Computational Modeling of Molecular Structures

Location and Time

Naka Hall 353; 4:00 pm – 5:15 pm, Monday and Wednesday, Spring Semester, 2018

Instructor

Prof. Jianlin Cheng (http://calla.rnet.missouri.edu/cheng/)

Objectives

As studying three-dimensional (3D) structures of proteins, protein complexes, RNAs and genomes is becoming more and more important in the post-genomic era, a comprehensive treatment of the principles, algorithms and data structures for computational molecular structure modeling is needed for training next generation computer scientists, data scientists, computational biologists and bioinformaticians with these topics. This course investigates common principles, data structures, algorithms, challenges, and solutions in computationally modeling (constructing) 3D structures of proteins, RNAs, chromosomes, and genomes. The computational algorithms, methods, data structures, molecular geometry, biophysical forces, and biological implications will be integrated together, in order for computational scientists and bioinformaticians to fully grasp the complexity and essence of computational structure modeling. A new problem solving based learning paradigm is used to teach the course. The course emphasizes the design and development of data structures, algorithms and tools in computational molecular structure modeling. This will help students build a solid algorithmic foundation to develop and use structure modeling methods and tools.

Course Website

http://calla.rnet.missouri.edu/cheng_courses/cscmms2018/

Text Book

No required textbook

Topics

1. Introduction to Computational Methods for Molecular Structure Modeling

2. Principles, Algorithms, Data Structures for Template-Based Protein Structure Modeling

3. Principles, Algorithms, Data Structures for Template-Free Protein Structure Modeling

4. Principles, Algorithms and Data Structures for Computational Modeling of Protein Complexes

5. Principles, Algorithms and Data Structures for Computational Modeling of Genome Structures

6. Principles, Algorithms and Data Structures for Computational Modeling of RNA Structures

Projects

- Develop a software tool of template-based protein modeling
- Develop a software tool of template-free protein modeling
- Benchmark three protein docking tools
- Develop a software tool of genome structure modeling

Course Format

A new problem-solving teaching format including three teaching components (lecture, student presentation, and discussion) will be used in the class. The class consists of two alternated phases.

Phase I: theory phase. An introduction lecture for each topic will be given by the faculty. The lecture will survey problems, methods, algorithms and data structures in each topic. Before or after a lecture, each student is required to read one classic paper and write a review summary as homework for the topic. Overall, the theory phase accounts for 1/3 to 1/4 class time.

Phase II: practice phase. Under the direction of the faculty, students will apply the techniques learned in the first phase to develop or benchmark computational methods for constructing the structure of a macromolecule (e.g. protein, protein complex, genome, or RNA) of each topic by working on a group software development project. In each topic, the faculty first introduces main problems to be solved and then engages students in discussions to come up tasks and solutions to the problems. Students are rotated to write a discussion memo / notes during discussions. Students then write a presentation document including the tasks, solutions and implementation plan and turn it in as homework assignment. In the following class, students present the implementation plan in the first half of a class. A faculty then leads students to discuss the feasibility, strength and weakness of the plan in the second half of the class. After the presentation, students revise the plan and post a revised plan to the project server. Then students start to implement the plan. At the end of each step, a formal progress report (e.g. a Word/PDF document) including results and assessment is turned in and the corresponding programs and results are posted at the project web site by students. The implementation and results will be assessed and discussed by faculty and students. At the end of the semester, students turn in a formal project report in a paper style and present the project to all the instructors of the class. All the students are required to do the group homework assignments (i.e. reports, implementation, and final presentation). Students are rotated to be the leader of each group assignment. The leader gives presentations with the help of other students. The final report and presentation should be done by all the students. Overall, the practice phase accounts for 2/3 to 3/4 class time.

Homework Assignments

Literature review, topic plan (in presentation style), topic implementation (software tool development), topic report, and final report and presentation.

Evaluation and Grading

Students are graded based on class discussion (individual, 15%), literature reading and review (individual, 10%), topic plan presentation (individual, 20%), topic implementation and topic report (i.e. results and assessment) (group, 45%), and a final presentation and report (group, 10%). A grade scale for graduate courses (A+, A, A-, B+, B, B-, C+, C, C-, and F) is applied.

Intellectual Pluralism

The University community welcomes intellectual diversity and respects student rights. Students who have questions concerning the quality of instruction in this class may address concerns to either the Departmental Chair or Institute Director or Director of the Office of Students Rights and Responsibilities (http://osrr.missouri.edu/). All students will have the opportunity to submit an anonymous evaluation of the instructor(s) at the end of the course.

Attendance Policy

Attendance is essential to understanding the course material and is required. As in the workplace, if you cannot attend a class session due to illness or emergency please call or e-mail before the class to inform the instructor of your absence.

Academic Integrity

Academic integrity is fundamental to the activities and principles of a university. All members of the academic community must be confident that each person's work has been responsibly and honorably acquired, developed, and presented. Any effort to gain an advantage not given to all students is dishonest whether or not the effort is successful. The academic community regards breaches of the academic integrity rules as extremely serious matters. Sanctions for such a breach may include academic sanctions from the instructor, including failing the course for any violation, to disciplinary sanctions ranging from probation to expulsion. When in doubt about plagiarism, paraphrasing, quoting, collaboration, or any other form of cheating, consult the course instructor.

ADA (Students with Disabilities)

If you anticipate barriers related to the format or requirements of this course, if you have emergency medical information to share with me, or if you need to make arrangements in case the building must be evacuated, please let me know as soon as possible.

If disability related accommodations are necessary (for example, a note taker, extended time on exams, captioning), please establish an accommodation plan with the MU Disability Center, S5 Memorial Union, 573-882-4696, and then notify me of your eligibility for reasonable accommodations. For other MU resources for persons with disabilities, click on "Disability Resources" on the MU homepage.