Molecular dynamics 2015

Exercises 8 to chapter 6: `mdmorse` : P control

1. (12 p) Implement Berendsen pressure control into `mdmorse`.

Use the read-in parameters `bpctau`, `desiredP` and `bpcbeta` into the code. The first one is the pressure control time constant τ_P, the second one the desired pressure P, towards which the pressure is controlled, and the third one the compressibility β (1/bulk modulus) of the material. Implement the change so that the control is not used at all if `bpctau=0`. Implement a pressure/virial calculation in the force routines, and then the control in the main routine. Use kbar as the external pressure unit.

Return the modified subroutines. Mark the pressure-related modifications in the code with comments with the string "`bpc`".

Test your code in the following way: Set $T = 300$ K and $P = 0$. Find the equilibrium box size for the system by simulating 10 ps and using $\tau_T = 300$ fs and $\tau_P = 300$ fs. Then perform two simulations where the box size (in file `mdmorse.in`) and the coordinates of atoms (in file `atoms.in`) are scaled 2% up and down (i.e. scaled by 1.02 and 0.98) from the equilibrium values you obtained from the first simulation. If your code works then all the three simulations should yield the same final box size and the instantaneous pressure fluctuating around zero. If your system explodes try using a longer time constant τ_P.

Return figures of the box size and instantaneous pressure as a function of time for all three simulations.

2. (8 p) Determine the thermal expansion coefficient of our copper model near NTP by simulating the system in constant pressure $P = 1$ atm $= 0.001013$ kbar [1] and at temperature range 200-400 K for 10-20 ps. Use the canonical value 5.0 Å for cut-off radius. Remember that the thermal expansion coefficient (in constant pressure) is defined by

$$\alpha_P = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P .$$

As always, when calculating averages from simulation data check how many points you have to skip from the beginning before starting to collect the average by plotting e.g. the system volume as a function of simulation time.

Compare your result to the literature value.

Return the curve $a_0(T)$ as a figure, explanation how you got α_P and of course its value.

1. Well, the results for $P = 0$ and $P = 1$ atm $= 0.001013$ kbar are practically the same.