The Materials Computation Center

Funded by NSF Division of Materials Research (ITR grant 03-25939)

Duane D. Johnson and R.M. Martin
at the Frederick Seitz Materials Research Laboratory
University of Illinois Urbana-Champaign

MCC Affiliates and Departments

(Chemistry) Todd Martinez (Co-Director) (CS) Eric de Sturler
(ECE) Jean-Pierre Leburton, Sanjay Patel (GE) David Goldberg
(MatSE) Pascal Bellon, Erik Luijten Duane D. Johnson (Director)
(MIE) Narayan Aluru (TAM) Robert Haber
(Physics) David Ceperley (travel program), Karin Dahmen, Alfred Hubler, Richard Martin

(MCC) Jeongnim Kim (Coordinator, NCSA/MCC), Amy Young (Webmaster)
(MRL) Kris Williams (Networking), Ramona Simpson (Secretary)
Interactions with others, e.g., Umberto Ravioli (ECE), G. Paulino (CEE), P. Guebelle (AAE)

Programs: Computational Science and Engineering Program (CSE)
National Center for Supercomputer Applications (NCSA) *summer schools*

The Materials Computation Center

http://www.mcc.uiuc.edu

Computational Materials Science has emerged as an important discipline that impacts all areas of science and engineering.

The MCC provides *world-class, multidisciplinary* education and research in Computational Materials Science (CMS) through a unique *collaborative* effort amongst faculty from 10 departments.

¬ The MCC fosters an interactive environment and facilities for students and researchers focused on **quality research, applications, software development, and education**:

- providing analysis, understanding, and prediction materials properties and serves as a bridge between theory and experiment.
- algorithms in conjunction with new theoretical developments, modern computer science approaches, and experiments, at the *forefront of scientific computing*.

To accomplish our long-term goals and address challenging problems in materials research there must be:

- **education** of future CMS scientists,
- **knowledge-transfer and networking** activities related to research,
- **creation and distribution of useful tools** for research applications.

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MCC has ***three main thrust areas*** based upon ***three main research themes*** for the computational, algorithmic and applications goals.

I. Collaborations/Networking Thrust: with groups around nation and world.

II. Education and Knowledge-Transfer Thrust involving:

–**Summer Schools and Graduate Education Materials:** Develop/disseminate CMS courses (web).
–**Research Workshops:** here and, e.g., with CECAM and PSI-k and APS. Support student travel.
–**Software Archive® at http://www.mcc.uiuc.edu**

III. Materials Research, Computation Tools and Algorithm Thrust

Theme 1: Quantum and Classical Simulations
Theme 2: Complex Systems and Transformations
Theme 3: Computer Science and Scaleable Parallel Methods for Materials Modeling

- Challenging problems that ***warrant extended multidisciplinary efforts***.
- Creation of ***computational tools*** that help address challenging problems.
  * Making freely available and maintaining documented, tested codes.
- Collaborative efforts to ***develop new, practical, and efficient algorithms***.
  * Well-written, modular codes with well-defined data structures.
  * Algorithms for parallel and scalable-parallel architectures. Scaling up algorithms.

The MCC Education and Knowledge-Transfer Activities

Examples, not comprehensive (see website)

Two-week Summer Schools *on web: lectures, labs, audio*

Board (D. Ceperley, D.D. Johnson, J. Kim, R.M. Martin, T.J. Martinez, E. de Sturler) chooses topic and organizer is found.

2004 "Computational Nanotechnology" organizer U. Ravioli
2003 "Theoretical and Computational Biology", organizer K. Schulten
2002 "Simulation of Electron Devices and MEMS", organizer N. Aluru
2001"Tools for multiple Length and Time Scales", organizers (board)

Other Outreach, Networking, and Workshops

"EU/US KKR Electronic-Structure Workshop (February 2004) organizers D.D. Johnson and H. Ebert (Technical U., Münich).

"Understanding Complex Systems Symposia" 2001-2004, organizer A. Hubler with K. Dahmen, D.D. Johnson, and others in physics, biology, etc (on-line lectures/voice).

"Novel Simulation Methods for Soft Condensed Matter Systems" (CECAM, Lyon, June 2004) organizer E. Luijten.

Most/All co-PIs have contributed as lecturers, organizers, etc., for these activities!

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The Materials Computation Center *Summer Schools*

on *Theoretical and Computational Biophysics*

with CRCD: David Ceperley, University of Illinois, EE-0088101

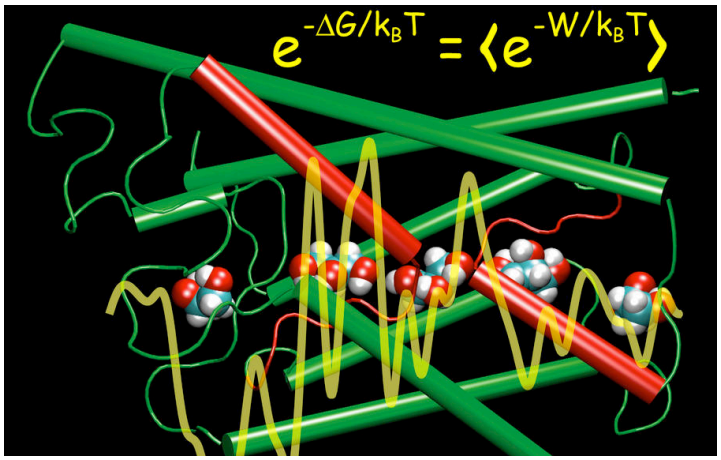
Education and Outreach (2003)

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 applications is achieved only with experience.

Our School on ***Theoretical and Computational Biophysics*** (co-organized by Klaus Schulten and others) taught the craft and art of modeling via ***learning by doing***. 93 participants came to Illinois to stretch proteins, pull water through molecular channels, mine genomic data, build their own computer cluster, study a favorite biomolecule… After morning lectures, afternoons were devoted to *learning by doing*, using 300 pages of tutorials in laboratories humming with computational biology software.

Web-published Lectures (with audio), Notes, and Labs, and contributing Lecturers may be found at

http://www.mcc.uiuc.edu



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

Attended by **71 US-based** and **22 non-US-based people**, with **25 women and 68 men, from 66 institutions**, consisting of 66 graduate students, 13 post-docs, 7 faculty, and 1 undergraduate student.

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The Materials Computation Center *Travel Program*

administered by David Ceperley (with advisory board and NSF)

Web-application at *http://www.mcc.uiuc.edu*

The MCC supports US-based students, postdocs, and faculty to travel to CECAM and PSIK activities.

Goals: Profit from related European activities and foster international contacts.

