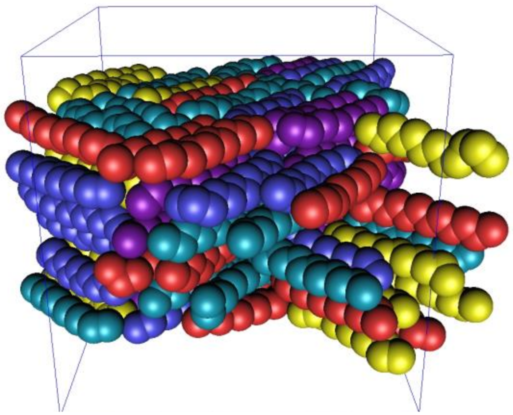
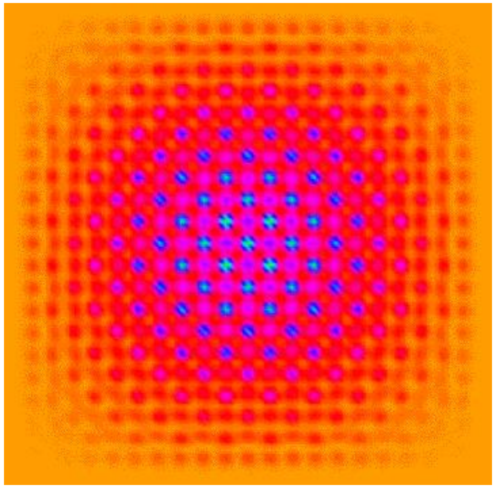
Theory and Modeling in Nanoscience

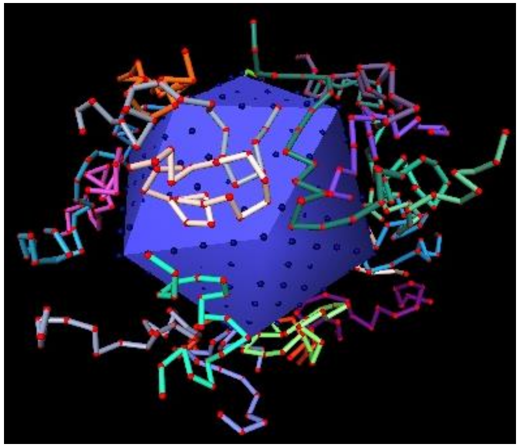


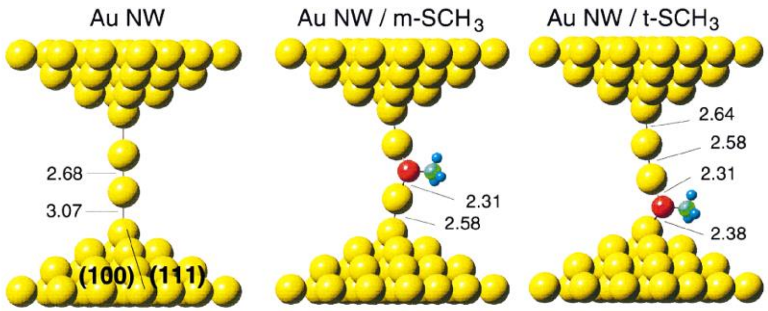
A BESAC/ASCAC Sponsored Workshop

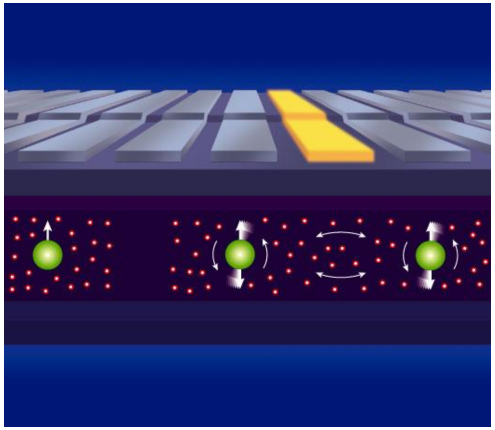
May 10-11, 2002

C. William McCurdy









Organizing Committee

Bill McCurdy, Co-Chair and BESAC Representative
LBNL

Ellen Stechel, Co-Chair and ASCAC Representative
Ford Motor Company

Peter Cummings
The University of Tennessee

Bruce Hendrickson
Sandia National Laboratories

David Keyes
Old Dominion University

Purpose of the Workshop

- Identify the challenges and opportunities for theory, modeling and simulation in nanoscience and nanotechnology.
- Investigate the role of applied mathematics and computer science in meeting those challenges.

