Laboratory of Computational Physics

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1 Hard-Core Molecular Dynamics in 2*d*

In this section we simulate the dynamics of a system of N identical spherical particles in two dimensions, subject to the hard-core central potential:

$$V(r) = \begin{cases} 0 & r > R \\ \infty & r \leq R \end{cases} \tag{1}$$

with $\sigma = 2R$ being the diameter of the particles. For convenience we decide to work with adimensional quantities and rescale all lengths by the size L of the box. In these units the volume of the box itself is rescaled to 1. For the same reason we take the mass of the particles to be the reference unit of mass. Periodic boundary conditions in both directions are implemented in order to reduce boundary effects due to the finite size of the system. This turns our box in a toroidal surface.

1.1 Thermalization

First we initialize the system positioning the particles (disks) on the sites of a regular square lattice

as in (Fig.1). This type of circle packing has a *packing density* η (i.e., the proportion of the surface covered by the circles) of:

$$\eta = \frac{N\pi\sigma^2}{4L^2} \tag{2}$$

which takes its maximum value for $\sigma = L/\sqrt{N}$:

$$\eta_{\max} = \frac{\pi}{4} \approx 0.78539816339... \tag{3}$$

The highest-density lattice arrangement of circles in the plane is actually the hexagonal packing arrangement, with a maximal packing density of $\eta_h = \frac{\pi}{2\sqrt{3}} \approx 0.9069$. In fact we see that, a system with large η, spontaneously tends to arrange itself in such a way (Fig.1).

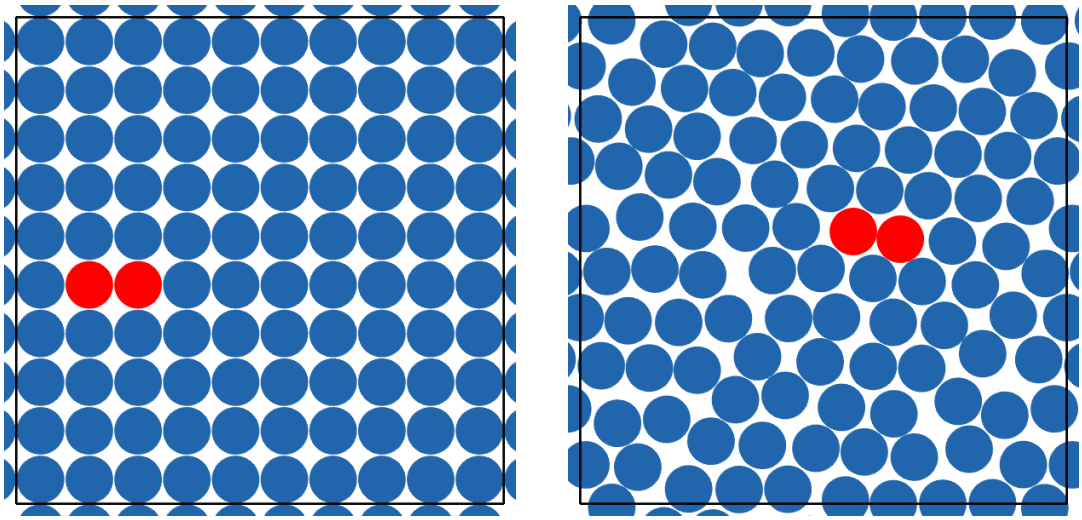

Figure 1. On the left we illustrate the initial spatial configuration of a system of 100 particles at temperature $T = 1$ and $\eta = 0.75$. On the right we show the same system after $2 \cdot 10^5$ collisions. The red disks indicate two particles colliding.

The momenta of the particles are initializated with uniform distribution inside the range $[-1, 1]$ with total momentum equal to zero (center of mass reference frame). After the initialization the momenta are rescaled in order to obtain the desired temperature. Kinetic energy and temperature are related by:

$$K = \frac{d}{2} N k_b T, \quad K = \frac{1}{2} m \sum_{i=1}^{N} |\vec{v}_i|^2 \tag{4}$$

$$\Rightarrow \quad T = \frac{1}{d\,N} \sum_{i=1}^{N} |\vec{v}_i|^2 \tag{5}$$

where we set $k_b = 1 = m$.

We now study the mixing properties of this type of system. We evolve a system of $N = 100$

particles from its initial configuration, for 10^4 collisions and measure the pressure (Fig.2) and the mean free path (Fig.3) every 10 collisions. This procedure is also repeated for $N = 400$.

