In this second issue of the LONI Institute (LI) newsletter, we welcome new members, provide LI and LONI news, explain HPC and LONI training, talk about the upcoming Mardi Gras conference, and put out the call for LI projects, where researchers of the State of Louisiana can ask for the help of an LI Computational Scientist.

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Mark Jarrell, new LONI Institute PI

We would like to express our best wishes to former PI, Jarek Nabrzyski, who left LSU to be the Director of the Center for Research Computing (CRC) at the University of Notre Dame.

We welcome Mark Jarrell, LI Faculty at LSU, as the new Principal Investigator of the LONI Institute. Mark's main area of interest lies in the physics of strongly correlated electronic materials, which include many nanostructures, high T_c superconductors, and heavy Fermion and magnetic materials.

New LI Members

We would like to welcome our new Faculty. The LI has hired another four full-time faculty, Dr. Scott Duke-Sylvester, Dr. Zhenyu Ouyang, Dr. Caz Taylor, and Dr. Rachel Vincent-Finley.

Dr. Scott Duke-Sylvester, Assistant Professor
Department of Biology
University of Louisiana at Lafayette
E-mail: smd3729 AT louisiana.edu
Website: http://biology.louisiana.edu

Dr. Duke-Sylvester received his MS in Mathematics and his PhD in Ecology and Evolutionary Biology and the University of Tennessee at Knoxville. While there, Scott worked on computational models of plant population dynamics in wetland ecosystems. The study system for this research was the Florida Everglades, for which he produced spatially explicit landscape scale models used to evaluate the effect of alternative Everglades restoration plans. Scott did his post-doctoral work at Emory University. While there, Scott branched out into studying the dynamics of infectious diseases (ID). In particular, Scott examined the spatial dynamics of raccoon rabies produced by cyclic patterns of increasing and declining density of the raccoon population

associated with seasonal breeding. At the ULL, he is currently moving into the evolution of infectious diseases. RNA viruses, such as rabies and west Nile virus, experience rapid rates of molecular substitution that occur on a time scale that is compatible with the ecological dynamics of disease spread. Scott is interested in how the evolutionary dynamics of a pathogen are influenced by the contemporaneous process of infection and disease spread.

Dr. Zhenyu Ouyang, Assistant Professor
Department of of Mechanical Engineering
Southern University
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Website: http://www.engr.subr.edu/ME/

Dr. Zhenyu Ouyang obtained his Ph.D. from Marquette University in Structural Engineering. Dr. Ouyang's research interests are in the areas of numerical modeling (Cohesive Zone Model), computational materials (Molecular Dynamics (MD) model), composite materials and structures, and solid and fracture mechanics.

Dr. Caz Taylor, Assistant Professor
Department of Ecology and Evolutionary Biology
Tulane University
E-mail: caz AT tulane.edu
Website: http://eebio.tulane.edu/people/faculty.php

Dr. Caz Taylor obtained her PhD from the University of California at Davis in Ecology in 2004. She received a postdoctoral fellowship from the National Science Foundation in Biological Informatics, which she completed at Simon Fraser University in British Columbia. Dr Taylor's general research interests include computational and mathematical modeling of population dynamics for spatially distributed plant and animal populations. Her particular interests are in the evolution of migration and population dynamics of migratory animals and in computer models to inform management and restoration of coastal wetlands.

Dr. Rachel Vincent-Finley, Assistant Professor
Computer Science Department, Southern University
E-mail: revf AT cmps.subr.edu
Website: http://www.cmps.subr.edu/

Dr. Rachel Vincent-Finley obtained her Ph.D. from Rice University in Computational and Applied Mathematics. Her primary research interests include numerical analysis, particularly the interface between numerical linear algebra and numerical solution techniques which occur in applications to biology, chemistry and biomolecular dynamics. More generally, she is interested in computational methods and high performance computing hardware and software methodology for molecular modeling including data structures and computer visualization.

In the third year of the LI, we are also welcoming Steven Baker (LaTech), Wei Huang (LSU), Salmen Javaid (UNO), Pavel Klimovich (UNO), Hongzhi Lan (Tulane), Kimberlee Lyles (SUBR), Narate Taerat (LaTech), Shuxiang Yang (LSU), and Linghang Ying (Tulane) as new LI Graduate Fellows. These graduate students will use the resources of the LI and LONI to advance their research.

For more information on the new LI members, please visit http://institute.loni.org/.

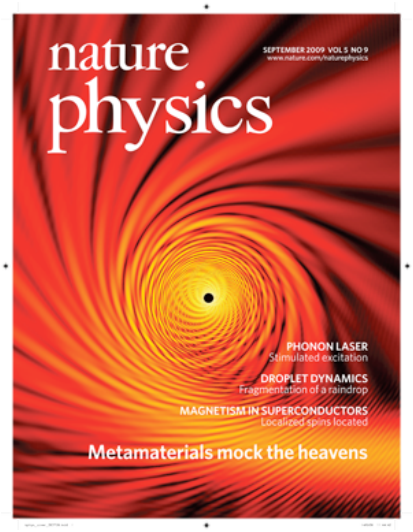
News from our members

Awards

David Mobley, LI Faculty at UNO, has been awarded the prestigious Hewlett-Packard Outstanding Junior Faculty Award in Computational Chemistry. Mobley was among four recipients presented the award at the national American Chemical Society meeting held August 16-20 in Washington, D.C. The awards are presented to junior tenure-track assistant professors who work in the area of algorithm and methods development. (Keep reading.)

In Spring 2009, Tevfik Kosar, LI Scientist Investigator at LSU, received the National Science Foundation's CAREER Award for his efforts. Kosar's CAREER-funded project is "Data-aware Distributed Computing for Enabling Large-scale Collaborative Science." NSF will fund this project for five years at $400,000. Through his work on the CAREER grant, Kosar will develop new computing systems that manage data more effectively with automated processes, which enables scientists to spend more time focusing on their research and less time dealing with data. (Read more.)

