# Molecular dynamics 2015

## Exercises 5 to chapter 5: `mdmorse`: calculating the forces

**1. (12 p)** Write the subroutine **`GetForces()`** in the file **`forces.f90/.c`** in `mdmorse`. It should calculate the interaction between atoms with the Morse potential with the input parameters `morseD`, `morsealpha`, `morser0` giving the parameter values. Use the neighbour list created previously. The resulting subroutine should output the accelerations in the array `a(i)` and the potential energies in the array `Epot(i)`. The units are as described in `main.f90/.c`.

**2.** (**8p**) Using subroutines written for the previous exercises (your own or the official solutions on the web page) , and the **`GetForces()`** routine you should now have a working MD code. Demonstrate that the code works by

**(a)** Running it with the test inputs for 10 ps. After the initial 50 fs, the total energy (column 6 on the "`ec`" output lines) should fluctuate or drift less than 0.01 eV over 10 ps with a time step `deltat` of 2 fs. The temperature (column 3) should fluctuate less than about 100 K from the average around 600 K.

**(b)** Running it as above, but with a free surface in all dimensions. Now the temperature and energy will be different, but the total energy should still be conserved within about 0.02 eV after the first 1 ps. Describe what happens.

*Be careful not to use too small `nmovieoutput`, so that you don't fill up the disk!*

Return the exercise as the file `forces.f90` and a plot of the total energy vs. time and the temperature vs. time for cases (a) and (b).

After passing these tests your code is probably correct. (*But you can never be absolutely sure...*)