Current Topics in Protein Structure Prediction
ChemBE 540.416/616 — Fall 2010

Instructor: Professor Jeffrey J. Gray
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Discussion: Thursdays, 3:00-5:30 p.m., Maryland 220

Overview: This course will consist of student-led discussions of current literature in protein structure prediction, protein-protein docking, and computational protein design. Related advanced computational approaches of the Rosetta3 protein structural modeling platform will be discussed and object-oriented software design concepts dissected. Students will present and critique C++ and Python code and scripts corresponding to related research projects.

Permission of instructor required.

Presentations: Each student is required to present in one or two of the discussion periods during the semester. The presentation can consist of one of the following:

1. **Research Presentation**: Presentation of recent research results including the background context, methods developed, results, work in progress, and future directions.
2. **Science Review**: A review of specific research topic in the broad area of protein structure prediction, *e.g.*, calculations and measurements of free energies of binding of a peptide to a solid substrate. Sometimes this can be the presentation of one particularly impactful or novel paper; in most cases this may be an overview summarizing several papers to show the current state of the field.
3. **Code Review**: Presentation of the code developed for a particular application. Paper copies of the main header and source files should be brought for the members of the class, and the whole source repository should be brought to the meeting for showing in an IDE on the projector. Ample time should be allowed for questions, discussions, and useful criticism. Some of the discussion may involve presentation of C++, Python, or shell script coding principles, practices and patterns.

Scheduling: Students should sign up for a discussion period by adding their name, the type of presentation, and the presentation title on the Gray Lab Google Calendar. The choice of topic must be approved by Prof. Gray.

Other requirements: Students are required to attend all class meetings and to participate in discussions with questions and feedback. Outside of the discussion meeting period, students are expected to be pursuing research in the structure prediction field. Students should meet periodically with Prof. Gray to discuss research directions, scientific results, and plans.