

Educational Outreach and Knowledge-Transfer

Software Archive

www.mcc.uiuc.edu/software/

MCC's web-based Software Archive contains research and education codes intended as a shared resource to foster vibrant interactions, to encourage communication between the developers and end users, and to eliminate redundant code and algorithm development. Summer School codes (see middle right) are popular downloads. To date, the Archive has delivered more than 2,000 downloads to 800 users.

The Software Archive is a community service, and we invite and encourage all interested parties to contribute at www.mcc.uiuc.edu/software/.

Educational outreach and communication within the field of Computation Materials Simulation are integral parts of the Materials Computation Center (MCC). Our activities include:

- organizing and hosting schools and workshops
- actively networking with researchers and students, locally and worldwide
- creating and distributing useful tools and algorithms for research and education
- hosting a Software Archive for the Materials Science community
- supporting travel to Europe by young US researchers, and
- mentoring undergraduates in REU projects

Sponsoring Research Workshops

Research and educational networking for young scientists

The Travel Program, administered by David Ceperley (Physics), supports US-based students, postdocs, and faculty to travel to CECAM and PSIK activities. The goal of the program is to enable young scientists, particularly those from smaller institutions, to profit from related European activities and to foster international contacts. In first six months, we received more than 40 travel applications and supported 18 trips for researchers from 10 different institutions. The typical award was \$800.



Alan Aspuru-Guzik, 2004 Travel Program Awardee, attended the QMC Winter School, Trieste, Italy.

"...an invaluable experience for my graduate education..."

To faculty and organizers:

If you are co-organizing a meeting, please contact us four months in advance so we can add your event to our list.

If you know junior scientists who would like to attend, let them know about the Travel Program.

To young scientists:

We are offering travel awards to support students and postdocs to attend PsiK 2005, September 17-21, 2005, Schwäbisch Gmünd, Germany. Details will be posted at www.mcc.uiuc.edu/travel/.

Fostering cross-disciplinary research activities

Now in its fourth year, the Understanding Complex Systems (www.how-why.com/ucs) symposium collects researchers from many academic disciplines to stimulate research involving complex systems.



The organizers, headed by Alfred Hübler (Physics), have grown the event from 35 talks in 2001, to 110 in 2004. This year's event offered hands-on tutorials and dozens of poster sessions to nearly 400 registered participants. Video conferencing and audio recordings further widen the possibilities for participation, both by speakers and by attendees.

Summer Schools

www.mcc.uiuc.edu/summerschool/

Each year, the two-week Summer School brings together leading faculty, students and researchers from different disciplines, with varied and necessary expertise. MCC has co-hosted schools on:

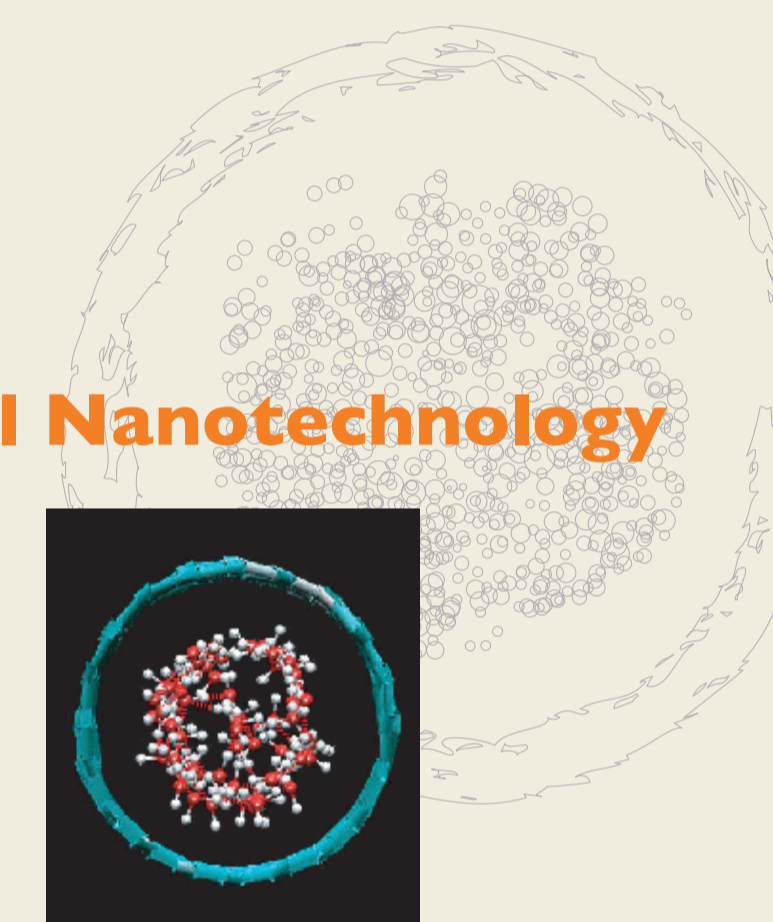
- 2004 Computation Nanotechnology
- 2003 Computational Biophysics
- 2002 Device Simulation/MEMS
- 2001 Computation at the Nanoscale

