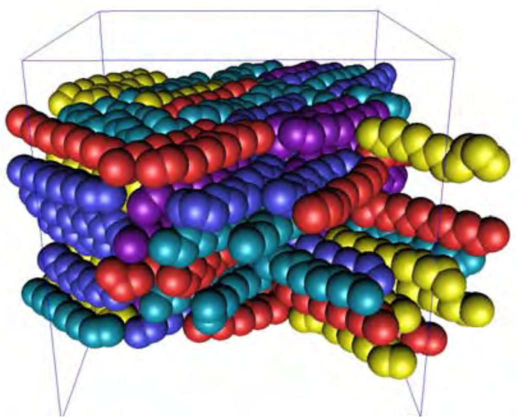
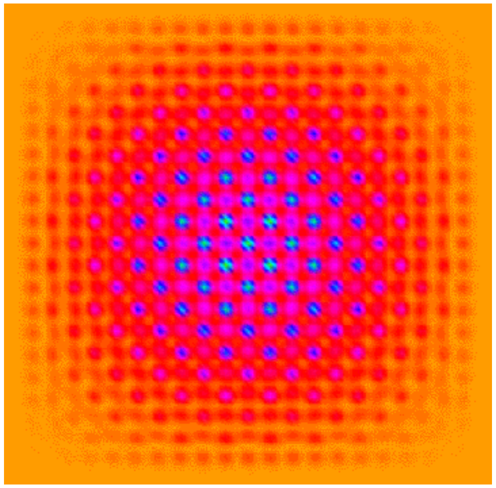
Theory and Modeling in Nanoscience

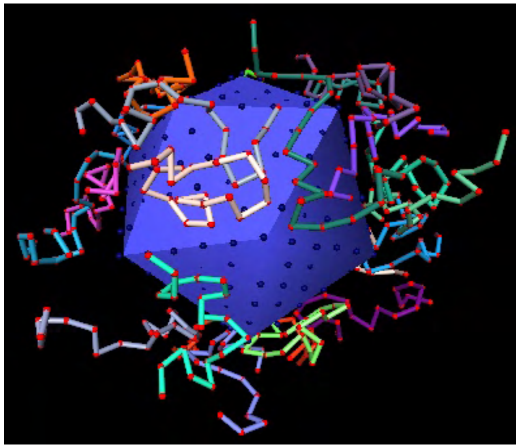


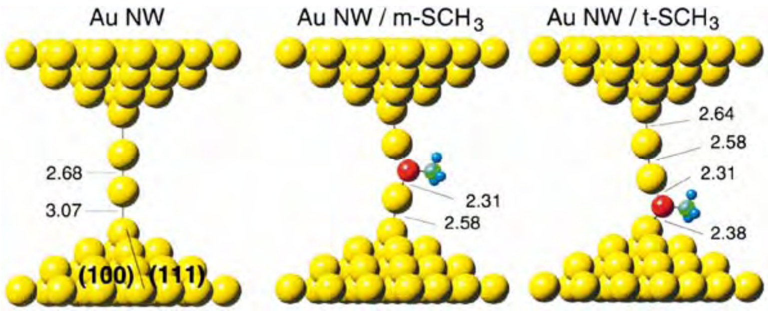
A BESAC/ASCAC Convened Workshop

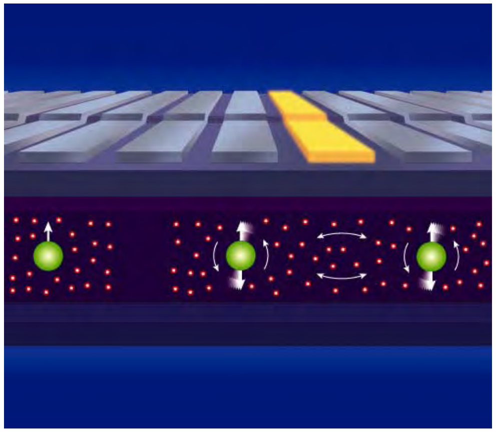
May 10-11, 2002

Ellen B. Stechel









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 (at that time)

Bruce Hendrickson
Sandia National Laboratories

David Keyes
Old Dominion University

A definition consistent with the National Nanotechnology Initiative

The study of structures, dynamics, and properties of systems in which one or more of the spatial dimensions is nanoscopic (1-100nm), thus resulting in dynamics and properties that are distinctly different (often in extraordinary and unexpected ways that can be favorably exploited) from both small molecule systems and systems macroscopic in all dimensions.