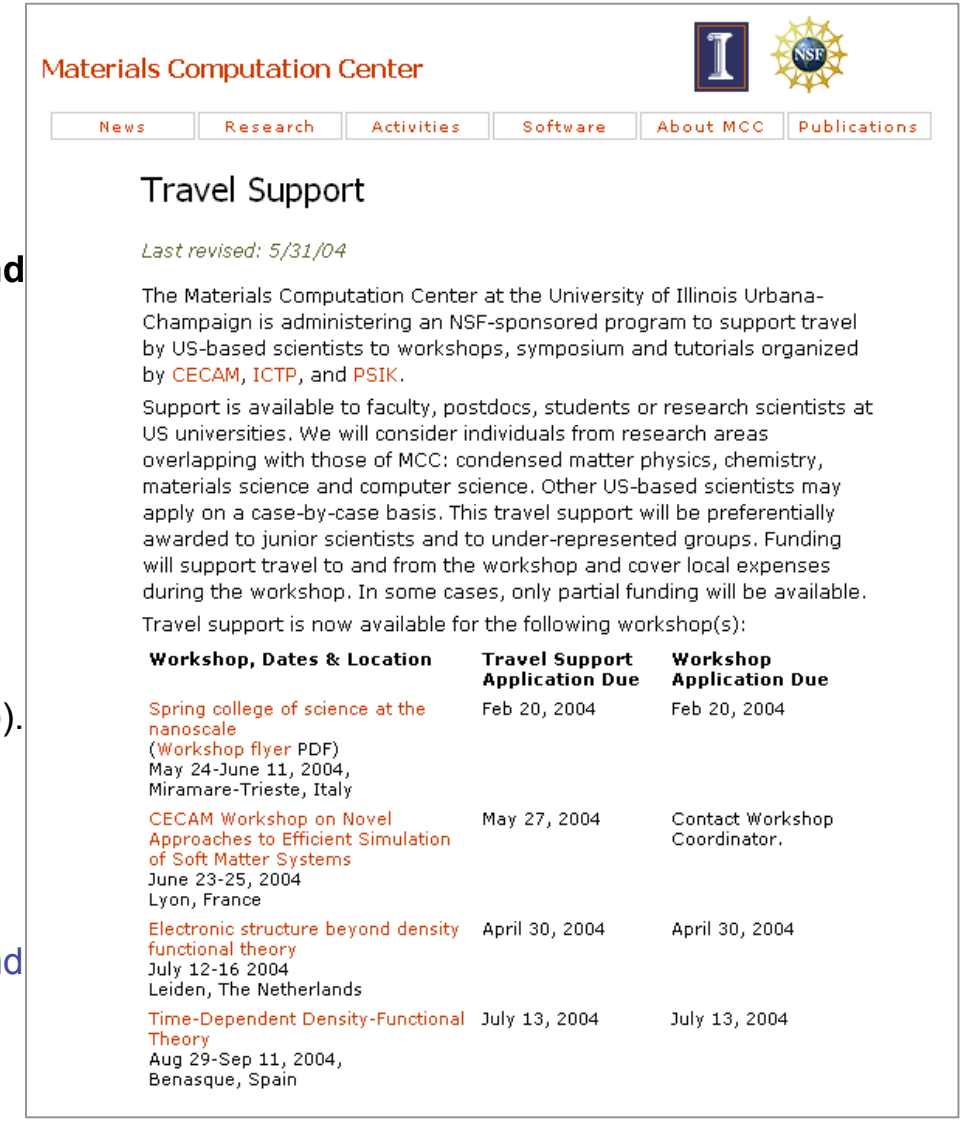
Younger scientists from smaller institutions particularly encouraged to apply.

Yearly budget is $23K. Typical award is $800.

If you are co-organizing a meeting:

- Let us know 4 months in advance to list it (see web).
- Inform junior scientists who would like to attend about our program.

In first 6 months, more than 40 travel applications and 18 supported trips from 10 different institutions.



Materials Computation Center

News | Research | Activities | Software | About MCC | Publications

Travel Support

Last revised: 5/31/04

The Materials Computation Center at the University of Illinois Urbana-Champaign is administering an NSF-sponsored program to support travel by US-based scientists to workshops, symposium and tutorials organized by CECAM, ICTP, and PSIK.

Support is available to faculty, postdocs, students or research scientists at US universities. We will consider individuals from research areas overlapping with those of MCC: condensed matter physics, chemistry, materials science and computer science. Other US-based scientists may apply on a case-by-case basis. This travel support will be preferentially awarded to junior scientists and to under-represented groups. Funding will support travel to and from the workshop and cover local expenses during the workshop. In some cases, only partial funding will be available.

Travel support is now available for the following workshop(s):

Workshop, Dates & Location	Travel Support Application Due	Workshop Application Due
Spring college of science at the nanoscale (Workshop flyer PDF) May 24-June 11, 2004, Miramare-Trieste, Italy	Feb 20, 2004	Feb 20, 2004
CECAM Workshop on Novel Approaches to Efficient Simulation of Soft Matter Systems June 23-25, 2004 Lyon, France	May 27, 2004	Contact Workshop Coordinator.
Electronic structure beyond density functional theory July 12-16 2004 Leiden, The Netherlands	April 30, 2004	April 30, 2004
Time-Dependent Density-Functional Theory Aug 29-Sep 11, 2004, Benasque, Spain	July 13, 2004	July 13, 2004

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Materials Computation Center *Sponsored Workshops*

Understanding Complex Systems Symposium – UCS 2004

With organizer: Alfred Hubler

Education and Outreach (2004)

This *MCC-supported* symposium, originated by Alfred Hubler in 2001, brings together researchers from many academic disciplines and industry to ***stimulate cross-disciplinary research activities involving complex systems***. This event has continued to grow steadily each year and this fourth year we had 400 participants over 4 days. The organizers provide information about funding opportunities for complex systems research and promote linkages for interdisciplinary proposals.

- **Speakers introduce key complex systems concepts in the context of their discipline.**
- **Invited plenary talks are on a 'Scientific American' level.**
- **Three hands-on tutorials are in parallel with technical sessions, covering the most recent research findings.**
- **Lectures are on-line with audio accompaniment.**

http://www.how-why.com/ucs2004/

Invited Speakers	Total Talks	Registered Participants	No. Days
2001	35	130	2
2004	**110**	**396**	**4**

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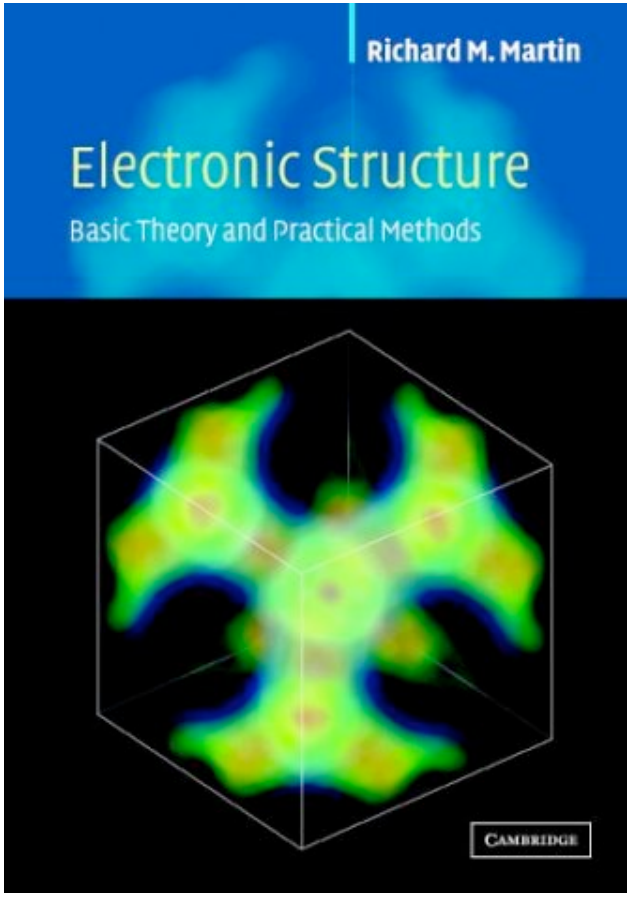
Resources for Electronic Structure

Organized by R.M. Martin (PI)

Dynamic resource hosted by the MCC



References point to extended material at the *MCC and ElectronicStructure.org*

ElectronicStructure.org

Resources for Electronic Structure

- Research Groups
- Research Centers
- Software
- Courses
- Other useful sites

- Book Website
- Figures & images

MCC

- Schools
- Events calendar
- Career Opportunities
- Software

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The MCC Software Archive©

http://www.mcc.uiuc.edu

Maintained by Amy Young (MCC webmaster)

Sponsor of a web-based *Software Archive*

For a shared resource for CMS community and to foster and encourage interaction and reduce redundancy.

