Computational Resources for Integrated Computational Materials

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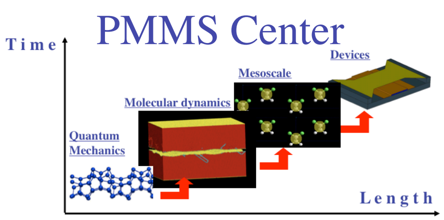

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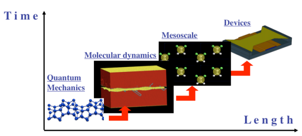
Simulation/computing tools and usage scenarios

Math software / databases analysis

Electronic Structure → MD → Mesoscale FP, DD, etc. → FEA/ Thermo

size/time

Basic level	Simulations/tool to help students understand difficult concepts or perform complex calculations
Advanced user level	Simulations relevant for industrial and research applications
Expert level	Students interested in computational science & engineering



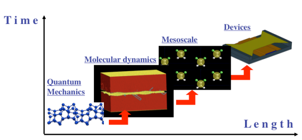
Basic level user scenario

- Objective
  - Help students better understand concepts taught in class
  - Perform calculations not possible without computing
  - Help achieve course's learning objectives

- Target
  - MSE core courses

- Students
  - No background on simulations or computing
  - Minimal overhead in getting students started with modeling

- Faculty
  - Little or no background on simulations/computational



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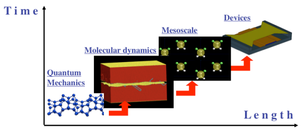
Basic level user: required resource features

- Simulation tools
    - User friendly
    - Easily and widely available
    - High-level, interactive visualization

- Instructional material tightly coupled with the tool
    - Lectures, notes and tutorials
        - Brief introduction to the physics of the simulation tool
        - Topic to be addressed
        - Detailed tutorial to run the simulation
    - Assignments and quizzes
    - Learning objectives



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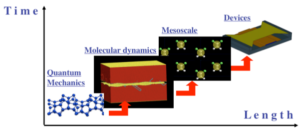
Advanced user level scenario

- Objectives
  - Train students in industrial/research grade computing and simulation
- Target use
  - Technical elective, senior design, and independent research courses
- Students
  - Expected to learn the details of the simulation tool
  - Develop basic knowledge of scientific computing
- Faculty
  - Some expertise in specific simulation



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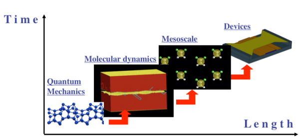
Advanced user level: required resource features

- Simulation tools
  - Powerful and flexible
  - Access to significant computational resources
  - User friendly and accessible

- Supporting material
  - Detailed tool descriptions
    - Model physics, numerical approximations
  - Examples of the use of simulation for industrial problems
  - Best practices
    - Reproducibility of results, documentation & data management
    - Verification and validation (V&V)
    - Uncertainty quantification



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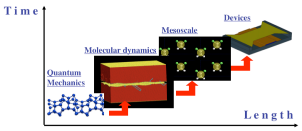
Expert scenario

- Objectives
    - High-level of expertise on physics and numerical aspects

- Target:
    - Technical elective courses, research

- Students
    - Background: basic programming skills
    - Outcome: able to add to or modify a computational tool
    - Outcome: trained in best practices in scientific computing

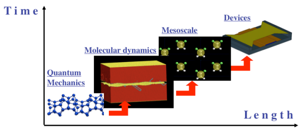
- Faculty/mentor
    - Some computational expertise



Expert scenario

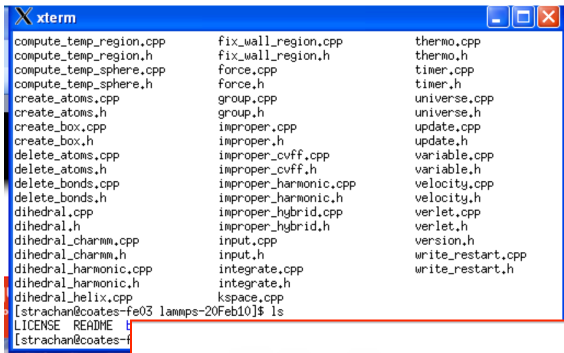
- Simulation tools
  - Open source or ability to add modules

