FINAL EXAM Spring 2013
TFY4235 Computational Physics
Version 1

This exam is published on Monday, May 6 at 09:00 hours. The solutions should be mailed to me at `Alex.Hansen@ntnu.no` *on Thursday, May 9 at 23:00 hours at the latest. The reports should be sent in PDF format.*

There are no constraints on any aids you may want to use in connection with this exam, including discussing it with anybody. But, the report and the programs you will have to write yourself. Please attach your programs as appendices to the report. Give as a footnote the names of your collaborators during the exam. The report may be written in either Norwegian (either variation) or in English.

In this exam, we will investigate the *Event-Chain Monte Carlo Algorithm,* [1] which belongs to a new class of Monte Carlo methods that are *rejection free.* We will implement the method for the *hard disk gas* and compare it to the Metropolis Monte Carlo algorithm [2].

Monte Carlo methods are fundamental to statistical mechanics. The earliest one is the *Metropolis algorithm* which we have discussed at length in the lectures. The earliest use of the Metropolis algorithm was to study the *hard disk gas* [2].

The hard disk gas consists of impenetrable disks that collide elastically (i.e., without losing kinetic energy). We assume that the disks have a radius σ. If then $r_{i,j}$ is the distance between two disks i and j, their interaction energy is given by

$$e(r_{i,j}) = \begin{cases} \infty & \text{if } r_{i,j} \le 2\sigma \;, \\ 0 & \text{if } r_{i,j} > 2\sigma \;. \end{cases} \tag{1}$$

The total interaction energy of a hard disk gas consisting of N disks is then given by

$$E(\vec{r}) = \sum_{i<j}^{N} e(r_{i,j}) \;, \tag{2}$$

where $\vec{r} = (r_1, r_2, \cdots, r_N)$ and $r_{i,j} = |\vec{r}_i - \vec{r}_j|$.

The Boltzmann factor for a given configuration $\vec{r}$ is given by

$$W(\vec{r}) = e^{-E(\vec{r})/k_B T} \;, \tag{3}$$

where k_B is the Boltzmann factor and T the temperature. We then see that the Boltzmann factor only takes on two values: $W(\vec{r}) = 1$ if no disks overlap and $W(\vec{r}) = 0$ if any two disks overlap. There is no temperature dependency. This makes the Metropolis very simple to implement for the hard disk gas:

- Choose a disk, say disk i,
- Move that disk a random distance $\delta\vec{r}_i$ in a random direction. (That is, set $|\delta\vec{r}| = \xi$ drawn from a uniform distribution on the interval $[0, \xi_{\max}]$.)
- If the move causes disk i to overlap with any other disk, reject the move — otherwise, accept it.

Simple as the Metropolis algorithm is for the hard disk gas, it has turned out to be very difficult to answer fundamental questions about it. For example, as the density of the gas increases, defined as

$$\eta = \frac{N\pi\sigma^2}{A} \;, \tag{4}$$

where A is the area in which the gas moves, it undergoes a phase transition where it freezes. It simply takes too long, even with modern computers, to study the system with enough precision to determine what kind of phase transition this is. The trouble with the Metropolis Monte Carlo algorithm is that as η increases, more and more Monte Carlo steps are rejected and in the end, the algorithm end up spending all its time making trial steps that go nowhere.

Enter Bernard, Krauth and Wilson [2] and their *event-chain Monte Carlo algorithm.* This algorithm is *rejection free,* which means that no time is wasted on dead-end moves. With this algorithm, Bernard and Krauth could finally, after 60 years, answer the question of what the nature of the hard disk transition is [3]. I will not go further into details on this here, as they are irrelevant for the exam — but have a look at Reference [3]. The answer turned out to be surprising.

The event-chain Monte Carlo algorithm is implemented as follows:

- Choose a disk i.
- Move this disk in the positive x direction until it hits a disk.
- Move this second disk in the same direction until it hits a third disk and so on, *until the disks have moved a total distance l* where l is a prechosen, fixed parameter.
- The last disk will stop before it has hit yet another disk.
- Repeat this algorithm, but this time in the positive y direction. Next iteration after this, return to the positive x direction and so on.

The algorithm is illustrated in Figure 1.

