Dear Members of the LONI Institute,

In this first issue of the LONI Institute (LI) newsletter, we would like to express our best wishes to Ed Seidel, as he is stepping down as the Principal Investigator to be the Director of the Office of Cyberinfrastructure at the National Science Foundation. Ed will continue to be an LSU faculty member and affiliated with the CCT and the LONI Institute.

In this issue we:

- Welcome new LI members
- Announce the first LI all hands Meeting
- Call for projects

New LI Members

We welcome Jarek Nabrzyski as the new Principal Investigator of the LONI Institute. Jarek is currently the executive director of the Center for Computation and Technology (CCT) at LSU. He has acted as interim HPC manager, which oversees the HPC environment at LSU and LONI, has become a Co-PI of the NSF TeraGrid project, and is taking on the official role of

Applications Integration Co-PI in the $12M NSF ESPCOR CyberTools project. Prior to joining the CCT, Jarek worked for more than 10 years at the Poznan Supercomputing and Networking Center in Poland, where he managed the scientific applications department. His research specialties include distributed applications, operations research and Grid and high-performance computing. Jarek, with his entrepreneurial skills, mentored several spin-off companies in Europe. Today, some of these companies work on a global market to transfer and apply knowledge obtained during research and development activities within Nabrzyski's team. Jarek has established international partnerships to advance Grid computing, networking and high-performance computing capabilities among academic and industrial organizations. He has served as a principal investigator or co-principal investigator on many international, European Union-funded projects and was the coordinator and co-principal investigator on the GridLab project, which developed the Grid Application Toolkit and the GridSphere portal framework. He serves as the European Commission's expert on Grid and distributed computing. Jarek has a Master's degree in information sciences and a Ph.D. degree in computer science from the Poznan University of Technology in Poland. He also has a diploma in management sciences.

We would like to also welcome our new Faculty, Computational Scientists, and Scientific Coordinator. The LI has hired six full-time faculty, four computational scientists, and a scientific coordinator.

Our new LI Faculty are Abdelkader Baggag (LaTech), Dentcho Genov (LaTech), Mark Jarrell (LSU), Damir Khismatullin (Tulane), David Mobley (UNO), and Christopher Taylor (UNO). The areas of expertise of these LI faculty include parallel numerical algorithms for large scale engineering applications, electromagnetic theory and its applications, the physics of strongly correlated electronic materials, cellular biomechanics, biophysics, biofluid mechanics, multiphase and non-Newtonian flow, computational drug design and lead optimization, modeling of biomolecular interactions and solvation, and the design of algorithms to analyze genomic data.

Our new LI Computational Scientists (CSs) are Hideki Fujioka (Tulane), Raju Gottumukkala (ULL), Abdul Khaliq (interim CS, LaTech), Shizhong Yang (SUBR),

and Zhiyu (Sylvia) Zhao (UNO). The areas of expertise of these LI CSs are computational efficient simulations of fluids in channels, developing complex codes in serial and parallel platforms, as well as developing tools to analyze data such as CT images, providing on-demand access to cyberinfrastructure for disaster management, reliability modeling, workflow modeling and analysis of distributed systems, design and simulation of TCAD/polymer TCAD, microelectronic, and microfluidic devices, semiconductor device fabrication and characterization, high performance computation algorithms, software design, ab initio plane wave and full potential material simulation, and bioinformatics: 3D structure alignment, protein structure searching form the Protein Data Bank, haplotype reconstruction from SNP matrices with incomplete and inconsistent errors, and genome comparison based on non-breaking similarity.

Our LI Scientific Coordinator is Bety Rodriguez-Milla. Her role is top coordinare the LI operational activities, such as serving as chief liaison between the LI campuses and sites, and between the LI and corporate/industrial partners.

In year 2 of the LI, we are also welcoming 5 new graduate students as LI Graduate Fellows. They are Christopher Clayton, Jeremy Dewar, A. Murat Eren, John Jack, and Jijun Lao. These graduate students will use the resources of the LI and LONI to advance their research.

For more information on the new LI additions, please go to http://institute.loni.org/.

First LI All Hands Meeting

This fall, we will be having our first LI All Hands Meeting where we introduce our Faculty and their research, as well as the on-going research at all the LI sites. We hope that all of you can attend. Location and details TBA.

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.

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 Dan Katz dsk@cct.lsu.edu by October 15th. 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.

About the Scientific Coordinator

I am Berta (Bety) Rodriguez-Milla, and I am the Scientific Coordinator of the LONI Institute.

I graduated this year from Syracuse University with a Ph.D. in Physics. My graduate work was on Computational and Condensed Matter Physics, more specifically, on the dynamics and statistical mechanics of disordered systems.

Here at the LI, I serve as the LI manager, and I am the chief liaison between the LI campuses and sites, as well as between the LI and corporate/industrial partners. Other activities include to develop and implement the application processes for students and associated faculty interested in participating in LI projects; to develop and maintain systems for tracking and reporting on LI projects and specific LI milestones; to develop, support and facilitate successful grant proposals involving one or more LI partners; to maintain close contacts with other centers, in Louisiana, the US and abroad, working with the Director and senior LI faculty and staff to forge partnerships where appropriate.

As part of being the LI manager, I will be in charge of writing the newsletters (such as this one), so if you have LI-related news, don't hesitate to send it to me at brodrig@cct.lsu.edu. You can also contact me for this and other issues, via mail. My address is 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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