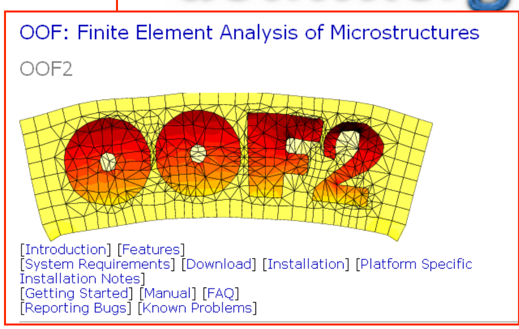
- Supporting resources
  - Access to advanced scientific computing tools
    - Compilers and debuggers
    - Version control software
  - Training material
    - High performance computing
    - Best practices in computing and simulations



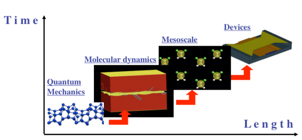
Resources: simulation codes and software

Open source

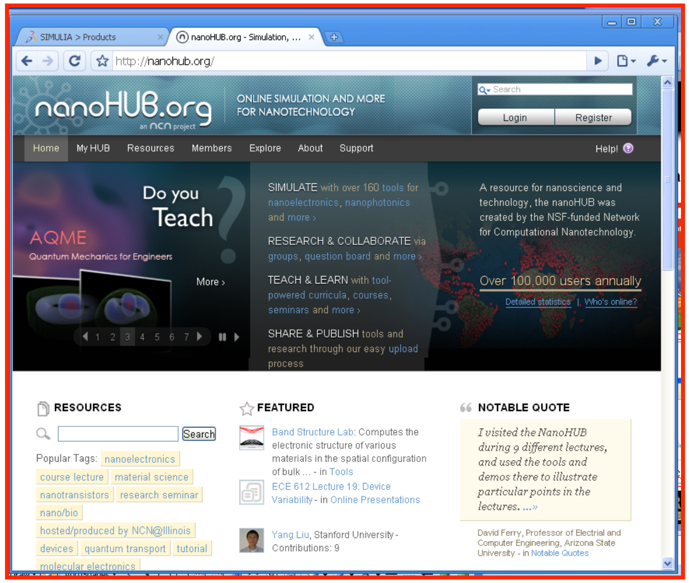




>MyCode.f

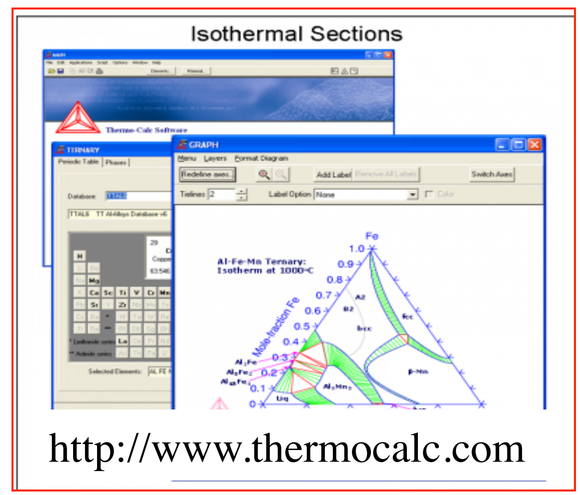


Cyber-enabled cloud scientific computing



NSF network: Purdue, UIUC, Northwestern, Berkeley/LBL, MIT, U of Florida, Norfolk, UT El Paso

Commercial



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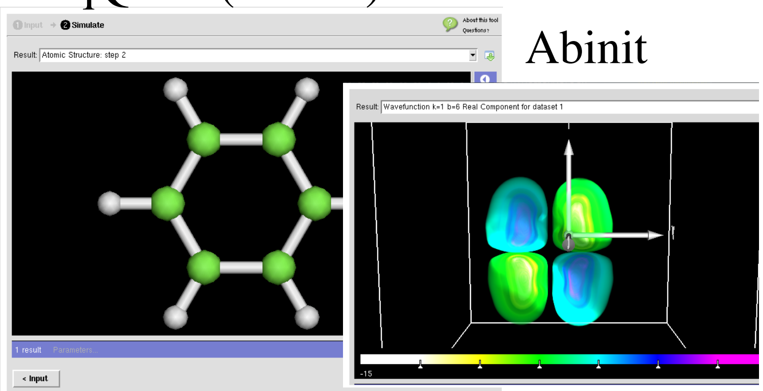
Materials codes in nanoHUB

