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

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
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
• 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
Open source

Cyber-enabled cloud scientific computing

Commercial

Resources: simulation codes and software

Open source

- abinit.org
- OOF: Finite Element Analysis of Microstructures
- >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
- http://www.simulia.com
- http://www.thermocalc.com
Materials codes in nanoHUB

**DFT tools**
- SeqQuest (Sandia)
- Abinit

**Molecular dynamics**
- LAMMPS, REBO, nanoMATERIALS

**Finite elements**
- OOF2

**Mesoscale**
- Virtual kinetics

**Dislocation dynamics**

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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
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
Example: learning module using online simulations

Two online Lectures

1. Introduce topic and simulation tool
2. Step by step tutorial to run a meaningful simulation and analyze the results
Compare MD results with tensile tests

Stress vs strain

MD simulation

Nanoscale vs. macroscopic samples

Experiment

- Cold worked (30 mins. @ 500° C)
- Annealed (30 mins. @ 650° C)
- Work hardening
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
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