Molecular dynamics 2015

Exercises 7 to chapter 6: `mdmorse` : T control
return date Wed 29.10., exercise session Fri 31.10. *(Note the exceptional times due to mid-term break.)*

1. (10p) Simulate the distribution of the velocity v of atoms in Cu at 300 K. Make a histogram of the velocities obtained, and compare with the analytical Maxwell-Boltzmann distribution [see e.g. Mandl, Statistical Physics, 2nd ed., equation 7.59a]. Plot the simulated and analytical distribution in the same figure, both using a linear and logarithmic scale on the y axis. Comment on the agreement of the two distributions.

Hint: use the actual (rather than desired) average temperature of your simulation run in the comparison.

Return the exercises as the plots or data requested (in ps or png format) and an answer to the questions asked.

2. (10 p) Implement Berendsen temperature control into `mdmorse`.

Use the readin parameters `btctau` and `desiredT` for this. The first one is the temperature control time constant, and the second one the desired temperature towards which the temperature is taken. Implement the change so that the control is not performed at all if `btctau=0.`

Test the control by simulating morse Cu with the default inputs but using

`desiredT=0.0, initialT=300.0` and `btctau=1000.0.`

How long does it take until the cell temperature has decreased below 10 K? How about when running with `btctau=100.0`?

Return the exercise as the modified subroutines and answers to the questions.