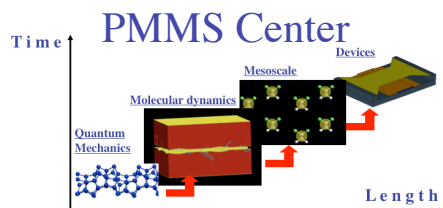


Computational Resources for Integrated Computational Materials

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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

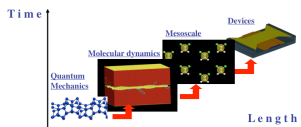
Simulations/tool to help students understand difficult concepts or perform complex calculations

Advanced
user level

Simulations relevant for industrial and research applications

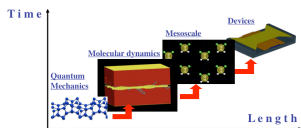
Expert
level

Students interested in computational science & engineering



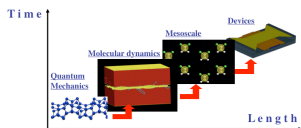
Basic level user scenario

- 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



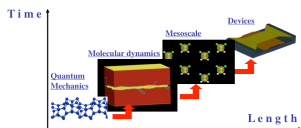
Basic level user: required resource features

- 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



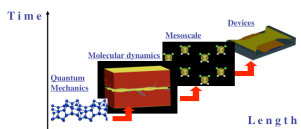
Advanced user level scenario

- 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



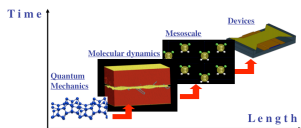
Advanced user level: required resource features

- 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



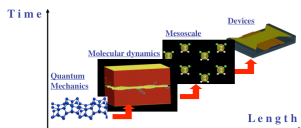
Expert scenario

- 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

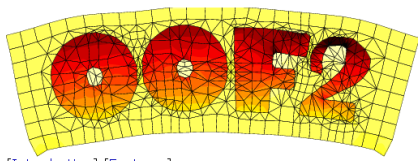
Open source

```
xterm
compute_temp_region.cpp
compute_temp_region.h
compute_temp_sphere.cpp
compute_temp_sphere.h
create_atoms.cpp
create_atoms.h
create_box.cpp
create_box.h
delete_atoms.cpp
delete_atoms.h
delete_bonds.cpp
delete_bonds.h
dihedral.cpp
dihedral.h
dihedral_charmm.cpp
dihedral_charmm.h
dihedral_harmonic.cpp
dihedral_harmonic.h
dihedral_helix.cpp
dihedral_helix.h
[strachan@coates-fe03 lammps-20Feb10]$ ls
LICENSE README
[strachan@coates-
```

abinit.org

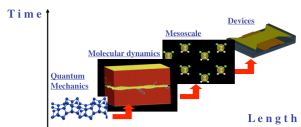
OOF: Finite Element Analysis of Microstructures

OOF2



[Introduction] [Features]
[System Requirements] [Download] [Installation] [Platform Specific
Installation Notes]
[Getting Started] [Manual] [FAQ]
[Reporting Bugs] [Known Problems]

>MyCode.f



Cyber-enabled cloud scientific computing

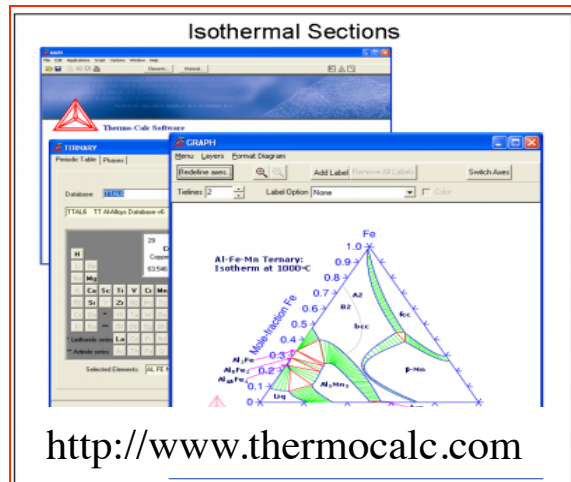


NSF network: Purdue, UIUC, Northwestern, Berkeley/LBL, MIT, U of Florida, Norfolk, UT El Paso

