



**February 20 – February 26, 2011**

### **LSU Offers High Performance Computing Training to Faculty, Staff and Students**

The LSU Center for Computation and Technology (CCT) in partnership with the LSU High Performance Computing (HPC) offers LSU faculty, staff and students a chance to learn computational skills to advance their current research.

All classes are free to attend, but registration is required. The training classes offered this Spring include:

Introduction to HPC, Account Allocation and Management - an introduction to the HPC environments for LONI (Louisiana Optical Network Initiative) and LSU;

Job Management with PBS/LoadLeveler - how to submit, check and customize parallel jobs in the LSU/LONI HPC Environment;

Introduction to MPI - an introduction to parallel programming concepts using MPI calls;

Molecular Dynamics, Programming to Production - fundamentals of molecular dynamics, general classical simulation protocol, and programming of a sample code to expose participants to computational chemistry;

Introduction to Hybrid Programming - using MPI to communicate from node to node and OpenMP to communicate within a node; and,

Introduction to Computational Package for Molecular Dynamics, CPMD coding.

In addition, a LONI HPC Workshop will be offered at Tulane University on March 24 & 25. This workshop is presented at the introductory level for new users, and will cover a general overview of LONI and its environment, and includes hands-on exercises on LONI supercomputers as well as demonstrations on how HPC skills can enhance computational research. User consultants will be onsite to discuss your particular interest or needs.

“CCT and HPC at LSU have provided over 100 tutorials and 20 workshops to students, faculty and staff in Louisiana since 2007. More than 1200 researchers attended the tutorials and 600 people participated in the workshops between January 2007 and

February 2011,” said Honggao Liu, Ph.D., LSU's CCT Deputy Director and HPC Director. “Through these training, workshops, and other support activities, we have enabled many researchers in the State to use local and national HPC resources to do their researches, enhanced the research strengths and competitiveness of the State’s research campuses, and brought more grants and revenue to the State.”

The Louisiana Optical Network Initiative, or LONI, is a state-of-the art, fiber optics network that connects Louisiana and Mississippi research universities to one another as well as to the National LambdaRail and Internet 2, providing the most powerful distributed supercomputer resources to the LSU academic community with over 85 teraflops of computational capacity.

HPC at LSU is a joint partnership between LSU's CCT and LSU's Information Technology Services (ITS), serves as a central point to access all HPC resources and user expertise for the University and LONI, and provides the infrastructure and support necessary to facilitate heroic research efforts, utilizing cutting-edge technology to push the limits of scientific discovery.

For more information on the training courses and for a list of pre-recorded tutorials available for self-paced learning, visit: <http://www.hpc.lsu.edu/training/>.

### **CCT Spotlight:**

#### **Peter Diener**



Peter Diener, Assistant Professor of Research in the Coast 2 Cosmos Focus Area at the CCT, is a native of Skovlunde, Denmark. He joined the CCT in the fall of 2003.

Peter is currently working on many different projects, but there are two main ones to highlight. The first one is binary black hole evolutions and the second is an investigation into new techniques for the self-force problem in relativity. "Astrophysics has always interested me and astrophysical black holes are just the most fascinating and cool objects in the universe," said Peter.

To unwind, one thing Peter likes to do is play disc-golf. He said, "I have had one hole in one in my disc-golf career. This was on a short 128 feet hole on a course in Denmark playing a New Year tournament in below freezing conditions." Since Peter enjoys disc-golf so much, it is no surprise that his favorite gadget is his new Flow, a gold line frisbee from Latitude 64. "It's cool looking and has lots of glide," he said.

Mongolia is a favorite vacation spot of Peter's. He enjoys reading books by Isaac Asimov and Peter Hoeg. Peter's favorite album is "Amarok," composed by Mike Oldfield. Peter also enjoys music by Brandi Carlile, who sings his favorite song, "The Story."

Peter's prescription for life is "to enjoy my work but also take time to relax and recharge the batteries."

### **Pats on the Back:**

- Qin Jim Chen, Patrick Hesp, Honggao Liu, and Steve Brandt received an award from the NSF (through the Louisiana Board of Regents) titled "Research and Education Cyberinfrastructure Investments to Develop the Coastal Hazards Collaboratory in the Northern Gulf Coast." The award is for \$1,348,656 for three years.
- Thomas Sterling visited Sandia National Laboratories to participate in the next of a series of technical meetings with research staff and leadership at the CSRI related to the X-caliber Project under the DARPA UHPC Program. Sterling is the Co-PI of the LSU technical contribution as a partnering institution of the SNL-led X-caliber Project. Although short, the visit was highly productive, advancing the goals of the project measurably.

