Stat. Mech. of Complex Systems

Project 1
Monte Carlo simulations of Hard Disks

The goal of this project is to implement a Makov-chain Monte Carlo (MC-MC) algorithm to simulate a system of hard disks (HD). Historically, this model was the first one addressed by numerical simulations, both using sampling techniques, as implemented by Arianna W. Rosenbluth and coauthors in 1953 [1], and the Molecular Dynamics pioneered by Alder and Wainwright in 1957 [2].

The Monte Carlo method starts with a rule for proposing *updates* or *trial moves* from a microstate x, to a different microstate y. Such trial moves are generated with probability $T(y|x)$. You could think about a microstate x as configuration of spins, if you are dealing for instance with an Ising model, or, as in the present case, the positions of particles composing a fluid (or eventually a solid).

We denote by $P(x)$ a probability distribution of configurations x. If one is considering a thermodynamic system equilibrated with a thermal bath at a temperature T, such probability is given by the Boltzmann distribution $P(x) = e^{-\beta E_x}/Z$, where $\beta^{-1} = k_B T$, Z is the canonical partition function and E_x is the energy associated to state x.

The MC-MC methods aim to generate states with the right probability $P(x)$ through the proposal of trial moves. Starting from any configuration, once a trial move has been selected, a decision has to be made in order to accept it or reject it. The probability of accepting such update $A(y|x)$, the *acceptance probability*, depends on the distribution one aims to sample. Thus, the *transition probability* from a state x to y can be written as the (independent) composition of these two process, the trail, and the acceptance:

$$W(y|x) = T(y|x)A(y|x) \tag{1}$$

Such transition probability constitutes the rule to generate a *Markov chain*, a stochastic process which determines the trajectory of our system: The trajectory corresponds to the chronological sequence of configurations obtained through the iteration of these updates.

In order to guarantee that the Markov chain generated by W relaxes towards $P(x)$, the Markov chain must be aperiodic and irreducible (conditions that we can prove to be true in the case of study) and impose the *global balance* condition:

$$\sum_x W(y|x)P(x) = P(y) = \sum_x W(x|y)P(y), \tag{2}$$

implying that the distribution $P(x)$ is stationary. In practice, we imposed the more restrictive *detailed balance* condition, meaning that there is a statistically null net flow between each pair of states x and y:

$$W(y|x)P(x) = W(x|y)P(y). \tag{3}$$

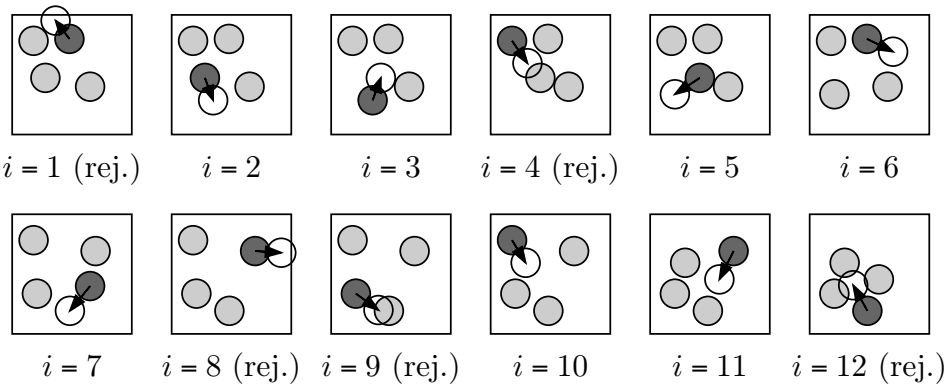

Fig. 2.24 Markov-chain Monte Carlo algorithm for hard disks in a box without periodic boundary conditions (see Alg. 2.9 (`markov-disks`)).

Figure 1: From [3].

