Introduction

Experience shows that if a pack of, for example, muesli is shaken well, the larger pieces (typically the brazil nut kernels) rise to the top. This project uses a Monte Carlo method to investigate this effect, by looking at the movement of shaken particles in a container under the influence of gravity.

The Monte Carlo method

It is important to realise that the Monte Carlo method does not model *processes* – it looks only at *configurations* of a system. In the Brazil nut problem, then, we are not going to apply Newton's laws and models of collisions between objects to follow the actual movements of particles. Instead, what we will do is to move particles at random, see whether the resulting arrangement of particles is both physically possible and an improvement on the previous one, and then decide whether to accept or reject the move. By 'improvement' we mean, in our case, that the gravitational potential energy is reduced. Note that many applications of Monte Carlo methods include a small probability of accepting a move that does not improve the configuration: this is often useful when exploring complicated energy surfaces and trying to find a minimum, as it offers the chance of escaping from a local minumum (such as A or A' in the figure) and continuing to explore the surface until the global minimum at B is found.

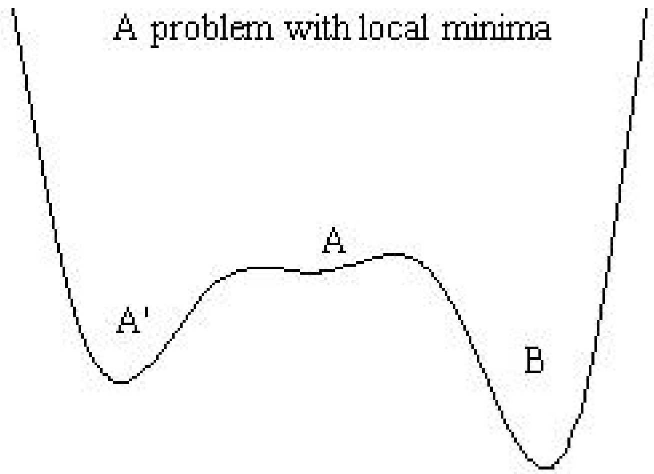

Figure 1: A problem with multiple minima.

The project

The project will model the situation in Flatland, where Brazil nuts are circular disks and all the other ingredients of muesli are smaller circular disks. The muesli is sold in infinitely tall rectangular containers (which makes carrying it home from the shops tricky, but means we don't need to worry about the muesli banging against the top of the container when shaken).

The following chunks of code are going to be needed:

- Code to check whether particle (i.e. a nut or any other bit of muesli) overlaps the sides or bottom of the box.
- Code to check whether two particles overlap.
- Code to find the largest nearest-neighbour distance between particles (that is, find the shortest distance from each particle to any other particle, and then find the largest of those distances.
- Code to draw the arrangement of particles.
- Code to determine the potential energy.

The Monte Carlo model then picks any particle at random, moves it a random distance horizontally and vertically, and if the move improves the energy and is physically possible (does not lead to overlaps), accepts it. There are several points to note.

- The algorithm does not follow the path of a particle – the particle just "jumps", which means that it might get from A to B even though there is no passage between A and B which is wide enough.
- Particles move sideways as well as vertically – imagine this to represent the effect of bouncing off the walls.
- Use the largest nearest-neighbour distance to control the step length. This will help to ensure that as many as possible of the moves attempted are accepted.

Start by putting one Brazil nut in, somewhere on the bottom of the box. Then add, say ten other particles, each half the radius of the nut, randomly positioned within the box horizontally but at steadily increasing heights. Use the Monte Carlo model to 'settle' all the particles, stopping when the change in potential energy in, say, 1000 attempted jumps makes only a small difference to the energy.

Then 'shake' the box – multiply the vertical coordinate of each atom by, say, 2. Settle again. See what has happened to the nut

Experiments

You may need to revise your code to get it to work fast enough. There may also be ways of choosing the maximum step length for the jumps efficiently. Once the program is working, you can see how different numbers of nuts and other particles behave, whether it makes much difference if you have a distribution of particle sizes, and so on. You should consider both whether the nuts rise to the surface and how long it takes them to do so.

References

[1] A. Rosato, K. J. Strandburg, F. Prinz, and R. H. Swendsen. Why the brazil nuts are on top: Size segregation of particulate matter by shaking. *Physical Review Letters*, 58(10):1038–1040, 9 March 1987.