Computational Nanoscience

Spring 2008
Physics C203 & NSE C242

Homework Assignment #2 - Due February 7

Molecular Dynamics Simulation of a Lennard-Jones Liquid

In this exercise, you will perform a full MD simulation based on the Verlet algorithm to calculate various properties of a simple liquid, modelled as an ensemble of identical classical particles interacting via the Lennard-Jones potential.

Please use the ljmd program on the **nanohub** for this work.

Setup

As an input temperature, choose T=80 K, which corresponds to the value 0.17 in the units of the code. Choose the number of particles to be initially 32, the dimensions to be 3, and select the box size so that the density is approximately 0.36 particles per cubic *sigma* Use a Lennard-Jones cutoff of around 2 *sigmas* for all of the calculations (why is this a reasonable choice for the cutoff?).

Some things to do:

- As usual, the first thing consists of adjusting the time step so that the energy is conserved within 1% or better. To check that, you will need a few trial runs (note that in general very short runs will suffice).
- Calculate the pressure, the temperature, the energy per particle and the diffusion coefficient (*with error bars* , using the code *average* as done in the first homework) for

the conditions specified above.
  - Is the energy negative? If so, why?
  - Did the temperature change with respect to the one you had chosen? If so, why?
  - Is it possible to obtain as a value for the temperature the one you wanted initially?
  - With what temperature do you have to start to achieve this?
  - What do you conclude from this?

- Look at the 10 plots of the pair distribution function: what can you conclude about the system ?

- Repeat the calculation with 128 particles but changing the box size to maintain the same particle density as before: do results change, qualitatively and/or quantitatively ? Does the time step required change ?

- Repeat the above calculation at T=40K, i. e. 0.085 in the code units (choose the appropriate number of particles): what changes do you observe with respect to the higher temperature ? In which quantities and/or aspects of the simulation ?

- For every run give a quantitative estimate of the length of the time step and the total duration of the run in seconds (the molar mass of Argon is 39.9).