Since $P(x) = e^{-\beta E_x}/Z$ we get

$$\frac{W(y|x)}{W(x|y)} = \frac{P(y)}{P(x)} = e^{-\beta(E_y - E_x)} \tag{4}$$

The simplest way to apply these MC-MC scheme is to use the Metropolis algorithm, which consist in choosing the trial probability to be uniform and and acceptance probability

$$A(x|y) = \min\left[1, \frac{P(y)}{P(x)}\right] = \min\left[1, e^{-\beta(E_y - E_x)}\right] \tag{5}$$

We consider a system of N hard disks of radius σ interacting with a potential: $U(r) = 0$ if $r \geq \sigma$ and $U(r) \to \infty$ if $r < \sigma$. Consider the centers of the disks located at $\vec{r}_i(t) = (x_i(t), y_i(t))$ at time t in a $L \times L$ box. We define the area fraction as

$$\phi = \frac{\pi\sigma^2 N}{4L^2} \tag{6}$$

We will always consider units in which $k_B = 1$. The microscopic dynamics are encoded in the updating rules used by the Metropolis algorithm and equilibrium measurements can be done after the relaxation of the system. From a state $\mu(t = 0) = (\vec{r}_1(0), ..., \vec{r}_N(0))$ the algorithm generates via a Markov process a new state $\mu(t = 1)$.

Implement the Metropolis algorithm for N hard disks with periodic boundary conditions following the steps below:

1. Trial move: Choose a particle i at random among the N particles in the system. Each component is virtually displaced using two uniform, independent, random numbers ξ_i^x, ξ_i^y, with $\xi_a \in [0, 1]$. The trail displacements are given by

$$x_i' = x_i + \delta(\xi_x - 0.5)$$

$$y_i' = y_i + \delta(\xi_y - 0.5)$$

Of course δ has to be much smaller than the smaller length scale in the system, here σ, which defines the unit of length, $\sigma = 1$. All lengths will be given in terms of σ. You can try $\delta = \sigma/10$. The random displacement $\vec{\delta}_i(t)$ can thus be written as

$$\vec{\delta}_i(t) = \delta\vec{\xi}_i(t), \tag{7}$$

where $\vec{\xi}_i(t) = (\xi_i^x, \xi_i^y)$ is a random vector with components independently drawn from a uniform distribution.

2. Acceptance: The trial move is accepted with probability

$$A(x|y) = \min\left[1, e^{-\beta(E_y - E_x)}\right]$$

i.e. with probability 1 if it does not generate any overlap between particles, and 0 (rejected) otherwise.

During the simulations we update the time variable by one after we have performed N times the two steps of the algorithm. This is called a Monte Carlo step (MCs) and it is the unit of time in the simulations: 1 MCs corresponds to N particle trial/acceptance (irrespective of wether they move or not). The Monte-Carlo dynamics can thus be written as

$$\vec{r}_i(t+1) = \vec{r}_i(t) + \vec{\delta}_i(t) p_{\rm acc}(t), \tag{8}$$

where the acceptance probability $p_{\rm acc}(t)$ is unity if no overlap is created, zero otherwise.

1. Using a random initial configuration, compute the mean-square displacement (MSD) of the particles using a system of $N = 1000$ disks

$$\Delta^2(t) = N^{-1} \sum_{i=1}^{N} \langle (\mathbf{r}_i(t) - \mathbf{r}_i(0))^2 \rangle \tag{9}$$

at $\phi = 0.05$ for $\delta/\sigma = 0.001, 0.003, 0.01, 0.03, 0.1, 0.3$. How does the diffusivity D depend on δ? [Plot MSD vs. t in log-log. Plot the MSD obtained for all the different values of δ in the same figure.] [**Plot** D vs. δ.]

2. How long does it take, in MCs (approximately), to the system to relax to an equilibrium state from an ordered initial configuration where all the particles sit on the sites of an triangular lattice for $\phi = 0.05$, 0.2, 0.5, (you can have a look at the MSD and the configuration snapshots to estimate how many MCs you need to reach equilibrium conditions)?

Show snapshots of the system (configurations, the position of each particle in the plane) in its steady state at $\phi = 0.05$, 0.2, 0.5,. Do you expect a qualitative change (a phase transition?) to occur as the system's density is varied?

What is the role played by temperature in this system?

