MASC 455-

Instructor: Priya Vashishta

Computational Materials I: Introduction to Atomistic Simulations

Fall 2021, 4 Units

Monday & Wednesday
Online, 2:00-3:50pm

- ✓ No prerequisite – Very simple math - only 1st and 2nd derivative and Gaussian Integral are used
- ✓ No homework. Four tests on course materials
- ✓ Three simulation projects on materials modelling
- ✓ No Final exam. Review of three projects
- ✓ In this course, you will learn,

- Basics of atomistic simulations using Molecular Dynamics & Monte Carlo methods
- How to model materials properties & processes
- Hands-on projects using USC High-performance computing center

Please contact Karen Woo Email: karenwoo@usc.edu for d-clearance

https://classes.usc.edu/term-20213/classes/masc/

USC Viterbi School of Engineering

MASC 455

Computational Materials Science and Engineering I: Introduction to Atomistic Simulation and Materials Modeling

Units: 4   Fall 2021

Time: Monday & Wednesday 2:00-3:50pm

Location: GFS 111

Instructor: Priya Vashishta
Office: VHE 608   Contact Info: priyav@usc.edu

Course Description

Computaitonal materials modeling and simulations have become critically important tools in materials science and engineering as well as in many other disciplines of engineering and technology. This course provides an introduction to the most widely used atomistic simulation techniques, namely molecular dynamics (MD) and monte carlo (MC) simulation methods. The focus of this course is to understand basic physical and engineering principles that underline MD & MC methods. In addition, the course offers an introduction to high performance computing (HPC) enrionment and Fortran programming for students that have little or no computing backgrounds. The course also has hands-on simulation projects using USC's high-performance computing center. The projects include material processes such as melting, thermal expansion, and characterization using structural and dynamical correlations. No prior experience or background of computer modeling and simulation is required to take this course.

Learning Objectives

In this course, students will learn

1. Basics of molecular dynamics and monte carlo simulation methods
2. How physical and materails properties are obtained using atomitics simulations.
3. How to design, organize and efficiently carry out atomisitc simulations using high-performance computing.

Prerequisite(s): None
Co-Requisite(s): None
Concurrent Enrollment: None
Recommended Preparation: Introductory differential and integral calculus
Course Notes Grading type: letter grade. All course notes will be provided on Blackboard.

Technological Proficiency and Hardware/Software Required

Personal laptop computer is necessary for the hands-on projects. Students will be provided MD and MC modeling and simulation computer programs to do their hands-on simulation projects.

Required Readings and Supplementary Materials

Computer Simulation of Liquids - Allen and Tildesley
Reading materials will be given in the class and posted on Blackboard.

Description and Assessment of Assignments

The learning outcome is assessed by four tests based on lectures and two simulation projects, and final simulations project review. There is no regurlar home work in this course. One test will be given roughly every month (four tests in total) on topics covered in the lectures during each period. Hands-on experience of the simulation methodologies using MC and MD projects provides solid understanding of materials and processes. During the final week each students will meet with instructor to review their simulation project reports. Instructor will provide comments and feedbacks.

Grading Breakdown

Assignment	Points	% of Grade
Test #1 : MD part 1	100	12.5%
Test #2 : MD part 2	100	12.5%
Test #3 : Linux and Fortran	100	12.5%
Test #4 : Ensembles	100	12.5%
MC Project	100	15%
MD Project	100	35%
TOTAL	600	100%

Assignment Submission Policy

MC project due is in two weeks after being assigned.
MD project due is in four weeks after being assigned.

Grading Timeline

Each test will be graded within two week. The grade will be posted on Blackbord.

Course Schedule: Weekly Breakdown

	Topics/Daily Activities	Readings and Homework	Deliverable/ Due Dates
Week 1	• Course overview, HPC account setup	"Correlations in the Motion of Atoms in Liquid Argon" A. Rahman, *Phys. Rev.* **136**, A405	
Week 2	• Atomic structure and interatomic bonding • Interatomic potentials. • Lennard-Jones potential: steric & attractive interactions, characteristic energy & length scales.	Allen and Tildesley Ch1	
Week 3	• Review on vector, matrix and differential and integral calculus • Discretization of equation of motion	Allen and Tildesley Ch1 Lecture Notes: Molecular Dynamic Basics I	
Week 4	• Dimensionsless coordinates of the system : Normalized equation of motion and interatomic potential	Allen and Tildesley Ch3 Lecture Notes: Molecular Dynamic Basics I	
Week 5	• Integraton methods : Verlet and velocity-Verlet algorithms.	Allen and Tildesley Ch3	

	• Algorithmic transformation and numerical error analysis	Lecture Notes: Molecular Dynami Basics I	
Week 6	• Boundary coditions : PBC and MIC • Initial configurations : crystal structu • Conservation laws: energy & momentum	Lecture Notes: Molecular Dynami Basics II	
Week 7	• Initial velocity : Random number generator • Radial and spherical coordinate transformation	Lecture Notes: Molecular Dynami Basics II	
Week 8	• Concepts of temperature, pressure i MD • Maxwell-Boltzmann distribution, Equipartition theorem • Temperature control schemes		
Week 9	• Introductio to Linux and Fortran programming • Computer and network architecture	Lecture Notes: Linux and Fortran	
Week 10	• **MD Project:** Project description, simulation setup and goal. • Simulation hands-on, data analysis a visualization	Assignemnt #1: MD project	
Week 11	• Canonical ensemble: specific heat, fluctuations	Allen and Tildesley Ch2	
Week 12	• Monte Carlo Method: Metropolis algorithm, Ising model, MC integrati method	Allen and Tildesley Ch4 Lecture Notes: Monte Carlo Basics	
Week 13	• **MC Project :** Project description, simulation setup and goal. • Simulation hands-on, data analysis	Allen and Tildesley Ch4 Assignement #2: MC project	MD project due
Week 14	• Atomistic characterization of materi pair-distribution function, mean-squ displacement • Structural phase tranformations	Allen and Tildesley Ch8 Lecture Notes: Molecular Dynami Basics III	
Week 15	• Temperature and pressure control ir MD simulations	Lecture Notes: Molecular Dynami Basics III	MC project due
FINAL	Project Review	N/A	Date: For the date ar time of the final for t class, consult the USC *Schedule of Classes* a classes.usc.edu.

Statement on Academic Conduct and Support Systems

Academic Conduct:

Plagiarism – presenting someone else's ideas as your own, either verbatim or recast in your own words – is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in *SCampus* in Part B, Section 11, "Behavior Violating University Standards" policy.usc.edu/scampus-part-b. Other forms of academic dishonesty are equally unacceptable. See additional information in *SCampus* and university policies on scientific misconduct, http://policy.usc.edu/scientific-misconduct.