MAT 306 Computational Techniques for Materials at the Nano-scale

Spring '24-'25

Intended Audience: A junior/senior level hands-on course for MAT and BIO majors, PHYS minors, or anyone interested in understanding the how molecular interactions at the nanoscale affect properties at the macro scale

Aims: To introduce various modeling techniques operative at the atomistic and mesoscopic time and length scales relevant to the understanding of the structure-property relationships of "materials" where a material is defined in the broad sense of anything that is utilized for a particular human defined purpose; to introduce a conceptual framework for the understanding of macroscopic observations of materials from a microscopic viewpoint; to include modeling and simulation on equal footing with experiments in attacking problems; to provide the background for choosing the appropriate technique suited to the system at hand.

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Hours: ***hands-on session*** – Mon 8:40–9:30 (G059); ***theory session*** – Tue 8:40–10:30 (G059)

Supplementary Textbooks: Leach, Molecular Modelling 2nd ed. Prentice Hall (2001). ISBN: 0-582-38210-6

Hinchliffe, Molecular Modeling for Beginners 2nded. Wiley (2008). ISBN: 978-0-470-51314-9

Frenkel & Smit, Understanding Molecular Simulation 2nd ed. Academic Press (2002). ISBN: 0-12-267351-4

Course Organization: hands-on sessions (1 hr/wk), structured instruction (2 hrs/wk), off-class assignments

Evaluation will be based two midterms (20 % each), homeworks (50 %) and class participation (10 %).

COURSE OUTLINE:

Week 1 (Feb. 10-11): The problem of time and length scales in molecular modeling; molecular graphics.

Hands-on session: Molecular graphics tutorial

Week 2 (Feb. 17-18): Useful concepts in molecular modeling: Coordinate systems; potential energy surfaces; degrees of freedom.

Hands-on session: Defining NAMD coordinate and potential files – psf generation tutorial

Week 3 (Feb. 24-25): Force fields and how to get a simple potential energy surface from a simple molecular dynamics (MD) run.

Hands-on session: Our first MD tutorial; butane

Week 4 (Mar. 3-4): Calculating forces from energies for simple energy functions.

Hands-on session: MD tutorial on forming distributions of torsional angles to reproduce the potential energy surface (PES) of a simple molecule

Assignment 1: Conformational map of cyclohexane

Week 5 (Mar. 10-11): How to extract barrier heights between the different conformations of a molecule.

Hands-on session: PES of a more complicated molecule (pentane)

Weeks 6 (Mar. 17-18): Principal component analysis and clustering of conformational states

Hands-on session: PCA/clustering of butane/pentane trajectories.

Assignment 2: PCA/clustering of cyclohexane trajectories

Week 7 (Mar. 24-25): Review for Midterm and **Midterm**

Hands-on session: Solving problems from exam archive

Spring break

Weeks 8 (Apr. 7-8): Normal mode analysis and its relation to spectroscopy

Hands-on session: NMA of molecules.

Assignment 3: Normal modes of motion of a nanoparticle

Week 9 (Apr. 14-15): Energy minimization; non-derivative, first- and second-derivative methods.

Hands-on session: Minimization of sample conformers of butane.

Week 10 (Apr. 21-22): The Boltzmann and the Maxwell-Boltzmann Distributions

Hands-on session: Deriving the velocity distribution of particles (in-class hand-out)

Assignment 4: Random number generation

Weeks 11 (Apr. 28-29): Ingredients of an MD simulation - I: the Verlet algorithm, choosing the time step.

Hands-on session: Running sample MD programs in NAMD on a hypothetical co-oligomeric system.

Assignment 5 – part 1: MD simulations of co-oligomeric systems – system setup

Week 12 (May 5-6): Ingredients of an MD simulation - II: Controlling the temperature; conservation of energy

Assignment 5 – part 2: MD simulations of co-oligomeric systems – trajectory analysis

Week 13 (May 12-13): Properties that may be calculated via MD simulations – the radial distribution function.

Hands-on session: Radial distribution function hand-out.

Assignment 6: Hydrophobicity

Week 14 (May 20,23): Properties that may be calculated via MD simulations – diffusion coefficient.

Hands-on session: Solving problems from exam archive

SOFTWARE:

- Various molecular visualization software (e.g. VMD: http://www.ks.uiuc.edu/Research/vmd/)
- Molecular Dynamics software (NAMD: http://www.ks.uiuc.edu/Research/namd/)
- Some calculations of your own (nothing fancy – just basic programming mainly in python to analyze data you produce from the package programs above)

LEARNING OBJECTIVES:

Interpret the problem of time and length scales in molecular modeling by relating the type of the problem to the available modeling technique.

Sketch simplified potential energy surfaces of molecular systems, identify their functionally relevant conformations and calculate the energies, given the parameters of a force field describing the molecules.

Apply simple statistical models from machine learning to identify conformational states of molecules.

Apply probability and statistics concepts to derive the Boltzmann and Maxwell distributions.

Relate the influence of conformations of a molecule on its properties by calculating the average properties of a given system based-on the Boltzmann distribution.

Perform normal mode analysis on nanoparticles and relate the output to vibrational spectroscopy experiments and the function of the nanomaterial.

Set-up and run molecular dynamics simulations on complex systems such as polymers and proteins.

Make physics-based descriptions of the main ingredients of a simulation such as the Verlet algorithm, periodic boundary conditions, selection of time step.

Calculate thermodynamic (e.g. temperature, pressure, heat capacity), and kinetic properties (diffusion constant, various relaxation times) from simulated trajectories.