My first MD code

October 9, 2018

Write a molecular dynamics code to integrate the motion of a particle of mass m in one dimension subject to a harmonic spring potential with the following form:

$$U(d) = \frac{1}{2}kd^2$$

with $k = 1$.

Use the Verlet algorithm and the following conditions:

- $q(0) = 2$
- $q(-\Delta t) = q(0)$

Consider different possible values of Δt. Which is the maximum value of Δt for which the simulation is stable? How do you expect the result to depend on k?

Now repeat the calculation assuming the particle subject to a Lennard-Jones potential:

$$U(d) = 4\epsilon\left(\left(\frac{\sigma}{d}\right)^{12} - \left(\frac{\sigma}{d}\right)^{6}\right)$$

with $\epsilon = 1$ and $\sigma = 1$. Find a value of Δt such that the simulation is stable. Can you relate it with the value obtained for the harmonic potential?