Participation

- Representation roughly split between 1) Nanoscience Theory and Modeling and 2) Applied Mathematics and Computer Science
- 55 attendees
  - 16 University
  - 31 National Labs
  - 3 Industry
  - 5 DOE
- BESAC and ASCAC members invited, and 20 additional invitations issued, mostly to university researchers
- Written contributions solicited from all attendees, and responses posted on website together with presentations:

http://www.nersc.gov/~hules/nano/

Agenda
Friday, May 10, 2002

Stanley Williams Hewlett-Packard Laboratories	“Big Theory as the Engine of Invention for Nanotechnology: Losing the Born-Oppenheimer Approximation”
Uzi Landman Georgia Institute of Technology	“Small is Different: Computational Microscopy of Nanosystems”
Steven Louie UC Berkeley	“Theory and Computation of Electronic, Transport and Optical Properties on the Nanoscale”
Dion Vlachos University of Delaware	“Bridging Length and Time Scales in Materials Modeling”
Phil Colella LBNL	“Computational Mathematics and Computational Science: Challenges, Successes, and Opportunities”
Jerry Bernholc North Carolina State University	“Quantum Mechanics on the Nanoscale: From Electronic Structure to Virtual Materials”
Sharon Glotzer University of Michigan	“Computational Nanoscience and Soft Matter”
Alex Zunger National Renewable Energy Laboratory	“Progress and Challenges in Theoretical Understanding of Semiconductor Quantum Dots”
Dinner Speaker: Bernd Hamann, University of California, Davis	“Massive Scientific Data Sets: Issues and Approaches Concerning Their Representation and Exploration”

Agenda
Saturday, May 11, 2002

Panel Paul Boggs, SNL/Livermore Jim Glimm, SUNY Stony Brook Malvin Kalos, LLNL George Papanicolaou, Stanford University Amos Ron, U. of Wisconsin-Madison Yousef Saad, U. of Minnesota	**The Role of Applied Mathematics and Computer Science in the Nanoscience Initiative** Panel Moderator: Paul Messina, ANL
Breakout Sessions Well Characterized Nano Building Blocks Complex Nanostructures and Interfaces Dynamics, Assembly and Growth of Nanostructures Crossing Time and Length Scales Fast Algorithms Optimization and Predictability	**Chair** James Chelikowsky, U. of Minnesota Sharon Glotzer, U. of Michigan Peter Cummings, U. of Tennessee George Papanicolaou, Stanford University Malvin Kalos, LLNL Paul Boggs, SNL/Livermore

