense collections of active particles? The answer to this question is highly relevant to a wide range of physical and biological phenomena from tissue formation to the dynamics of vibrated granular layers. We present a numerical study of the phases and dynamics of a dense collection of self-propelled particles with soft repulsive interactions and polar alignment in a two-dimensional confined geometry. The phase diagram consists of a polar liquid phase at low packing fraction and high self-propulsion speed, and an active jammed phase at high density and low self-propulsion speed. The liquid phase exhibits local alignment and giant number fluctuations typical of the Vicsek class of models. The dynamics of the jammed phase is dominated by oscillations along the low frequency modes of the underlying packing. We show analytically that at long times the energy is carried entirely by the lowest available excitations of the system. Recent experiments on epithelial cell monolayers using force traction microscopy have revealed stress distributions that resemble those observed in granular materials. We measure and compare the local stresses in our active system, with added attraction, to both granular materials and the tissue experiments.

This work was done in collaboration with Yaouen Fily and M. Cristina Marchetti and supported by the NSF through grants DMR-0806511 and DMR-1004789. The computations were carried out on SUGAR, a cluster supported by NSF-PHY-1040231.