

University of Virginia, Department of Materials Science and Engineering  
Fall 2011, Tuesday and Thursday, 8:00 - 9:15 pm, Thornton Hall A 119

**MSE 4270/6270: Introduction to Atomistic Simulations**

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**Course web site:** <http://people.virginia.edu/~lz2n/mse627/>

**Abstract:** The course introduces students to atomic-level computational methods commonly used in Materials Science, Physics, Chemistry, and Mechanical Engineering. The molecular dynamics and Monte Carlo methods are discussed in depth, from the introduction to the basic concepts to the overview of the current state-of-the-art. Some of the emerging methods for mesoscopic and multiscale modeling are also discussed in the context of real materials-related problems (mechanical and thermodynamic properties, phase transformations, microstructure evolution during processing). Success stories and limitations of contemporary computational methods are considered.

The emphasis of the course is on getting practical experience in designing and performing computer simulations. Pre-written codes implementing atomistic computational methods will be provided. Students will use and modify the pre-written codes and write their own simulation and data analysis codes while working on their homework assignments and term projects. A set of example problems for term project will be provided, although students are encouraged to choose a project relevant to their thesis research.

Recent research articles in the area of atomistic modeling will be discussed, with each student presenting one or two article. Students will learn to assess the quality and significance of published computational results.

**4270/6270 split:** The two groups will have joint lectures and largely overlapping homework, with some of the homework problems identified as optional (extra credit) for undergraduate students. The expectation for term projects performed by graduate students is that new non-trivial scientific results are obtained and discussed in the context of current published data. Term projects by undergraduate students may reproduce (with some innovative additions) results reported in literature.

**Grading:** Term project 50%  
Homeworks 40%  
Presentation/discussion of published research articles 10%

**Homework:** cooperation among students (preferably through course e-mail list) is permitted.

**Main text:** Handouts and lecture notes posted on the course web site:  
<http://people.virginia.edu/~lz2n/mse627/>

**Books placed on reserve circulate in the Engineering Library:**

1. M. P. Allen and D.J. Tildesley, Computer simulation of liquids (Clarendon Press: Oxford, 1990, 1987). Call number: QC 145.2 .A43 1990 or QC145.2 .A43 1987
2. D. Frenkel and B. Smit, Understanding molecular simulation: from algorithms to applications (Academic Press: San Diego, 1996). Call number: QD461 .F86 1996
3. M. Metcalf and J. Reid, Fortran 90/95 explained (Oxford University Press: Oxford, New York, 1999). Call number: QA76.73 .F28 M49 1999

**Additional books:**

Jörg-Rüdiger Hill, Lalitha Subramanian, and Amitesh Maiti, Molecular modeling techniques in material sciences (Taylor & Francis/CRC Press: Boca Raton, FL, 2005). Call number: TA401.3 .H55 2005

Handbook of Materials Modeling, edited by Sidney Yip (Springer, Berlin, New York, 2005).

D. Raabe, Computational materials science: the simulation of materials microstructures and properties (Wiley-VCH: Weinheim, New York, 1998). Call number: TA403.6 .R23 1998

M. Meyer and V. Pontikis, Computer simulation in materials science: interatomic potentials, simulation techniques, and applications (Kluwer Academic: Boston, 1991). Call number: TA 403.6 .N42 1991

V. Bulatov, T. Diaz de la Rubia, R. Phillips, T. Kaxiras, and N.M.Ghoniem, Multiscale Modelling of Materials (Mat. Res. Soc. Symp. Proc. v. 538, MRS: Warrendale, Pa., 1999). Call number: TA405 .M887 1999

W. G. Hoover, Computational statistical mechanics (Elsevier: Amsterdam, New York, 1991). Call number: QC 174.8 .H66 1991

K. Ohno, K. Esfarjani, and Y. Kawazoe, Introduction to computational materials science: from ab initio to Monte Carlo methods (Springer-Verlag: Berlin, New York, 1999). Call number: TA404.23 .O36 1999

H. Kitagawa, T. Aihara Jr., Y. Kawazoe, Mesoscopic dynamics of fracture: computational materials design (Springer-Verlag: Berlin, New York, 1998). Call number: TA409 .M458 1998

K. Binder and D.W. Heermann, Monte Carlo simulation in statistical physics: an introduction (Springer: Berlin, New York, 1997). Call number: QC174.85 .M64 B56 1997