A Context for the Workshop: Recent Developments in Theoretical Methods

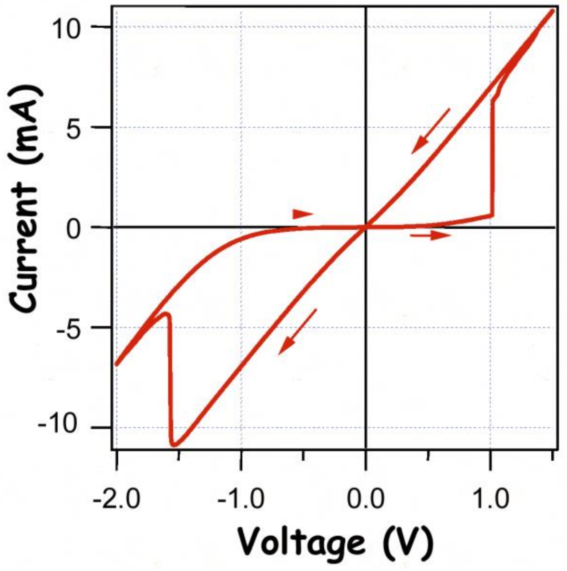
- Nanoscience arose from the appearance of new experimental techniques over the last ~15 years
- The applicable techniques of Theory and Modeling have undergone a revolution in the same period
  - Density Functional Theory for electronic structure
  - *Ab initio* Molecular Dynamics (Car-Parrinello)
  - Classical Molecular Dynamics with fast-multipole approaches
  - New methods for Classical Monte Carlo simulation
  - New Quantum Monte Carlo methods for electronic structure
  - New mesoscale methods including dissipative particle dynamics and field-theoretic polymer simulation
  - Etc.
- Advances in computational power have yielded ~ 4 orders of magnitude improvement since 1988.

Some Fundamental Theoretical Challenges Identified by the Workshop

- To bridge electronic through macroscopic length and time scales
- To determine the essential science of transport mechanisms at the nanoscale
- To devise theoretical and simulation approaches for nano-interfaces
- To simulate with reasonable accuracy the optical properties of nanoscale structures and to model nanoscale opto-electronic devices
- To simulate complex nanostructures involving “soft” biologically or organically based structures and “hard” inorganic ones as well as nano-interfaces between hard and soft matter
- To simulate self-assembly and directed self-assembly
- To devise theoretical and simulation approaches to quantum coherence, decoherence, and spintronics
- To develop self-validating and benchmarking methods

A Central Challenge

- *"Within five to ten years, there must be robust tools for quantitative understanding of structure and dynamics at the nanoscale, without which the scientific community will have missed many scientific opportunities as well as a broad range of nanotechnology applications."*

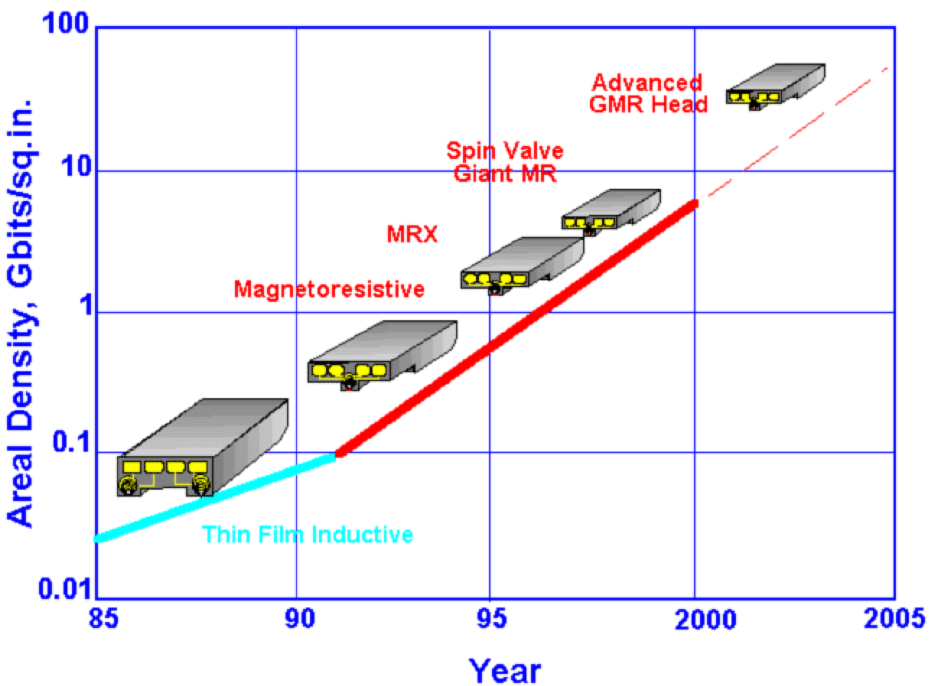


Calculated current-voltage curve for a novel memory-switchable resistor with 5μ × 5μ

