New Jersey Institute of Technology
Digital Commons @ NJIT

Chemical and Materials Engineering Syllabi | NJIT Syllabi

Spring 2020

CHE 775-102: Molecular Simulations in Chemical Engineering

Gennady Gor

Follow this and additional works at: https://digitalcommons.njit.edu/cme-syllabi

Recommended Citation
Gor, Gennady, "CHE 775-102: Molecular Simulations in Chemical Engineering" (2020). *Chemical and Materials Engineering Syllabi*. 106.
https://digitalcommons.njit.edu/cme-syllabi/106

This Syllabus is brought to you for free and open access by the NJIT Syllabi at Digital Commons @ NJIT. It has been accepted for inclusion in Chemical and Materials Engineering Syllabi by an authorized administrator of Digital Commons @ NJIT. For more information, please contact digitalcommons@njit.edu.

ChE 775: Molecular Simulations in Chemical Engineering
Spring 2020

Instructor: Dr. Gennady Gor, Assistant Professor web: `http://porousmaterials.net`
Office/Lab: 364/321A Tiernan Hall, Phone: 973-596-2944, E-mail: gor@njit.edu
Class: Thursday, 6:00-9:05 PM; Room: FMH321 Office hours: by appointment only
Text: Required: Allen, M. P. and Tildesley, D. J. Computer Simulation of Liquids, Oxford, 1989
Additional: McQuarry, D. A. Statistical Mechanics, University Science Books, 2000
Dill, K. and Bromberg, S., Molecular driving forces: statistical thermodynamics in biology, chemistry, physics, and nanoscience (Second Edition). Garland Science, 2010

Course Objectives

Taking this course, a motivated student will learn:
1. What quantities can be calculated using molecular simulations
2. How statistical mechanics relates the microscopic properties to the macroscopic ones
3. How molecular dynamics and Monte Carlo methods work
4. How to implement one of these methods for a basic system
5. How to use these methods implemented in popular open source tools
6. How to use High Performance Computing facilities (available at NJIT) to run molecular simulations
7. How to search and study literature on molecular simulations
8. How to write reports on computational projects

Course Outline

This course aims to kill two birds with one stone: (1) to cover the basics of classical statistical mechanics and (2) explain how the most common methods of molecular modeling work. Understanding the latter is not possible without knowing the former. The course will include several computational assignments. It will include a short introduction to Python 3, NumPy and SciPy, so that we all "speak the same language".

Today molecular simulations became a significant complement to "paper-and-pencil" theory and experimental research. Moreover, often molecular simulations can substitute experimental research being much cheaper, safer and faster. Molecular simulations are used in numerous various fields, e.g. they are applied to study problems related to drug design, protein folding and aggregation; wetting phenomena and hydration thermodynamics; nucleation and growth processes; the thermophysical properties of complex fluids, such as ionic liquids and liquid crystals; the phase behavior of polymeric, colloidal, and self-assembled systems; and the synthesis, design and characterization of advanced materials, etc.

Pre-Requisites: There are no formal pre-requisites. The course is aimed for Ph.D. students, but M.S. students are also encouraged to enroll. Although the course is theoretical, it is expected that students focused on experimental work will also benefit. Experimentalists often have to deal with the literature data, obtained using molecular simulations, and this course will help them in making sense of the simulation results. The course is about the methods and not about any specific systems, so it could be of interest for students outside of ChemE, e.g. physics, chemistry, mechanical engineering, etc.

Course Format: the course consists of lectures and practical sessions. Each weekly meeting typically includes both. Therefore, students should bring their laptops to every class.
Homework: There will be several homework assignments during the semester, which will be collected and graded. The assignments will be posted on Canvas.
Exams: There will be two exams in the form of the research mini-projects. The projects will be implemented in teams of 2-4 students. The individual grade for each of the team members will be calculated as the team grade, multiplied by the participation coefficient calculated based on peer-evaluations from all the team members. Midterm exam (project) will require implementing a basic molecular simulation code in Python, using it to calculate thermodynamic properties, analyzing the result and writing a report. The grade will take into account all the aspects of the assignment. The final exam (project) will require running a molecular simulation to solve a outstanding research problem within the scope of interests of Computational Laboratory for Porous Materials. The final project will be implemented using an existing open-source MC or MD code. It will require getting familiar with the literature on the topic, setting up and running the simulations, analyzing data and writing a report in a form of a paper. Note that excellent final reports can become publishable research papers.
Projects Examples:
Midterm projects:
1. MD simulations for LJ particles (2D or 3D) in microcanonical ensemble
2. MC simulations for hard disks in canonical ensembles
3. MC simulations for hard disks or hard spheres in canonical ensemble
4. MC simulations for LJ particles (2D or 3D) in canonical ensemble
Final projects:
1. Simple fluids: Calculation of bulk VLE for pure fluids and mixtures of practical interest using MC simulations in Gibbs ensemble (in RASPA)
2. Macromolecules: Calculation of solvation free energies of polymers in organic solvents (in LAMMPS)
3. Biomolecules: Calculation of adhesion forces between aminoacids and minerals of practical interest in aqueous environment (in LAMMPS or GROMACS)

Grading

Homeworks	30%
Midterm project	30%
Final Project	30%
Participation	10%
	100%

Percent	Grades	Points
above 85%	A	4.0
above 75%	B+	3.5
above 65%	B	3.0
above 55%	C+	2.5
above 45%	C	2.0
below 45%	F	0.0

The "participation" part of the grade will be based on participation in the in-class discussions. Attendance is expected. Unexcused absence will decrease the participation part of the grade.
The NJIT Honor Code will be upheld and any violations will be brought to the immediate attention of the Dean of Students.

Topics

- General overview of classical molecular simulations methods and a spectrum of research problems which can be solved using them. Overview of the topics for the course projects.
- Use of HPC resources at NJIT and beyond
- LAMMPS: an open source molecular dynamics simulations package
- RASPA: an open source Monte Carlo simulations package
- Review of basic physics needed for classical molecular simulations: classical mechanics, quantum mechanics and thermodynamics
- Review of basics of statistical mechanics. Statistical ensembles: Microcanonical, Canonical, Grand canonical. Fluctuations.
- Simple examples of applications of statistical mechanics: Lattice model for ideal solution, Flory-Huggins model for polymer solution, Boltzmann statistics, Ideal gas model
- Classical Statistical Mechanics, Classical partition function, Real classical fluids, Virial EOS, Second virial coefficient
- Interatomic potentials and their implementation for molecular simulations
- Basics of molecular dynamics (MD) simulations and its implementation, Verlet and leap-frog algorithms, MD for Lennard-Jones system
- MD for complex systems, MD algorithms for non-rigid, non-spherical molecules
- Distribution function theory, Definition and calculations of thermodynamic properties, Radial distribution function, Virial pressure
- Integral equation theory, Ornstein-Zernike, Percus-Yevick, Carnahan-Starling
- Basics of Monte Carlo methods, Markov process, Metropolis algorithm
- Monte Carlo in canonical ensemble and grand canonical ensemble, Widom insertion method,
- Monte Carlo simulations in Gibbs ensemble, Free energy calculations

Exams

Date	**Exam**
March 22	Midterm Exam (Midterm report submitted by the end of the Spring recess)
May 8-14	Final Exam (Submission of the final version of the report for the final project)

Note: the final grades are due May 16