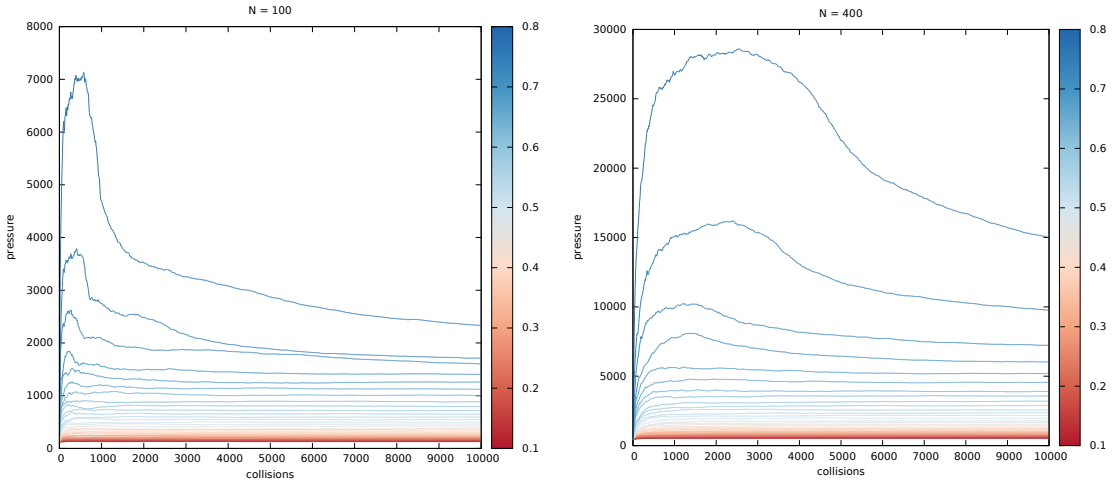

Figure 2. Plot of the pressure of an hard-core interacting gas of $N = 100$ particles on the left, and $N = 400$ on the right. The various colors of the curves represent the value of η of the simulation. The mixing rate of the system (as a function of the number of collisions) grows with η and the number of particles.

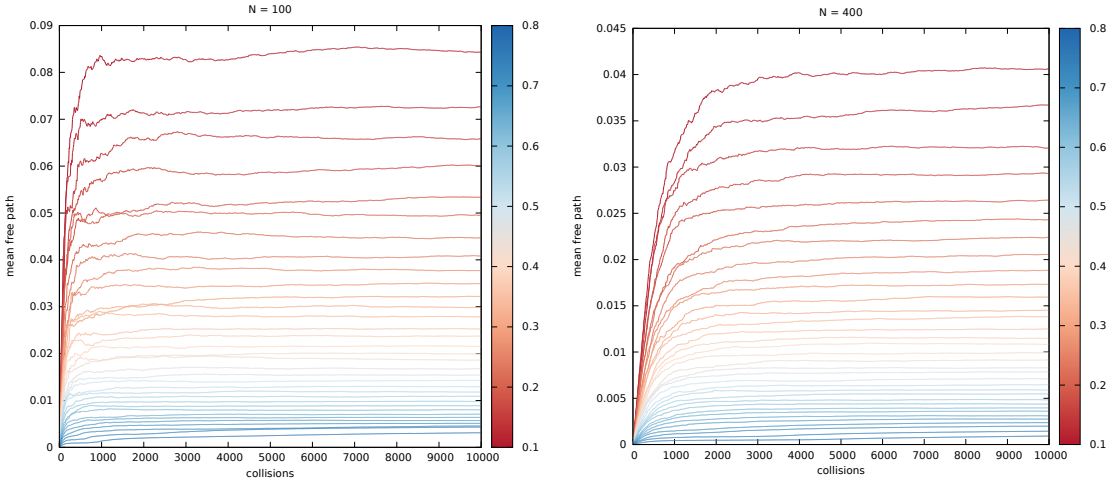

Figure 3. Plot of the mean free path of an hard-core interacting gas of $N = 100$ particles on the left, and $N = 400$ on the right.

A many-body system reaches thermalization only when every particle has interacted with every other particle at least once. Since hard-core particles interact only when they collide with each other, the mixing of this type of systems depends only on the number of collisions and not directly on the elapsed time.

We see that larger systems (system with a large number of particles) need more collisions to mix completely, expecially at high densities η, while smaller systems mix faster. At high densities we also note a peak in the pressure curve near the start of the simulation. This is due to the fact that we used an initial arrangement not ideal for the close packing of particles. The particles are initially very close to each other and interact frequently, but after a few collisions they rearrange in such a way as to maximize the distance between them, therefore reducing the pressure (Fig.1).

