Molecular Simulation

Chemical Engineering I5800 Prof. Joel Koplik, Physics Department & Levich Institute

(ST-1M19, 650-8162, jkoplik@ccny.cuny.edu)

Course Web Site: http://www-levich.engr.ccny.cuny.edu/courses/molecular_simulation/

The purpose of this course is to present the theoretical background and provide hands-on experience with molecular-scale numerical simulations of soft condensed matter and fluid mechanical systems. Monte Carlo, Molecular Dynamics and related methods will be covered, with some emphasis placed on applications to simulations of liquids and fluid flow. The course is meant to be accessible to graduate students in physics, chemistry and engineering. The prerequisites are an undergraduate degree in any of these fields, some knowledge of statistical mechanics, and some experience with basic fortran programming. The homework will be oriented towards computational practice, and will involves exercises such as modifying a standard MC or MD program for a particular problem, or writing data analysis routines.

Outline:

1. Intermolecular forces
2. Monte Carlo integration
3. The Metropolis Monte Carlo method
4. Smart MC techniques
5. Molecular Dynamics fundamentals
6. MD optimization, thermostats, and ensembles
7. Correlation functions and transport coefficients
8. Simulating fluid flows
9. Phase equilibria and interfaces
10. Long-range forces
11. Brownian dynamics

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Textbook:

D. Frenkel and B. Smit, *Understanding Molecular Simulation*, 2nd ed. (Academic, 2002)
M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, 2nd ed. (Oxford, 2017)

Other MD books:

J. M. Haile, *Molecular Dynamics Simulation : Elementary Methods* (Wiley, 1992)
A. R. Leach, *Molecular Modeling*, 2nd ed. (Prentice-Hall, 2001)
D. Rapaport, *The Art of Molecular Dynamics Simulation*, 2nd ed. (Cambridge, 2004)
T. Schlick, *Molecular Modeling and Simulation* (Springer, 2002)
M. E. Tuckerman, *Statistical Mechanics: Theory and Molecular Simulation* (Oxford, 2010)

Statistical Mechanics books:

D. Chandler, *Introduction to Modern Statistical Mechanics* (Oxford 1987)
D. Goodstein, *Thermal Physics* (Cambridge, 2015)
K. Huang, *Statistical Mechanics* (Wiley, 1987)
D. A. McQuarrie, *Statistical Mechanics* (University Science Books, 2000)
F. Reif, *Fundamentals of Statistical and Thermal Physics* (McGraw-Hill, 1965)