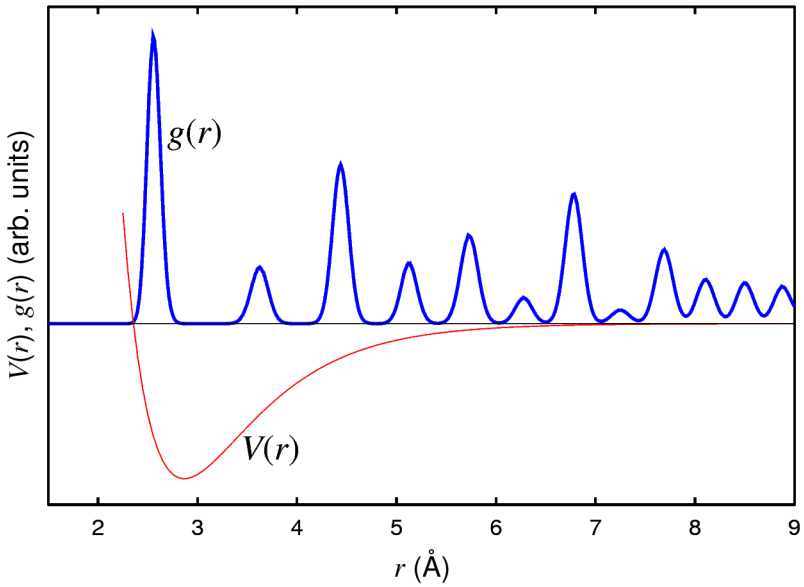
Molecular dynamics 2015

Exercises 6 to chapter 5: `mdmorse` : effect of cut-off radius and time step

1. (**10p**) Simulate a Cu fcc system with periodic boundary conditions and at temperature of 300 K for 10 ps using `mdmorse`. Do the simulations with the following values for the potential cut-off radius (`rpotcut` in `mdmorse`): r_c = 4.0, 4.5, 5.0, 6.0, 8.0 Å. Investigate the energy conservation by calculating the average fluctuation[1] in total energy. Remember to skip say 200 timesteps from the beginning of the simulation when calculating the averages. Why do the fluctuations behave as they do as a funtion of r_c? *Hint:* See the figure below, where the pair correlation function $g(r)$ of Cu at 300 K is plotted. Also plotted is the Morse potential used in the simulations.

Hints: Check that the temperature really is 300 K from your simulation output; no hassle with the infamous factor of two. For all simulations set the neighbourlist cut-off radius (`rskincut`) to 1 Å larger than the potential cut-off. The default value of `MAXAT*MAXNEIGHBOURS` (100000) in `modules.f90/global.h` should be sufficient.



2. (**10p**) Check the effect of the time step `deltat` on energy conservation in the code `mdmorse`. Use time steps of 1, 3, 10, 30 and 100 fs to simulate thermal motion in Cu at 300 K over 10 ps. Plot the total energy as a function of time for each time step in the range in which it still behaves sensibly. What happens with the atoms for the largest time steps?

Return the appropriate figures and answers to the questions.

Remember that data visualization is your friend. Never just calculate the final results without first checking how the system configuration looks like (`dpc` and `rasmol`) and how the temperature and energies behave as a function of time.

1. Variance or the like.