1.2 Momentum Distribution

After thermalization is reached, the system acquires time translation invariance and the distribution of the momenta of the particles converge to the Boltzmann distribution:

$$f(v) = \sqrt{\left(\frac{m}{2\pi k_b T}\right)^3} 4\pi\, v^2 \exp\left[\frac{-m\, v^2}{2k_b T}\right] \tag{6}$$

and for the single components:

$$f(v_i) = \sqrt{\frac{m}{2\pi k_b T}} \exp\left[\frac{-m\, v_i^2}{2k_b T}\right] \tag{7}$$

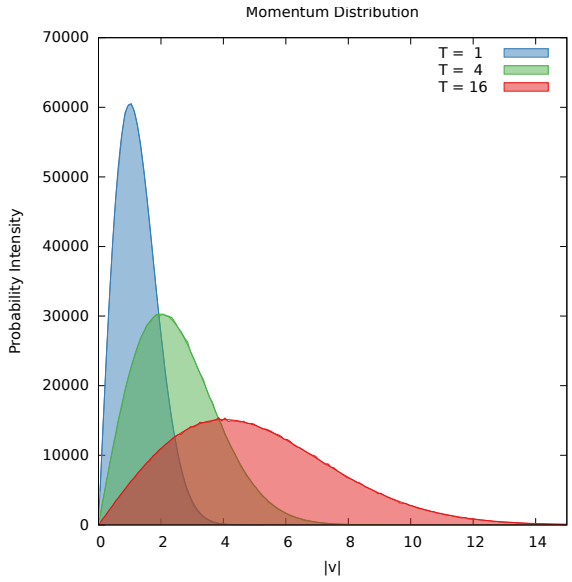

Figure 4. Histogram of the module of the momenta for $N = 100$ particles. The measurements are taken after 10^5 collisions from the start of the simulation, and after that every 500 collisions for a total of 10^4 datasets each containing the momenta of N particles. The system is initialized at temperatures $T = 1, 4, 16$.

We repeat the simulation for three different values of the temperature ($T = 1, 4, 16$) which we set by hand at the beginning. The temperature can now be read from a fit of the histograms of (Fig.4) and compared with the one obtained from (5):

T	T_{fit}
1	1.011343 ± 0.005696
4	4.028977 ± 0.007747
16	16.134445 ± 0.023048

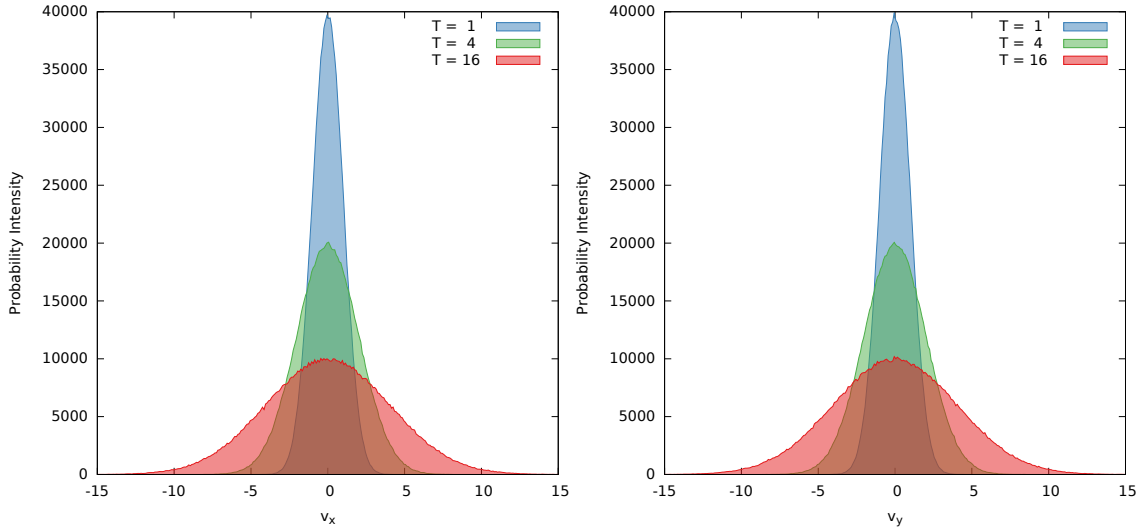

Figure 5. Histograms of the x and y components of the momenta for $N = 100$ particles.

1.3 Phase Transition