MECHENG 599-004 Special Topics Course:

Atomistic Computer Modeling of Materials

Tuesday and Thursday 10:30—noon, Fall 2009
DOW 2150

Computational hardware and algorithms have evolved to the point where they present a compelling alternative to the traditional experiment-based approach to materials research and development. This course will cover the core methods used to simulate matter at the atomic scale, and will offer hands-on experience with a number of research-caliber simulation codes on multi-processor clusters. A variety of applications will be highlighted, ranging from the mechanical properties of solids to the discovery of new materials for energy storage.

Syllabus:

1. Preliminaries: Structure of matter and Inter-atomic potentials
2. Molecular dynamics
3. Monte Carlo methods
4. Electronic structure methods: Hartree-Fock & Density Functional Theory
5. Transition state theory
6. Accelerated dynamics and multi-scale modeling

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