3. Consider now the system in a closed box, of size $L_x \times L_y$ in which the particle-wall interactions

are hard core, of the same nature as the particle-particle ones. How do you have to adapt the Metropolis algorithm to take into account the confining geometry? (hint: see figure below)
4. We want to study the sedimentation of hard disks. This means adding gravity, and let them fall to the bottom of the container. How do you have to modify your Metropolis algorithm to account for a constant gravity field of amplitude g? Write the transition probabilities in the presence of gravity. Explain the role of temperature in presence of gravity.

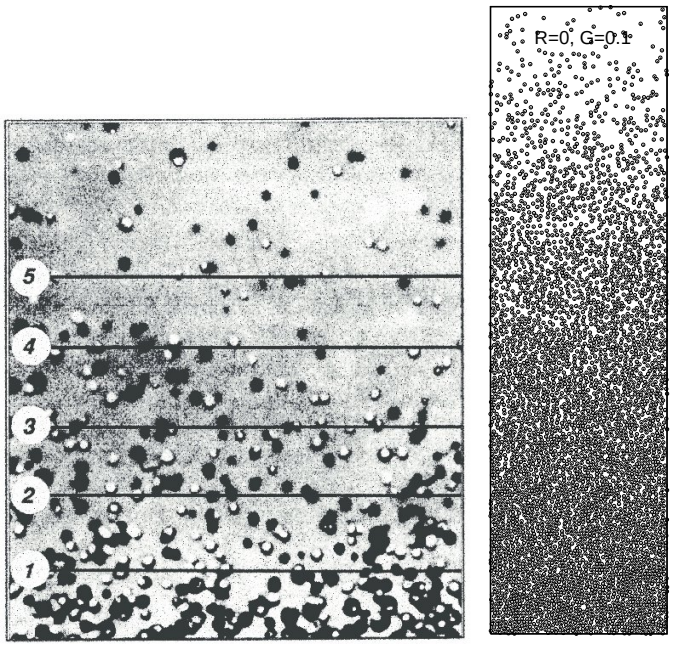

Figure 2: Left: A micrograph taken by J. Perrin of the sedimentation-diffusion equilibrium of resin (gamboge) spheres suspended in water. From: Randriamasy F. *Les grandes experiences de Jean Perrin.* Revue du Palais de la Decouverte 1992; 20: 18-29. Right: Monte Carlo simulations of $N = 10000$ hard disks in a gravity field $g = 0.1$ in reduced units.

5. Jean Perrin's virtual experiment [1]: Using an elongated closed box $L_x \times L_y$, with $L_y = 10L_x$ in a constant gravity field g along the y-axis, simulate a system of hard disks with $N = 1000$, $m = 1$ at $T = 1$. Choose L_x wisely. **Plot the equilibrium configurations** of the system for $g = 0$, 0.01, 0.1, 1, 10. Comment the snapshots.
6 (bonus). Give the particle density profile $\rho(y)$ along the vertical direction of the sedimenting system in equilibrium conditions. Which value of the parameters would you choose to put this prediction from equilibrium stat. mech. into test?
7 (bonus). Measure the steady density profile $\rho(y)$ along the vertical direction of the sedimenting system. In order to do so, you will need to:

1. 'Slice' your system into horizontal stripes of width b (to be chosen, $b > \sigma$ but $b \ll L_x$).

[1] Jean-Baptiste Perrin was awarded the Nobel Prize in Physics in 1926 "for his work on the discontinuous structure of matter, and especially for his discovery of sedimentation equilibrium." His work on Brownian motion verified Albert Einstein's theory and confirmed the atomic nature of matter.

2. Measure the mean density $\rho(y)$ of each slab at a heigh y.

3. Repeat (average) over several steady configurations. Then plot $\rho(y)$ and compare with the expected form.

4. Try several values of b and check that your results converge into a well defined density profile $\rho(y)$.

5. Repeat this analysis for $T = 0.1, 1, 10$.

References

[1] Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., & Teller, E. (1953). Equation of state calculations by fast computing machines. *The journal of chemical physics*, 21(6), 1087-1092.

[2] Alder, B. J., & Wainwright, T. E. (1957). Phase transition for a hard sphere system. *The Journal of chemical physics*, 27(5), 1208.

[3] W. Krauth, *Statistical Mechanics: Algorithms and Computations*, Oxford university press, 2006.