DFT tools

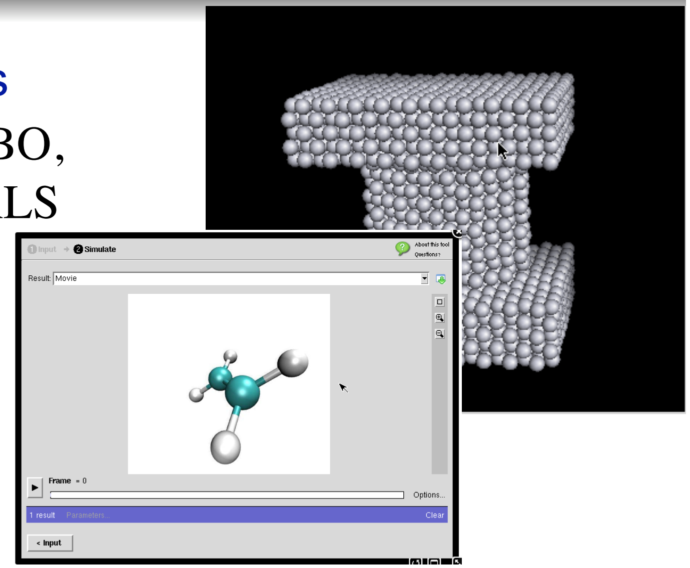
SeqQuest (Sandia)

