

CBE 422 Final Project Guidelines

The final project (term paper) for CBE 422 is due on Dean's Day (Tuesday 5/14). The project topic selection is due on Tuesday 4/30 by email to azp@princeton.edu. The project can be one of the following:

A literature review of 10-15 pages on a topic of relevance for CBE422 - you will need to consult and discuss original literature sources (scientific papers) in this case, not just textbooks. Some example project titles:

- Determination of critical points and finite-size scaling in Monte Carlo simulations
- Methods for long-range electrostatic energy summation: Ewald sums, PPPM, etc.
- The Nobel Prize in Chemistry in 2013: Multiscale models for complex chemical systems
- Ab initio computation of rates of chemical reactions
- Molecular-dynamics studies of protein stability and folding
- Crystal structure predictions for pharmaceuticals by molecular modeling
- Early history of Monte Carlo and Molecular Dynamics methods
- The Car-Parinello ab initio molecular dynamics methods and its applications

OR: An actual computation - Monte Carlo, Molecular Dynamics, or ab initio, e.g.,

- Vapor-liquid equilibria for the Lennard-Jones fluid using Gibbs ensemble Monte Carlo (using your own code)
- Molecular dynamics calculation for Lennard-Jones fluid: diffusion coefficient versus temperature (using your own code)
- Spectroscopic properties of conjugated alkenes (e.g. ethylene, butadiene, hexatriene) and comparison with experiments using Hyperchem
- Conformational states of oligopeptides using Hyperchem
- Protein-ligand interaction energies using Hyperchem

There are, of course, many other possibilities – however, please make sure to check with me first, before starting on a project.

Since the project counts as much as 2.5 problem sets in the final grade, expect to spend a little more than twice as much time on it relative to the average CBE422 homework assignment. The project will be graded on (a) comprehensive coverage of the topic, if literature review (b) critical analysis skills, inherent degree of difficulty of project, for both cases (c) quantity and quality of results, if an actual computation and (d) aesthetics of presentation.