Part B: Triatomic reaction dynamics with Lennard-Jones potentials

You will now use the velocity Verlet algorithm to study the dynamics of systems with three atoms (A, B, and C), first of all when the atoms interact via a L-J potential function and then when the atoms interact via a LEPS potential. To make things simple, we will restrict the dynamics of the atoms to be along a line, i.e. only colinear configurations of the atoms will be allowed. It is, first of all, instructive to visualize the potential energy surface. There are only two independent variables in this problem, the distance between atoms A and B, and the distance between atoms B and C. The interaction potential can, therefore, be represented as a surface in 3-D space. With a L-J potential between each pair of atoms, the total potential is

$$V(r_{AB}, r_{BC}) = V_{AB}^{LJ}(r_{AB}) + V_{BC}^{LJ}(r_{BC}) + V_{AC}^{LJ}(r_{AB} + r_{BC})$$

where

$$V_{ij}^{LJ}(r) = 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right],$$

The parameters in the LJ potential function will be different for different types of atoms, for example the parameters will be different for Ar-Ar interaction than a Ar-Kr interaction.

B1: The Lennard-Jones potential

a) To keep things simple, we will assume all three atoms are of the same kind, and choose units in such a way that the numerical values of ϵ_{ij} and σ_{ij} are unity. Plot the potential as a function of the two variables. In Mathematica you can use the SurfacePlot and/or the ContourPlot functions. Choose an appropriate region to plot, such as r_{AB} and r_{BC} from $[0.9, 2.0]$. What configuration of the three atoms gives a minimum potential energy (i.e. what values of r_{AB} and r_{BC})?

b) Explore the energy dependence of the dynamics. Start from the example we worked in class. Choose unit masses, $m_A = m_B = m_C = 1.0$, a time step of 0.02, and a total time of 4.0. Plot the dynamics for initial positions of particles A, B, and C of -3.0, 0.0, and 1.3 respectively. Give particle A an initial velocity of 1.0, and let B and C be initially at rest. Describe in words what the initial conditions chosen here correspond to.

c) Change the initial velocity of atom A to 0.2. The total time of the simulation needs to be increased. A time of 15.0 would be appropriate in this case. When do you see an exchange reaction and when does a three atom complex form? This is also a function of the phase of the vibration of the BC molecule when the A atom hits. Try changing the phase of the $B-C$ vibration without increasing the amount of vibrational energy in the BC molecule before the collision (how can that be done easily?).

d) Increase the velocity of the A atom to 5. At this high energy the attractive part of the interaction between A and B-C is quite irrelevant and the collision is well described as a collision of hard spheres (analogous to billiard balls).