### **CCT in the News:**

#### **HPCC Conference Celebrates 25 Years**

Source: [insideHPC](#)

### **Lectures this week:**

#### ***TUESDAY—***

There will be a lecture on [“Dye Binding, Folding and Aggregation of Alzheimer's and Type 2 Diabetes Amyloid Forming Peptides Probed by All-Atom Molecular Dynamics \(MD\) Simulations” \(Computational Biophysical faculty candidate\)](#) by Chun Wu, University of California, Santa Barbara. The lecture will take place Tuesday, Feb. 22 at 1:00 p.m. in 210 Choppin Hall.

There will be a lecture on [“Composite And Hidden Order In F-Electron Materials And The Lessons We Are Learning”](#) (sponsored by LONI/LASiGMA) by Piers Coleman, Rutgers University. The lecture will take place Tuesday, Feb. 22 at 2:00 p.m. in 338 Johnston Hall

**WEDNESDAY**— There will be a lecture on ["Probing and Optimization of Functional Small and Bio-Molecules by All-Atom Molecular Dynamics \(MD\) Simulations"](#) (Computational Biophysical faculty candidate) by Chun Wu, University Of California, Santa Barbara. The lecture will take place Wednesday, Feb. 23 at 11:00 a.m. in 210 Choppin Hall.

**THURSDAY**— There will be a lecture on [“Electrostatic Mechanisms in Biology and Chemistry”](#) (Computational Biophysical faculty candidate) by Jana Shen, University Of Oklahoma. The lecture will take place Thursday, Feb. 24 at 1:00 p.m. in 338 Johnston Hall.

**Please Note:**

- The University will be closed Tuesday, March 8, 2011 for Mardi Gras holiday.
- Effective February 1, 2011, Mailing Services will **require** the use of Charge Slips with outgoing mail that we apply postage to. Charge slips include a bar code that allows Mailing Services to bill departmental budget codes in one easy step. This process will increase the efficiency and effectiveness of current and future mail operations. Please download the domestic and international forms at <http://pas.lsu.edu/mailling-services/forms>, and follow the instructions at the bottom of the forms. For any questions about this process, please contact Paul Ramirez ([pramire@lsu.edu](mailto:pramire@lsu.edu), 578-6086).
- This summer, CCT will host its second Research Experience for Undergraduates (REU), a nine-week program that gives students an opportunity to join interdisciplinary research groups and use the advanced cyberinfrastructure available on campus to work collaboratively on computational science projects. Each participating student will receive a stipend of \$4,500, free housing in University dormitories, and up to \$500 in travel expenses. Interested undergraduate students from any academic discipline are welcome to apply. Applications are due February 28, 2011, and students will be notified of whether they have been accepted by March 31. For more information or to see details on how to apply, please visit <http://reu.cct.lsu.edu/>.
- Prior approval is required for Special Meal Requests. Employees who make meal purchases without prior approvals may find that they must cover the cost of any monies spent for an unapproved event out of pocket, especially now that state funds are under a spending freeze. Please contact Susie Poskonka ([susie@cct.lsu.edu](mailto:susie@cct.lsu.edu)) prior to any special meal with visitor(s) to file the appropriate request for approval. Prior

approval could take up to one week, so please plan accordingly.

- Please remember to send your news concerning grants, awards, conferences, or other pertinent information to CCT Event Coordinator Jennifer Claudet at [jennifer@cct.lsu.edu](mailto:jennifer@cct.lsu.edu)
- Follow CCT with social media to access photos and see news, events or updated information. These pages are public; you do not need an account to view the information.
  - [Facebook group](#) : LSU Center for Computation & Technology
  - [Twitter](#) : LSUCCT
  - [YouTube channel](#) : LSUCCT

### **Upcoming Grant Deadlines:**

**Note:** Please check the [CCT deadline Web site](#), since it is updated daily.

#### [Research Experiences for Teachers \(RET\) in Engineering and Computer Science](#)

Supplements and Sites

February 28 2011 10:00 am

At Most \$ 500,000.00 available

#### [High Performance Computing System Acquisition: Enhancing the Petascale Computing Environment for Science and Engineering](#)

March 07 2011 10:00 am

At Most \$ 30,000,000.00 available

#### [Cyberinfrastructure Training, Education, Advancement, and Mentoring for Our 21st Century Workforce \(CI-TEAM\)](#)

March 16 2011 10:00 am

At Most \$ 1,000,000.00 available

#### [Cyber-Physical Systems \(CPS\)](#)

March 21 2011 10:00 am

At Most \$ 5,000,000.00 available

**\*\*\*NSF has revised proposal submission requirements** - a quick review of the changes are noted in this announcement:

[http://www.nsf.gov/pubs/policydocs/pappguide/nsf11001/gpg\\_sigchanges.jsp](http://www.nsf.gov/pubs/policydocs/pappguide/nsf11001/gpg_sigchanges.jsp)

Check the NSF website for announcements - [www.nsf.gov](http://www.nsf.gov)