On the Archive Page

Welcome to the MCC Software Repository

For information about posting your code on the Archive, email mcc@uiuc.edu

Software posted is made available to (and from) the Computational Materials Community. The software will be either readily accessible or access will be controlled by the author(s) of the software. You will be asked to register for each software you wish to download.

Instructional Analysis DFT_Electronic_Structure
Classical/Quantum_Simulation Summer_School

- *Software can be found by specific search of type or area*
- *Authors **retain ownership** and, if desired, **control over dissemination**.*

Please consider contributing to the Software Archive.

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The MCC Software Archive

http://www.mcc.uiuc.edu

Maintained by Amy Young (MCC webmaster)

Examples Instructional

CLAMPS
Classical Many-Particle Simulator
Author: ***David Ceperley***, UIUC
Date of submission: 10/10/2000

OHMMS
Object-Oriented High-Performance Multiscale Materials Simulator
Author: ***Jeongnim Kim, MCC***
Date of submission: 12/12/2001

Examples DFT_Electronic_Structure

PARSEC
Pseudopotential Algorithm for Real-Space Electronic Calculations.
Author: ***Jim Chelikowsky***, U. of Minnesota
Date of submission: 6/14/2002

TDDFT
TD-DFT in the LDA approximation using real-time and real-space methods, i.e.without basis sets.
Author: ***George Bertsch***, U. of Washington
Date of submission: 6/10/2002

The MCC Software Archive

http://www.mcc.uiuc.edu

Maintained by Amy Young (MCC webmaster)

Examples Classical/Quantum_Simulation

CEIMC
Coupled Electronic-Ionic Monte Carlo
Author: ***Mark Dewing***, NCSA
Date of submission: 1/1/2002

Digital Material
An extensible modeling and software infrastructure for support of the representation and simulation of structure and evolution across multiple length and time scales.
Author: ***James Sethna***, Cornell University
Date of submission: 5/30/2002

Examples Summer_School_Codes

Labs from "Spanning Multiple Length and Time Scales (2002)"

Eric de Sturler Lab and Lectures
Iterative methods for eigenvalue problems
Author: ***E. de Sturler, MCC***
Date of submission: 2/5/2002

Tim Germann Lab and Lectures
Hyperdynamics Lab
Author: ***Tim German, LANL*** (MCC)
Date of submission: 2/7/2002

Software Archive has many more

Funded by NSF DMR 03-25939

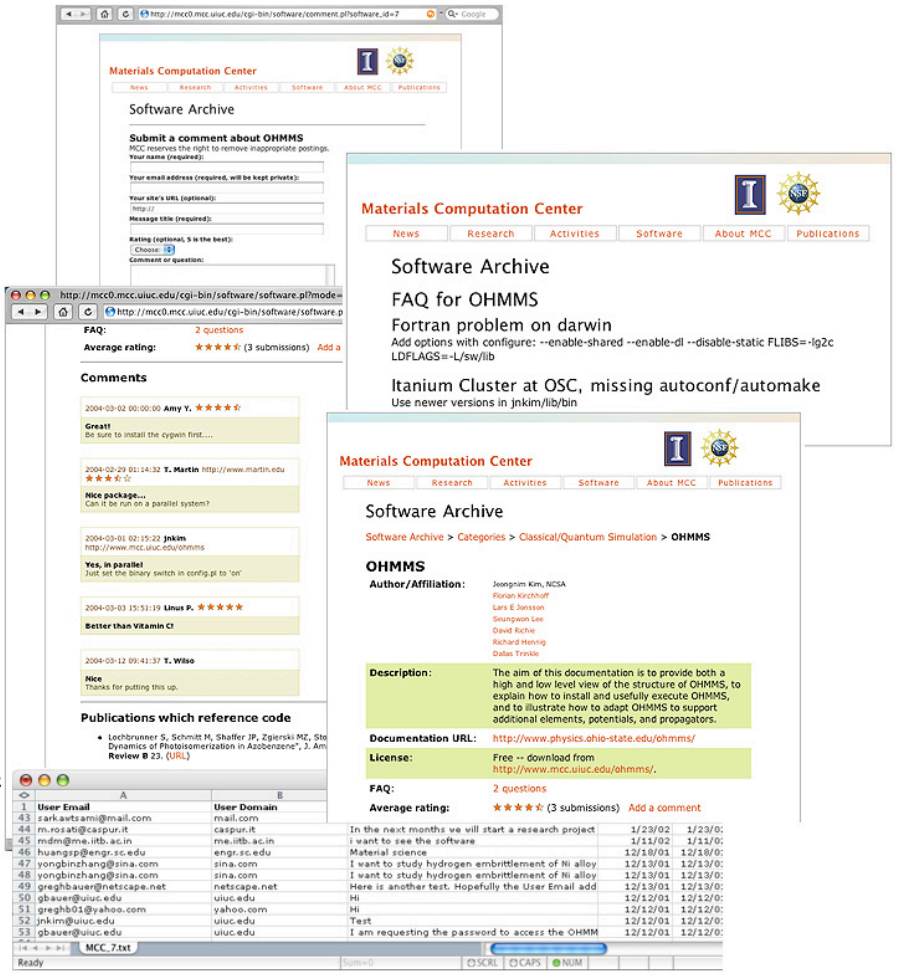
Expanding functionality

Additional benefits to Users:
- can submit tips for other users (install instructions, platform specific questions, etc.)
- can submit comments/ratings

New features for Authors:
- view download stats over the web, or download tab-delimited files
- maintain dialogue with users via FAQs and

Comments
- provide list of publications based on software
- can supply additional files (older versions, supporting docs, images, etc.)

Both are currently supported.



Materials Research, Computational Tools, Algorithms, and Resources

In what follows, the MCC activities are highlighted, with some examples and inter-collaboration required for development and applications.

