Periodic Boundary Conditions

Software project May / June 2013, continued

1 Boundaries 1

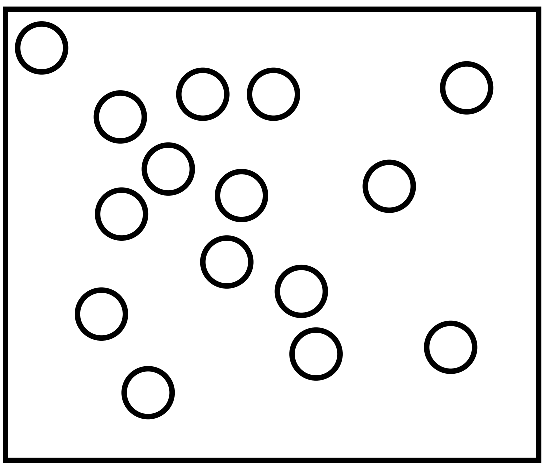
1 Boundaries

Some systems have boundaries, but we do not care about the details. For gas in a cylinder, the boundaries determine the volume and properties such as pressure, but these are average properties. Except for those particles near the edges, most particles will have no interaction with the walls. If we have 10^{20} particles, very few of them feel the walls directly.

In a large simulated system with 10^5 particles, the walls will be much more important. Most naïve approaches to represent walls will introduce some unwanted effects. Imagine you have springy walls. This is not so easy to program, it requires some choices for spring constants and energetic properties are hard to calculate. The wall would store potential energy like a spring. If your walls have mass and motion, than they would also have kinetic energy.

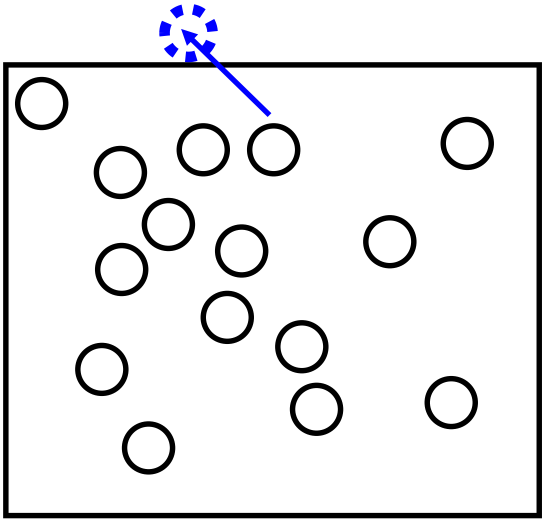
One might consider walls have infinite mass and infinite elasticity. If a particle hits a wall, it bounces off without loss of energy. If it hits a wall in a 2D system its initial velocity of $\begin{bmatrix}\dot{x}\\ \dot{y}\end{bmatrix}$ its velocity might instantaneously change to $\begin{bmatrix}-\dot{x}\\ \dot{y}\end{bmatrix}$. This would preserve kinetic energy ($\frac{1}{2}mv^2$), but not momentum (mv).

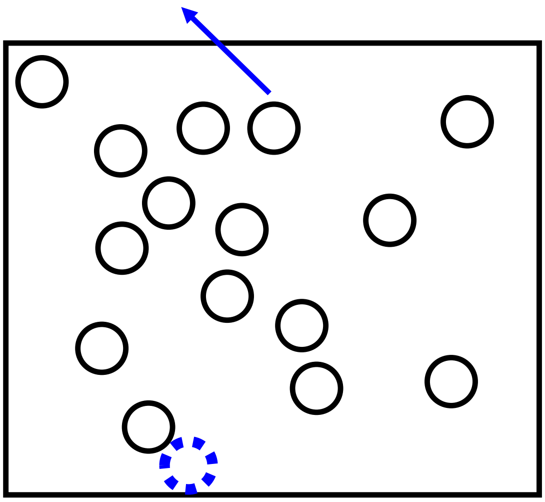
One may note that in many systems, we do not care about momenta and maybe we do not even have velocities in the model. There is a reason why boundaries are very bad. Consider a box of particles. A particle in the middle of the system has half a dozen neighbours and interactions with each of them. A particle near the edge has three or four neighbours and a smaller energy contribution. All properties of the system that depend on energy will be incorrect. The smaller the system, the worse the boundary



effects will be. A better approach is to try to simulate an infinite system.

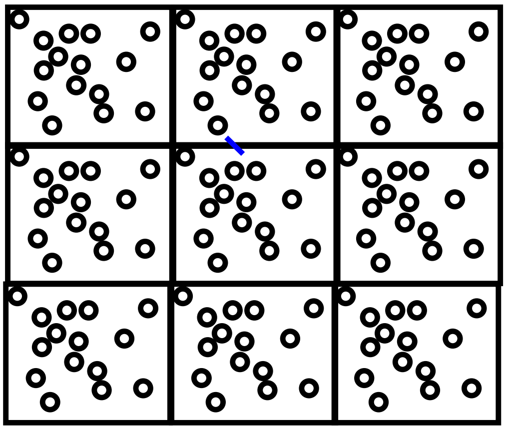
2 Periodic boundaries

With periodic boundaries we simulate one part of an infinite system. The ideas are the same, in 1, 2, 3 or *n*-dimensional spaces. They are the most common approach to simulating particle systems, but also appear in places such as ecological simulations. When implementing them, remember to treat each dimension separately. If a particle moves out of the top of the box  it comes back in the bottom.

.

If one is looking at distances between particles, you must account for periodicity. This means a particle's neighbours may be on the other side of the box. A particle may sit in the top left corner, but the near neighbours include the particle on the bottom right.

The interactions are what you would intuitively expect, but imagine you had velocities in your system. A particle moves out of the box with a positive *y* velocity and comes back in the bottom and keeps moving. Kinetic energy and momentum are both preserved. This is elegant and makes the physics easier. Conceptually, it is easy to see the system as infinite



3 Problems

Periodic boundary conditions introduce artificial periodic effects. Imagine the box is 10 nm and there is one special particle, such as an ion with a large charge. There is another particle a nm away. This particle interacts with the special particle at distances of a, a+10 nm, a + 20 nm and so on. This means you have artificial periodicity in your system or something like crystal behaviour. This usually not treated in an elegant way. Instead, one normally ignores interactions between particles which are more than r_{cut} (cutoff distance) from each other. Without cutoffs, a particle would also interact with copies of itself. This does not lead to any strange energies, it is just non-physical.

The use of a cutoff is not pretty, but there are some rules. If you write code like,

```
for (i = 0; i < n; i++)
     for (j = i+1; j < n -1; n++)
          r_ij = x_i – x_j
          if (r_ij > r_box / 2)
               r_ij = r_box – fabs (r_ij)
          .. repeat for y dimension
```

than you have implemented a cutoff distance. No interaction distance can be larger than half the box size.

To discuss

- Is it clear why there is an implicit cutoff distance ?

- Electrostatic interactions have the form $\frac{q_1 q_2}{4\pi\epsilon_0 r_{12}}$ which is long-range on the atomic scale. What will be the problem if you have a box of 2 nm, but interactions are significantly non-zero at 1½ nm ?