Computational Nanoscience
NSE C242 & Phys C203
Spring, 2008

Lecture 22: Pop Quiz!

(yes, really)

NAME _____

Computer Simulation

"The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved." (P.A.M. Dirac)

1) What are the Advantages and Disadvantages of Doing Computer Simulations

a) Advantages

b) Disadvantages

Sources of Error

2) Give at least 2 real examples for each of these types of errors common to computer simulation.

a) Systematic Errors

b) Statistical Errors

Molecular Dynamics vs. Monte Carlo

3a) What is the difference between the MD and MC approaches?

3b) Give several examples of simulations where you would choose one over the other, and explain why.

Molecular Dynamics

4a) In molecular dynamics, is it possible to develop an algorithm that accurately predicts the trajectory of all particles at both short and long times? Explain your answer.

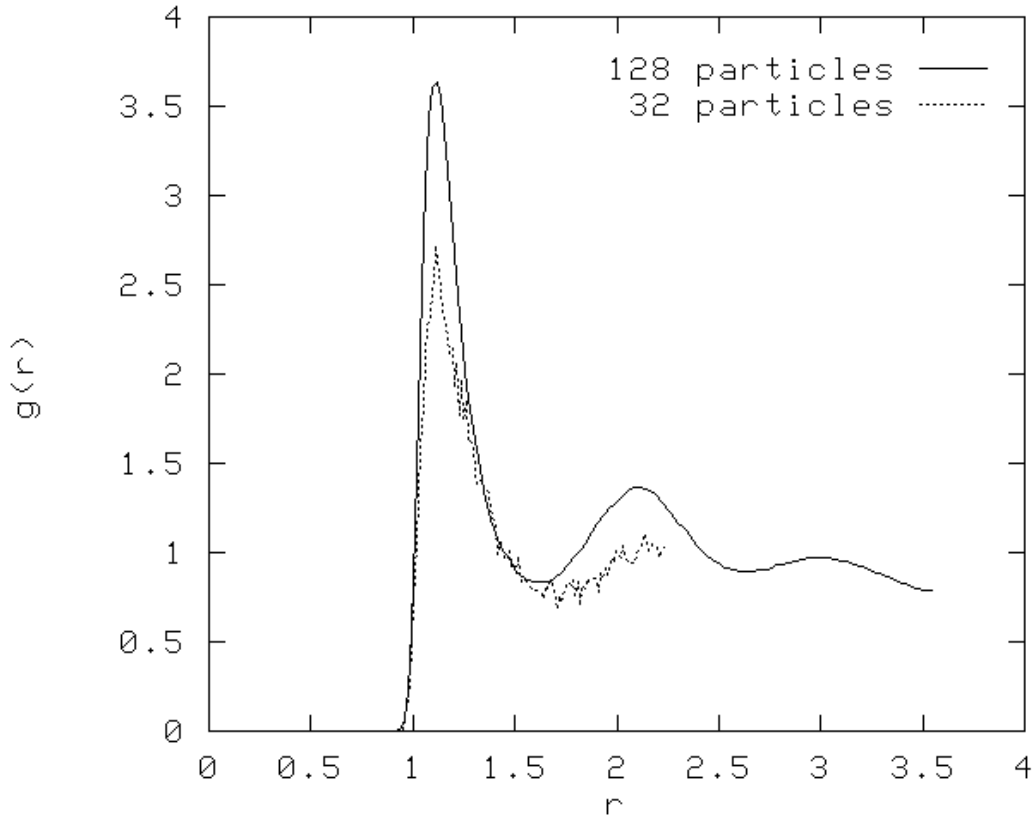
4b) What is the most expensive (computationally) part of a molecular dynamics simulation?

Molecular Dynamics

5) Here is a pair distribution plot for a 32 and 128 particle system interacting via an LJ potential. Is the system a liquid or solid?

a) Liquid or solid, and why?

b) Comment on the difference between 32 and 128 particles



Monte Carlo

6a) Why is it importance to obey detailed balance? How does the Metropolis algortihm obey detailed balance?

6b) Explain how you might use Monte Carlo methods to look for phase transitions. What problem will you run into? How do finite size effects affect your simulation?

