Multiscale Modelling for Polymer Mechanics
TU/e – Mech. Eng. – 4LM30

Exercise 2 (February 7, 2020)

(Markus Hütter, Lambèrt van Breemen)

Single polymer chain in 3D

The main task consists is writing an MD-code that simulates the motion of a linear polymer chain consisting of N particles (="monomers"). Each particle moves in 3D according to

$$m\dot{\boldsymbol{v}}_i = -\frac{\partial \Phi(\boldsymbol{r}_i)}{\partial \boldsymbol{r}_i} = \boldsymbol{F}_i \ , \tag{1}$$

with $\boldsymbol{r}_i$ and $\boldsymbol{v}_i$ the vectors denoting the position and velocity of particle i, respectively, while $\boldsymbol{F}_i$ stands for the force on particle i. The interaction energy between any two connected particles is given by

$$\Phi_{pp}(r) = \frac{k}{2}\left(r - l_0\right)^2 \ , \tag{2}$$

with r the distance between the two particles, and k the spring constant.

- For the numerical implementation, choose $N = 10$, $m = 1$, $l_0 = 1$, $k = 1$. For the initial condition, set all particles on a straight line with distance l_0 between neighbours, and the initial velocities should be random (using `randn`) with a root-mean-square of 0.3, but zero on average. Note: you need to make sure that the initial velocity vectors averaged over all particles is identical to zero (why?).

- Solve the dynamics with a time step $\Delta t = 0.01$. Use the velocity-Verlet scheme.

- Continuously plot the evolution of the structure to judge graphically what is happening:
  `plot3(x(:,1),x(:,2),x(:,3),'ro')`

- At the end of the simulation, plot the total energy (sum of kinetic and potential energy) of the entire system as a function of time.

- Measure, as a function of time, the end-to-end distance of the chain, and plot that at the end of the simulation.
  If time permits: For the period where you are in steady state, make a histogram of the visited end-to-end distances.

- *If time permits:* Define a measure for the "mobility" of the particles. Try to quantify whether the mobility of a particle at the end of the chain differs from the mobility of a particle in the middle of the chain.

- Change from the velocity-Verlet scheme to the Euler scheme, and redo (some of) the simulations. Take note of your observations and rationalize them.

- For all measurements: Try to rationalize them, and compare them with your initial expectations.

Hints for the numerical implementation:

- Make use of separate functions to calculate (i) the forces, (ii) the updated positions, and (iii) the updated velocities, respectively.

- To store the positions and velocities of all particles, generate matrices `r` and `v` of dimension $N \times 3$, where the i-th row stands for particle i.

- For the function, called `forceall` here for simplicity, that calculates the interaction force on each particle due to the presence of all the others, proceed as follows. Input to the function `forceall`: $N \times 3$ position matrix `r`, spring constant k, and bond length l_0; output of `forceall`: forces acting on each particle, in the form of a $N \times 3$ matrix `f`.
  In `forceall`, there will be a loop over all particle pairs. For calculating the interaction force per particle pair, make use of another function `forcepair`.
  In order to increase the efficiency of the force calculation (i.e., cut the computational cost by a factor of two), you may want to use Newton's 3$^{\text{rd}}$ law, "actio = reactio".