MONTE CARLO SIMULATIONS OF TWO DIMENSIONAL HARD PARTICLE SYSTEMS

Melvin Lasky and Marvin Bishop
Department of Mathematics/Computer Science
Manhattan College
Manhattan College Parkway
Riverdale, New York 10471

Abstract

Engineering and science students should be exposed to techniques of computer modeling of materials. Monte Carlo methods provide an opportunity for students to develop computer skills while also deepening their knowledge of the behavior of materials. The graphics capabilities of the Maple software package allow one to easily visualize the change in ordering which takes place at higher densities. This kind of project is ideal for students who are interested in modeling.

Introduction

In a previous publication in this journal Harnett and Bishop [1] presented a Monte Carlo simulation of a one dimensional hard particle system. In this article their methods are extended to two dimensions. We also demonstrate how the graphics capabilities of the Maple software package can be combined with a C++ simulation program to investigate the onset of ordering in hard disk systems.

An important property of multi-particle systems in any dimension is the pair correlation function [2], G(R**)** which measures the relative number of particles at a distance |**R**| from the center of a reference particle. The change in the shape of the pair correlation function mirrors the underlying particle arrangements. It is well-known [3] that in the gaseous state there is little order and that particles are distributed at random whereas in the solid state the particles pack into long-ranged ordered crystals. The appearance of multiple, well defined peaks in the pair correlation function at higher densities, indicates the onset of localization behavior.

Method

A periodic two dimensional hard particle system has been studied with a Monte Carlo computer simulation [4-7] method. In this kind of simulation a random walk, which asymptotically converges to the exact result after a large number of steps, is performed. The particles are started at fixed positions in a lattice and then moved by the standard Metropolis Monte Carlo method [4] until an equilibrated state is achieved. The details of this type of computation for any dimension are given in Bishop, Whitlock and Klein [8] but the key ideas for two dimensional systems can be summarized as follows. The number of particles, N = 100, and the number density, ρ, of interest are input parameters. The particles are started on a triangular lattice which determines the length, Lx, and the width, Ly, of the rectangular simulation box:

$$Lx = [2\ N / (3^{1/2}\ \rho)\ ]^{1/2} \qquad (1a)$$

$$Ly = 3^{1/2}\ Lx / 2 \qquad (1b)$$

Figure 1 illustrates the triangular starting lattice when ρ = 0.40.

The calculation proceeds by attempting to move, in turn, each of the particles in the simulation box. A pass is defined as a sequence of steps in which an attempted move is made for each of the N particles. To move a particle from its original location, ($X_{original}$, $Y_{original}$), two uniform random numbers, RN_1 and RN_2, between 0 and 1 are generated and used to select a new trial position,

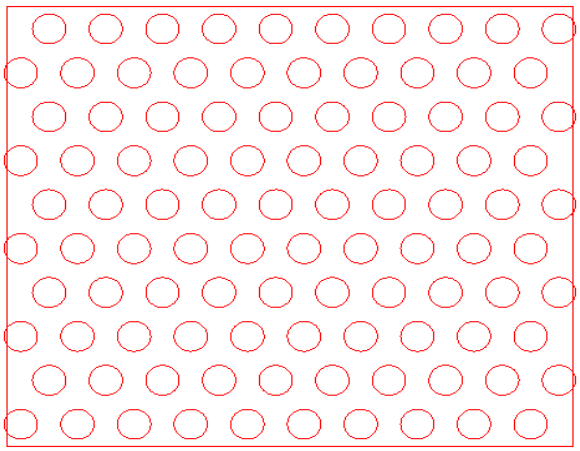

Figure 1: The starting triangle lattice for ρ = 0.40.

$$X_{trial} = X_{original} + (2 * RN_1 - 1) * MAXDX \quad (2a)$$

$$Y_{trial} = Y_{original} + (2 * RN_2 - 1) * MAXDY \quad (b)$$

Here, MAXDX and MAXDY are the maximum magnitude of an allowed displacement in the X and Y directions, respectively, measured from the particle's center of mass. It is the largest possible move. In the current simulations MAXDX and MAXDY have been set to 0.1 in reduced units for which a particle has a diameter of 1.0. A move is rejected whenever a particle overlaps another particle; e.g. the separation between their centers becomes less than 1.0. If the new position is not accepted, the test particle remains at its current location. The acceptance ratio, the number of accepted moves divided by the number of total moves, is monitored. The acceptance ratio was 0.89 when ρ = 0.4 and 0.54 when ρ = 0.8. Standard periodic boundary conditions [9] are employed. This means that if a particle is moved such that if X and/or Y becomes either less than 0 or larger than Lx or Ly, respectively, an identical particle is placed in the box at position modulo Lx and/or Ly. This procedure maintains the number of particles in the box and makes the simulation more representative of bulk matter.