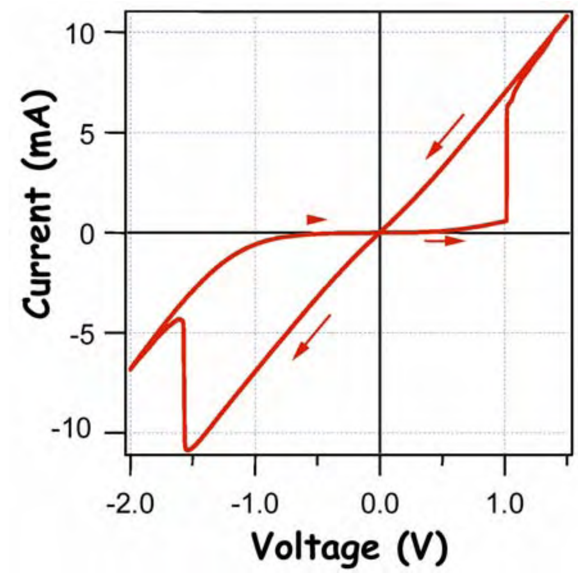
Purpose of the Workshop

- To identify **challenges and opportunities** for theory, modeling, and simulation in nanoscience and nanotechnology.
- To investigate the growing and promising role for **applied mathematics and computer science** in meeting those challenges.
- To make the case for **new investment** in theory, modeling, and simulation in nanoscience and nanotechnology in DOE.

A Central Challenge

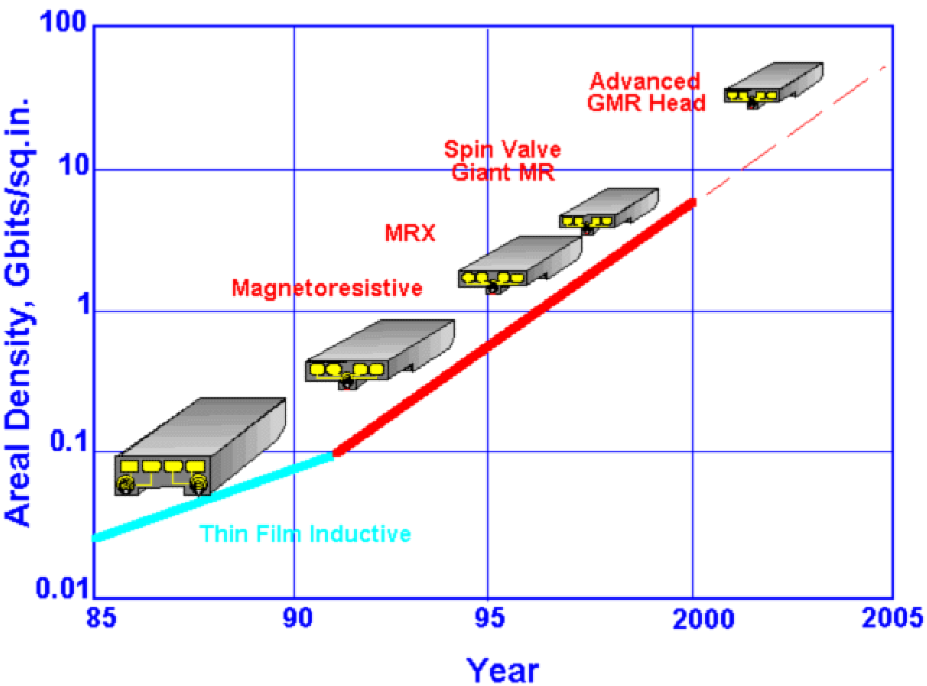
"Within five to ten years, there must be robust tools for quantitative understanding of structure and dynamics at the nanoscale, without which the scientific community will have missed many scientific opportunities as well as a broad range of nanotechnology applications."

