Note on Periodic Boundary Conditions

A cube of silicon that has a side length of one millimeter contains approximately 5×10^{19} atoms. To perform an MD simulation of such a system is beyond the capabilities of current computers. The largest simulations performed to date contain on the order of one billion atoms, which would correspond to a silicon cube with a side length of about 0.3 μm. To run MD simulations over long enough periods of time to obtain sufficient statistics for thermal transport calculations, systems with hundreds or thousands of atoms are typically considered. The actual number of atoms considered should be taken to be the smallest number for which no computational cell size effects are evident.

In a cubic crystal with n atoms per side of the simulation cell, the percentage of atoms on the surfaces scales as approximately $6n^2/n^3 = 6/n$. For a system with $n = 10$, about 60% of the atoms will be on surfaces, and experience a different environment than the interior atoms. In many cases, the goal of an MD simulation is to investigate bulk phase behavior, so that a system with surfaces is unsuitable. To allow for modeling of the bulk phase, periodic boundary conditions and the nearest image convention are used. The idea is to reproduce the simulation cell periodically in space in all directions, and have a pair of particles only possibly interact between their images that are the closest together (i.e., a particle only interacts with another particle once, and not with itself). This idea is shown schematically in Fig. 1 for a two-dimensional system. Success of this technique requires that the potential cutoff be no larger than one half of the simulation cell side length. In very large systems, where some particles will never interact with certain others, schemes exist that can significantly reduce computation times, and allow for the parallelization of the MD code.

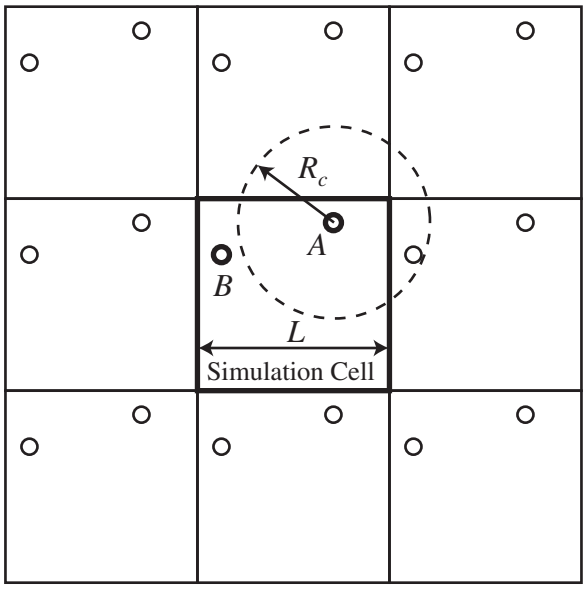

Figure 1: Schematic of the implementation of periodic boundary conditions in a two-dimensional system. The potential cutoff, R_c, must be less than or equal to one half of the simulation cell size, L. Note that the nearest image of atom B for atom A is not in the simulation cell, but in the right side periodic image.

There are a number of points of interest regarding the implementation of periodic boundary conditions.

1. It is possible for a particle near the boundaries to leave the simulation cell. When this occurs, we need to consider the image of that particle that has entered the simulation cell. This switch is achieved by either adding or subtracting the size of the simulation cell to the particle coordinates. For each particle i, we need to do the following check after the positions have been advanced:

$$\begin{aligned} &\text{if } (x_i < 0) \text{ then } x_i = x_i + L_x \\ &\text{if } (x_i > L_x) \text{ then } x_i = x_i - L_x, \end{aligned}$$

then repeat for the y and z directions. This procedure leads to the apparent jumping around of particles when an MD simulation is visualized. The particles are of course not jumping around – we are just seeing different images of the same particle.

2. When a pair of particles has been identified as a possible interaction, the closest distance between them must be identified (this is the nearest image convention). This distance may not correspond to the atoms in the actual simulation cell, as shown in Fig. 1. To find the nearest image, we note that the maximum distance between two particles in the x direction is $L_x/2$, and implement the following scheme:

$$\begin{aligned} &\Delta r_{ij,x} = r_{i,x} - r_{j,x} \\ &\text{if } (\Delta r_{ij,x} > L_x/2) \text{ then } \Delta r_{ij,x} = \Delta r_{ij,x} - L_x \\ &\text{if } (\Delta r_{ij,x} < -L_x/2) \text{ then } \Delta r_{ij,x} = \Delta r_{ij,x} + L_x \end{aligned}$$

Repeat this check for the y and z components, then find the separation between the two particles.