- *Portable* Materials Simulations Toolkits
  J. Kim, D.M.Ceperley, D. D. Johnson, and R. M. Martin

- Hijacking *Game Consoles* for Computational Chemistry
  T. Martínez, E. de Sturler, and S. Patel

- Electronic-Structure Tools & Applications
  TD-DFT and Nanodevices: **R.M. Martin and J-P Leburton (w/ I. Vasiliev and J. R. Chelikowsky)**
  TD-DFT Chemistry: **Todd J. Martinez (GP: Johnson and Goldberg, Linear-Algebra: de Sturler)**

- *Multiscaling Method* via *Genetic Programming*
  D.D. Johnson, D.E. Goldberg., P. Bellon, T. Martinez

- *"Dynamical" Methods*: e.g. *Geometric Monte Carlo*
  P. Bellon and E. Liujten

See Poster Session for these and more.

Portable Materials Simulations Toolkits

J. Kim, D. D. Johnson, D.M.Ceperley, and R. M. Martin

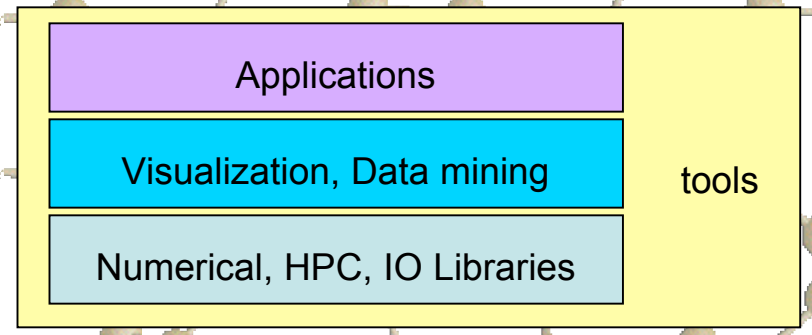
Motivations and goals:

- **No Standard Environment exists.**
  > Reduce researcher's "learning curve" for useful applications of techniques/codes.
- **Combine ever-better hardware with new software engineering technology**
  > Powerful materials simulation tools
- **Use of standard, open-source software**
  >Dynamic, maintainable and adaptable scientific code development
- **Use of standard IO**
  >Communications between diverse appl.
- **Use of standard tools**

e.g., Compilers: C/C++, OpenMP
Documentation: deoxygen
Cmake and GNU autoconf/automake/libtool

>Portability in changing HPC environment

- **Use of standard tools**
  >*Availabilty via Software Archive©*



Guiding principles:

- **Standard libraries and components.**
- **Open-source development**

Current status:

- **OHMMS, qmcplusplus, atomicHF, TBPW…**
- **Standard IO based on XML/HDF5**
  e.g. HDF at http://hdf.ncsa.uiuc.edu
- **Data analysis and visualization tools:**
  e.g. DataSpork© and MatSimViz©
- **Open source utility tools**

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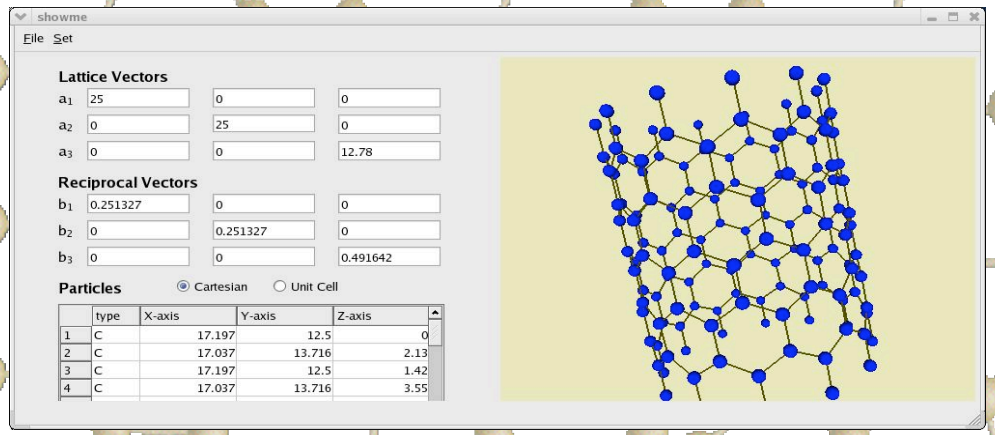
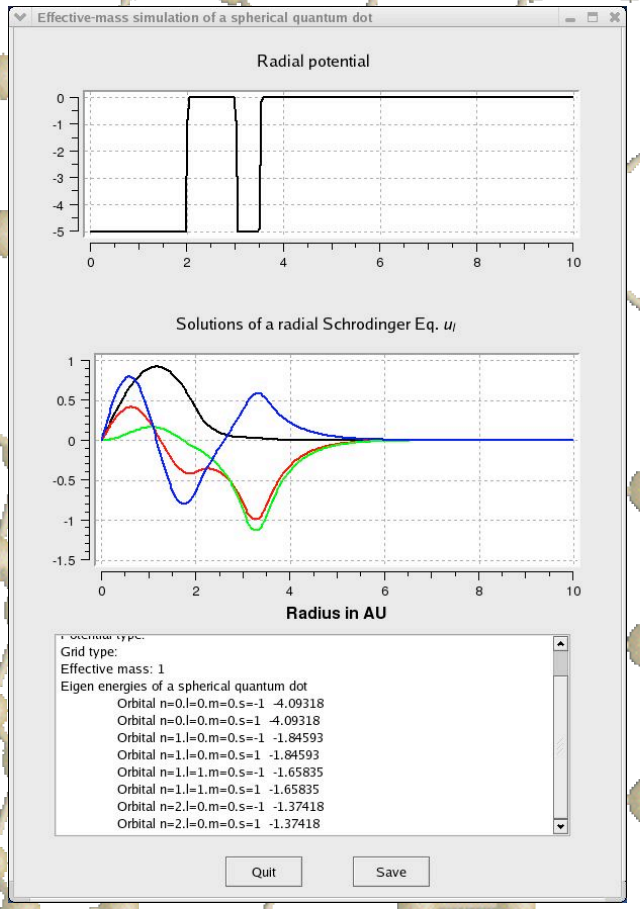
Portable Materials Simulations Toolkits

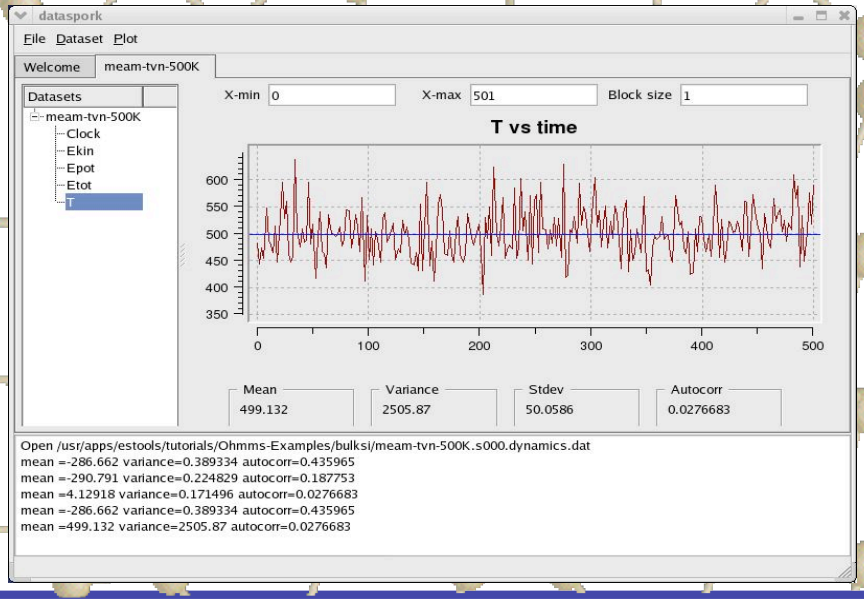
Preparing materials simulations



Visualizing simulations



Analyzing and mining data



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Hijacking Game Consoles for Computational Chemistry

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

See Poster

YOU Choose!