Abinit



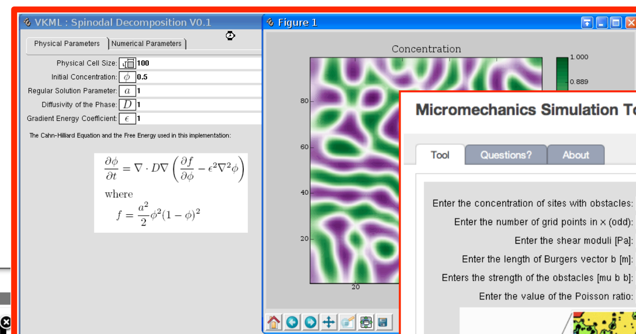
Molecular dynamics

LAMMPS, REBO,
nanoMATERIALS

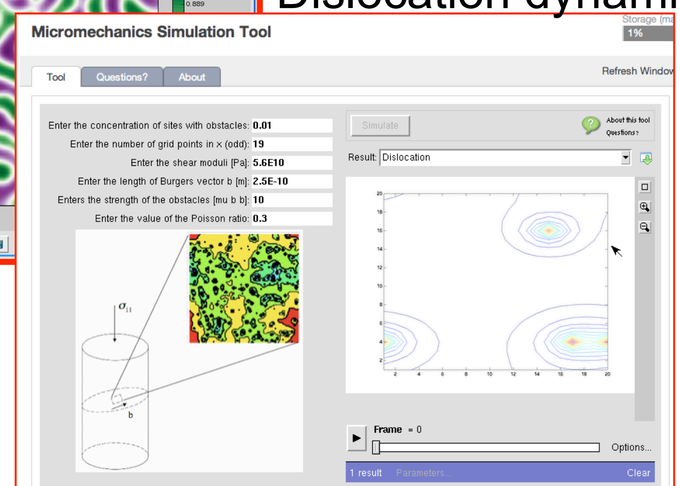


Mesoscale

Virtual kinetics

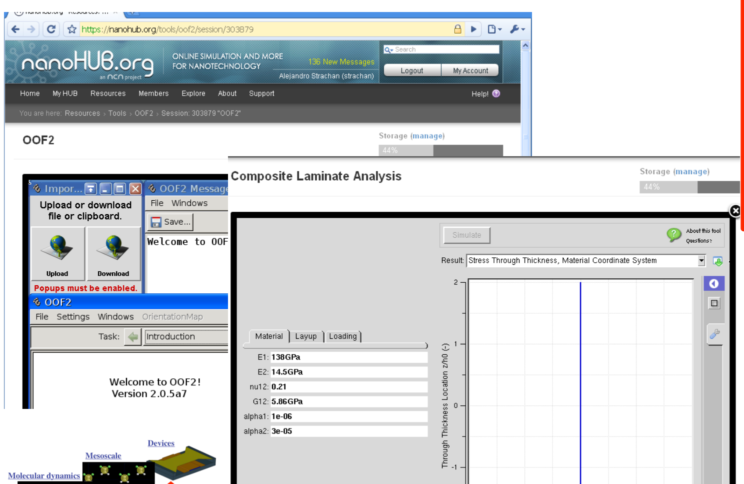


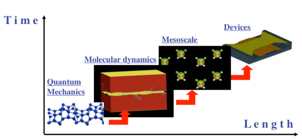
Dislocation dynamics



Finite elements

OOF2





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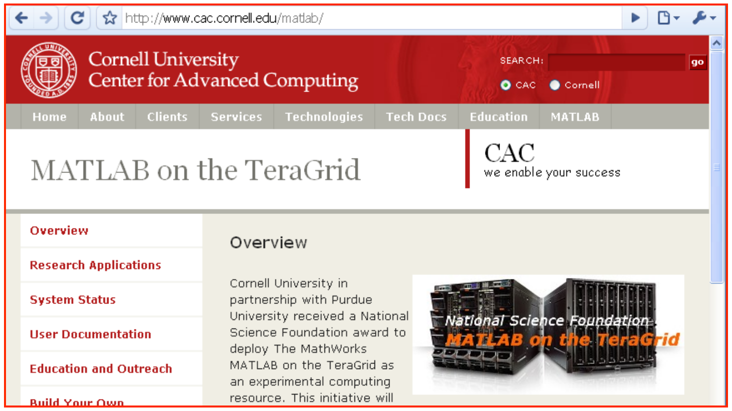
General purpose resources

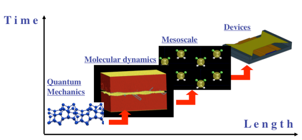


Cornell MATLAB Resource - http://www.cac.cornell.edu/matlab/

- 512 cores with MATLAB Parallel Computing Toolbox licenses
- Submit from your desktop MATLAB program

- Full-featured Linux desktop
- For researchers and educators
- Accessible from any web browser
- Still running after you close your browser
- Development resources
- Access to Grid resources
- File storage provided by nanoHUB

http://nanohub.org/tools/workspace



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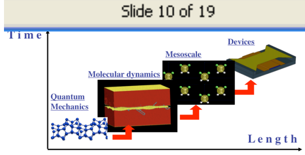
Example: learning module using online simulations

Objectives:

- introduce students to the atomic-level processes responsible for plastic deformation in metals
- help them develop a more intuitive understanding of how materials work at molecular scales

Contents:

- Two introductory lectures
- Laboratory assignment
- Learning objectives



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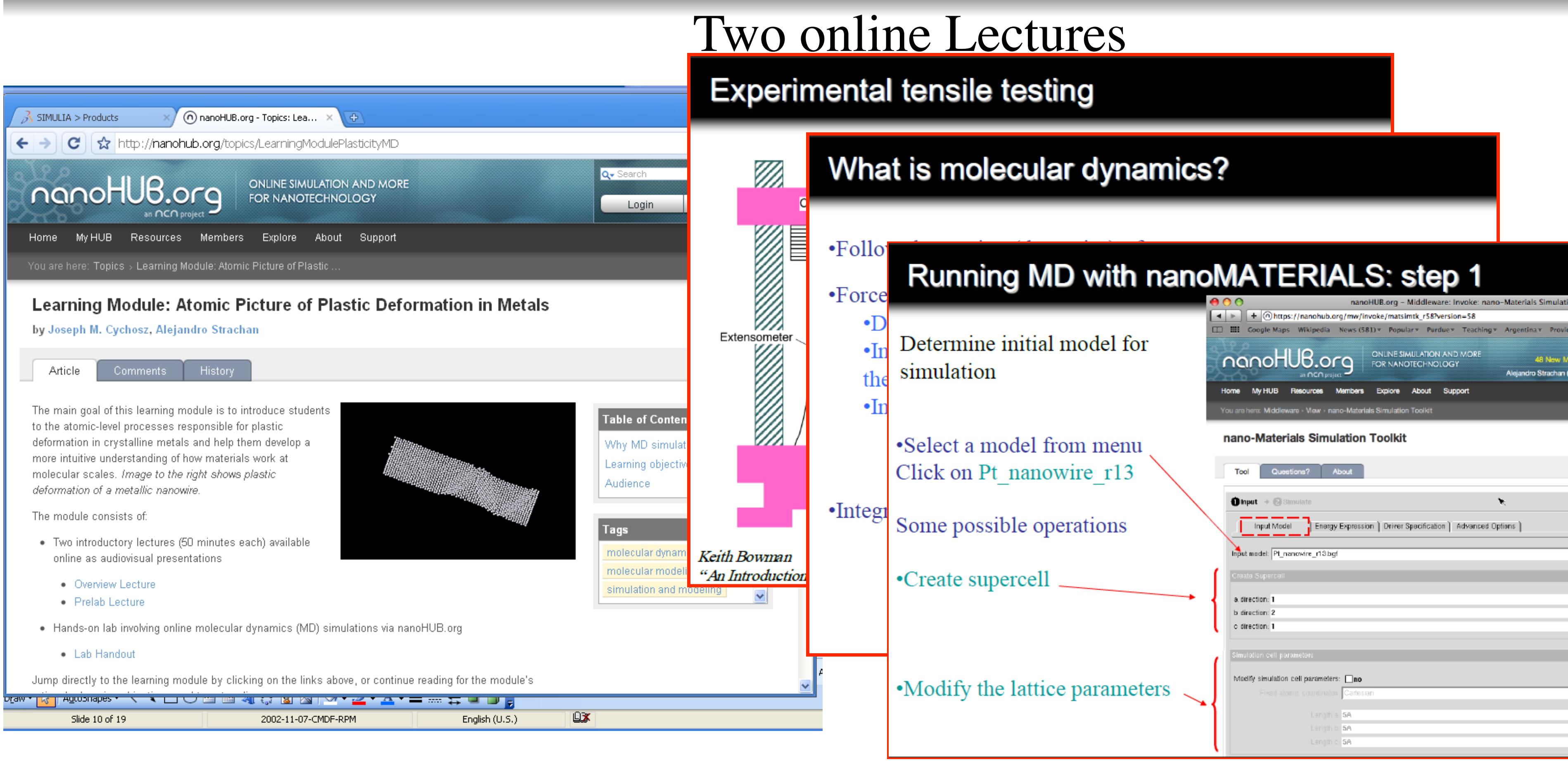
Example: learning module using online simulations



