Computational Biochemistry

Lecture 1 Introduction

Teaching Format & Style

- 50% lectures + 50% labs
- Everything will be taught in English.
- Reports and presentations are required to be formulated in English.
- Encourage discussions, both in-class and after-class.

Lectures and labs

Lectures:

Week 5 – 8

Tuesday	10:00 – 11:40 am
Friday	10:00 – 11:40 am

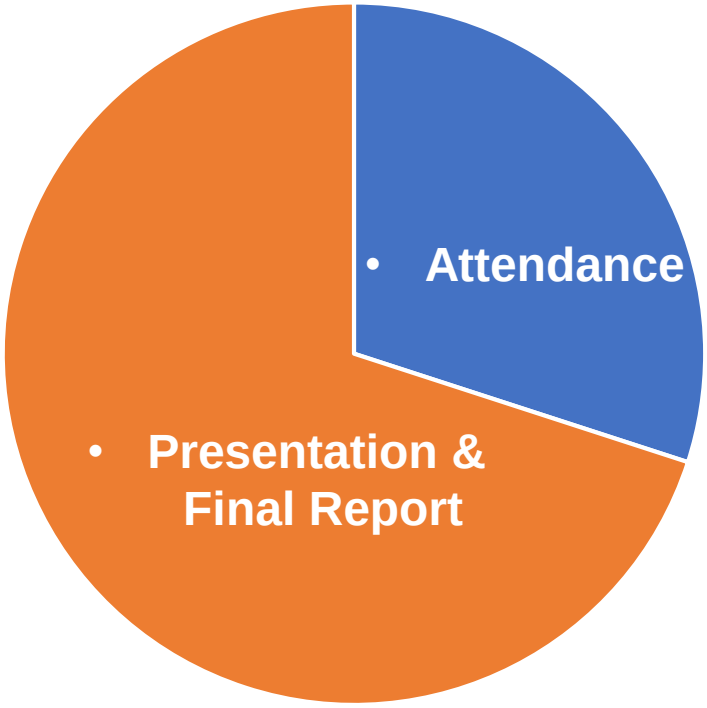
Labs:

