CHEM 8520: Computational Chemistry

Spring Minimester II, 2020 (3 Semester Credit Hours)

Instructor: Xinqiu Yao, 523 Science Annex, (Email: xyao4@gsu.edu)

Lecture Time and Location: March 03 – April 23
Tuesday & Thursday, 2:30 PM – 5:00 PM, PSC 311 & Online

Office Hours: By appointment

Course Prerequisite: Physical Chemistry I and II

Suggested Reading:

Andrew R. Leach --- Molecular Modelling: Principles and Applications (Pearson, 2001)
Frenkel and Smit --- Understanding Molecular Simulation: From Algorithms to Applications (Academic Press, 2001)
Allen and Tildesley --- Computer Simulation of Liquids (Oxford, 2017)
McCammon and Harvey --- Dynamics of Proteins and Nucleic Acids (Cambridge, 1988)
Tamar Schlick --- Molecular Modeling and Simulation: An Interdisciplinary Guide (Springer, 2010)
Branden and Tooze --- Introduction to Protein Structure (Garland Science, 1999)

Software Used: R (Bio3D), VMD, AMBER, Autodock, PyMol

Course Description: Computational Chemistry is a 3-credit minimester course that covers the introduction to structural bioinformatics, molecular modeling and dynamics simulation, docking and drug discovery, and principles of computational methodologies and their applications. Students will develop fundamental knowledge of computational chemistry and gain hands-on excises of using software and programming to solve chemical and biophysical problems. The broader goal is to help students establish the attitude of appreciating biomolecular motions and their relevance to function.

Grading: Final grading will be based on homework assignments (30%), in-class assignments (50%), and final report (20%). Late completion of DataCamp assignment is acceptable with a penalty of 5/100 points per day delayed. No late submission of other assignments will be accepted.

Tentative Course Outline and Schedule:

Week 1: **(3/3, Tuesday) Welcome to Computational Chemistry**
What is computational chemistry, course description, introduction to Linux
Lab1: Practice Linux and complete worksheet
Homework1: Complete the *Introduction to Shell* course on DataCamp (due 3/10)

(3/5, Thursday) Basic Probability Theory and Introduction to R
Random variables, probability, probability (density) distribution, Gaussian distribution, mean and variance, what is R, basic R commands, vector and matrix, plotting and simple statistics with R, further reading and where to find helps
Lab2: Practice R and complete worksheet
Homework2: Solve problem set (due 3/12)
(Optional) *Foundations of Probability* DataCamp course

Week 2: **(3/10, Tuesday) Structural Bioinformatics (Part 1)**
What is structural bioinformatics, dynamics is the key to link structure and function, fundamentals of biomolecular structure, Protein Data Bank (PDB), visualization (introduction to VMD), structural data manipulation with R (introduction to Bio3D)
Lab3: Explore PDB, practice VMD and Bio3D

(3/12, Thursday) Recap and Lab3 Extension
Lab: Continue to practice R and Bio3D
Homework3: *Introduction to R* DataCamp course (due 4/2)
(Optional) *Intermediate R* DataCamp course

Week 3-4: **Spring Break**

Week 5: **(3/31, Tuesday) Structural Bioinformatics (Part 2)**
Protein dynamics is the missing link between structure and function, collecting data for dynamics analysis, structural superimposition and comparison, principal component analysis (PCA)
Homework 4: Answer questions on iCollege (due 4/7)
Bonus: Complete one or more optional DataCamp assignments by 4/30

(4/2, Thursday) Lab 4: Structural Analysis of the DHFR Family
Requirement: R, RStudio, Bio3D and related packages, MUSCLE, DSSP, VMD, and Seaview are all properly installed on a local computer

Week 6: **(4/7, Tuesday) Classical Molecular Mechanics**
Statistical mechanics basics, potential energy function, force field, energy minimization
Homework 5: Answer questions on iCollege (due 4/14)

(4/9, Thursday) Lab 5: Introduction to AMBER
Requirement: Linux shell (for Windows) and VPN are installed

Week 7: **(4/14, Tuesday) Molecular Dynamics Simulation**
Equation of motion, numerical integration, periodic boundary condition, temperature and pressure, typical workflow, state of the art, trajectory analysis
Homework 6: Answer questions on iCollege (due 4/23)

(4/16, Thursday) Lab 6: Analysis of DHFR simulation trajectory
Final report: Summarize results in the lab sessions and write a report (due 4/30)

Week 8: **(4/21, Tuesday) Molecular Docking and Virtual Screening**
Homework 7: Answer questions on iCollege (due 4/28)

(4/23, Thursday) Lab 7: Introduction to Autodock Vina and PyMol Plugin
Requirement: Autodock, Autodock Vina, MGLTools, PyMol, and the PyMol Vina plugin are all properly installed

NOTE:
1. All lectures after Spring Break will be videos available on iCollege.
2. All labs after Spring Break will be done via synchronous virtual meetings.
3. There will be no final exam. Instead, students are required to summarize their results during the lab sessions and write a report (due 4/30).