22.53 Statistical Processes and Atomistic Simulations

Fall 2000

Lecture Outline

I. Overview [1]*

Part A. Simulation Methodology

II. Elements of Molecular Dynamics [4]

III. Elements of Monte Carlo [2]

IV. Interatomic Potential Functions [6]

Lab Sessions on code development and property calculations [2]

Part B. Statistical Processes

V. Phase space sampling [1]

VI. Thermodynamic Behavior and Stability [4]

VII. Free Energy Calculations [4]

VIII. Strength, Deformation, Toughness [6]

IX. Linear Response Theory of Fluctuations and Transport [4]

Part C. Selected Applications [4]

Recent topics in materials modeling - melting, glass transitions, stability, defect mobility, and fracture.

*number in [ ] denotes number of lectures (hour each) devoted to the topic.

Sept.	6, 8, 11, 13, 15, 18, 20, 22, 25, 27, 29	(11)
Oct.	2, 4, 6, 9x, 11, 13, 16, 18, 20, 23, 25, 27, 30	(12)
Nov.	1, 3, 6, 8, 10x, 13, 15, 17, 20, 22, 24x, 27, 29	(11)
Dec.	1, 4, 6, 8, 11, 13	(6)

x denotes holiday

total no. of class meetings: 40

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Subject will be taught on the basis of class lectures. There will be regular problem sets, a term project, a written quiz, and an oral exam at the end of the term.

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General References:

K. Binder, ed., *Applications of the Monte Carlo Method in Statistical Physics*, Springer-Verlag, Berlin, 1984.

G. Ciccotti and W. G. Hoover, eds. *Molecular Dynamics Simulation of Statistical Mechanical Systems*, North-Holland, Amsterdam, 1986.

M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, Clarendon Press, Oxford, 1987.

D. Frenkel and B. Smit, Understanding Molecular Simulation - From Algorithms to Applications, Academic Press, San Diego, 1996.

Farid F. Abraham, "Computational Statistical Mechanics: Methodology, Applications, and Supercomputing", Advances in Physics 35, 1 (1986).

http://long-march.mit.edu/22.53/

22.53 course locker