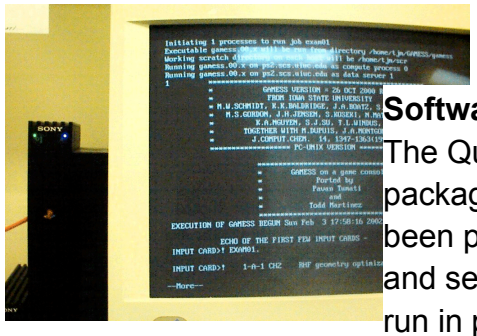
- Expensive, high-performance, proprietary computers.
- Beowulf clusters build of commodity-off-the-shelf parts.

or

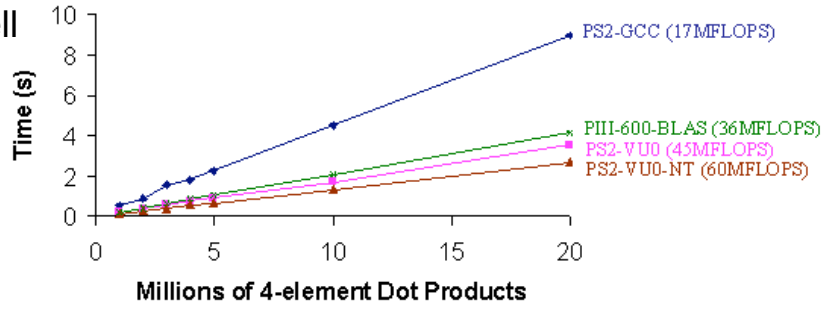
- **Video game consoles, providing higher potential performance at a lower cost by using GPU**, since today's video games are physics simulations, and graphics involves many of the same linear algebra operations used there**.**

- Sony sold 60M PS2 consoles in 2002, while Compaq, Dell and IBM *together* sold only 50M PCs.

- **We have harnessed the power of Sony's Playstation2 (PS2) for scientific calculations.**
- ***The PS2 processor can do up to 5x as many floating point operations per second as a Pentium III*.**
- We are developing quantum chemical and linear algebra software to use game consoles as *supercomputers* ***that even high schools can afford*!**



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



PS2 Performance: The PS2 outperforms the fastest Pentium III (2001) in linear algebra tests. Hardware-optimized linear-algebra routines for the PS2 will be made publicly available through the Software Archive.

Work has led to collaboration with IBM – RA at IBM for summer 2004!

17-20 June 2004
Website: http://www.mcc.uiuc.edu

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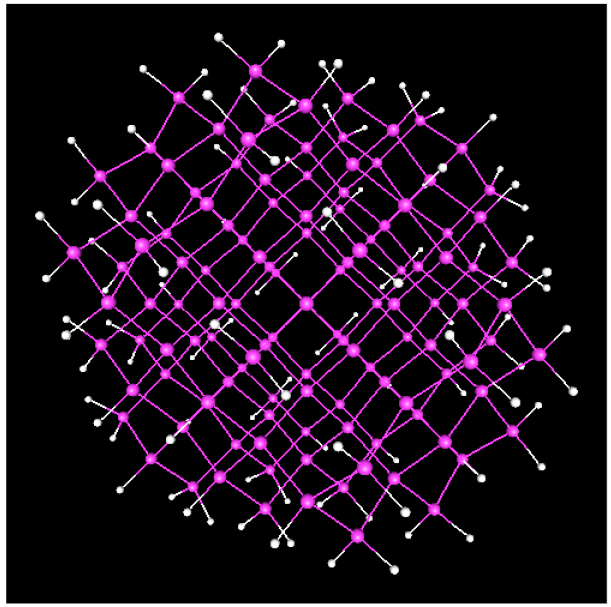
Electronic-Structure Tools & Applications

- Pedagogical Codes
- Density Functional Theory
- Time-Dependent DFT
- Quantum Monte Carlo

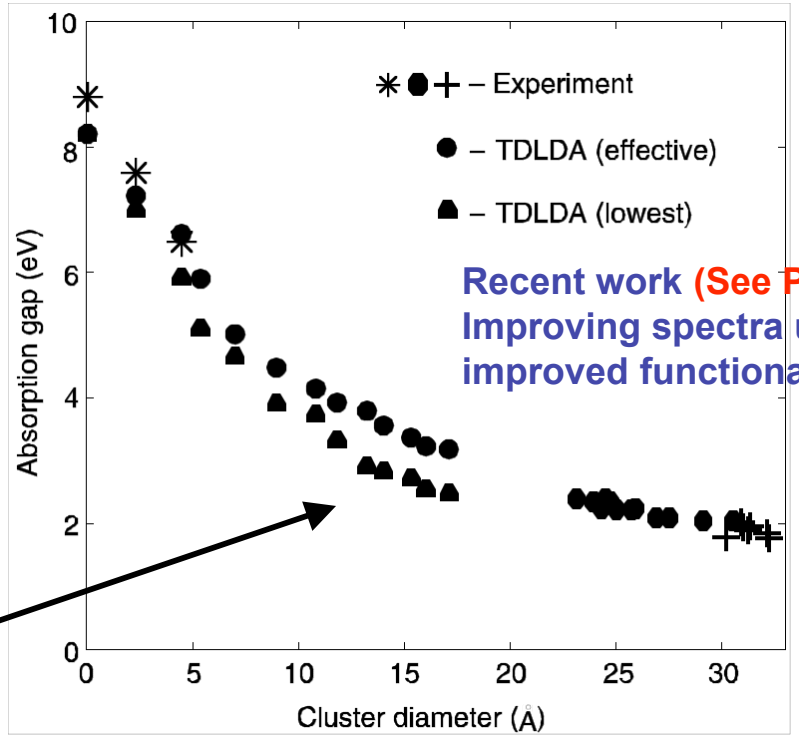


Example of cluster: $Si_{123}H_{100}$ or $Ge_{123}H_{100}$

Example using DFT and TDDFT

Predicted TDFT optical gaps vs. Si-cluster size

I. Vasiliev, R. M. Martin, J. R. Chelikowsky



Recent work (See Poster)
Improving spectra using improved functionals

New Thrust (R. Haber, D.D. Johnson, R.M. Martin, *with CPSD-ITR tools*)
Using methods from Discontinuous Galerkin FEM to solve TD-DFT

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Electronic-Structure Tools & Applications

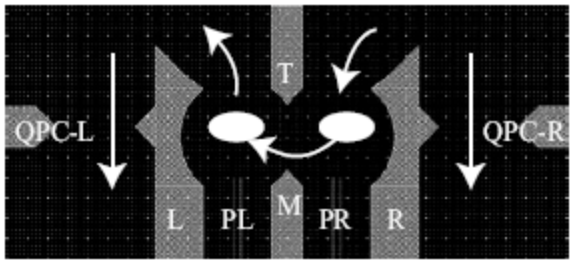
R.M. Martin and J-P Leburton

New Methods and Connections

Simulation of electrons by *QMC* with all interactions and applied gate potentials simulated by classical *Green Function MC*.