Commercial

Abaqus Unified FEA

Complete Solution for Realistic Simulation



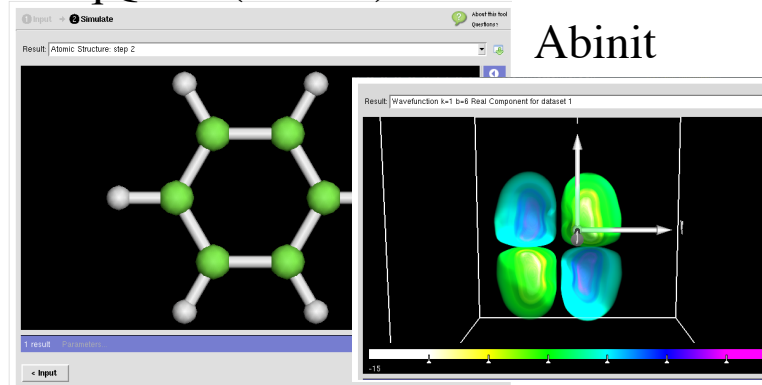
<http://www.thermocalc.com>

PURDUE
UNIVERSITY

Materials codes in nanoHUB

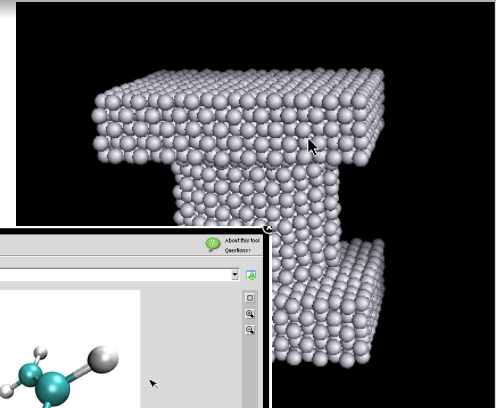
DFT tools

SeqQuest (Sandia)



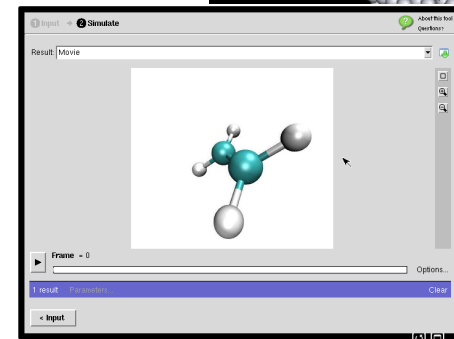
Molecular dynamics

LAMMPS, REBO,
nanoMATERIALS



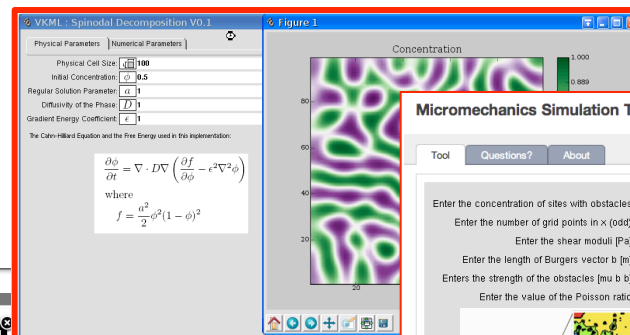
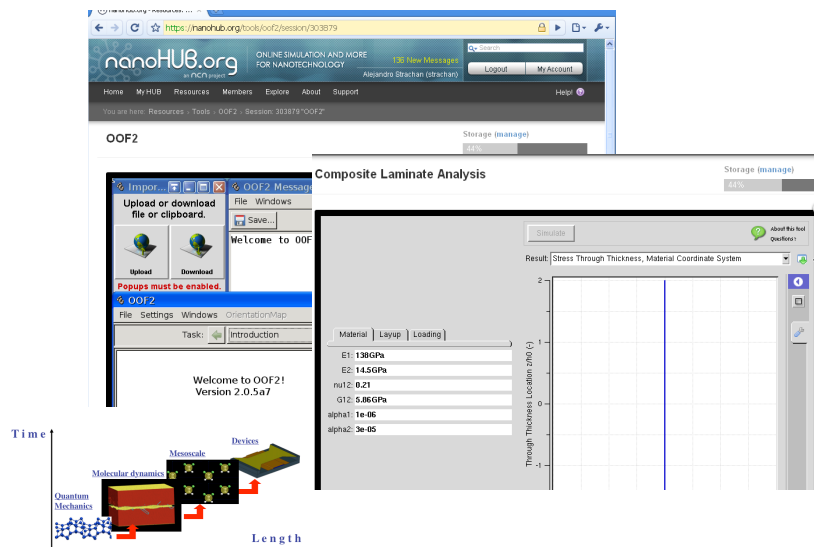
Mesoscale