Week 7 – 10

Wednesday	2:00 – 5:40 pm

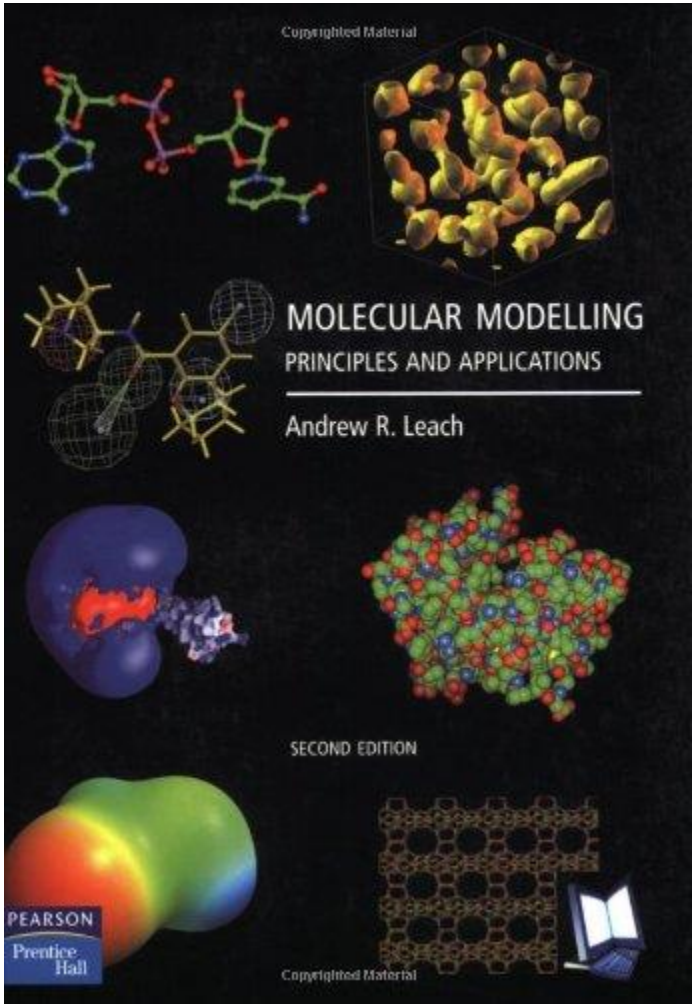
Grading

Final Grade Composition



- Presentations are based on your projects in the lab, and held in the last lab session.
- Students will be divided into 2 to 3 groups.
- Final reports are also based on your project. They are due by the end of April.

Reference book



Contact Information

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QQ group:

736588065

- please edit your name tag in the group to your real name.

TA:

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Self-introduction

Education & Experience:

Postdoc	Complex Carbohydrate Research Center	University of Georgia
Ph.D.	Chemistry	University of Georgia