Nanoscale quantum device: Comparison of DFT vs QMC

Top View

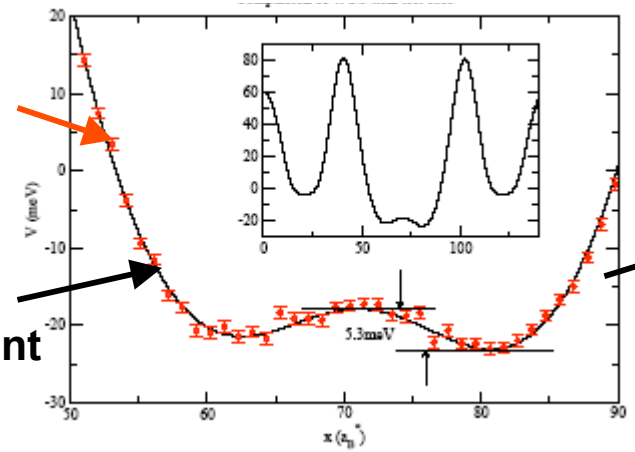


Actual device

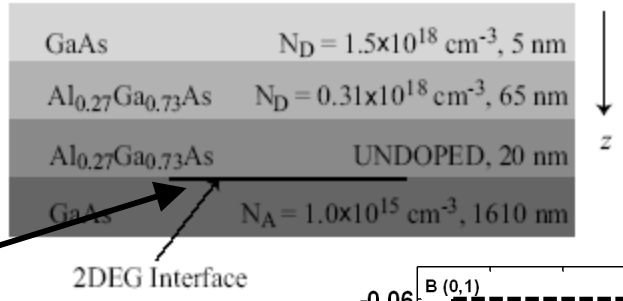
Potential Profile in the dot

GFMC

Finite Element



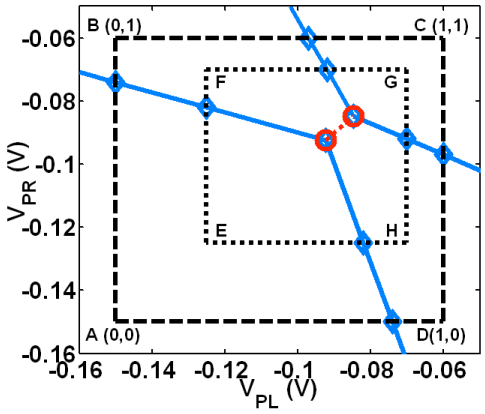
Side view



Transition in double dot

- **LDA (Leburton)**
- **QMC in progress**

See Poster



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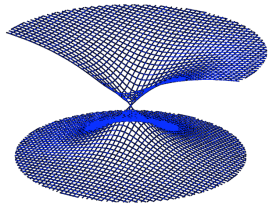
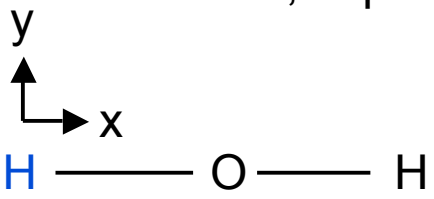
Intersections in Time-Dependent DFT

Todd J. Martinez

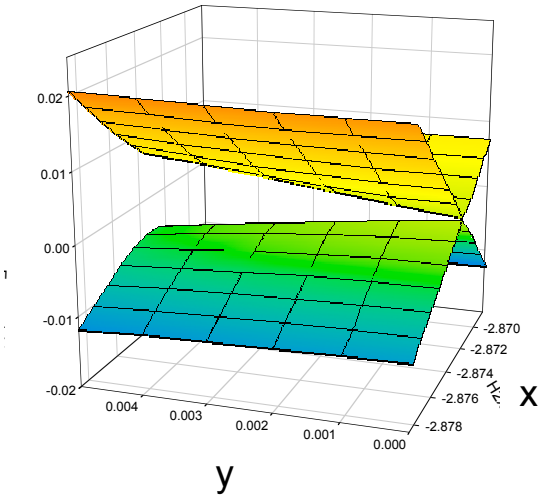
Conical Intersections are important in excited state dynamics.

- Does TDDFT work in this case?
- If not, improve functionals and formalism.

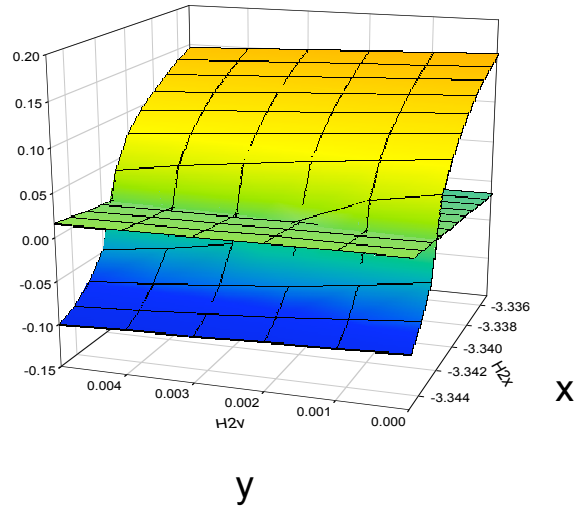




Other molecules are similar
(ethylene, butadiene, stilbene)



Ab Initio (CASSCF)



TDDFT (B3LYP)

Energetics well-predicted
Wrong dimensionality!
•Current Functionals?
•Berry Phase?
•Multireference TDDFT?

All functionals have same behavior
(e.g. LDA, BLYP, PBE, PW91)

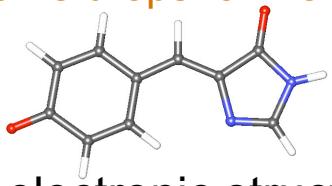
Funded by NSF DMR 03-25939

Optical Response in Complex Environments

Todd J. Martinez

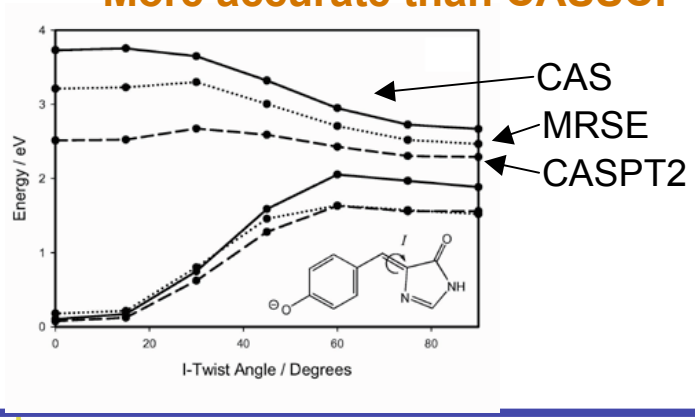
Nanoscale wavelength conversion (GFP)

- Chromophore does not fluoresce in solution
- Can we understand/design nanoscale optical devices?
- Excited-state lifetime drops10x from vacuum to in solution of H_20!



