Opportunities and Challenges in Computational and Theoretical Nanoscience

Peter T. Cummings

Department of Chemical Engineering, Vanderbilt University
and
Nanomaterials Theory Institute and Chemical Sciences Division
Oak Ridge National Laboratory

Fall Creek Falls Conference
Delivering Computational Science for the Nation
Fall Creek Falls, TN
October 17-18, 2004

UT-BATTELLE
Oak Ridge National Laboratory

Introduction

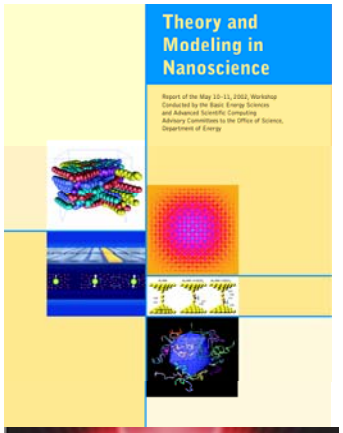
- Nanoscale science and engineering
  - *Ability to work at molecular level, atom by atom, to create large structures with fundamentally new properties and functions**
    - At least one dimension is of the order of nanometers
    - Functionality is critically dependent on nanoscale size
  - *Promise of unprecedented understanding and control over basic building blocks and properties of natural and man-made objects**
- National Nanotechnology Initiative
  - *http://www.nano.gov*
    - $710 million in FY 2003
    - 21st Century Nanotechnology Research and Development Act
      - *$3.7B over 4 years*
      - *Passed unanimously by Congress*

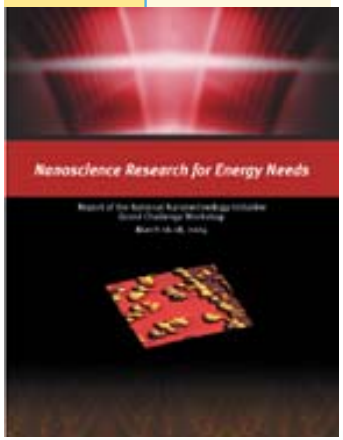
***M. Roco, FY 2002 National Nanotechnology Investment Budget Request**

UT-BATTELLE
Oak Ridge National Laboratory

Introduction

- Theory, modeling and simulation (TMS)
  - *Expected to play key role in nanoscale science and technology*