•Introduce topic and simulation tool

•Step by step tutorial to run a meaningful simulation and analyze the results

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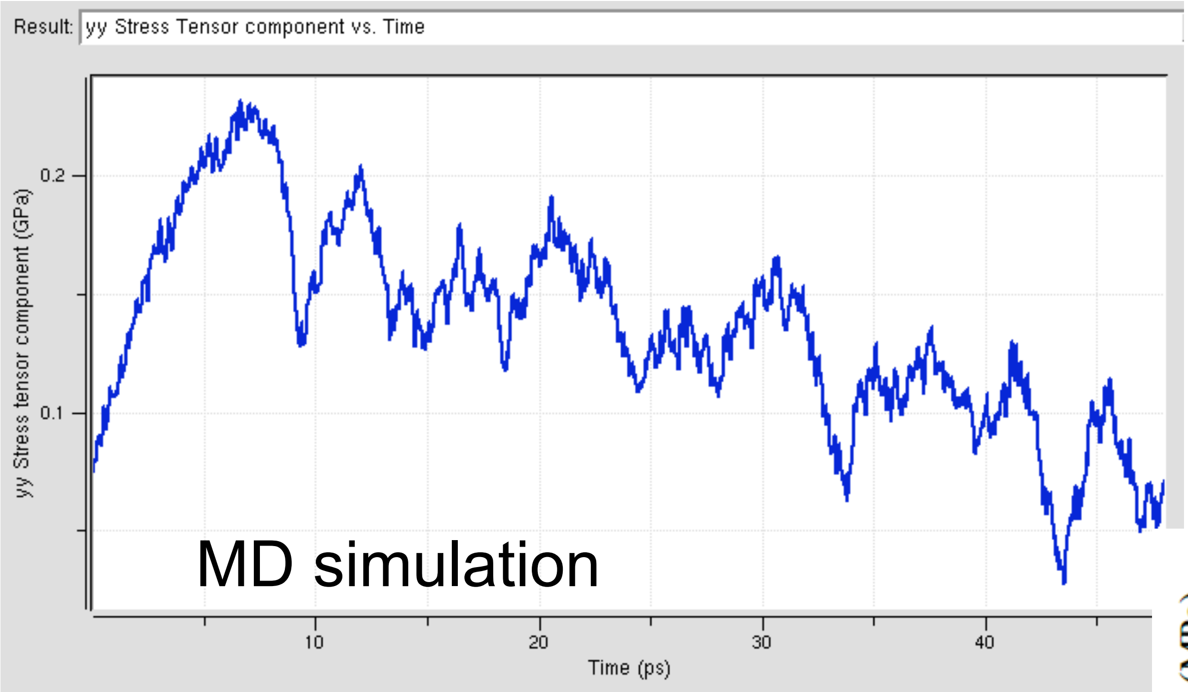
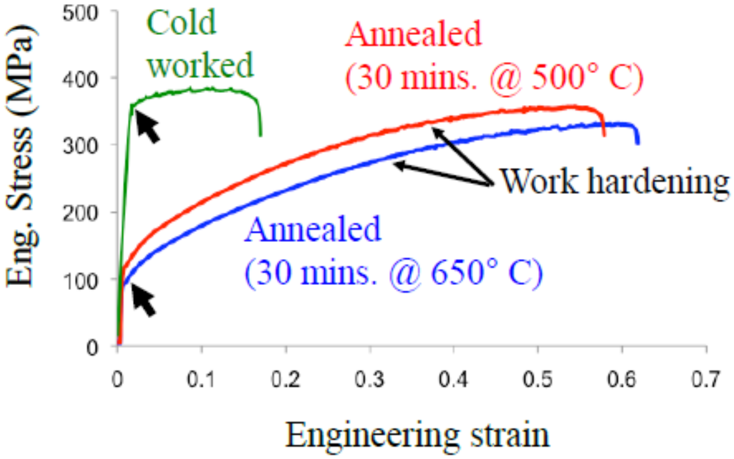
Compare MD results with tensile tests