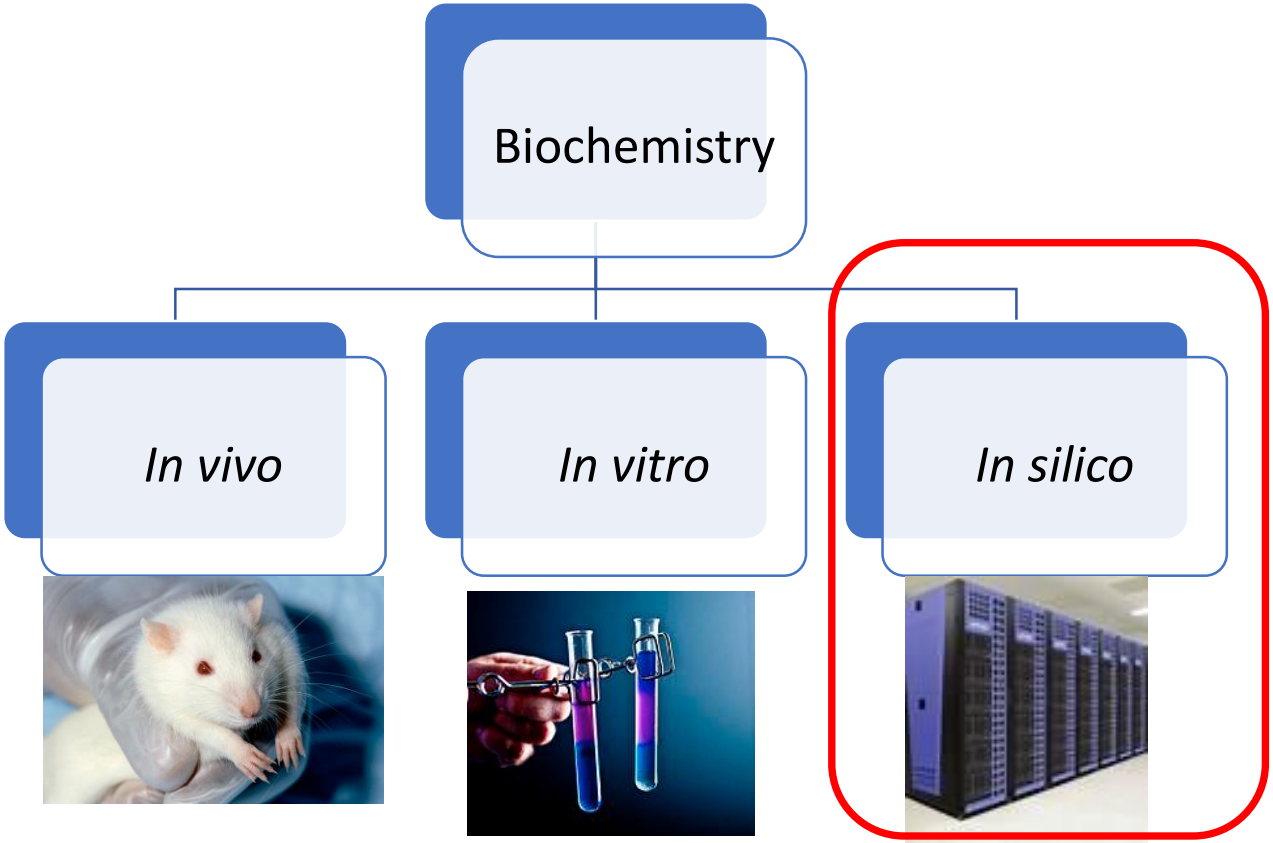
華中農業大學
HUAZHONG AGRICULTURAL UNIVERSITY

Research Interests:

1. Force field parameter development for molecular mechanics.
2. Drug design involving carbohydrate molecules.
3. Carbohydrate-protein interactions.

Introduction

- What is Computational Biochemistry ?



Computational biochemistry is a branch of biochemistry that uses computer simulation to assist in solving biological problems. It uses methods of theoretical chemistry, incorporated into efficient computer programs, to simulate and calculate properties of biological molecules and processes.