GFP Chromophore

- **Dynamics is expensive** - Need new methods for electronic structure of excited states in condensed phases and large molecular assemblies.
- **Use multi-reference re-parameterized QM/MM semiempirical methods.**
  - **Locations of intersections well-predicted by reparameterized potential.**
  - Comparable to Multi-reference-perturbation theory
  - **More accurate than CASSCF for 1/10th the expense!**



Connections

Use **Genetic Programming** to reparameterize potentials to avoid unphysical pathways but match *ab initio* database.

> See Poster with Bellon, Goldberg, Johnson, Martinez

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Funded by NSF DMR 03-25939

New "Multiscaling" Method via *Genetic Programming*

D.D. Johnson, D.E. Goldberg., P. Bellon, T. Martinez

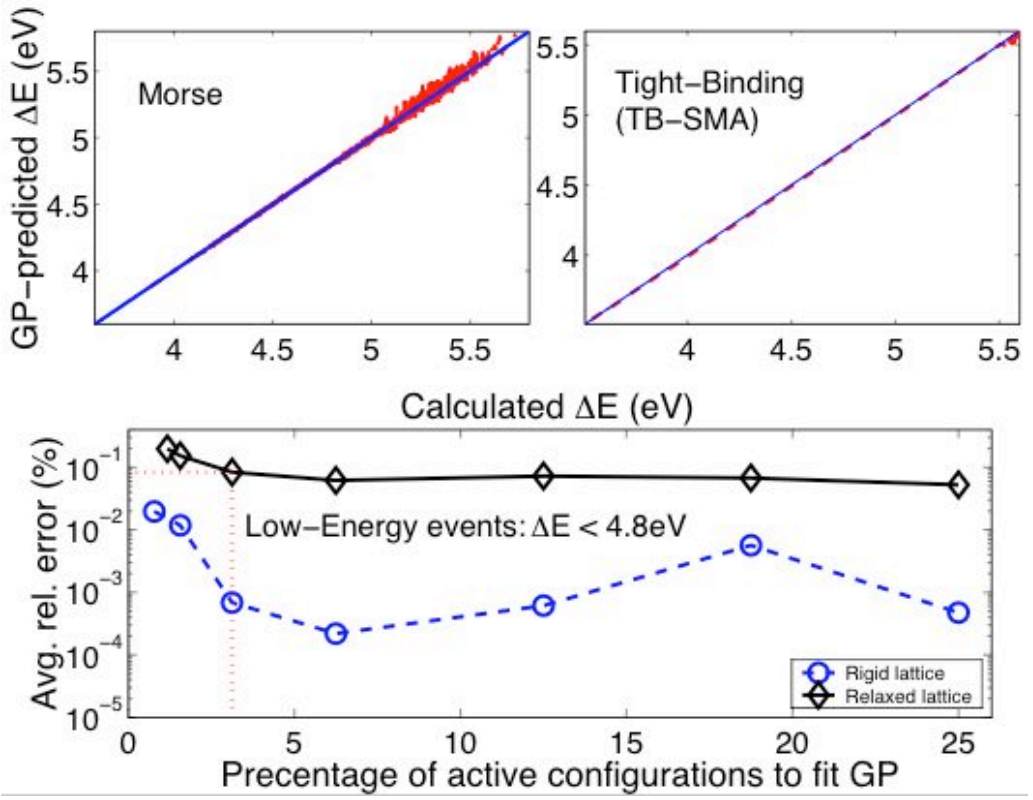
Genetic-Programming is a Genetic Algorithm that evolves a program!

Can diffusion barriers be machine-learned from only a few calculations?

E.g. vacancy-assisted migration of surface binary alloy (see Poster). With 1st and 2nd n.n. environments giving barriers, 8192 barrier need to be determined for **Kinetic Monte Carlo** simulations.

- Using GP **all** barriers are obtain with **0.1-1% error from 0.3-3%** direct barrier calculations.

- **Kinetic MC can now be done with *in-line function* "table".**
  - ~100x faster than table calculation.
  - 4-8 orders faster than "on-the-fly"
  - Simulate *real* seconds via KMC.



Connections (see Poster)

- Use GA/GP methods to get re-parameterized semi-empirical QC potentials to yield *ab initio* result.
- Use GP for system-specific KMC.

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Dynamical Systems: Irradiation-induced self-organization of chemical order in alloys

Pascal Bellon

Background

- Energetic irradiation yield disordered zones (size L≈1 to 10 nm) in ordered alloys.
- Competition between irradiation-induced disorder and thermally-activated reorder.
- Steady states depend on degree of order controlled by temperature and flux.

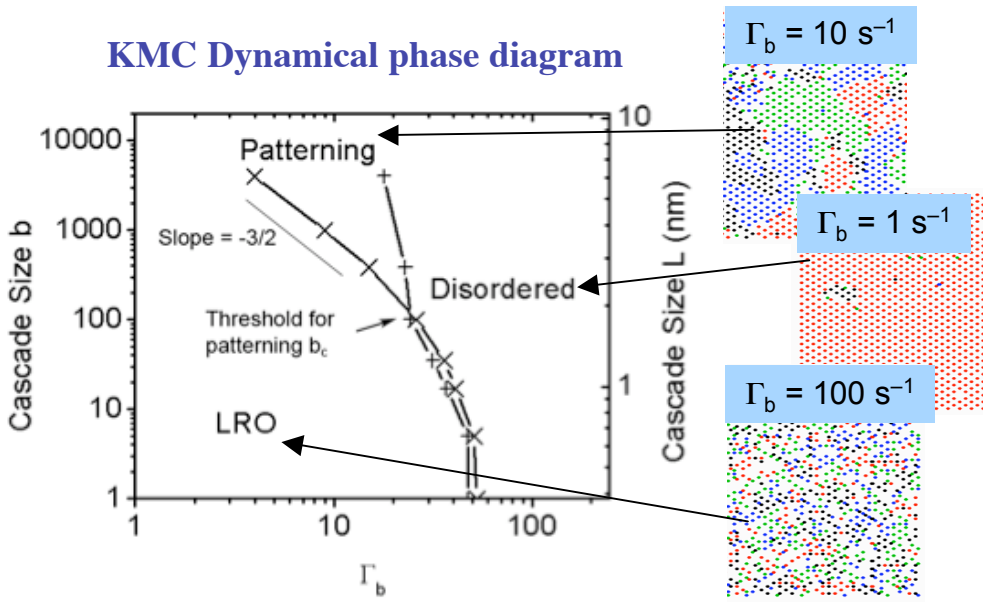
Key results using *Kinetic Monte Carlo*

- **Patterning when cascade size > $L_{critical}$**
- **Found dynamical phase diagrams**:
  LRO, patterns of order, and disordered.
- KMC and analytical method agree.

Demonstrated impacts

- **Key role of extrinsic length scales on self-organization in driven systems.**
- Applications? Fe-Pt magnets w/ A1-$L1_0$ or $L1_2$-$L1_0$ nanocomposites.

Maps of {111} B atoms under irradiation rate Γ_b.



Connections

- Genetic Programming for system-specifics.
- Contributed KMC code for *Software Archive.*
- KMC tutorial with 2-D KMC lab was developed for *Summer School* (Johnson).

