IN-CLASS WORK: MOLECULAR DYNAMICS SIMULATIONS

12. Potential Energy

If you had finished the in-class work 11b, you may use your program, if not, please start with ~kvollmay/classes.dir/phys338.dir/phys338_s2015.dir/md.dir/md12_start.py Add to the MD program a function which determines the potential energy per particle

$$V/N = \frac{1}{N} \sum_{i=1}^{N} \sum_{j>i} V_{\text{cutshift}}$$
(13)

where for $r_{ij} < 2.5 V_{\text{cutshift}} = V_{ij} - V_{ij}(2.5\sigma)$, $V_{ij} = 4 \epsilon \left(\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right)$ and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. For $r_{ij} \ge 2.5 V_{\text{cutshift}} = 0$. Include the minimum image convention similar to how it is used for the determination of the acceleration. Run the simulation for 500 MD steps. Print also V/N every nprint=5 steps. Let us together have a look at your result for V(t).

13. Kinetic Energy and Temperature

13a. Add to your program from 12. a function which determines the kinetic energy $E_{\text{kin}} = 0.5 \sum_{i=1}^{N} \mathbf{v}_{i}^{2}$. Print E_{kin} also every nprint=5 MD steps. Look at your result.

13b. Temperature T is related to the kinetic Energy. How? Determine and look at T(t). Get me, when you found the answer.

14. Maxwell-Boltzmann Distribution

Copy into your working directory

~kvollmay/classes.dir/phys338.dir/phys338_s2015.dir/md.dir/maxboltest_start.py

14a. Run the program and look at the resulting $P(v_x)$. Add to the program the determination of the expected Maxwell-Boltmann distribution

$$G(v_x) = \frac{1.0}{\sqrt{2\pi\sigma}} \exp\left(-v_x^2/(2\sigma^2)\right)$$

where

$$\sigma = \sqrt{\langle v_x^2 \rangle} = \sqrt{\frac{kT}{m}}$$

and compare $P(v_x)$ and $G(v_x)$.

14b. Play with each of the constants, how they change $P(v_x)$ and the comparison with $G(v_x)$.

15. Temperature Bath

Add to your program from 13b a constant temperature bath by periodically redrawing all velocities from the Maxwell-Boltzmann distribution of the desired temperature. Look at your results and play with the bath temperature.

Upcoming Deadlines:

- April 10 (extended): Results section of second paper (Results will be graded)
- April 14: Mini-Project II (in class & graded) and title and abstract of main projectpaper
- April 21, 23, 28: 5, 5, 3 Talks
- April 21: First Version of Second Main Project Paper
- May 6 (our final): Final Version of Second Main Project Paper