MAT 306 Computational Techniques for Materials at the Nano-scale

Spring 2023

Intended Audience:
A junior level hands-on course for MAT, BIO, and CS majors, PHYS and CHEM minors, or anyone who would like to roll up their sleeves for modeling materials and obtain their characteristic properties "in silico."

Objective:
The goal of this course is to introduce various modeling techniques operative at a broad range of 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.

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Learning Assistant: *TBA*

Course Data: Hours/Class: Mon 12.40-14.30; Tue 08.40-09.30/FENS G059
Office hours: *TBA*
Zoom link: https://sabanciuniv.zoom.us/j/92296434574

Textbook:

Leach, A.R., *Molecular Modelling*, 2nd Ed. Prentice Hall, 2001. ISBN: 0-582-38210-6

References:

Hinchliffe, A., *Molecular Modeling for Beginners*, 2nd Edition. Wiley, 2008. ISBN: 978-0-470-51314-9

Weeks Commencing/Topics:

Feb 27 and Mar 6
The problem of time and length scales in molecular modelling; molecular graphics.
Useful concepts in molecular modeling: Coordinate systems; potential energy surfaces; degrees of freedom
(Assignment – 1)

Mar 13 and 20
Force fields and how to get a simple potential energy surface from a simple molecular dynamics (MD) run
Calculating potential of mean force from MD simulations
(Assignment – 2)

Mar 27 and Apr 3
How to extract barrier heights between the different conformations of a molecule
Energy minimization; non-derivative, first derivative and second derivative methods.
(Assignment – 3)

Apr 10 **Exam I**

Apr 17 and 24
Ingredients of an MD simulation
- the Verlet algorithm; choosing the time step
- conservation of energy; controlling the temperature

(Assignment – 4)

May 8 and May 15
(May 1 International Workers' Day; *May 2 Q&A session*)
Thermodynamic properties that may be calculated via MD simulations
Calculation of kinetic properties from an MD simulation
(Assignment – 5)

May 22 **Exam II**

May 29
Deliberations on learning objectives and future recommendations

Software

NAMD and VMD both of which may be reached at http://www.ks.uiuc.edu/

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 simple potential energy surfaces for systems of up to five particles and identify the global energy minimum and local energy minima on it;

Calculate the energy of conformations of simple molecules of up to five particles, given the parameters of a force field describing the molecule;

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;

Set-up and run molecular dynamics simulations on complex systems such as polymers and proteins; apply principal component analysis to extract a few coarse-grained intrinsic features;

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.

Class Policies

It will be the students' decision to follow **online lectures**, held in classrooms, **via Zoom or in the classroom**.
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*"We may have to revise the course plan according to the countrywide reassessment to be made regarding higher education. This is expected to happen at the beginning of April. The **content** to be delivered is **certain** but the **method of course delivery, the number and dates of exams**, and some other details are **subject to change**."*

Grading

Assignments: (5 of them), total is for 50% of the final grade
Interim exam: (2 of them), each 25% of the final grade