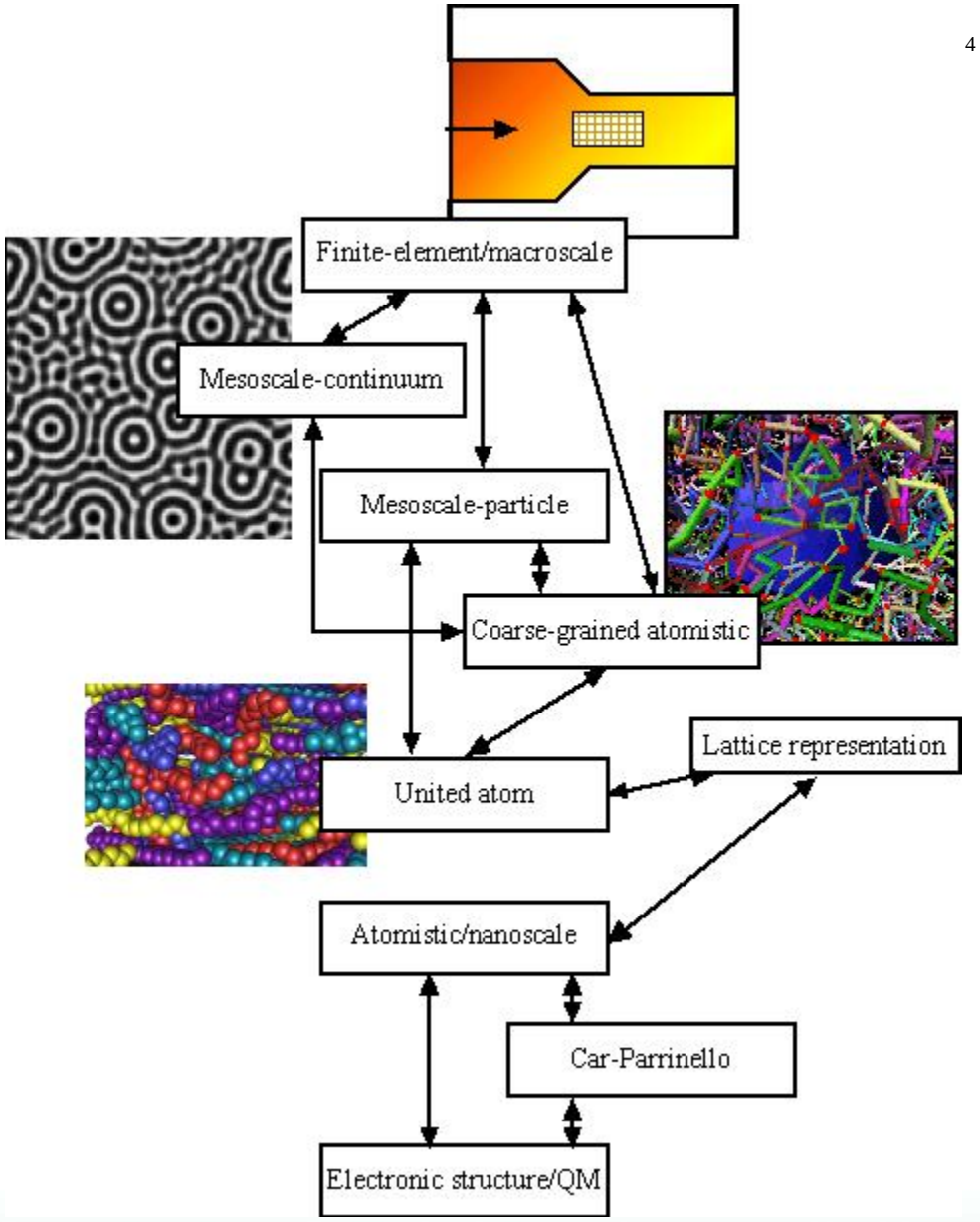


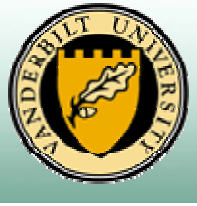


- "Nanotechnology Research Directions: IWGN Workshop Report. Vision for Nanotechnology Research and Development in the Next Decade," edited by M.C. Roco, S. Williams, P. Alivisatos, Kluwer Academic Publisher, 2000
  - *Also available on-line at http://www.nano.gov*
  - *Chapter 2, Investigative Tools: Theory, Modeling, and Simulation, by D. Dixon, P. T. Cummings, and K. Hess*
    - Discusses issues and examples
- McCurdy, et al. "Theory and Modeling in Nanoscience: Report of the May 10-11, 2002, Workshop Conducted by the Basic Energy Sciences and Advanced Scientific Computing Advisory Committees of the Office of Science, Department of Energy
  - *Published by DOE*
  - *Also available on the web at http://www.sc.doe.gov/bes/Theory_and_Modeling_in_Nanoscience.pdf*
- Alivisatos, *et al*., "Nanoscience Research for Energy Need: Report of the March 2004 National Nanotechnology Initiative Grand Challenge Workshop
  - *Published by DOE and NNI*
  - *Also available on the web at http://www.sc.doe.gov/bes/reports/NREN_rpt_print.pdf*

Introduction

- Heirarchy of methods relevant to nanoscale science and technology
  - *Connection to macroscale*





