

Computational Methods in Materials Science

MATS 588, Spring 2015
Instructor: **Alex Greaney**

Lecture: Wngr. 285, Tu.& Th., 09:00–09:50
Lab: Dear. 19, Tu.& Th., 14:00–15:50

Course Credits: 4 credits. This course is comprised of two fifty minute lectures and two one hour and fifty minute sessions of instruction in the computer lab.

Prerequisites, Co-requisites and Enforced Prerequisites: ME 112 or prior experience programming with *MATLAB*, *Mathematica* and/or scripting languages such as *Python* or *Perl*.

Course Content: An introduction to computational methods used in materials science, ranging from atomistic methods, including density functional theory and molecular dynamics, to the continuum and including Monte Carlo methods. The aim of this class is to teach materials simulation methods through hands-on lab projects in which students use computational methods to explore and reinforce important concepts in materials science. A second, and equally important aim of the class is to teach how and when to use modeling and simulation effectively, when to avoid simulation, and how to critically assess simulation results (one's own or others').

Topics covered: List of topics covered by fortnightly mini project

- **Weeks 1-2:** *The Ising model, and Monte Carlo methods*
 - *Concepts:* Difference between model and simulation; order parameters; phase transitions and critical slowing down; pseudo random numbers and stochastic sampling.
 - *Calculations/Tasks:* Students write their own Ising model simulation in *Matlab*, culminating with use of it to compute the vacancy self-correlation correction factor that arises in vacancy mediated lattice diffusion coefficient.
- **Weeks 3-4:** *Molecular statics*
 - *Concepts:* Fundamentals of empirical interatomic potentials; pair vs. many body potentials; elastic compliance for a cubic material and the Cauchy pressure; the dynamical matrix; and building continuous distributions from discrete data.
 - *Calculations/Tasks:* Computation of elastic constants, the phonon dispersion, and specific heat capacity (using LAMMPS).
- **Weeks 5-6:** *Molecular dynamics*
 - *Concepts:* fundamentals of integration of atom trajectories; the Verlet algorithm; Lyapunov instability and phase space; thermostats, thermodynamic ensembles, and thermodynamic averaging; and correlation functions.
 - *Calculations/Tasks:* Compute melting/freezing hysteresis in a simple system; construct pair-pair distributions, and compute temperature dependent vibrational spectrum from the velocity autocorrelation function. Tasks completed in small teams.
- **Week 7-8** *Introduction to Density Functional Theory*
 - *Concepts:* The Kohn-Sham ansatz; XC functional for local density approximation; basis sets; self consistent solution to the electron density; and convergence.

- *Calculations/Tasks*: Using DFT compute the energy barrier for surface diffusion, and adatom-adatom binding energies. Use these in the Ising model to simulate 2D nucleation and growth. Determine transition from compact to dendritic (fractal) growth. Required DFT calculations distributed amongst the class.

- **Week 9-10** *Final independent project.*

- *Concepts*: During the last two weeks the lectures will focus on “When is modeling useful?” and the ethics of modeling; validation of simulation; issues surrounding data management; and high performance and high throughput computing.
- *Calculations/Tasks*: Work will be devoted to an independent final project. This will be chosen by the student in consultation with instructor and must relate to the student’s research. Students will also have to present a 5 minute “research proposal” on their final project.

Measurable Student Learning Outcomes:

1. Demonstrate a sound understanding of what is, and what is not, meaningful computer simulation. Knowing what new insight can we learn through simulation and what simulation can not teach us.
2. Demonstrate understanding of the fundamentals of Monte Carlo methods
3. Demonstrate practical understanding of molecular dynamics (MD) and the anatomy of an MD simulation
4. Demonstrate working understanding with density functional theory and its practical application to predict configurational energies, band gaps, and wave functions.

Evaluation of Student Performance: There is no final exam. Grading is based entirely on 5 project reports and an oral presentation with the following weighting: 15% Project 1, 20% Project 2, 20% Project 3, 20% Project 4, 20% Project 5 5% In class presentation of research proposal. Project reports are due at 2pm on Tuesday of week 3 and every subsequent fortnight.

Learning Resources: The required textbooks for this class is:

- Richard LeSar, “Introduction to Computational Materials Science: Fundamentals to Applications”

As the class covers the introduction to a wide spectrum of methods there are few text books that cover all of the topics nicely. An important aspect of the class is that you learn methods by doing them, reinforce concepts by seeing them in action in your simulations. Listed here are some texts that will enable you to go deeper into the topics covered in class:

- Ellad Tadmor and Ronald Miller, “Modeling Materials: Continuum, Atomistic and Multiscale Techniques”
- Daan Frenkel “Understanding Molecular Simulation”

- Richard Martin: “Electronic Structure: Basic Theory and Practical Methods”
- William H. Press, Saul A. Teukolsky and William T. Vetterling, “Numerical Recipes”
- K. Ohno, “Computational Materials Science: From Ab Initio to Monte Carlo Methods”

Office Hours: Office hours will be held in 304 Dearborn Hall on Tuesday 10–11am, and Thursday 4–5pm.

Academic Dishonesty: Oregon State University provides clear definition and sanctions for academic dishonesty. As a result, academic dishonesty of any kind is not tolerated. For suspected academic dishonesty, a meeting with the student will take place and a formal report to the Chair of the Department, to the student’s dean, and to the Student Conduct Office may follow. Students caught cheating, plagiarizing, or participating in any form of academic dishonesty may receive an F or other penalty on the assignment or test and possibly in the course. If you have any questions about the definition of academic dishonesty or the extent of sanctions that may result from dishonest behavior, it is important to access information on the OSU Student Conduct Website at:
<http://oregonstate.edu/studentconduct/offenses>

Statement Regarding Students with Disabilities: Accommodations are collaborative efforts between students, faculty and Disability Access Services (DAS). Students with accommodations approved through DAS are responsible for contacting the faculty member in charge of the course prior to or during the first week of the term to discuss accommodations. Students who believe they are eligible for accommodations but who have not yet obtained approval through DAS should contact DAS immediately at 737-4098.