

Syllabus for MCB 5896: Introduction to Molecular Dynamics Simulations, Fall 2019

1 Credit

BPB 201

Instructor(s)

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Overview

This course is intended to be a practical introduction to the method of molecular dynamics simulations. Students will be guided in using the GROMACS software program for performing simulations of biomolecular systems, VMD for visualizing simulation trajectories and Python for analyzing and plotting simulation data. The course will be conducted in four hands-on sessions over the span of four weeks.

Reference Material

- GROMACS Manual <http://manual.gromacs.org/2019.3/download.html>
- Understanding Molecular Simulation, Frenkel and Smit, Academic Press, 2002
- Molecular Modeling and Simulation, Schlick, Springer, 2006

Grading

Grading will be based upon class attendance, participation and a final presentation of the results of a short-term MD project.

Policy Statements

Policy Against Discrimination, Harassment and Related Interpersonal Violence

Student Conduct Code

Academic Integrity Statement

Academic misconduct is dishonest or unethical academic behavior that includes, but is not limited to, misrepresenting mastery in an academic area (e.g., cheating), failing to properly credit information, research, or ideas to their rightful originators or representing such information, research, or ideas as your own (e.g., plagiarism).

Course Schedule (Subject to change) The course will meet four times for 4 hours per class with mixed lecture and directed computer exercises

Oct 30 Session 1 – MD Basics

- Force Fields
- Energy Minimization
- Integrators
- File Formats
- Interacting with the UCONN HPC environment

- Nov 6 Session 2 – MD Production and Analysis
- Equilibration
 - Benchmarking
 - GROMACS Tools
 - Python
 - MD Analysis
 - Matplotlib
 - Visualization in VMD
- Nov 13 Session 3 – Complex System Setup
- CHARMM-GUI
 - CGenFF
 - Membranes and Membrane Proteins
 - Protein-ligand
 - Modeling missing segments
- Nov 20 Session 4 – Advanced Topics
- Enhanced Sampling
 - Free Energy Methods
 - Mini-Project Presentations