Virtual kinetics

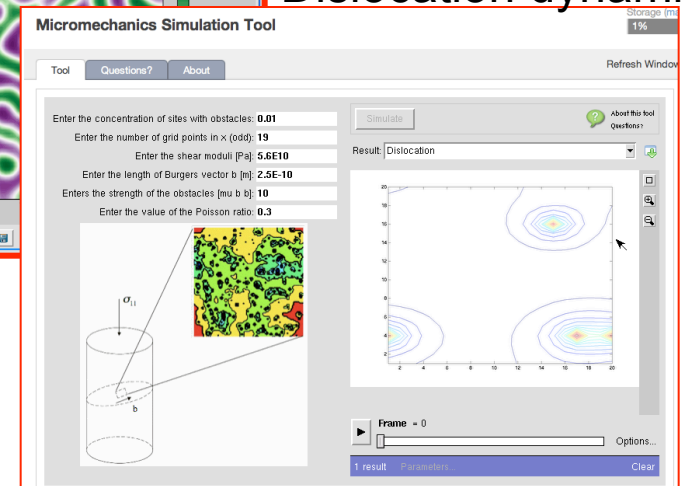


Finite elements

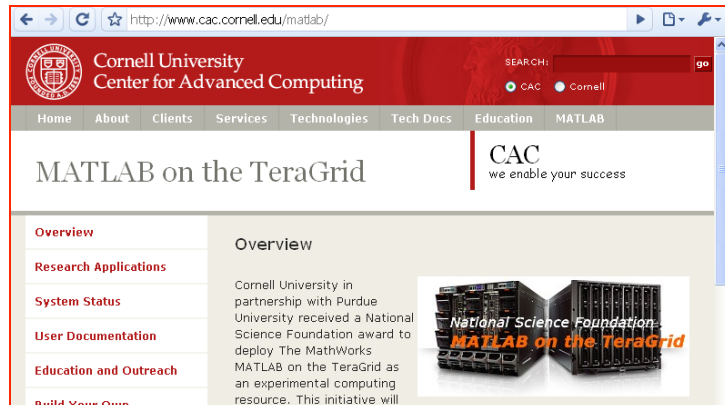
OOF2



Dislocation dynamics



General purpose resources



Cornell MATLAB Resource -

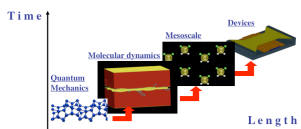
<http://www.cac.cornell.edu/matlab/>

- 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>



Example: learning module using online simulations

SIMULIA > Products nanoHUB.org - Topics: Lea...
http://nanohub.org/topics/LearningModulePlasticityMD

nanohUB.org
an ncn project
ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

Home My HUB Resources Members Explore About Support

You are here: Topics > Learning Module: Atomic Picture of Plastic ...

Learning Module: Atomic Picture of Plastic Deformation in Metals

by Joseph M. Cychosz, Alejandro Strachan

Article Comments History

The main goal of this learning module is to introduce students to the atomic-level processes responsible for plastic deformation in crystalline metals and help them develop a more intuitive understanding of how materials work at molecular scales. *Image to the right shows plastic deformation of a metallic nanowire.*

The module consists of:

- Two introductory lectures (50 minutes each) available online as audiovisual presentations
 - Overview Lecture
 - Prelab Lecture
- Hands-on lab involving online molecular dynamics (MD) simulations via nanoHUB.org
 - Lab Handout

Jump directly to the learning module by clicking on the links above, or continue reading for the module's

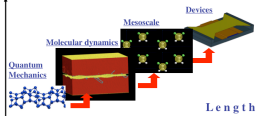
Slide 10 of 19 2002-11-07-CMDF-RPM English (U.S.)

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



Example: learning module using online simulations

Two online Lectures

Experimental tensile testing

The screenshot shows the nanoHUB.org website. The main heading is 'Learning Module: Atomic Picture of Plastic Deformation in Metals' by Joseph M. Cychosz, Alejandro Strachan. Below the heading, there is a table of contents with links to 'Why MD simulation', 'Learning objectives', and 'Audience'. There are also tags for 'molecular dynamics', 'molecular modeling', and 'simulation and modelling'. A list of lecture topics is provided: 'Two introductory lectures (50 minutes each) available online as audiovisual presentations', 'Overview Lecture', 'Prelab Lecture', and 'Hands-on lab involving online molecular dynamics (MD) simulations via nanoHUB.org'. A 'Lab Handout' link is also present. At the bottom, there is a navigation bar with 'Slide 10 of 19', '2002-11-07-CMDP-RPM', and 'English (U.S.)'.