DoE Investment in Nanoscience

- Five nanoscale science research centers (NSRCs)
  - *Oak Ridge National Laboratory*
    - Center for Nanophase Materials Sciences
  - *Lawrence Berkeley National Laboratory*
    - Molecular Foundry
  - *Sandia National Laboratory/Los Alamos National Laboratory*
    - Center for Integrated Nanotechnologies
  - *Argonne National Laboratory*
    - Center for Nanoscale Materials
  - *Brookhaven National Laboratory*
    - Center for Functional Nanomaterials
  - *Funding: >$300M startup, >$90M/yr ongoing programmatic*
- Each NSRC includes theory/modeling/simulation effort
  - *Nanomaterials Theory Institute at ORNL*
    - See poster by Schulthess/Cummings/Stocks
- Extraordinary science problems in which experiments are divergent
  - *Electron transport/molecular electronics*
  - *Nanotribology*
  - *….*

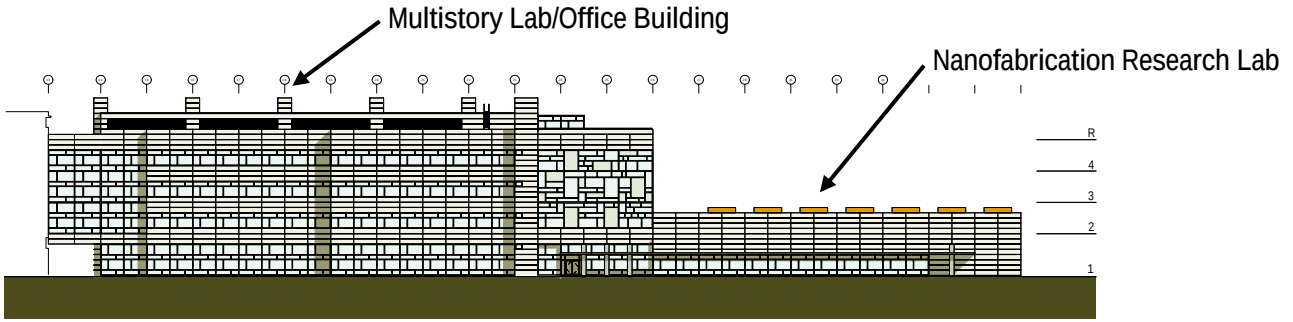
Center for Nanophase Materials Sciences

Oak Ridge National Laboratory

Specializing in neutron science, synthesis science, and theory/modeling/simulation

- Neutron Science
  - *Opportunity to assume world leadership using unique capabilities of neutron scattering to understand nanoscale materials and processes*
- Synthesis Science
  - *Science-driven synthesis will be the enabler of new generations of advanced materials*
- Theory/Modeling/Simulation
  - *The Nanomaterials Theory Institute*
- Scientific thrusts in 10 multidisciplinary research focus areas
- Access to other major ORNL facilities
  - *Spallation Neutron Source*
  - *High-Flux Isotope Reactor*
  - *Center for Computational Sciences*
- Began Sept, 2003; to be occupied beginning April, 2005
  - *$60M for building and equipment; $18.5M/yr ongoing*