Materials Computation Center
University of Illinois Urbana-Champaign
Funded by NSF DMR 03-25939

New "Dynamical" Methods: *Geometric Monte Carlo*

for MC simulation of complex fluids

E. Luijten

J. Liu and E. Luijten, Phys. Rev. Lett. ***92****, 035504 (2004)*

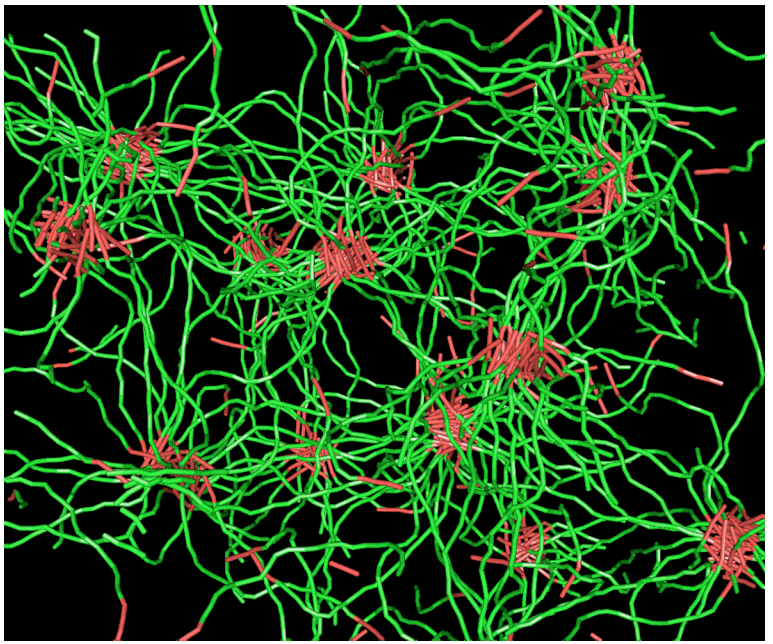
Science: Simulation of soft-condensed systems and complex fluids; mostly driven by electrostatics (colloids, polyelectrolytes, hydrogels, translocation, …)

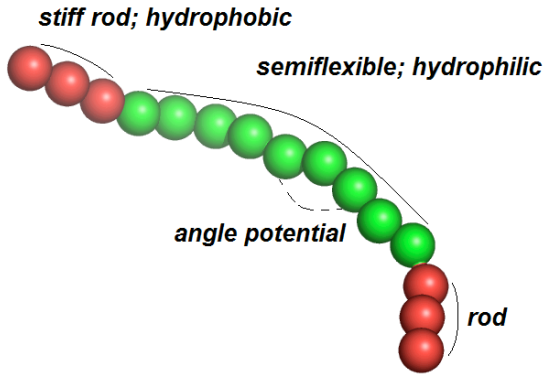
- First full continuum analog of lattice cluster algorithms (Swendsen-Wang, Wolff).
- Rejection-free for arbitrary pair potentials.
- Accelerates size-asymmetric-fluids simulations by orders of magnitude vs. Metropolis MC.

Outreach: Organizing CECAM workshop on "Novel Simulation Methods for Soft Condensed Matter Systems" (Lyon, June 2004).

Illustration: Tri-block Copolymer Gels

- Triblock copolymer solutions form gels at remarkably low concentration.
- Challenge: reproduce and understand in simulations.
- Tools: *dl_poly, lammps*
- Percolation precedes gelation upon decrease of temperature.





L. Guo and E. Luijten, invited contrib. to J. Polym. Sci. B

Announcing: New *Apple G5 Xserve* Cluster

- 640 Xserve units
- Dual 2GHz G5 processors per unit
- 4GB RAM and 80GB disk per unit
- 7TB RAID for cluster
- Ethernet and high-speed, fully-switched interconnection network
- May be operated as 512-unit and 128-unit clusters
- Mac OS X operating system

This **parallel computer** is joint effort on campus for *dedicated machine for computational materials science*, with R_{peak}~8 Gflops/node **(range of 2.5-5 Teraflops overall)**, and maintained by the professionals at the CSE.

Funded by NSF DMR 03-25939

Major User Groups for Apple Cluster

- **Beckman Institute**
  - Theoretical Biophysics Group, Computational Electronics Group, and Integrated Systems Lab
- **Computational Science and Engineering**
  - CSE Program and Center for Simulation of Advanced Rockets
- **Computer Science**
  - Parallel Computing Group and instructional use
- **Electrical & Computer Engineering**
  - Computational Electromagnetics Group, Plasma Processing Group, and Power Systems Group
- ***Materials Research Laboratory****
  - **Materials Computation Center**

* In support of MCC needs and future

Funded by NSF DMR 03-25939

Why Apple?

- Superior performance and relatively low power and cooling requirements of G5 processor
- Compact, well-engineered packaging
- Standard, stable software environment
- Positive experience with cluster loaned from Apple
- Attractive, aggressive pricing and eagerness of Apple to work with us
- Strong marketing support from Roberta Knapp and technical support from Paul Whitlock and Mike Bombich of Apple

The MCC External Advisory Board

Meets at least once a year to review the MCC program and to offer the **Advisory Board** a critical review with the purpose of improving the center objectives and means to achieve them.

expertise in MCC research areas but not collaborators

Warren Pickett (Physics, U. California, Davis)
Electronic-structure of condensed matter systems

Glenn Martyna (Div. Of Physical Science, Chemistry, IBM)
Theoretical and biophysical chemistry

Peter Voorhees (Materials Science and Engineering, Northwestern)
Thermodynamics and Kinetics of Phase Transformations

Rich Lehoucq (Computer Science, Sandia National Laboratory, Albq.)
Large-scale eigenvalue problems and applications (ARPACK)

MCC Advisory Board

D.D. Johnson (MatSE), R.M. Martin and Karin Dahmen (Physics), T. Martinez (Chemistry), Jeongnim Kim (MCC/NCSA), Eric de Sturler (Computer Science)

Funded by NSF DMR 03-25939

The Materials Computation Center

Duane D. Johnson and R.M. Martin (NSF-DMR/ITR grant 03-25939)

see http://www.mcc.uiuc.edu

Through unique, multidisciplinary collaboration we are producing novel, advanced algorithms and computational methods in ***3 research (broad impact) areas***.

I. Collaborations/Networking Thrust: with groups around nation and world.

Numerous examples, but, besides, NCSA, Psi-K, CECAM, FSATOM, etc., there is CPSD-ITR, IBM, Gerd Ceder (MIT) *electronic-structure database*….

II. Education and Knowledge-Transfer Thrust involving:

– **Summer Schools, Education Materials, Research Workshops, and Software Archive® for shared resources.**

*** If you want to contribute to Software Archive, even your link,** email mcc@uiuc.edu

*** If you have Summer School idea and want to organize, please contact us!**

III. Materials Research, Computation Tools and Algorithm Thrust

(1) Quantum and Classical Simulations; (2) Complex Systems and Transformations; (3) Computer Science and Scaleable Parallel Methods for Materials Modeling

– **Challenging problems that *warrant extended multidisciplinary efforts*.**

– **Creation of *computational tools*.**

– **Collaborative efforts to *develop new, practical, and efficient algorithms*.**