What is molecular dynamics?

Running MD with nanoMATERIALS: step 1

Determine initial model for simulation

Select a model from menu
Click on Pt_nanowire_r13

Some possible operations

Create supercell

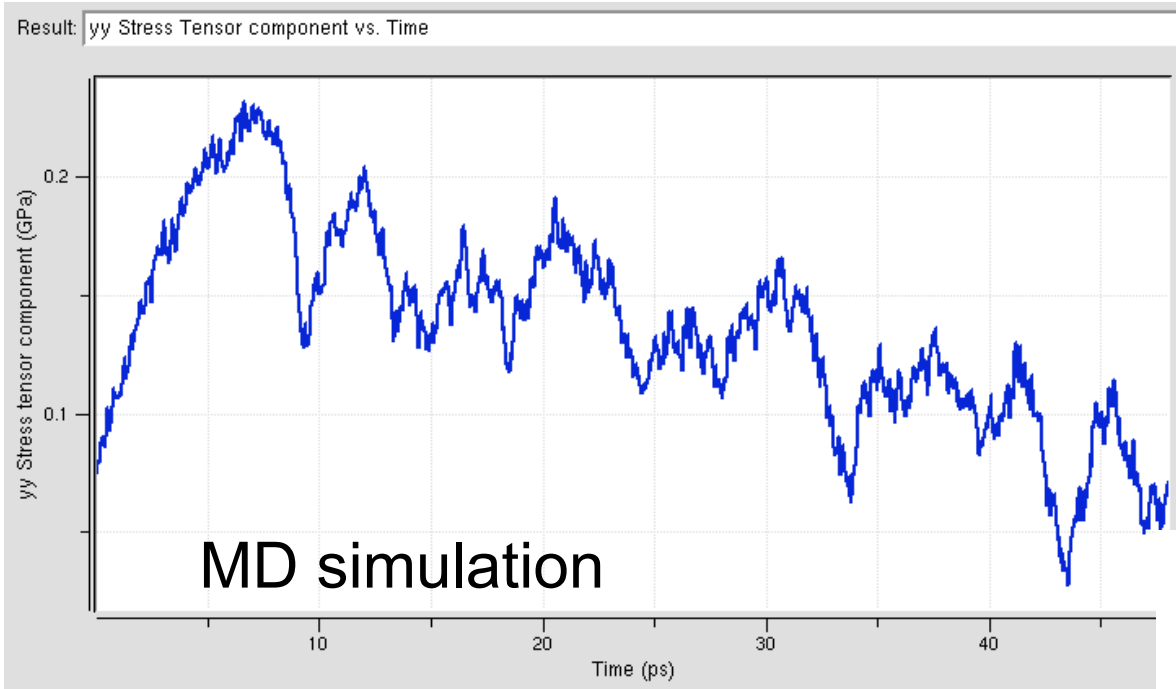
Modify the lattice parameters

The screenshot shows the nanoMATERIALS simulation toolkit interface. The 'Input Model' tab is selected, and the 'Create Supercell' section is visible. The 'Input model' field is set to 'Pt_nanowire_r13.bgl'. The 'Create Supercell' section has fields for 'a direction: 1', 'b direction: 2', and 'c direction: 1'. The 'Simulation cell parameters' section has a checkbox for 'Modify simulation cell parameters' which is currently unchecked. The 'Length' field is set to '5A'.

