APS March Meeting 2016
Baltimore, Maryland
http://www.aps.org/meetings/march/index.cfm
Monday, March 14, 2016 11:15AM - 2:15PM –
Session B12 FIP DBIO: Large Scale Neuroscience Projects 308 - Maria Spiropulu, California Institute of Technology

11:15AM B12.00001 Computational Neuroscience Today TERRY SEJNOWSKI, Salk Institute for Biological Studies — No abstract available.

11:51AM B12.00002 The BRAIN Initiative, MIYOUNG CHUN, Kavli Foundation — No abstract available.

12:27PM B12.00003 Big neuron, HANCHUAN PENG, Allen Institute for Brain Science — No abstract available.

1:03PM B12.00004 The Global Brain (Simons Collaboration), DAVID TANK, Princeton — No abstract available.

1:39PM B12.00005 Panel Discussion —

Wednesday, March 16, 2016 2:30PM - 5:30PM –
Session P14 FIP DCOMP: International Cooperative Efforts for Electronic Structure Methods 310 - Aldo Romero, West Virginia University

2:30PM P14.00001 The European Theoretical Spectroscopy Facility: an illustration for the power of collective research, LUCIA REINING, CNRS-Ecole Polytechnique — As researchers and citizens, we should contribute to facing the grand challenges of our epoch. It is important to work on problems such as climate change or limited resources. However, maybe the biggest challenge is to find ways to unite our forces and develop models of collaborative problem solving. This is mandatory to deal with complex problems, and it can boost efficiency in any case. Code development is just one example where a constructive and well-organized collaboration can take us much further than individual attempts. On the background of this general idea, we will analyze the impact of the European Theoretical Spectroscopy Facility (ETSF, www.etsf.eu) on the day-to-day research of its members, on the theoretical and computational tools that are produced, and on a wider field of theoretical or experimental research. We will see that much can be learnt from this attempt to consider ideas in competition, with people in collaboration.

3:06PM P14.00002 The ABINIT software project, GIAN-MARCO RIGNANESE, Univ Catholique de Louvain — The ABINIT software project aims at providing the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) thanks to a first-principles approach. The ground state properties are calculated in the framework of the Density-Functional Theory (DFT). The excited states properties are computed within the Many-Body Perturbation Theory (MBPT). Finally, the response properties are obtained from Density-Functional Perturbation Theory (DFPT). The ABINIT software project was started in 1997 as an open software project, without a definite goal, developed using several software engineering techniques to allow international collaboration of many different groups. The first publicly available version of ABINIT was released in December 2000 under the GNU GPL. The software has already been described in various articles [1-4]. The last stable version of the package (7.10.4) has now a 70 MBytes size, consisting in nearly 1400 files written in F90 (830000 lines) and including documentation, tutorials and more than one thousand tests. The code is developed by an always opened community (around fifty people) and it is used by more than a thousand individuals worldwide.

References
1. X. Gonze et al., Comp. Mat. Sci. 25, 478492 (2002).

3:42PM P14.00003 The Road to Interoperable Simulation Software: Examples Using the Qbox Code, FRANCOIS GYGI, University of California Davis — The diversity of available simulation software implementing various methods—from atomistic classical molecular dynamics to quantum many-body perturbation theory—makes it highly desirable to couple these codes in a seamless fashion. We discuss the approach taken with the Qbox code to couple first-principles molecular dynamics with advanced sampling algorithms and with GW electronic structure calculations.
http://qboxcode.org
http://www.quantum-simulation.org

1Supported by DOE Office of Basic Energy Sciences

4:18PM P14.00004 The CECAM Electronic Structure Library: community-driven development of software libraries for electronic structure simulations, MICAEL OLIVEIRA, Universite de Liege — The CECAM Electronic Structure Library (ESL) is a community-driven effort to segregate shared pieces of software as libraries that could be contributed and used by the community. Besides allowing to share the burden of developing and maintaining complex pieces of software, these can also become a target for re-coding by software engineers as hardware evolves, ensuring that electronic structure codes remain at the forefront of HPC trends. In a series of workshops hosted at the CECAM HQ in Lausanne, the tools and infrastructure for the project were prepared, and the first contributions were included and made available online (http://esl.cecam.org). In this talk I will present the different aspects and aims of the ESL and how these can be useful for the electronic structure community.
The Yambo code: a comprehensive tool to perform ab-initio simulations of equilibrium and out-of-equilibrium properties

Density functional theory and many-body perturbation theory methods (such as GW and Bethe-Selpeher equation) are standard approaches to the equilibrium ground and excited state properties of condensed matter systems, surfaces, molecules and other several kind of materials. At the same time ultra-fast optical spectroscopy is becoming a widely used and powerful tool for the observation of the out-of-equilibrium dynamical processes. In this case the theoretical tools (such as the Baym-Kadanoff equation) are well known but, only recently, have been merged with the ab-Initio approach. And, for this reason, highly parallel and efficient codes are lacking. Nevertheless, the combination of these two areas of research represents, for the ab-initio community, a challenging perspective as it requires the development of advanced theoretical, methodological and numerical tools. Yambo is a popular community software implementing the above methods using plane-waves and pseudo-potentials. Yambo is available to the community as open-source software, and oriented to high-performance computing. The Yambo project aims at making the simulation of these equilibrium and out-of-equilibrium complex processes available to a wide community of users. Indeed the code is used, in practice, in many countries and well beyond the European borders. Yambo is a member of the suite of codes of the MAX European Center of Excellence (Materials design at the exascale). It is also used by the user facilities of the European Spectroscopy Facility and of the NFFA European Center (nanoscience founcdries & fine analysis). In this talk I will discuss some recent numerical and methodological developments that have been implemented in Yambo towards to exploitation of next generation HPC supercomputers. In particular, I will present the hybrid MPI+OpenMP parallelization and the specific case of the response function calculation. I will also discuss the future plans of the Yambo project and its potential use as tool for science dissemination, also in third world countries.

Friday, March 18, 2016 11:15AM - 1:03PM –
Session Y4 FIP: Physics and Physicists in Cuba

11:15AM Y4.00001 The Role of Science Cooperation in World-Wide Social Progress, DAVID GROSS, Univ of California - Santa Barbara — No abstract available.


12:27PM Y4.00003 Science and Technology Diplomacy with Cuba, FRANCES COLON, US Department of State — President Obama’s announcement of U. S. policy change toward Cuba and increased freedom of interaction with the Cuban people opens unprecedented and long-awaited opportunities for the scientific and engineering communities in the U. S. and in Cuba to establish and expand collaborative efforts that will greatly advance U.S. and Cuba science and technology agendas. New rules for export of donated-only items for scientific use will bring researchers closer to the level of their professional peers around the world. Increasing Cubans’ access to information will result in greater interactions between scientific communities and enable the sharing of ideas and discoveries that can fuel entrepreneurship on the island. The scientific community has expressed an extraordinary level of interest in the wide range of scientific opportunities that the new policy presents, in collaborating with their Cuban counterparts, and in supporting the development of scientific capacity in Cuba. In response to numerous expressions of interest and inquiries from the scientific community, the Office of the Science and Technology Adviser to the Secretary of State (STAS) has engaged in public outreach to inform the U.S. science and technology community of the implications of the new policy for collaborative research, emerging scientific opportunities, and the standing limitations for engagement with the people of Cuba.