ChE 702: (ST) Statistical Thermodynamics and Molecular Modeling
Spring 2017

Instructor: Dr. Gennady Gor
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Class: Tuesday, 6:00-9:05 PM; Room: FMH205 Office hours: by appointment only
Text. Required: McQuarry, D. A. Statistical Mechanics, University Science Books, 2000
Additional: Allen, M. P. and Tildesley, D. J. Computer Simulation of Liquids, Oxford, 1989
Dill, K. and Bromberg, S., Molecular driving forces: statistical thermodynamics in biology, chemistry, physics, and nanoscience (Second Edition). Garland Science, 2010

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 2.7, 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.

Homework: There will be regular homework assignments during the semester, which will be collected and graded. The assignments will be posted on Moodle.

Exams: There will be two exams in the form of the mini-research projects. Midterm exam will require running a small molecular simulation project using the existing open-source code, analyzing the result and writing a report. The grade will take into account all the aspects of the assignment. The final exam will require implementing a very basic molecular simulation code, using it to solve a certain problem and writing a report in a form of a paper. Note that an excellent final report for some of the final projects can become a real research paper.

Grading

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

Percent	Grades	GPA
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.

Course Objectives

Taking this course, a motivated student will learn:

1. What quantities can be calculated using molecular simulations
2. Classical statistical mechanics, which is the theoretical basics of molecular simulations
3. Simple algorithms for two main molecular simulation methods, Molecular Dynamics and Monte Carlo
4. How to implement one of these algorithms for a basic system
5. How to use these methods implemented in popular open source tools

Schedule

1. January 17: Review of classical mechanics and thermo and statistics

   - Review of classical mechanics
   - Newtonian, Lagrangian, Hamiltonian approaches
   - Review of quantum mechanics
   - Review of classical thermodynamics
   - Review of the probability theory

   Reading: MQ. Ch.1, D. Ch.1, D. Ch.11

2. January 24: Statistical ensembles

   - Method of Lagrange multipliers
   - Microcanonical ensemble
   - Canonical ensemble

   Reading: MQ. Ch.1, MQ. Ch.2, D. Ch.4

3. January 31: Statistical ensembles. Fluctuations.

   - Grand canonical ensemble
   - Other ensembles
   - Fluctuations

   Reading: MQ. Ch.3

4. February 7: Simple examples

   - Lattice model for ideal solution
   - Flory-Huggins model for polymer solution
   - Boltzmann statistics
   - Ideal gas model

   Reading: MQ. Ch.4, MQ. Ch.5, D. Ch.15, D. Ch.27, D. Ch.32,

5. February 14: Classical stat. mech., Real fluids

   - Classical Statistical Mechanics
   - Classical partition function
   - Real classical fluids
   - Virial EOS
   - Second virial coefficient

   Reading: MQ. Ch.7, MQ. Ch.12

6. February 21: Real fluids (cont.)

   - Second virial coefficient
   - Calculations of virial coefficients using diagrams

   Reading: MQ. Ch. 12

7. February 28: Interatomic potentials and their implementation for molecular simulations

   - Interatomic potentials
   - Implementation for molecular simulations

   Reading: AT Ch.1, D. Ch.24

8. March 7: Basics of molecular dynamics (MD) simulations and its implementation

   - Verlet and leap-frog algorithms
   - MD for Lennard-Jones system using Gromacs

Reading: AT Ch.3

9. March 21: MD for complex systems

   - MD algorithms for non-rigid, non-spherical molecules
   - MD with Gromacs: tutorial for more advanced systems
   - In-class exercise for MD simulations of complex systems

10. March 28: Distribution function theory

    - Definition and calculations of thermodynamic properties
    - Radial distribution function
    - Virial pressure

    Reading: MQ. Ch.13

11. April 4: Integral equation theory

    - Ornstein-Zernike
    - Percus-Yevick
    - Carnahan-Starling

    Reading: MQ. Ch.13

12. April 11: The basics of Monte Carlo method

    - Markov process
    - Metropolis algorithm
    - Monte Carlo in canonical ensemble

    Reading: AT Ch.4

13. April 18: Monte Carlo simulations in other ensembles

    - Monte Carlo simulations in grand canonical ensemble
    - Free energy calculations
    - Widom insertion method

14. April 25: Implementation of Monte Carlo algorithm

    - Monte Carlo simulations for bulk Lennard-Jones system
    - Monte Carlo simulations for confined fluids

15. May 2: Monte Carlo simulations using open source codes

Exams

Date	**Exam**
March 19	Midterm Exam (Midterm report submitted by the end of the Spring recess)
May 5-11	Final Exam (Submission of the final version of the report for the final project)

Note: the final grades are due May 16