- Introduce topic and simulation tool
- Step by step tutorial to run a meaningful simulation and analyze the results

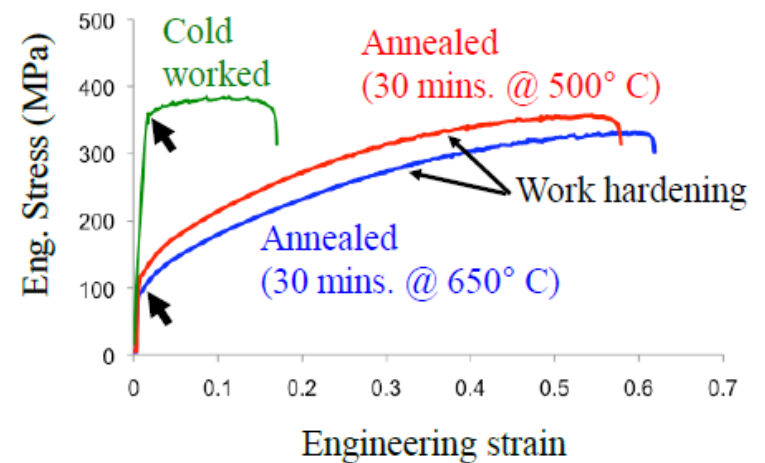


Compare MD results with tensile tests

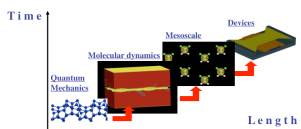


Stress vs strain

Experiment

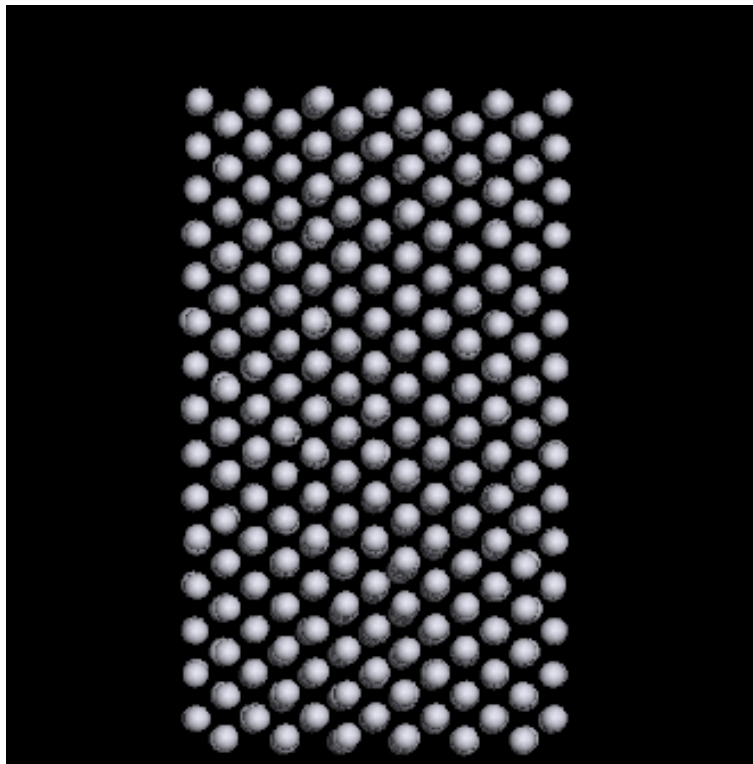


Nanoscale vs. macroscopic samples

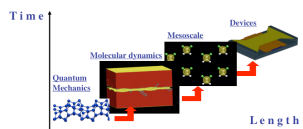
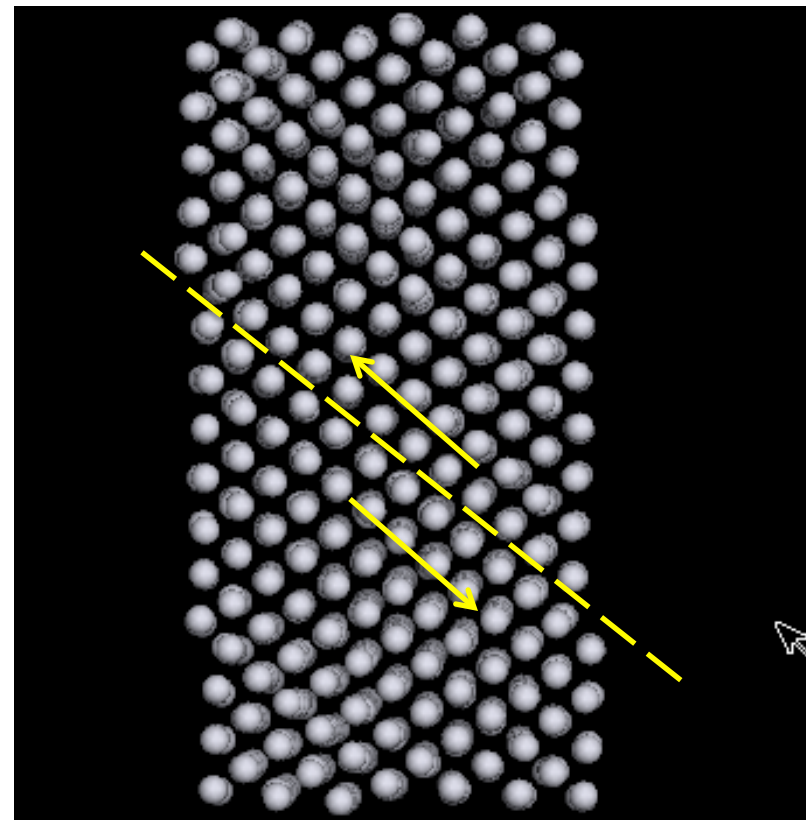