Nanomaterials Theory Institute



Center for Nanophase Materials Sciences

http://www.cnms.ornl.gov


August, 2004
04

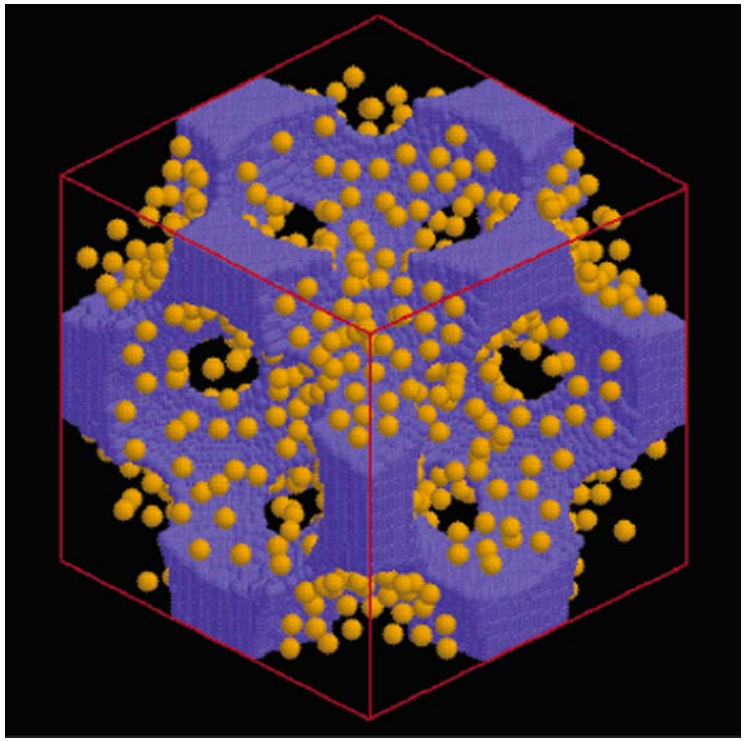
Scientific Challenges

- Experimental challenges to theory
  - *Carrot-like morphology of SiO_x nanowire assemblies*
    - One of five different morphologies obtained in different temperature ranges during molten-gallium-catalyzed synthesis in a three-phase reactor

– *Pan, Z.W., S. Dai, D.B. Beach and D.H. Lowndes, Temperature dependence of morphologies of aligned silicon oxide nanowire assemblies catalyzed by molten gallium.* Nano Letters*, 2003. 3(9): p. 1279-1284.*

Scientific Challenges

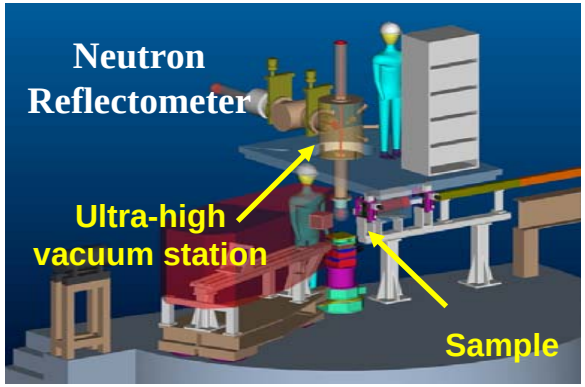
- Theory challenges to experiment
  - *Simulation-based prediction of structure for a carbonaceous material that has large capacity for adsorbing hydrogen*
    - Relevant to hydrogen initiative



– *Cao, D.P., P.Y. Feng and J.Z. Wu, Molecular simulation of novel carbonaceous materials for hydrogen storage. Nano Letters, 2004. 4(8): p. 1489-1492*

National Leadership Computing Facility

Spallation Neutron Source (SNS)
Center for Nanophase Materials Science (CNMS)



User Community

Facility

Instrumentation

Nanoscience Virtual User Center

Materials : Math : Computer Scientists

- *Open Source Repository*
- *Object Oriented Tool Kit*
- *Focused User Laboratories*
- *Education*

