# Physics 371: Problem Set 4

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**Due date: 15th of March, 2013.**

## Molecular dynamics for a Lennard-Jones system (in C++)

1. Write a function which reads in the input variables of a molecular dynamics simulation of a Lennard-Jones system. The input variables are the temperature, density, number of particles, a flag to determine the type of lattice, e.g. simple cubic, face-centered cubic, body-centered cubic (later also the number of time steps).
2. Write a function which sets upthe initial positions of a molecular dynamics simulation.
3. Write a function which sets up the initial velocities of a molecular dynamics simulation.
4. Write a molecular dynamics algorithm based on the Verlet algorithm.

*Calculate the average kinetic energy, potential energy and their standard deviations. Also produce plots of the kinetic, potential, and total energiesi and check if energy is conserved.*

## Monte Carlo for a Lennard-Jones system (in C++)

Based on the setup for the molecular dynamics program, write a Monte Carlo code for a Lennard-Jones system.

*Calculate the acceptance ratio. Calculate the average potential energy and compare it to the result of a molecular dynamics run with the same parameters (density, number of atoms, temperature).*