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/
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
Computational 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 underlie MD & MC methods. In addition, the course offers an introduction to high performance computing (HPC) environment 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 materials properties are obtained using atomistics simulations.
3. How to design, organize and efficiently carry out atomisitic 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 regular 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

<table>
<thead>
<tr>
<th>Assignment</th>
<th>Points</th>
<th>% of Grade</th>
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</thead>
<tbody>
<tr>
<td>Test #1: MD part 1</td>
<td>100</td>
<td>12.5%</td>
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<tr>
<td>Test #2: MD part 2</td>
<td>100</td>
<td>12.5%</td>
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<tr>
<td>Test #3: Linux and Fortran</td>
<td>100</td>
<td>12.5%</td>
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<tr>
<td>Test #4: Ensembles</td>
<td>100</td>
<td>12.5%</td>
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<tr>
<td>MC Project</td>
<td>100</td>
<td>15%</td>
</tr>
<tr>
<td>MD Project</td>
<td>100</td>
<td>35%</td>
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<tr>
<td>TOTAL</td>
<td>600</td>
<td>100%</td>
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</tbody>
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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

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