K. Binder, Monte Carlo and molecular dynamics simulations in polymer sciences (Oxford University Press: Oxford, New York, 1995). Call number: QD 381.9 .E4 M66 1995

T. Saito, Computational materials design (Springer: Berlin, New York, 1999). Call number: TA404.8 .C66 1999

W. H. Press, et al., Numerical Recipes in Fortran 90 (or C): The Art of Scientific and Parallel Computing, Cambridge University Press, is available on-line from <http://www.nr.com/>

## Topics that are covered include:

- Introduction
  - Spatial and temporal hierarchy of microstructure and dynamics in materials
  - Types of models: quantum mechanical, atomistic, mesoscopic, continuum
  - Multiscale approaches
- Atomistic models: Molecular dynamics
  - The basics of classical molecular dynamics
  - Initial conditions, creating lattice structures, introducing defects
  - Defining and maintaining temperature and pressure
  - Boundary conditions (free, periodic, stochastic, conducting, non-reflecting)
  - Methods for constant temperature or/and pressure simulations
  - Tricks of the trade (neighbor lists, force/energy tables, potential cutoffs, etc.)
- Monte Carlo methods
  - The basics of Monte Carlo
  - Monte Carlo integration, thermodynamic averages
  - Importance sampling, Metropolis scheme
  - Lattice Monte Carlo, Ising model
  - Multi-state Potts models (grain coarsening, recrystallization)
  - Kinetic Monte Carlo (surface processes, thin film growth)
- Interatomic potentials
  - Introduction, Born-Oppenheimer approximation
  - Pair potentials and their limitations
  - Calculation of elastic constants from potential function
  - Potentials for ionic systems, ceramics
  - Many-body potentials for metals
  - Many-body potentials for covalently bounded systems
  - *Forces from “first principles” (time permitting)*
- Analysis of the simulation results
  - Equilibrium properties (energy, temperature, pressure, velocity distributions)
  - Structural properties (geometrical tessellation, pair correlation functions, atomic-level stresses)
  - Dynamic properties (diffusion, time correlation functions)
- *Examples of mesoscopic methods (time permitting)*
  - *Discrete dislocation dynamics*
    - *Strain and stress fields for edge and screw dislocations in an isotropic medium*
    - *The equation of motion in Newtonian Dislocation Dynamics*
    - *Examples from 2D and 3D simulations*
    - *Current problems*
  - *Coarse-grained models for organic materials*
- Bridging the scale gaps between different simulation levels
  - Simultaneous integration of the models
  - Sequential integration of the models (hierarchical approach)
  - Examples of combined methods (MD-FEM, MD-MC, etc.)

- *Computer use (if needed)*
  - *Introduction to UNIX and Networking*
  - *Visualization (Java-applets, animated gifs, VRML, animations with Tecplot)*
- Codes to be provided
  - MSE627-MD code for MD simulations
  - MSE627-CG crystal generator (FCC, BCC, diamond)
  - MSE627-MC Ising model for binary alloys

### **Discussion of published research articles**

Each student will lead one or two discussions of recent research papers in the area of atomistic simulations (~10-15 min). Although a few papers will be proposed by instructor, students are encouraged to propose papers that are interesting or relevant to their research work (but not to the term project). Papers should be posted on the course web site at least one week before the discussion.

### **Term project**

**Objective:** To get experience in designing and performing computer simulations.

#### ***Parts of the project:***

- Design (or adapt an idea from literature) a simulation that is of scientific or computational interest to you
- Justify what computational approach is appropriate
- Write a computer code (or add parts to MSE627-MD code)
- Perform simulations and analyze the results
- Prepare a report; include electronic copies of your code
- Make a short presentation to the class (mini-symposium)

#### ***Tentative timeline:***

September 15<sup>th</sup> - have project approved by instructor

October 13<sup>th</sup> – turn in introduction (with references to relevant papers) and discuss progress with instructor (optional)

December 9<sup>th</sup> and 10<sup>th</sup> – turn in a report; give a presentation to the class at a mini-symposium

#### ***Sample projects:***

A set of example problems for term project will be given. A problem chosen for the term project should have some science content and be doable in the timeframe of one semester. Students are encouraged to choose a project relevant to their thesis research. If the intention is to continue computational work in the future, the term project may be a well-defined part of a larger research project.