University of Virginia, Department of Materials Science and Engineering

Spring 2025, Tuesday and Thursday, 3:30 - 4:45 pm, Jesser Hall 171

MSE 4270/6270: Introduction to Atomistic Simulations

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Course web site: https://CompMat.org/mse6270/

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 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%
Homework 50%

Homework: Discussions among students are permitted *at the conceptual level*, particularly through the course e-mail list.

Main text: Handouts and lecture notes posted on the course web site:
https://CompMat.org/mse6270/

Online textbooks available through UVa library:

1. M. P. Allen and D. J. Tildesley, Computer simulation of liquids, 2nd edition (Oxford University Press, 2017)
https://academic.oup.com/book/27866
2. D. Frenkel and B. Smit, Understanding molecular simulation: from algorithms to applications, 2nd edition (Elsevier Science & Technology, 2001)
https://ebookcentral.proquest.com/lib/uva/detail.action?docID=307221
(access to the online books may require login to UVa account)

Additional books:

S. Yip, Molecular Mechanisms in Materials: Insights from Atomistic Modeling and Simulation (MIT Press, 2023). https://direct.mit.edu/books/monograph/5676/Molecular-Mechanisms-in-MaterialsInsights-from

R. LeSar, Introduction to Computational Materials Science (Cambridge University Press, 2013).

J. G. Lee, Computational Materials Science, An Introduction (CRC Press, 2011).

M. J. Buehler, Atomistic Modeling of Materials Failure (Springer, 2008).

J.-R. Hill, L. Subramanian, and A. Maiti, Molecular modeling techniques in material sciences (Taylor & Francis/CRC Press: Boca Raton, FL, 2005).

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

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

M. Meyer and V. Pontikis, Computer simulation in materials science: interatomic potentials, simulation techniques, and applications (Kluwer Academic: Boston, 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).

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

K. Binder, Monte Carlo and molecular dynamics simulations in polymer sciences (Oxford University Press: Oxford, New York, 1995).

T. Saito, Computational materials design (Springer: Berlin, New York, 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 https://numerical.recipes/

M. Metcalf and J. Reid, Modern Fortran Explained (Oxford University Press: Oxford, New York, 2011)

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*
  - *Mesoscopic models for nanofibrous and carbon nanotube 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.)

- 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 discussion of a research paper in the area of atomistic simulations (10 min). Although a few papers may be proposed by the instructor, students are encouraged to propose papers that look interesting to them or are relevant to their research work (but not to the term projects). 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(s) (or add parts to MSE627-MD code)
- Perform simulations and analyze the results
- Prepare a report; include electronic copies of your code
- Present your results to the class (mini-symposium)

Tentative timeline:

February 1st – decide in the topic/title of your project and inform the instructor

March 1st – prepare the first draft of the introduction (with references to relevant papers) and discuss progress with instructor (optional)

Early May (dates TBD) – turn in report; give 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.