CENG4000P Course Syllabus

Title: Introduction to Molecular Dynamics Simulation

Code: CENG4000P

Credit: 3 Credits

pre-requisites: No pre-requisites

Instructor's Name: Chen, Shensheng

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Office Hours: By appointments

Teaching assistants:

Zongpei WU (zwudb@connect.ust.hk) and Haoke ZHOU (hzhouck@connect.ust.hk)

Course Description

This course (CENG 4000P) is designed to provide both a solid understanding and practical experience in molecular dynamics (MD) simulations, which are increasingly vital in many scientific and engineering fields today. Students will learn the foundational principles of MD simulations and acquire the skills needed to design, execute, visualize, and analyze MD simulations. The course will also feature hands-on MD projects that tackle real-world challenges in chemical and biomolecular engineering, such as water in oil, ion transport in battery applications, and protein folding in biological systems.

Assessments:

Assessment Task	Contribution to Overall Course grade (%)
Class attendance	20%
Homework	20%
Mid-term	30%
Final Project	30%

Required Texts and Materials

[Optional] Additional Resources

Recommended textbooks: *Understanding Molecular Simulation: From Algorithms to Applications,* by Daan. Frenkel and Berend Smit (3rd edition) is available as an online book through the HKUST library (https://www.sciencedirect.com/book/9780323902922/understanding-molecular-simulation). The textbook serves as supplementary reading material to reinforce the lecture notes.

Some useful online resources:

Lammps tutorial: https://lammpstutorials.github.io/

OpenMM Tutorial: https://openmm.org/