6c) What is Kinetic Monte Carlo? What is the biggest source of error in a KMC simulation?

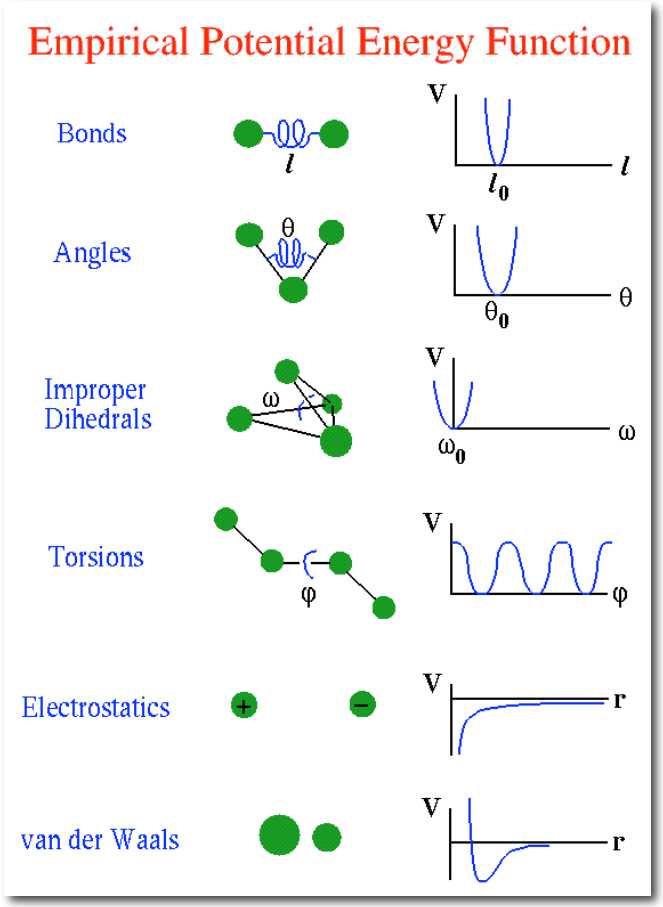
Boundaries

7a) Tell me everything you know about periodic boundary conditions (PBC).

7b) Give at least 2 examples of simulations where you should employ PBC and 2 examples where you should not (or at least need not).

Interatomic Potentials

8) Here are the main degrees of freedom in typical classical potentials. As we have learned, not everything can be optimized for all properties. Give at least three physical examples of simulations and state for each case which potential terms are most important to get "right".



http://cmm.info.nih.gov/intro_simulation/node15.html

Quantum Mechanics

9a) In what situations should we use a quantum mechanical calculation?

9b) What's a pseudopotential and when do we use it and when do we question its use?

9c) Tell me everything that you know about basis sets for representing the electronic wavefuction in a quantum mechanical simulation.

Basis Sets

10) What is the difference between a plane wave basis and a gaussian basis?

Quantum Mechanics

11a) Tell me everything you know about the difference between Hartree-Fock and Density Functional Theory.

11b) In DFT there are many functionals. What are the differences between them? How do you know which one to use?

Quantum Monte Carlo

12a) What does adding correlation do? What is the leading order effect in the wavefunction?

12b) How is diffusion Monte Carlo different from Hartree-Fock, variational Monte Carlo, and post-Hartree Fock methods?

Codes

13) We have worked with 8 codes so far in this class. Tell me, briefly, whatever you can about each one:

Average

Lennard-Jones Molecular Dynamics

LAMMPS Molecular Dynamics

Hard-Sphere Monte Carlo

Ising (pronounced *Eye-Sing*) Monte Carlo

Quantum Chemistry (GAMESS)

DFT for Solids (Siesta)

QMC

Last Question

14) How would you simulate the following systems/properties. Please list which code(s), approach(es), and any details you can think of.

a) Mechanical energy transfer rate between two carbon nanotubes.

b) Band gap as a function of diameter, crystal growth direction, and surface termination of Si nanowires.

c) Phase transition in liquid Argon.

d) Strength of nanoscale materials with defects.