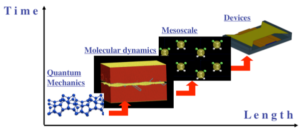


Stress vs strain

Experiment

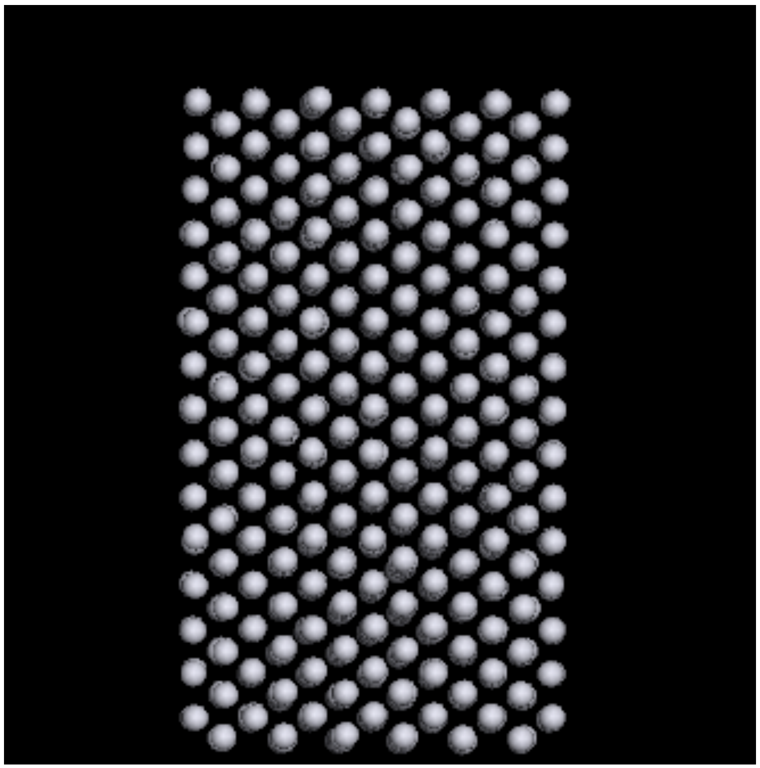


Nanoscale vs. macroscopic samples

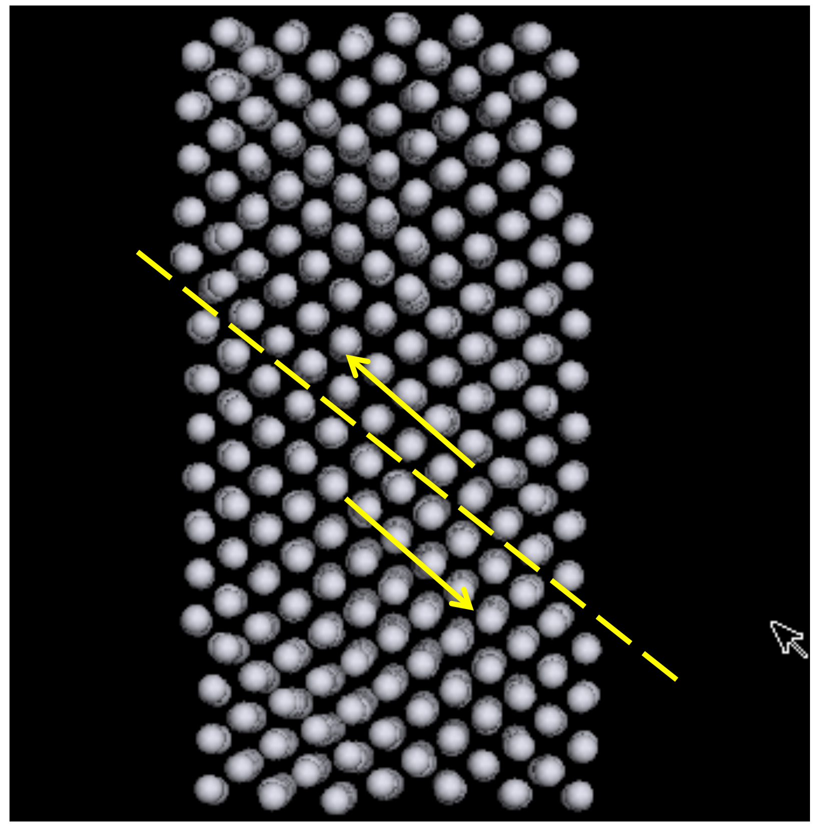


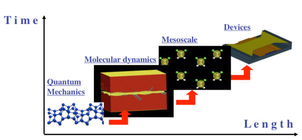
Explore atomistic processes

Initial structure



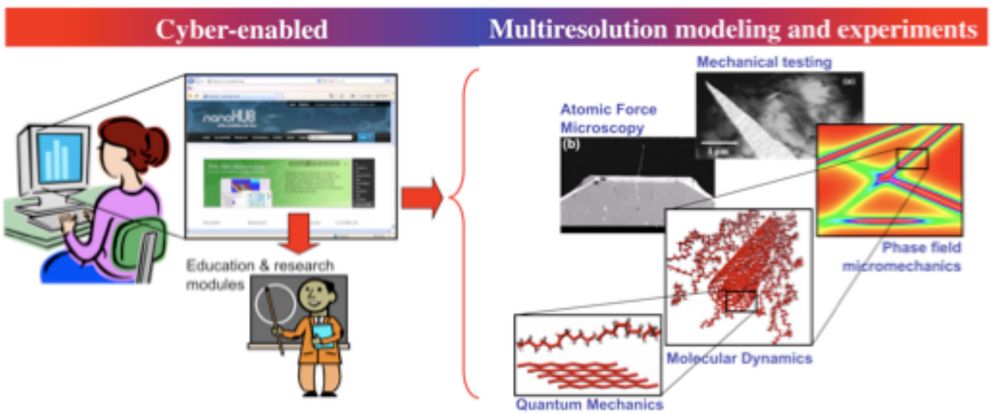
Final structure





Leveraging integrated computing research efforts

NSF: cyber-enabled predictive models for polymer nanocomposites: multiresolution simulations and experiments