Explore atomistic processes

Initial structure

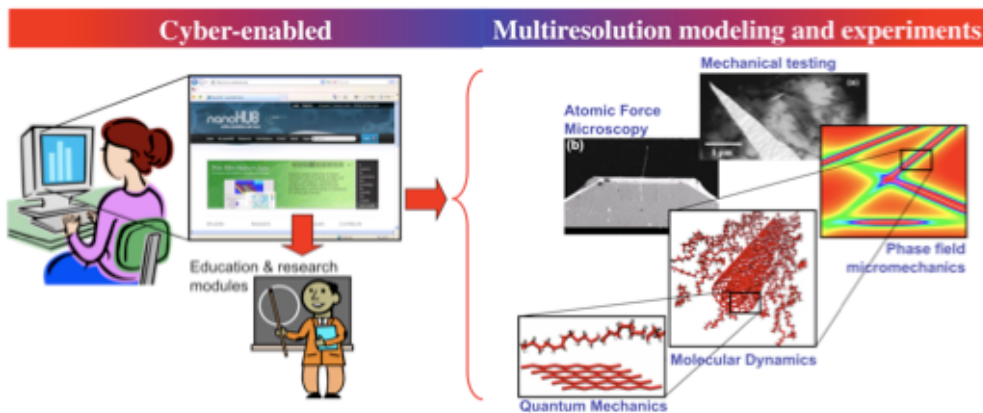


Final structure



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

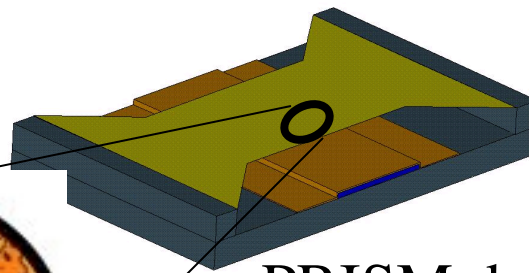


www.newairplane.com

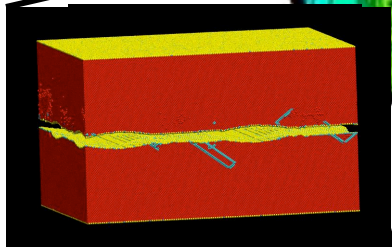
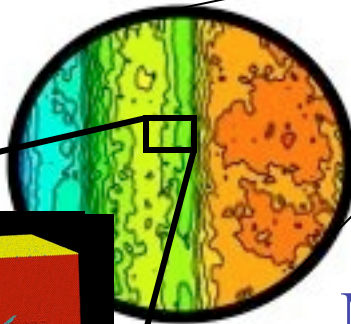


Leveraging integrated computing research efforts

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



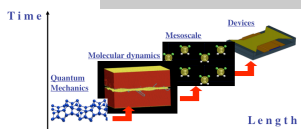
PRISM device:
Contacting RF capacitive switch



Mission:

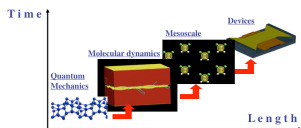
- Accelerate the incorporation of MEMS in civilian and defense applications
- Increase our understanding of failure and reliability

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



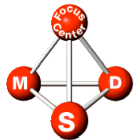
Summary

- 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

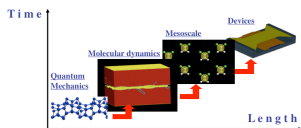


Thanks

Michael McLennan, Gerhard Klimeck, Mark Lundstrom, George Adams, David Johnson



MARCO focus center on
Materials Structures and
Devices



DoE-NNSA ASC



DoE-BES



Network for Computational
Nanotechnology