Notable Publications



The paper, "Mimicking celestial mechanics in metamaterials", by Dentcho Genov (LI Faculty at LaTech), et al., is featured on the cover page of Nature Physics. The article was published online in Nature Physics on 20 July 2009, and is now in print (Nature Physics 5, 687-692 (2009)).

Genov's groundbreaking work links the newly emerging field of artificial optic materials with celestial mechanics in order to investigate celestial phenomenon in a controlled laboratory environment. Metamaterials are artificial structures that display properties beyond those available in naturally occurring materials. (Read more.)

The paper was also featured in many electronic and national media, including: sciencedaily.com, PhysOrg.com, ESciencenews.com, AZoNano.com, etc. The largest Bulgarian newspaper "Trud" published a full-page interview and another article about the paper. Also, there will be an upcoming article in the New Scientist. Genov is also being nominated for the 2010 Edition of "Who's Who in America".

LONI News

LONI Receives Funding for TeraGrid Research. The TeraGrid, a backbone of national cyberinfrastructure, received $30.2 million in extension funding from the National Science Foundation to continue providing an integrated, persistent computational resource for the national research community. The project, led by the University of Chicago, is titled "TeraGrid Extension: Bridging to eXtreme Digital (XD)," and extends TeraGrid operations through 2011. Included in the extension is $1.05 million that will come to the Louisiana Optical Network Initiative, or LONI, to extend the support and network connections that allow TeraGrid users to access LONI's computational resources through March 2011. (Keep reading.)

LSU Launches New Supercomputing Cluster. LSU's new supercomputing cluster, Philip, will support research requiring high-performance processing and very large memory resources. The new system allows researchers to take advantage of shared memory programming techniques, and gives researchers the means to experiment with and take advantage of new computing models. (Read more.)

HPC and LONI Training

HPC @ LSU offers High Performance Computing training to LSU and LONI users. They provide introductory courses on a variety of subjects that range from Linux, VI, and LaTeX, to MPI, OpenMP and other true parallel programming topics.

Their training courses are free of charge, and are held on the Access Grid and through a web streaming solution so that remote sites may attend. You can find the upcoming training sessions at http://www.hpc.lsu.edu/training/.

If you have questions about HPC training, would like to suggest a new training course, or would like to have training for you and your group on a previously taught topic, or software package that is installed on the LONI clusters, please email Kathy Traxler at ktraxler AT cct.lsu.edu.

Announcements

Upcoming workshop. Louisiana Tech University is hosting the first 2009-2010 LONI HPC Workshop. The workshop curriculum will cover basics needed to get started with HPC and parallel programming. It will also cover many of the software packages on the supercomputers and how to access them. Lunch will be provided each day. The workshop will be held at Louisiana Tech with no virtual attendance, you must be present to attend. There are only 25 seats available so register soon. For more information, the topics to be presented and to register please visit: http://www.hpc.lsu.edu/training/20091006/index.php.

Mardi Gras Conference. From February 11 to February 14 of next year, LSU will host the 17th Mardi Gras conference. The theme this year is Computational Materials Science and Algorithms. Invited speakers will be drawn from a variety of disciplines in both materials science and applied mathematics. There will be sessions on computational algorithms and hardware, strongly correlated materials, biological materials, multiscale modeling, classical simulation methods, and catalysis and reactions. The meeting will culminate in a bus trip to New Orleans for parade watching. Some travel support is available for LONI institute students and postdocs.

Call out for projects involving LI Computational Scientists

One of the goals of the LONI Institute is to foster interdisciplinary and interuniversity research. For this, we would like you to propose projects that involve the LI Computational Scientists (CSs).

The LONI Institute proposal (p. 12) states: “A crucial component of the *LI* is a strong contingent of advanced staff computational scientists… The *LI* will recruit 6 Ph.D. level computational scientists, typically with preexisting postdoctoral experience, to help State research groups take advantage of advanced cyberinfrastructure deployed across LONI and the nation. Distributed across the 6 participating campuses, these staff will be experts in the use of LONI hardware and cyberinfrastructure, including parallel computing, networks, visualization, grids, computational mathematics, and data management. These staff will work

closely together using HD video on all campuses, and will meet biweekly at LSU. Each of the computational scientists will be assigned 4-5 projects, with duration of 1-2 years each, so that significant progress can be made. These projects will be based on applications from all State campuses, with the applicants being encouraged to commit some internal resources. At least 50% of the projects will be in computational biology and materials science applications; however, we expect projects from other areas of importance to the State, in disciplines ranging from astrophysics, CFD, coastal science, medicine, engineering, digital arts and humanities, and business. This is a total of 70-90 projects over 5 years. Application teams from all State campuses and all companies will be eligible to apply for *LI* partnerships to develop applications that make use of LONI hardware and the staff."

Please send your proposals (up to 1 page) requesting time from the LI CSs to Bety Rodriguez brodrig AT cct.lsu.edu by December 15th, 2009. In your proposal, explain what you want to do, about what effort (in FTE-months) you think will be required, and how the project will benefit the LI. The scientific committee will then review the proposals, rank them according to potential contribution to the LI deliverables, and decide which projects should be supported and at what level by February 1st, 2010. PIs of currently supported projects are also eligible to apply for continuing support.

About the Newsletter

If you have LI-related news, don't hesitate to send them to Bety Rodriguez at brodrig AT cct.lsu.edu. You can also contact her for this and other issues, via mail at 216 Johnston Hall, Center for Computation and Technology, Louisiana State University, Baton Rouge, LA, 70803, or by phone at (225) 578-8990.

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