ME/MS: Computational Nanomechanics

Fall 2011

Instructor and Class Information

Instructor: Dr. Harold Park, Assistant Professor of Mechanical Engineering
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Phone: 617.353.4208
Office Hours: TBD
Class Hours: Tuesdays and Thursdays 8:00 AM - 10:00 AM
Classroom: TBD
Prerequisites: (1) Linear algebra; (2) Ordinary differential equations

Course Summary

This course offers a detailed introduction to the computational techniques that are needed to study the mechanical behavior and properties of nanomaterials. Specifically, the course focuses upon developing numerical discretizations to differential equations that govern the dynamics of nanomaterials, and that form the basis for modern molecular and multiscale modeling. The course also focuses on the development of novel multiple scale, or hybrid atomistic-continuum coupling techniques that enable spatial and temporal resolution at length and time scales that are not achievable by the single scale analyses alone. Finally, we will discuss new multiscale computational techniques that can capture the critical size and surface effects that cause the mechanical behavior and properties of low-dimensional nanostructures such as nanowires to differ greatly from their bulk counterparts.

Textbook

None.

Reference Books

- *Nonlinear Finite Elements for Continua and Structures* by T. Belytschko, W.K. Liu and B. Moran, Wiley 2000
- *Crystals, Defects and Microstructures* by R. Phillips, Cambridge University Press 2001

Class Policies

- Homework not turned in by the end of class (i.e. 10:00 AM) on the due date will be considered to be late. Late homework will be reduced by 10 percent for each class that goes by without turning it in. Homeworks that are more than 2 classes late will not be accepted.
- All complaints related to grading of homework and programming assignments must be reported to the instructor immediately after the grades are announced.

Approximate List of Topics to be Covered

Elements of nonlinear continuum mechanics and finite elements, including hyperelastic theory, deformation measures, strong and weak forms; introduction and overview of molecular dynamics/molecular statics, including interatomic potentials, equations of motion, energy minimization methods, surface energy and surface stress, equations of motion in different ensembles; quasicontinuum method and the Cauchy-Born rule, strain energy density, stress and modulus measures; surface Cauchy-Born model, and derivation from bulk Cauchy-Born theory, concurrent atomistic to continuum coupling methods.

Grading

- Homeworks and programming assignments: 100 percent