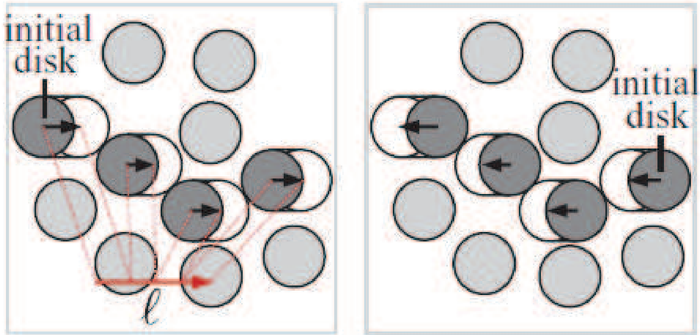

Figure 1 *Event-chain Monte Carlo algorithm for hard disks. The left panel shows a collective move with the total displacement l as a fixed parameter of the algorithm. The move is never rejected. The right panel shows the return move, demonstrating microscopic reversibility. (From [4].)*

We will in this exam compare the Metropolis Monte Carlo algorithm and the event-chain Monte Carlo algorithm. Implement both for a gas living in a square box of size $L \times L = A$ and having periodic boundary conditions in both the x and y directions. Let the gas consist of N hard disks with radius σ. The density then becomes $\eta = N\pi(\sigma/L)^2$. Do not be overambitious with respect how high you can go with η (The freezing transition occurs at around $\eta \approx 0.7$ — stay well below this limit.) Place the disks initially so that they do not overlap. Run the Monte Carlo algorithm long enough so that all traces of the initial configuration are gone before making any measurements.

The periodic boundary conditions are most efficiently implemented as follows. We place the box such that its edges run parallel with the x and y axes. We place one corner at the origin, $(x, y) = (0, 0)$. The other three corners are then at $(0, L)$, $(L, 0)$ and (L, L). Suppose that disk i has x coordinate x_i. It moves to a new position x'_i which may lie outside the range $x = 0$ to $x = L$. However, the following transformation brings it back inside the interval,

$$x'_i \to x'_i = \text{mod}(x'_i + 2L, L) \ . \tag{5}$$

The same construction works (of course) in the y direction.

Task 1 Measure for both the Metropolis and the event-chain Monte Carlo algorithms the average distance each disk moves per attempted one-disk move as a function of η. In the Metropolis Monte Carlo algorihm, this means also counting rejected moves (during which the disk moves a distance equal to zero) and in the event-chain Monte Carlo algorithm, if n disks move so that they in total move a distance l, the move per disk was l/n in a time step.

Task 2 Measure the radial distribution function $g(r)$ for the hard disk gas using both the Metropolis Monte Carlo algorithm and the event-chain Monte Carlo algorithm for different densities η. This is how to do this. Around the center of each disk, draw $m+1$ concentric circles with radii from $r = \sigma$ to $r = r_{\max}$ so that m annular zones of equal area are formed. Count the number of disks whose centers are within each annular ring. Do this for each disk and for many different realizations (Monte Carlo times). Record the numbers in a histogram $H(k)$, where $1 \le k \le m$. Then $g(r)$ is approximated by $H(k)/H(1)$. Do the results from the Metropolis Monte Carlo algorithm and the event-chain Monte Carlo algorithm match?

We show in Figure 2, $g(r)$ as measured by Metropolis et al. [1] in 1953.

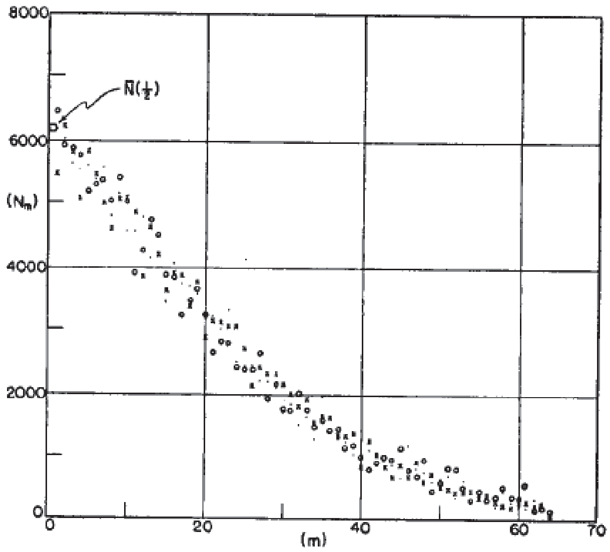

Figure 2 *Here is the radial distribution function $g(r)$ for the hard disk gas as measured by Metropolis et al. [2] in 1953.*

You should determine the parameters that go into the system, L, σ, N, $\xi_{\max}$, m, $r_{\max}$ and l yourself. Do remember that this is not a simple problem numerically when η is large. Good luck!

References

[1] E. P. Bernard, W. Krauth and D. B. Wilson, Phys. Rev. E, **80**, 056704 (2009).

[2] N. Metrolopis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller and E. Teller, J. Chem. Phys. **21**, 1087 (1953).

[3] E. P. Bernard and W. Krauth, Phys. Rev. Lett. **107**, 155704 (2011).

[4] E. P. Bernard and W. Krauth, Phys. Rev. E **86**, 017701 (2012).