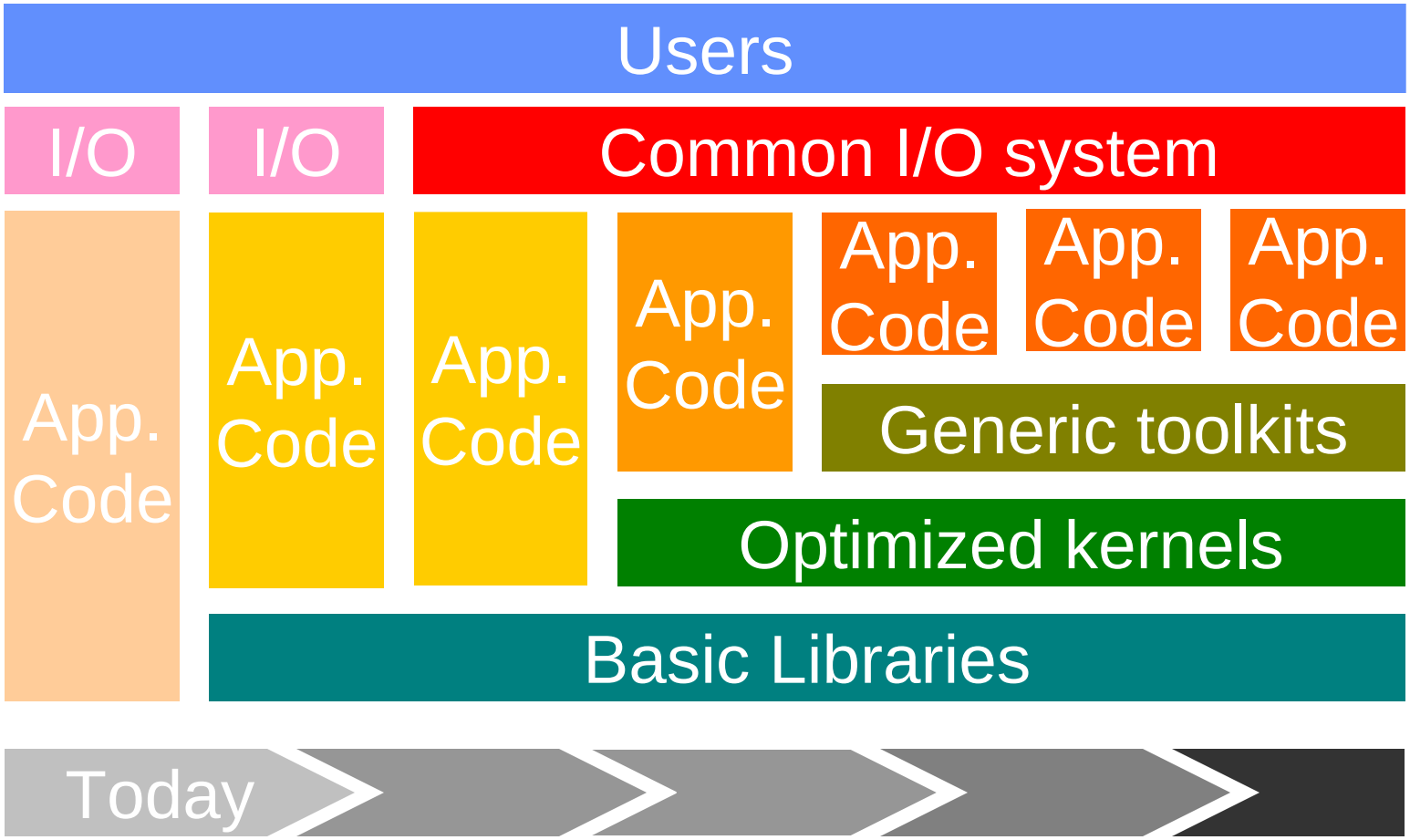
User Community

UT-BATTELLE
Oak Ridge National Laboratory

Strategies for Nanoscience on NLCF

- Criteria for access to NLCF
  - *Ground-breaking science*
    - Must answer an outstanding question in nanoscience
      - *Peer review*
  - *Availability of codes that scale on the NLCF*
    - Endstation/instrumentation strategies
      - *Development of scalable versions on NLCF of widely used community codes, leading to common kernels*
        - Examples in electronic structure and molecular dynamics (MD)
        - E.g., 12 billion-atom MD simulation of nanotribology
  - *Urgency*
    - Compelling reason for answering the question 1-2 orders of magnitude faster than capacity computing allows
      - *E.g., stability of amorphous polymer nanostructures in next-generation microprocessors*
      - *E.g., solution of design/operation question for experimental capability*
        - Rapid peer review

Toolkit for Computational Nanoscience



See poster by Schulthess, Cummings, Stocks

UT-BATTELLE
Oak Ridge National Laboratory