- Ultimate mechanical properties of nanocomposites
- Poly-imides and PMMA with CNTs and graphene

Boeing – Purdue: atoms to aircraft

- Prediction of onset of irreversible deformation and damage propagation in epoxy formulations
- Cyclic loading and damage accumulation

www.newairplane.com

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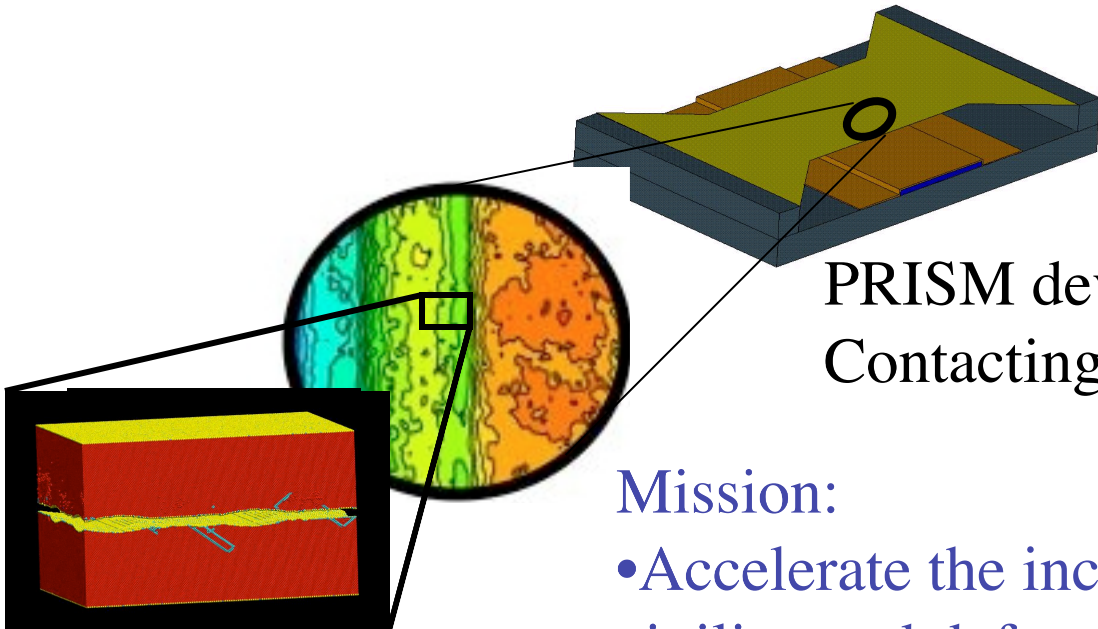
Leveraging integrated computing research efforts

Center for *Prediction of Reliability, Integrity and Survivability of MEMS*



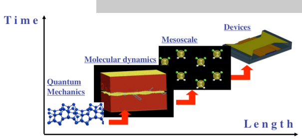
PRISM
Center for Prediction of Reliability, Integrity and Survivability of Microsystems

PRISM device:
Contacting RF capacitive switch

Mission:

- Accelerate the incorporation of MEMS in civilian and defense applications
- Increase our understanding of failure and reliability

- High fidelity simulations from atoms to device
- Uncertainty quantification and experimental validation



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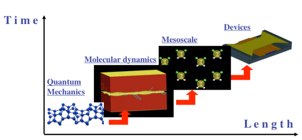
Summary

- Access to tools and training material to non-experts
  - Lower the barriers for incorporation of computing in core courses

- Close the gap between simulation tools and instructional material
  - Learning modules for learning and teaching
  - Examples/tutorials of modeling and simulations relevant for industrial applications (benefits reproducibility of results)
  - Leverage research efforts

- Encourage best practices in modeling and simulation
  - Reproducibility of results and documentation
  - Verification and validation, uncertainty quantification



Thanks

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National Science Foundation
WHERE DISCOVERIES BEGIN

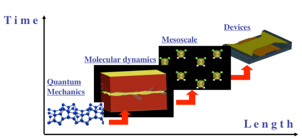
DoE-NNSA ASC

PRISM
Center for Prediction of Reliability, Integrity and Survivability of Microsystems

DoE-BES

Office of Science

MARCO focus center on Materials Structures and Devices



BOEING

Network for Computational Nanotechnology

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