058:295 advanced topics of mechanical systems: multiscale modeling
Fall semester, 2004

2004 Catalog Data: 058:295, 3 s.h.

Lecture time: T Th 9:30AM – 10:45AM, 2128 SC

Catalog Description: Introduction to molecular dynamics, Monte Carlo method and continuum mechanics simulations at the nanoscale; Cauchy-Born rule and exponential Cauchy-Born rule for quasicontinuum methods; Coupling methods between molecular dynamics and continuum mechanics

Prerequisites: 058:115 or 058:143 or equivalent background in computational mechanics, computational chemistry or computational physics

Textbook: S. P. Xiao, class notes, 2004
Reference(s): some published articles

Instructor: Shaoping Xiao, assistant professor of Mechanical and Industrial Engineering

Student Group: This course is designed for PhD students

Course Goals: The main objective of the course is to introduce the basic concepts of numerical techniques at the nanoscale. The recently developed hierarchical and concurrent multiscale methods at the nanoscale are emphasized. Students are exposed to the forefront of computational nano- mechanics and material science.

Learning Objectives:

1. Gain an understanding of molecular dynamics and its applications.
2. Understand how to apply the (exponential) Cauchy-Born rule in quasicontinuum methods when using continuum mechanics at the nanoscale.
3. Understand the basic ideas of hierarchical and concurrent multiscale methods for coupling molecular dynamics with continuum mechanics.
4. Apply multiscale methods to obtain mechanical properties of nanostructures such as graphite sheet, diamond etc.
5. Learn about the forefront of computational nano- mechanics and material science research.

Topics(class hours)

1. Introduction and motivation (3)
2. Molecular modeling assumption, interatomic potential function (MM2, MM3, LJ etc.), Lagrangian and Hamiltonian formulations (3)
3. Molecular mechanics simulation and conjugate gradient method, molecular dynamics simulation and periodic boundary conditions. (6)
4. Introduction to Monte Carlo Method (6)
5. Overview of nonlinear finite element methods. (3)
6. Quasicontinuum method, Cauchy-Born rule and exponential Cauchy-Born rule. (3)
7. Introduction to multiscale methods such as CGMD, MAAD etc. (3)
8. Bridging scale method (3)
9. Bridging domain coupling method and its static and dynamics solutions (3)
10. Applications of multiscale methods such as crack propagation in a silicon block and bending of graphite sheet. (3)
11. Presentations of team projects (3)
12. in-class midterm; Individual presentation and discussion. (6)

Total: 45 class hours

Evaluation plan

3 Homeworks (projects)	30%
in-class midterm	20%
individual presentation	15%
team project	35%

The final grade of the students will be based on three homeworks or small projects, one individual in-class presentation, in-class midterm and the contribution to the team project. Each student will be required to search a recently published paper which is related to this course. He/she will be required to give an Individual in-class presentation and answer questions. The instructor will provide several possible topics for team projects. Each team will consist of 3 or 4 students (depending on the number of teams and students). Teams will meet with instructor regularly and give a presentation at the end of the semester. There is no final exam but final reports for the team projects will be due at the end of the class.