Calculated current-voltage curve for a novel memory-switchable resistor with 5µ × 5µ junctions. (Stan Williams, Hewlett-Packard)

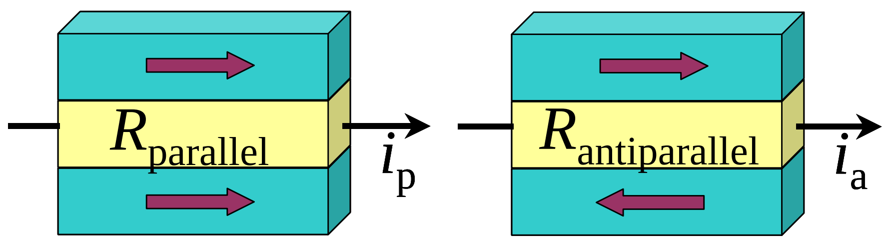


Ample Precedent for the Role of Theory and Modeling in Nanoscience

- 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 challenge of Mathematization of Nanoscience

"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

Participation

- Representation roughly split between
  - Nanoscience Theory and Modeling
  - Applied Mathematics and Computer Science
- 55 attendees
  - 16 University
  - 31 National Labs
  - 3 Industry
  - 5 DOE
- Invitations to:
  - BESAC and ASCAC members,
  - National Labs
  - 20 additional -- mostly to university researchers
- Written contributions solicited from all attendees,
  - Responses & presentations posted on website

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 Univ ***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	**Chairs** ***James Chelikowsky***, U. of Minnesota ***Sharon Glotzer***, U. of Michigan ***Peter Cummings***, U. of Tennessee ***George Papanicolaou***, Stanford Univ ***Malvin Kalos***, LLNL ***Paul Boggs***, SNL/Livermore

Output of the Workshop

- Presentations and Short White Papers
  - http://www.nersc.gov/~hules/nano/
- Published Report
  - Written in the context of other documents that define and support the National Nanotechnology Initiative
    - A broad range of applications that will benefit the principal missions of the DOE
      - ✓ Ranging from new materials enabling energy efficiencies to improved chemical and biological sensing
  - Not a roadmap
  - Not complete
  - Not a research agenda
  - Support for a case for new investment
    - Science Driven
    - Strong Collaboration
- Approved by BESAC and by ASCAC

A Context for the Workshop: Parallel Dramatic Advances: Experiment, Theory & Computation

- Nanoscience emerged from the appearance of extraordinary experimental advances over the last ~15 years
- Parallel revolutionary advances in Theory, Modeling, and Algorithms in the same period
  - Density Functional Theory for electronic structure
  - *Ab initio* Molecular Dynamics (Car-Parrinello)
  - 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
  - Fast-multipole approaches
  - Multigrid algorithms
- Advances in computational power have yielded ~ 4 orders of magnitude improvement since 1988.
  - Gordon Bell Prize in 1988 (1 Gflop/sec) and 2001 (11TFlops/sec)

Some Fundamental Theoretical Challenges & Opportunities 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” in-organic 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

Simulation needs to lead the way – sometimes no equations to lead the way

Time to solutions will be a good measure – time from formulation of the problem to formulation of mathematical models to algorithms and software – then time to solution

The Growing & Promising Role for Applied Mathematics

- There is a strong, recent history of the impact of applied mathematics on theory and modeling of molecules and materials
  - Mathematical homogenization, Fast multipole methods, FFTs, sparse linear algebra, multigrid methods, adaptive mesh refinement, optimization methods (global minimization), etc.
- There are some clear and directly relevant opportunities
- But the challenge for the report was that:

  "*Some of the mathematics of likely interest (perhaps the most important mathematics of interest) is not fully knowable at the present …*"

- Uncontested consensus
  - Collaborative efforts between applied mathematicians and scientists in nanoscience will yield significant advances central to success

Some Identified Opportunities for Impact and Discovery from Applied Mathematics

"To make tractable the problems that are currently impossible"

- 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, Linear scaling~N) ,...
- Optimization and Predictability
  - Multi-dimensional minimization algorithms, stochastic optimization methods, analytic techniques for propagating errors, comprehensive error bounds.

Potential Barriers and Considerations for Progress in Theory and Modeling in Nanoscience

- *"Opportunities will be missed if new funding programs in theory, modeling, and simulation in nanoscience do not aggressively encourage highly speculative and risky research."*
- Theoretical advances in separate disciplines are converging on this intrinsically multidisciplinary field.
- The traditional separation of experiment, theory, applied mathematics, and computer science and separation by sub-discipline will impede progress if the separation persists.
- *"A new investment in theory, modeling and simulation in nano-science should facilitate the formation of (multidisciplinary) 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 and computer science, particularly in collaboration with theorists in nanoscience, will almost certainly play a critical role in meeting those challenges.
- *"Many opportunities for discovery will be missed if the new tools of theory, modeling, and simulation are not fully exploited to confront the challenges of nanoscience."*

The Office of Science is in a Unique Position to Build a Successful 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.