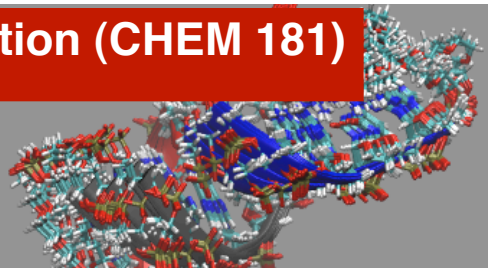
Summer 2011

Introduction to Molecular Simulation (CHEM 181)



Course Description

This course enables Chemistry and other science students to utilize computational tools for molecular simulation. Students completing this class will be able to understand the theory behind molecular dynamics and force-fields. In addition, students will be able to construct and execute molecular simulations using standard tools such as CHARMM, NAMD, VMD and other tools. Students will demonstrate an ability to analyze and present the data obtained from such simulations. This course is four (4) units. Students should expect to spend about three hours a day on coursework and assignments, and another five or so hours a week consulting with the instructor.

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Course Goals

After successfully completing this course, students will understand the fundamentals of computer simulation: structure and coordinate files, basic theory of force fields, Newtonian molecular dynamics, equilibration and heating versus equilibrated systems, different solvation models, measurement, calculation, and display of dynamical information, visualization methods of both molecular systems and data, and an introduction to non-equilibrium molecular dynamics.

Student Responsibilities

Students are responsible for completing all on-line tutorials and assignments (generally two formal assignments per week), any quizzes or other short assessment assignments, and the final project. Before the end of the first week, all required programs and files must be installed on the student's personal computer. Students are also required to attend the on-line chats or discussions that Dr. McCallum schedules for the course.

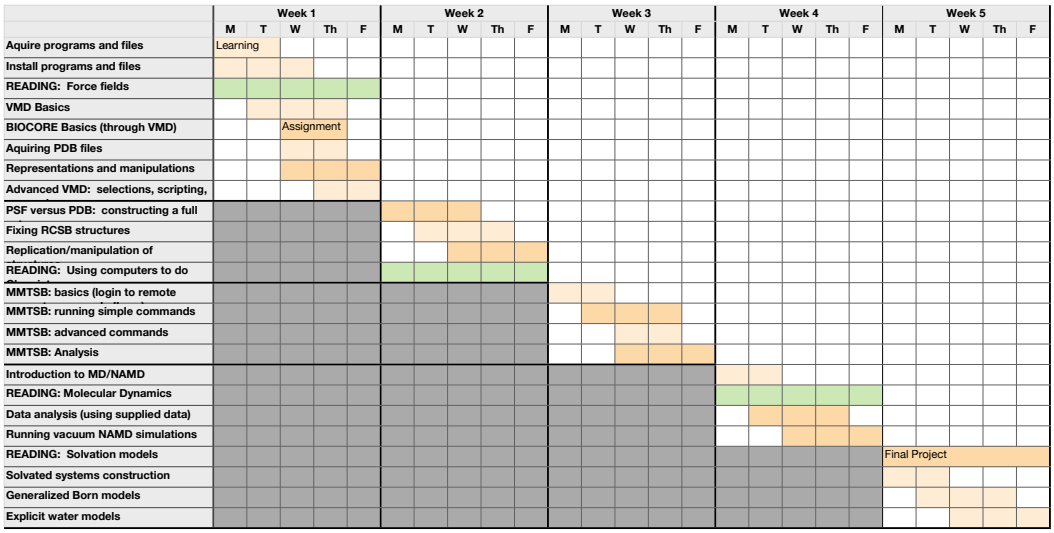
Student Learning Outcomes

- Understand the different file types required to describe molecules (proteins, peptides, etc) in a simulation
- Acquire, construct, and manipulate structural files using shell- and GUI-based (for example, VMD) tools
- Use VMD to manipulate and visualize molecular structure files (static and dynamic)
- Understand fundamental features of force-fields used in molecular dynamics
- Understand how to interpret and visualize molecular dynamics data
- Understand different solvation models and when they are useful
- Use actual molecular dynamics packages NAMD and CHARMM to run simulations and acquire data
- Understand basics of MMTSB toolset programming
- Understand simulation timing requirements

Retention of Student Work

Student work shall be retained both locally and remotely (BIOCORE) in order to fulfill assessment requirements and to help improve later versions of this course.

Course Schedule



Grading breakdown	Weekly Assignments	53 %
	Quizzes	13 %
	Final Project	33 %

There are two assignments per week, due Wednesday/Thursday and Friday/Monday. Each of these is worth 20 points. The Final Project is due the last day of class, and is worth 50 points.