Materials Computation Center

Providing world-class, multidisciplinary education and research in Computational Materials Science through a collaborative effort amongst faculty from 10 departments
University of Illinois at Urbana-Champaign • Funded by NSF DMR 03-25939 • www.mcc.uiuc.edu

As the Computational Materials Science discipline affects all fields of Science and Engineering, the Materials Computation Center (MCC) is actively developing powerful, leading-edge tools to analyze and predict the properties of materials. MCC provides an intellectual and interactive environment for students, teachers, and researchers focused on world-class, multidisciplinary education and research in Computational Materials Science.

We achieve the MCC goals through:

- multidisciplinary education and research across traditional boundaries
- active networking of researchers and students, locally and worldwide
- creating useful tools and algorithms for research and education
- hosting a Software Archive for the Materials Science community
- applications to challenging problems in materials research.

MATERIALS RESEARCH, COMPUTATIONAL TOOLS & ALGORITHMS

Research falls into three areas:
- Quantum Simulations
- Complex Systems and Phase Transformations
- Computer Science and Scaleable Parallel Methods for Materials Modeling

EDUCATION AND KNOWLEDGE-TRANSFER

By sponsoring the Visitor Program and Summer School series, MCC brings together leading faculty, students and researchers from different disciplines, with varied and necessary expertise. MCC has hosted schools (www.mcc.uiuc.edu/summerschool) on:

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

Other recent outreach activities include:
- an APS course on computational methods
- a three-day symposium, Understanding Complex Systems
- co-sponsoring REUs for multiple departments

COLLABORATION & NETWORKING

MCC is actively collaborating with similar efforts in Europe, such as PSI-k and CECAM, and with DOE, DOD, and NIST Laboratories. Equally important is the education focus of the MCC. As a part of the Center, we have developed graduate-level training modules on various topics in computational materials science: These modules and other codes are distributed through MCC’s Software Archive. (www.mcc.uiuc.edu/software/)

THE 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.

The Software Archive is a community service, and we invite and encourage all interested parties to contribute.