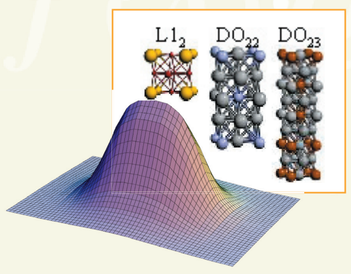
Training the Computational Materials Science Community

Summer Schools

An important training activity is the annual Summer School, held on the campus of the University of Illinois at Urbana–Champaign. Participants include faculty, students, and postdoctoral researchers. Instructors from come from industry, labs, and universities around the country and abroad.

2005



Left: H_2 Density, taught by Don Hamann. Right: DFT energies, covered D. Johnson

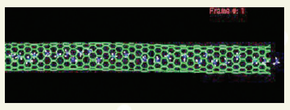
Introduction to Electronic Structure and Thermodynamics Calculations of Real Materials

Participants obtained hands-on experience for the accurate use of *ab initio* electronic structure methods for calculating properties of real molecular, semiconductor and metallic systems. Participants learned via open-source TBPW, SIESTA and ABINIT codes, for use back at their home institutions, and taught by the software developers themselves. During week two, participants experienced *ab initio* thermodynamics via cluster expansion methods. They received hands-on training to determine reliable structural energies in real alloys and to utilize such information to predict phase stability and diffusion, taught by key developers in the field. Presentations (audio, video, and slides synchronized by DoD) are available on the MCC Summer School website.

Support from co-PI: David Ceperley, NSF (CRCD) EE-0088101.

School participants learn from each other:
Graduate students Amy Berta (UW-Madison) and Federico Iori (University of Modena-Reggio, Emilia, Italy) work on a tutorial problem during the second week of instruction.

2004



Simulating gas diffusion in a carbon nanotubes using molecular dynamics in the lab taught by Susan Sinnott

Introduction to Computational Nanotechnology

Computational applications in nanotechnology requires working knowledge of interdisciplinary approaches, involving physics, chemistry, engineering, and computer science. This year's school provided theoretical instruction and practical computational experience on such topics as density functional theory and band structure calculations, numerical methods, carbon nanotubes, nanoelectronic and molecular devices, transport with non-equilibrium Green's functions, nanofluidics and Nano-Electro-Mechanical Systems, and charge transport in ionic channels. Several computer sessions were based on software residing of the nanoHUB portal of the NSF Network for Computational Nanotechnology (NCN) at www.nanohub.org.

Co-support obtained from NSF NCN by U. Ravaioli and CRCD by D. Ceperley EE-0088101.

2003

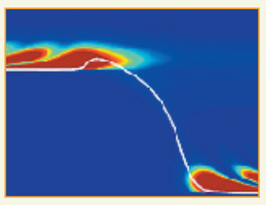
Diverse participants:
- **71 US-based, 22 international**
- **25 women, 68 men**
- **66 institutions**
- **66 graduate students**
- **13 post-docs, 7 faculty**

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. Although theoretical and computational skills can be learned by training, meaningful applications is achieved only with experience. 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.

Support from co-PI: David Ceperley, NSF (CRCD) EE-0088101. Co-support obtained from NIH by K. Schulten.

2002



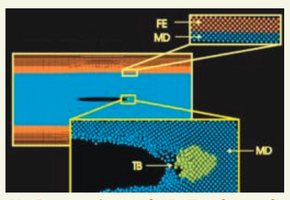
Potential change across interface in nano-transistor, M. Lundstrom.

Computational Approaches for Simulation of Electron Devices and MEMS

Electron devices and Micro-Electro-Mechanical Systems (MEMS), i.e. micro-machines, are ubiquitous in computers and nano-technology devices, such as biosensors. Modeling devices for design purposes require theoretical and computational skills and meaningful applications achieved with experience. This school taught the background and provided software to model MEMS via learning by doing. Participants came to conduct electrons through carbon nanotubes and nano-transistors, and move electrons through molecular resistors.

Support from co-PI: David Ceperley, NSF (CRCD) EE-0088101.

2001



N. Bernstein et al., B. Tuttle et al.

Tools for Multiple Length and Time Scale Simulations

What properties arise from cracks or interfaces? Participants simulate atomic-scale effects using Molecular Dynamic (based on empirical or quantum potentials) and continuum methods (e.g., finite-elements) determining properties and responses and their origins. This school introduced and developed the concepts and tools for simulating atomic, molecular, and bulk systems to predict experimental properties of materials. We also developed knowledge of necessary theoretical and high-performance computing skills, as well as meaningful applications through experience. Students, post-docs and faculty came from worldwide to defect and diffuse material, accelerate and extend time, couple atomic and continuum scales, and handle bigger systems sizes using high-performance computing.

Support from co-PI: David Ceperley, NSF (CRCD) EE-0088101.

Quotes from Participants

ABOUT THE INSTRUCTORS

"Your scientific passion encouraged me a lot. You are a greater tutor than I thought."

"It was first time that I learned DFT from a lecture. My brain was refreshed and well ordered."

"I especially found going through OUTPUT files with him helpful since I learned what he searches for in output and what he finds helpful."

COLLABORATION WITH OTHERS

"Teamwork in lab truly encourages networking."

"I found it helpful learning with discussing with different neighbors each times."

"I met a lot of important people in the field and people around the world. The lab sessions are practical and useful. I just hope that there would be more social events and a longer summer school."

Over the past five years, the Summer Schools included:
- *15–36% women*
- *5–10% faculty*
- *22–37% international participants*

CONTINUING TO LEARN

"I have a feeling I will be reading his lecture for many months to come..."

"One of the best parts about this school has been learning other computational techniques that I didn't know were out there."

"Great information!! Having handouts is very helpful. It is even more helpful that the handouts are all on the website and that we can download them and the lab materials. I'm also looking forward to seeing the videos online. This will really help me continue to learn all of this information after I leave the summer school."

"Great presentation! His talk gave a lot of great information to look over at home. The toolbox is a great idea and hopefully many others will add to it."

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Materials Computation Center

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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. The MCC provides an intellectual and interactive environment for students, teachers, and researchers focused on world-class, multidisciplinary education and research in Computational Materials Science.

www.mcc.uiuc.edu

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