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

"I felt that I would actually learn to do things and not just learn that they existed."

— Ana Vila Verde, physics graduate student
University of Minho, Portugal
2003 Summer School Participant

Other recent outreach activities include:

- an **APS course on computational methods**
- a three-day symposium, **Understanding Complex Systems** (**www.how-why.com/ucs**)
- co-sponsoring REUs for multiple departments

COLLABORATION & NETWORKING

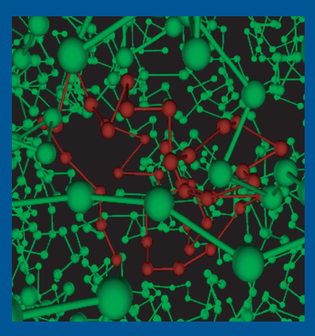
MCC is actively collaborating with similar efforts in Europe, such as PSI-k and CECAM, and with DOE, DOD, and NIST Laboratories. Equally important is the education focus of the MCC. As a part of the Center, we have developed graduate-level training modules on various topics in computational materials 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.

POLYMER SHAPES IN MULTICOMPONENT SOLUTIONS



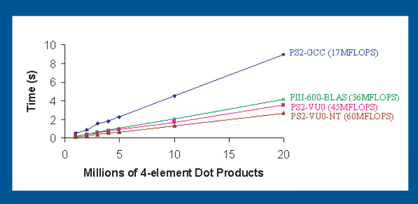
Erik Luitjen
We develop and apply new algorithms for simulations to study polymer shape changes in solutions containing several types of polymers. At certain temperatures and concentrations, such a solution exhibits phase separation. We found that phase separation leads to a radical change of the polymer shapes.

HIJACKING THE SONY® *PLAYSTATION 2*® (PS2) FOR COMPUTATIONAL CHEMISTRY

Todd J. Martínez , Sanjay Patel, and Eric de Sturler

We are developing quantum chemical and linear algebra software to use new generations of game consoles as supercomputers that even high schools can afford.

The Quantum Chemistry package GAMESS has been ported to the PS2, and several PS2s can be run in parallel using MPI.



The PS2 (blue) outperforms the fastest 2003 Pentium III (green) in linear algebra tests.

EDUCATION AND OUTREACH

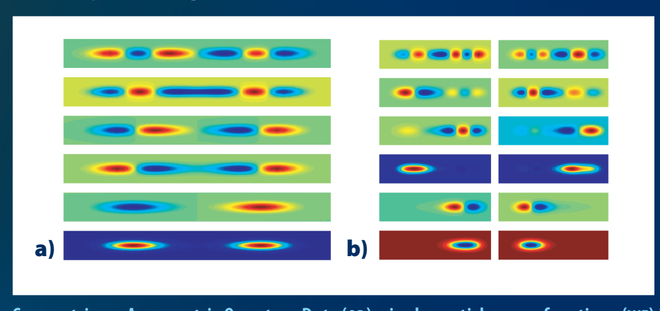
Our two-week 2003 Summer School on Theoretical and Computational Biophysics (organized by Klaus Schulten with eight other lecturers) taught the craft and art of modeling to over 90 participants from 23 countries. (www.mcc.uiuc.edu/summerschool/)

Over 390 researchers and students attended the Understanding Complex Systems tutorials, hosted by the MCC and the Center for Complex Systems Research. (www.how-why.com/ucs2004)

SPINTRONICS IN QUANTUM DOTS

J.-P. Leburton and R. M. Martin

We focus upon understanding of many-body effects in semiconductor quantum dots (QDs) for applications in quantum information processing.

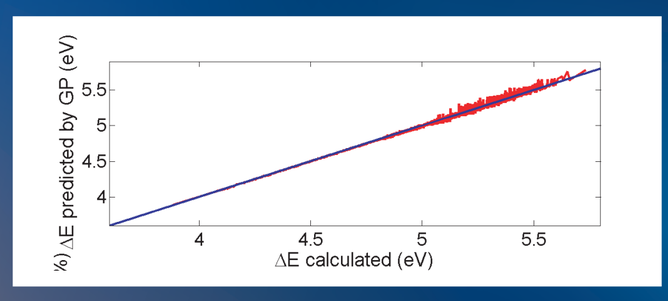


Symmetric vs. Asymmetric Quantum Dots (QD): single particle wave functions (WF) in a symmetric (a) and asymmetric (b) coupled QD. In a) the WFs are identical for both spins, while in b), the left and right panels are for spins up and down.

MACHINE-LEARNING TO PERFORM MULTI-TIMESCALE KINETIC MODELING

Duane D. Johnson and David Goldberg

We have devised a machine-learning strategy to get kinetic barriers based on concepts of evolution: Genetic Programming (Genetic Algorithms that evolve computer programs) is used to regress functions that predicts all diffusion barriers from a extremely limited set of calculated barriers.



Predictions vs. calculations: The GP-predicted (red) versus calculated energy barriers (blue) for 8196 barriers at surface of fcc $Cu_{50}Co_{50}$ alloy. GP used as few as 25 barriers to learn all barriers, whereas simple basis-set regression is not possible.

For details and other research results, visit www.mcc.uiuc.edu/research/nsfnuggets/.

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