Since the successive positions of the particles are not independent, it takes many passes to converge from the initial state to an equilibrated state. Only the equilibrated passes are employed in the final calculations. Hence, some number of passes must be discarded; we have discarded 10,000 passes and continued the runs for an additional equilibrated 20,000 passes. Even after the equilibrated regime is attained there is still serial correlation between each pass in the MC process. We have addressed this problem by computing G(R) only at fixed intervals of 50 passes. Hence, G(R) is averaged over 400 samples in our simulations.

The pair correlation function is calculated by computing a histogram of the average number of particle separations as a function of separation distance (see Allen and Tildesley [9]). This histogram is normalized by dividing by the differential "volume" occupied by the particles, $\pi ((R + \Delta R)^2 - R^2)$, and the actual number density of particles, ρ.

Sample Monte Carlo codes are available from many sources; see for example, Gould and Tobochnik [7], and Allen and Tildesley [9]. We have developed the simulation using the Dev C++ compiler on a PC.

Results

Figure 2 presents a snapshot of the system at ρ = 0.4 and its corresponding pair correlation function. We have employed Maples' plottools package to draw disks centered on the system particles. Also we have used the plot facility of Maple to obtain the G(R) plots presented. Figure 3 presents the same information at a density of 0.8.

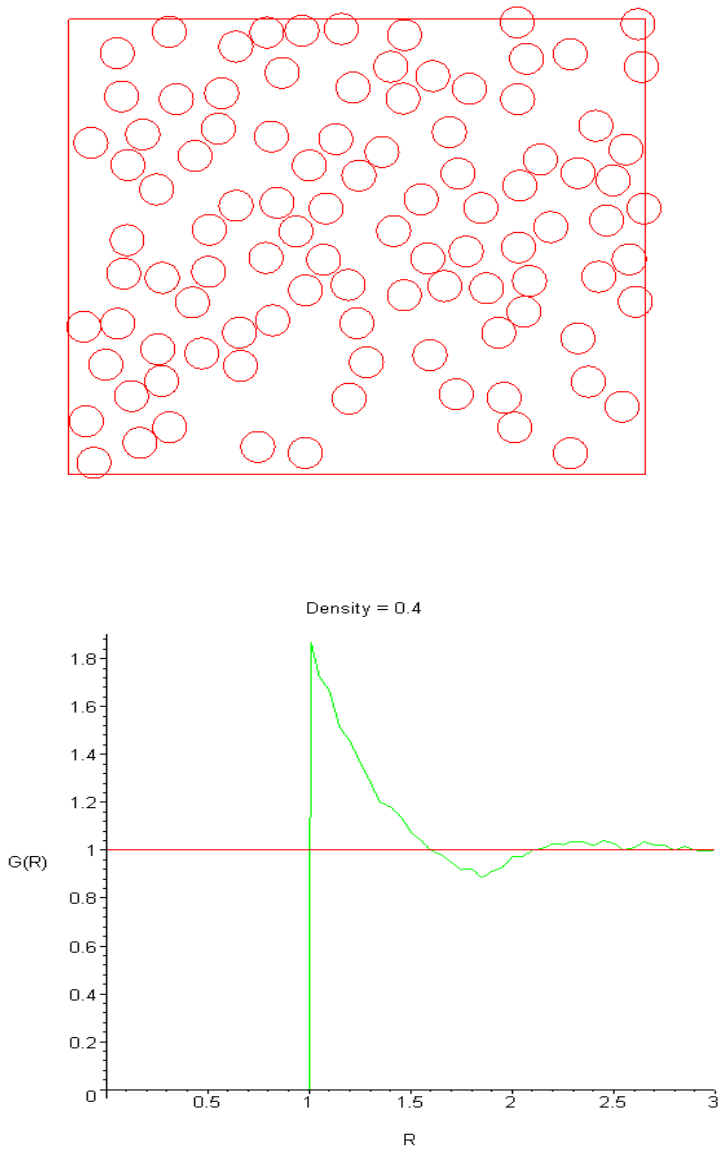

Figure 2: A typical configuration of a 100 particle system and its pair correlation when the density is 0.4.

