ME 418: Multi-scale Modeling and Simulation in Fluid Mechanics

Instructor : Prof. Sinan Keten
Office : Tech A133
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Class Times : MoWe 12:30PM – 1:50 PM
Class Location : Tech M120

Course Objectives:

1) Learn theory and fundamental principles of molecular simulation techniques and theoretical frameworks.
2) Apply molecular simulation tools to explain nano-scale fluid phenomena with relevance to biological and bioinspired systems.
3) Learn computational methods developed for studying physical systems at multiple length and time scales.

Topics to be covered:

a. Diffusion: Microscopic and macroscopic perspectives, mechanisms
b. Multi-scale theories in complex fluids: Coarse-graining approaches
c. Time-scale issues and advanced sampling methods
d. Transport in nanoconfined systems
e. Continuum approaches: Case studies on multi-physics problems

Homework: There will be three homework assignments during the term, due in two weeks. The purpose of the homework is to provide the student with an opportunity to apply theoretical and computational concepts to multi-scale problems.

Project: Students will have the opportunity to apply the concepts that they have learned in class to a research problem of their own interest. Projects typically include a multi-scale simulation aspect and some preliminary theoretical concepts on the expected observations. Topics can include and not be limited to diffusion, self-assembly, coarse-graining, nanofluidics, granular flow, and biological / bioinspired systems.

Grading: Homework (45%), Paper Review & Discussion (%10), Project (45%)

Textbook: There is no required textbook. Some resources relevant to this class are:
Molecular Dynamics: *Computer Simulation of Liquids* – Allen and Tildesley, *Atomistic Modeling of Materials Failure* – Markus J. Buehler, *Understanding Molecular Simulations* Frenkel and Smit
Statistical Mechanics: *Molecular Driving Forces* – Dill and Bromberg, *Intermolecular and Surface Forces* – Jacob Israelachvili

Software: LAMMPS compiled on Quest will be used for the simulations. Students will use and develop simple scripts for input generation, post-processing and data analysis.

COURSE OUTLINE	Date	Topics	Events
Lecture 1	Monday, January 7, 2013	Computing, Scales and Dynamics	
Lecture 2	Wednesday, January 9, 2013	Molecular Dynamics Method	
Lecture 3	Monday, January 14, 2013	Review of Statistical Mechanics	
Lecture 4	Wednesday, January 16, 2013	Molecular Interactions and Property Calculation	
Lecture 5	Monday, January 21, 2013	Diffusion Processes	**HW1**
Lecture 6	Wednesday, January 23, 2013	LAMMPS: In-class exercise	
Lecture 7	Monday, January 28, 2013	Energy Landscape Concepts	
Lecture 8	Wednesday, January 30, 2013	Advanced Sampling Methods	
Lecture 9	Monday, February 4, 2013	Coarse-graining Approaches	
Lecture 10	Monday, February 6, 2013	Coarse-graining Approaches	
Lecture 11	Wednesday, February 11, 2013	Dissipative Particle Dynamics	**HW2**
Lecture 12	Monday, February 13, 2013	Guest Lecture	
Lecture 13	Wednesday, February 18, 2013	Transport in Biological Channels	
Lecture 14	Monday, February 20, 2013	Transport in Nanochannels	
Lecture 15	Wednesday, February 25, 2013	Paper Discussion	
Lecture 16	Monday, February 27, 2013	Paper Discussion	
Lecture 17	Wednesday, March 4, 2013	IMFEM (Guest Lecture)	**HW3**
Lecture 18	Monday, March 6, 2013	IMFEM (Guest Lecture)	
Lecture 19	Wednesday, March 11, 2013	Wrap-up	
Lecture 20	Monday, March 13, 2013	Project Presentations	

Project Report will be due March 15. There will be no Final Examination.