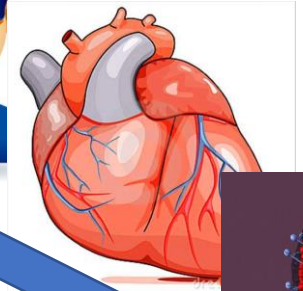
Size of the system

Universe

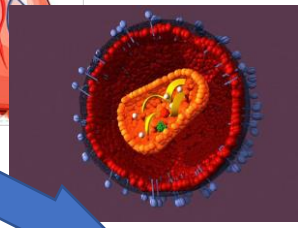
Solar system

Planet

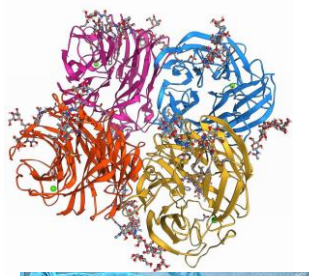
human



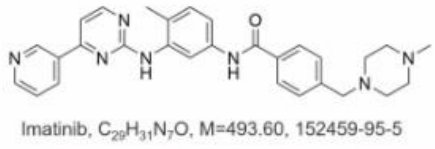
organ



cell



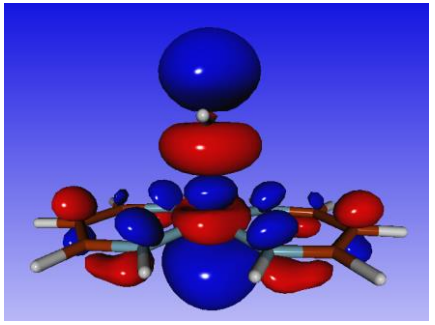
Protein
DNA

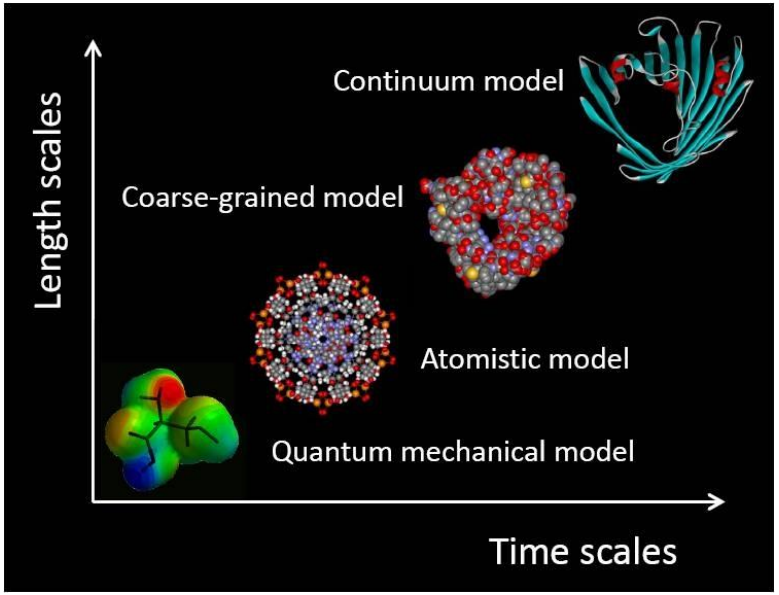


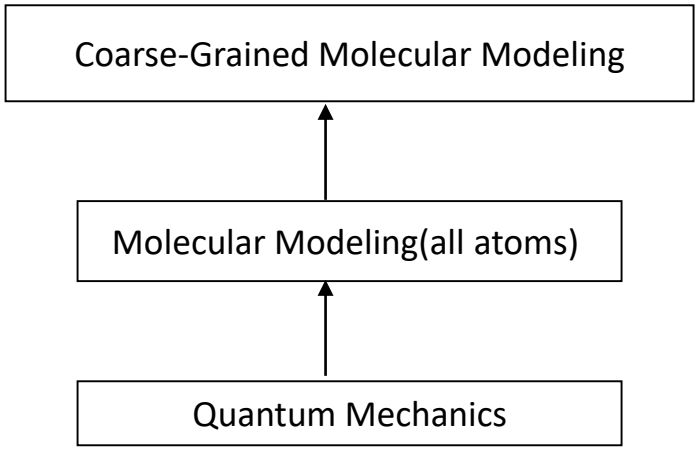
Drug
Molecule

Size of the system

- Atoms or larger —— molecular mechanics
- Electrons —— quantum mechanics







Importance of computational biochemistry

- Provides atomic detail of the system.
- Predict/Study mechanism of the biological process.
- Efficient and convenient.
- Visualizable.

Computational and theoretical studies of biological molecules have advanced significantly in recent years and will progress rapidly in the future. These advances have been partially fueled by the ever-increasing number of available structures of proteins, nucleic acids, and carbohydrates, but at the same time significant **methodological improvements** have been made in the area of **physics relevant** to biological molecules. These advances have allowed for **computational studies** of biochemical processes to be performed with greater accuracy and under conditions that allow for direct comparison with experimental studies.

-- Oren M. Becker

Importance of computational biochemistry

- Nobel Prize in Chemistry 2013

Martin Karplus

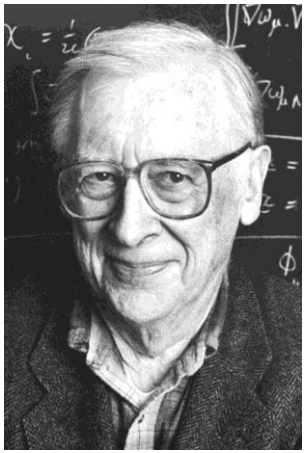
Michael Levitt

Arieh Warshel

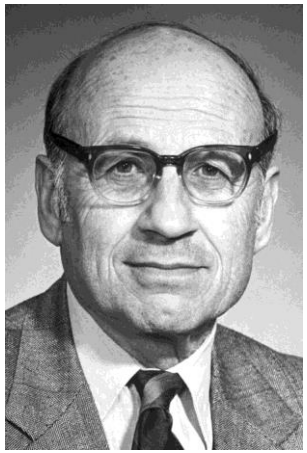
For the development of multiscale models for complex chemical systems.

Importance of computational biochemistry

- Nobel Prize in Chemistry 1998



John A. Pople



Walter Kohn

John A. Pople
"for his development of computational methods in quantum chemistry."

Walter Kohn
"for his development of the density-functional theory."

Methods in computational biochemistry

- Quantum mechanics (QM)
- Molecular mechanics (MM)
- Molecular dynamics (MD)
- Combinations of methods:
  QM/MM-MD
- Docking
- Bioinformatics
- Machine learning

… …

Objects in computational biochemistry

- Small molecule – biomolecule interactions
- Protein-protein interactions
- Protein-nucleic acids interaction
- Mechanisms of biological reactions, i.e. enzymatic reactions

… …

Resources for computational biochemistry