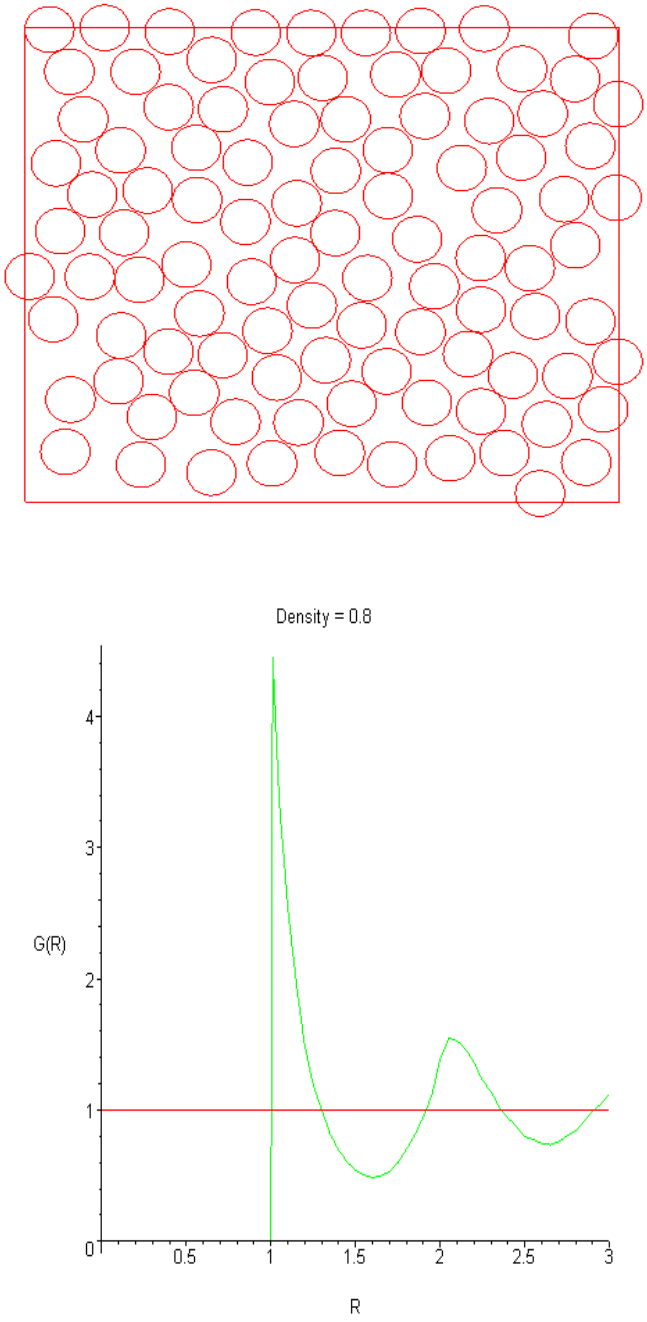

Figure 3: A typical configuration of a 100 particle system and its pair correlation when the density is 0.8.

One can easily notice the larger free space at the lower density. This fact is mirrored in the behavior of G(R) which develops a sharper first peak and a well developed secondary peak as the density increases from 0.4 to 0.8. The secondary peak indicates strong correlations between second-nearest neighbors. G(R) is zero when $R \leq 1.0$ since particles cannot penetrate each other. When G(R) attains a value of 1.0 the fluid is uniform in its structure.

Conclusion

We have investigated two dimensional periodic hard disk systems by Monte Carlo simulations and have indicated how the pair correlation function reveals the underlying

molecular structure of materials. Graphic tools such as those employed here provide a clear demonstration of some aspects of the behavior of materials and thus strongly enhance student understanding and intuition.

Acknowledgements

We wish to thank the Manhattan College Computer Center for providing computer time. We also wish to thank Professor Paula Whitlock for many useful conversations about Monte Carlo calculations.

References

1. J. Harnett and M. Bishop, "Monte Carlo Simulations of One Dimensional Hard Particle Systems", Comp. Edu. J., XVIII, 73 (2007).

2. M. Bishop and C. Bruin, "The Pair Correlation Function: A Probe of Molecular Order", Am. J. Phys., 52, 1106 (1984).

3. D.A. McQuarrie, Statistical Mechanics, (Harper and Row, New York, 1976).

4. N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, "Equation of State Calculations by Fast Computing Machines", J. Chem. Phys., 21, 1087 (1953).

5. D. P. Landau and R. Alben, "Monte Carlo Calculations as an Aid to Teaching Statistical Mechanics", Am. J. Phys., 41, 394 (1973).

6. M.H. Kalos and P.A. Whitlock, "Monte Carlo Methods Volume I Basics", 2nd edition, (Wiley., Berlin, 2008).

7. H. Gould and J. Tobochnik, "An Introduction to Computer Simulation Methods: Part 2", (Addison and Wesley, Reading, 1988).

8. M. Bishop, P.A. Whitlock and D. Klein, "The Structure of Hyperspherical Fluids in Various Dimensions", J. Chem. Phys., 122, 074508 (2005).

9. M.P. Allen and D.J. Tildesley, "Computer Simulation of Liquids", (Oxford University Press, Oxford, 1993).

Biographical Information

Melvin Lasky received his B.S. Cmpe. and M.S.Cmpe. from Manhattan College. He is currently working in the Manhattan College Computer Center.

Marvin Bishop is a Professor in the Department of Mathematics and Computer Science at Manhattan College. He received his Ph. D. from Columbia University, his M.S. from New York University and his B.S. from the City College of New York. His research interests include simulation and modeling and parallel processing.