

CHE 210D: Principles of Modern Molecular Simulation Methods

UCSB Department of Chemical Engineering

meeting times: TR 9:30-10:45am, Engineering II 3301

web page: www.engr.ucsb.edu/~shell/che210d/

course announcements: thermopia.blogspot.com (You can subscribe to updates via email.)

Course description

The goal of this course is to equip students of a variety of research interests with the basic skills necessary to design and carry out molecular simulations: (1) formulation of both atomistically detailed and simplified molecular models, (2) basic and advanced algorithms for computing thermodynamic and kinetic behavior, (3) modern analysis techniques and visualization packages, (4) physical intuition for developing and interpreting new simulation “experiments”, and (5) knowledge of computational issues and methods for improving efficiency.

This course focuses more on concepts, algorithms, and tools than on specific programming styles and languages, although enrolling students should have had at least minimal exposure to coding or mathematical software (e.g., have used any of Matlab, Mathematica, C, C++, Visual Basic, or Fortran). From early in the course, a strong emphasis will be placed on students performing and visualizing their own simulation projects.

Topics discussed in the course include: ab initio methods, classical semi-empirical force fields, energy minimization, molecular dynamics techniques, Monte Carlo methods, free energy algorithms, advanced sampling strategies, coarse-graining and multiscale methods, and rare events algorithms. Case studies in soft condensed matter, materials, and biophysics will be presented throughout the lecture material.

Instructor

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Course text

Molecular Modelling: Principles and Applications (2nd edition)

Andrew R. Leach, Prentice-Hall (2001).

Other highly recommended text

Understanding Molecular Simulation (2nd edition)

Berend Smit and Daan Frenkel, Academic Press (2001).

Coursework

Coursework will consist of a series of exercises in which students write their own small simulation programs based on methodologies discussed in lecture, run these, and provide analysis of results. At the end of the course, students will complete a project in which they simulate a system of interest, based on current topics in the literature, using methodologies discussed in class. The course will present Python as a particularly powerful and freely available programming platform for scientific computing and highly encourage its use..

Course outline

- 1) Overview of molecular simulation methods**
capabilities, kinds of models and simulations performed, case studies
- 2) Review of probability and statistical mechanics**
continuous and discrete probability distribution functions, microstates and macrostates, statistical mechanical ensembles
- 3) Introduction to scientific computing with Python**
overview and capabilities of Python, SciPy, Numpy; basic coding tutorial, numerical tools in Python
- 4) Introduction to molecular editing and visualization software**
viewing simulation structures and movies, features of common freely available tools and Python scripting
- 5) Quantum chemical methods**
Born-Oppenheimer approximation, hydrogen and multielectron atoms, Hartree-Fock theory and basis sets, charge-fitting, density functional theory, ab initio MD
- 6) Classical semi-empirical force fields**
bonded and nonbonded interactions, multipole expansion & van der Waals interactions, combining rules, parameterization, common forms (AMBER, CHARMM, etc), polarizability, implicit solvation (PBSA and GBSA)
- 7) Exploring the energy landscape and its minima**
energy landscape concepts, steepest descent minimization, conjugate gradient method, Newton and quasi-Newton methods, normal mode analysis
- 8) Molecular dynamics: basic principles**
phase space and distribution functions, integrators for Newton's equations, timestep and timescale considerations, stability
- 9) Computation of thermodynamic and transport properties**
equilibration and block averages, correlation times, pressure and temperature estimators, radial distribution functions, measuring transport properties
- 10) Practical aspects of simulations**
periodic boundaries, initialization, force computation, storage, potential truncation, long-range interactions
- 11) Molecular dynamics: advanced techniques**
constraints, multiple time steps, thermostats and barostats, Langevin dynamics, simulated annealing
- 12) Monte Carlo: basic principles**
canonical phase space distribution, separation of kinetic and configurational integrals, move sets, Markov processes and detailed balance, acceptance criteria, random number generation, comparison to MD
- 13) Monte Carlo: other ensembles**
fluctuations, NPT ensemble, grand canonical ensemble, microcanonical ensemble, Gibbs ensemble
- 14) Monte Carlo: advanced move sets**
lattice polymer moves, configurational bias, hybrid MC/MD
- 15) Histogram-reweighting free energy techniques**
connection between histograms and ensemble probabilities, measuring histograms, potentials of mean force, reweighting, Bennet's method, Ferrenberg Swendsen reweighting and WHAM, phase equilibria
- 16) Monte Carlo: biased sampling and related free energy techniques**
basic idea and formalism, umbrella sampling, multicanonical method, stratification, Wang-Landau method, transition matrix methods
- 17) Other free energy techniques**
perturbation theory, Widom particle insertion method, thermodynamic integration, absolute free energies, ideal gas and Einstein crystal reference states, alchemical transforms, Gibbs-Duhem integration
- 18) Advanced sampling techniques**
simulated tempering, replica exchange MD/MC and variants, non-Boltzmann sampling in MC, non-Boltzmann sampling in MD, basin-hopping and variants, multiple time steps
- 19) Coarse graining and multiscale techniques**
kinds of simplified models, advantages of simple vs. detailed, development and parameterization of simple models, inverse MC, force-matching, relative entropy
- 20) Rare event methods**
transition state theory, transition path sampling, finding transition states, computing rate coefficients & rates