2004 Summer School on Computational Nanotechnology

This year's School includes 66 participants, 15% of which are women. The attendees come from India, France, Nigeria, Taiwan, Korea, Singapore, Italy, Scotland, and Spain; two-thirds are from across the US. Most are graduate students, but several faculty and staff are also attending.

—Umberto Ravaioli

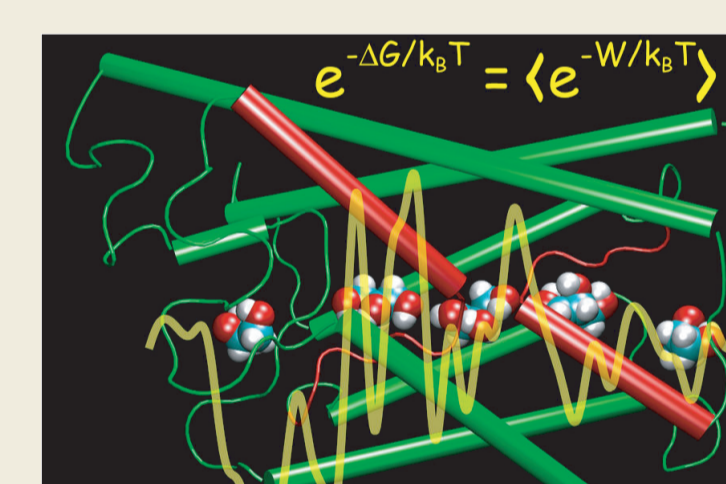
Professor of Electrical and Computer Engineering and Summer School Organizer



Visualization of MD result of H₂O in carbon nanotube by N. R. Aluru (UIUC), one of the 2004 Summer School invited speakers.

2003 Summer School on Theoretical and Computational Biophysics

Medical and biological sciences require modeling to understand life processes and measured data. Modeling molecular processes of biological cells is a craft and an art. While theoretical and computational skills can be learned by training, meaningful application is achieved only with experience.



Learning to simulate the thermodynamic structure and properties of proteins and bio-molecules.

Our Summer School on Theoretical and Computational Biophysics (co-organized by Klaus Schulten and others) taught the craft and art of modeling via learning by doing.



Lectures (with audio), notes, and labs may be found at www.mcc.uiuc.edu.

93 participants came to Illinois to stretch proteins, pull water through molecular channels, mine genomic data, build their own computer cluster, and study a favorite biomolecule.

Developing Tools and Educational Codes in Computational Materials Science

MCC is developing robust and efficient tools for visualization, analysis, and education. Software is created using many open-source tools, and is designed to run on a wide variety of platforms.

Code development by J.N. Kim, D. M. Ceperley, R. M. Martin and D.D. Johnson

MCC codes were the foundation for an APS short course (March 2004) on computational methods, given by Jeongnim Kim and Richard Martin, and for Summer School lectures and labs. Many codes are available on the Software Archive.