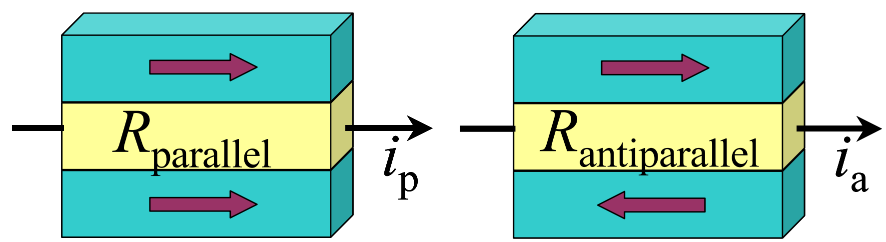
junctions. (Stan Williams, Hewlett-Packard)

Ample Precedent for the Role of Theory and Modeling in Nanoscience

- The giant magnetoresistance (GMR) effect was discovered in 1988 and within a decade was in wide commercial use in computer hard disks and magnetic sensors
- The unprecedented speed of application resulted largely from advances in theory and modeling that explained the quantum-mechanical processes responsible for the GMR effect.



Magnetic head evolution. (IBM)



Schematic of GMR indicating change in resistance accompanying magnetization reversal upon sensing an opposing bit.

The Role of Applied Mathematics

- There is a strong, recent history of the impact of applied mathematics on theory and modeling of molecules and materials
  - Fast multipole methods, FFTs, sparse linear algebra, multigrid methods, adaptive mesh refinement, optimization methods (global minimization), etc.
- But the challenge for the workshop was that: "*Some of the mathematics of likely interest (perhaps the most important mathematics of interest) is not fully knowable at the present …*"

Some Candidates for Improvement and Invention in Applied Mathematics

- Bridging length and time scales
  - Mathematical homogenization, “space sharing” methods, application of the “multigrid” and “proper orthogonal decomposition” paradigms, formulation of bi-directional coupling between scale-adjacent models,…
- Fast Algorithms
  - FFTs in electronic structure, parallel (sparse) linear algebra approaches, Kinetic Monte Carlo Method, Fast Multipole (scaling~N) ,…
- Optimization and Predictability
  - Multi-dimensional minimization algorithms, stochastic optimization methods, analytic techniques for propagating errors, comprehensive error bounds,

Issues for a New Program in Theory and Modeling in Nanoscience

- Theoretical efforts in separate disciplines are converging on this intrinsically multidisciplinary field

- *"Opportunities will be missed if new funding programs in theory, modeling, and simulation in nanoscience do not aggressively encourage highly speculative and risky research."*

- *"A new investment in theory, modeling and simulation in nanoscience should facilitate the formation of such alliances and teams of theorists, computational scientists, applied mathematicians, and computer scientists."*

Consensus Observations of the Workshop

- The role of theory, modeling, and simulation in nanoscience is central to the success of the National Nanotechnology Initiative.
- The time is right to increase federal investment in theory, modeling, and simulation in nanoscience.
- Fundamental intellectual and computational challenges remain that must be addressed to achieve the full potential of theory, modeling, and simulation in nanoscience.
- New efforts in applied mathematics, particularly in collaboration with theorists in nanoscience, are likely to play a key role in meeting those challenges.

The Office of Science is in a Unique Position to Build a New Program in Theory and Modeling in Nanoscience

- Much of the Nation’s experimental work in nanoscience is supported by DOE.
- New nanoscience facilities are being built at DOE national laboratories.
- DOE supports the core portfolio of applied and numerical mathematics for the Nation.
- DOE has unique resources and experience in high performance computing and algorithms.

- *“I am never content until I have constructed a mechanical model of what I am studying. If I succeed in making one, I understand; otherwise I do not. . . . When you measure what you are speaking about and express it in numbers, you know something about it, but when you cannot express it in numbers your knowledge about it is of a meagre and unsatisfactory kind.” —William Thompson (Lord Kelvin), 1824–1907*