MONTE CARLO SIMULATIONS OF TWO DIMENSIONAL HARD PARTICLE FLUIDS

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Abstract

Computer modeling is an important skill for engineering and science students to acquire. Monte Carlo simulations of two dimensional fluids provide an opportunity for students to develop their computer skills while deepening their knowledge of the behavior of materials. Using the Maple software package, students can easily create animations of particle movements.

Introduction

In a series of previous publications in this journal investigating two dimensional hard disks, Lasky and Bishop [1] presented their Monte Carlo (MC) simulations of homogeneous systems, Merriman and Bishop [2] examined 50:50 binary mixtures in which the larger component had twice the diameter of the smaller one and Havlicek and Bishop [3] studied binary mixtures with 25:75, 50:50 and 75:25 compositions and diameter ratios of 1/2 and 2/3. Havlicek and Bishop [3] obtained the equation of state from their calculations. In this work we revisit the homogeneous fluid and compute its equation of state. Our results are compared to other simulations and theory.

A hard disk system contains N particles, each with a diameter of σ, in a box with sides Lx and Ly. The number density, ρ, is given by

$$\rho = N / (Lx\ Ly) \qquad (1)$$

When the starting configuration of the particles is a square lattice, Lx = Ly, but if the particles are started in a triangular lattice,

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

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

Figures 1a and 1b illustrate these starting states when N = 100 and ρ = 0.50

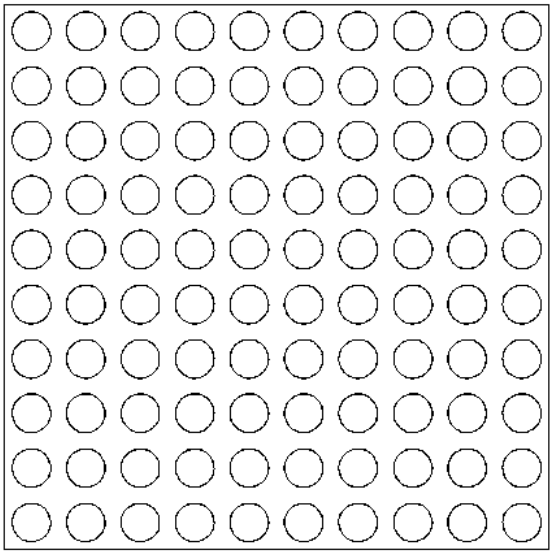

Figure 1a Square Lattice.

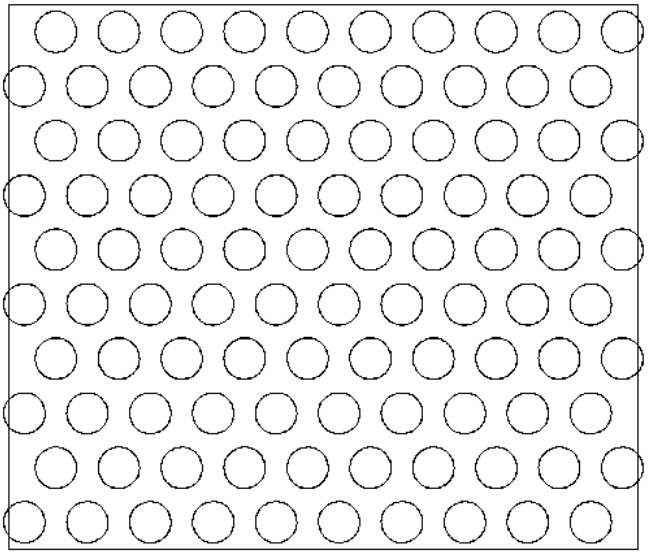

Figure 1b Triangular Lattice.

The equation of state [4] is given by the compressibility factor, $Z = P/\rho k_B T$, where P is the pressure, k_B is Boltzmann's constant and T is the absolute temperature. In an ideal gas the particles do not interact and then Z = 1. In the case of the homogeneous hard disk fluid, Z is related [5] to the pair correlation function at contact by

$$Z = 1 + \rho\,(\pi/2)\,\sigma^2 G(\sigma) \qquad (3)$$

Here, σ is the contact diameter, the separation between the centers of the particles when touching. The pair correlation function at contact is G(σ). A pair correlation function [6], G(R**),** measures the relative distribution of particles at a distance |**R**| from the center of a reference particle.

Method

The details of our MC computer simulation are contained in the papers of Lasky and Bishop [1] and Merriman and Bishop [2]. The particles are started at positions in a lattice and then moved by the standard Metropolis Monte Carlo method [7-11] until a random, equilibrated state is achieved. A move is rejected whenever a particle overlaps another particle; e.g. the separation between their centers becomes less than σ. If the new position is not accepted, the test particle remains at its current location and the next particle is selected for a test move. Once all N particles have been tested a single pass (or MC step) is complete.

The Maple software package allows one to easily create an animation indicating how the particles change their configuration. At the starting lattice stage and after every fixed interval of passes (a number specified by the user) a frame is generated and written to a file. Using Farley and Tiffany's four step method [12], each frame is then used to make an animation. This animation shows different stages in the simulation. Figure 2a illustrates the initial configuration of the particles in a square lattice, and Figure 2b shows the configuration of the same lattice after 50 MC steps. The behavior of the shaded particle is typical of how particles "melt" from the lattice and move in the resulting fluid.

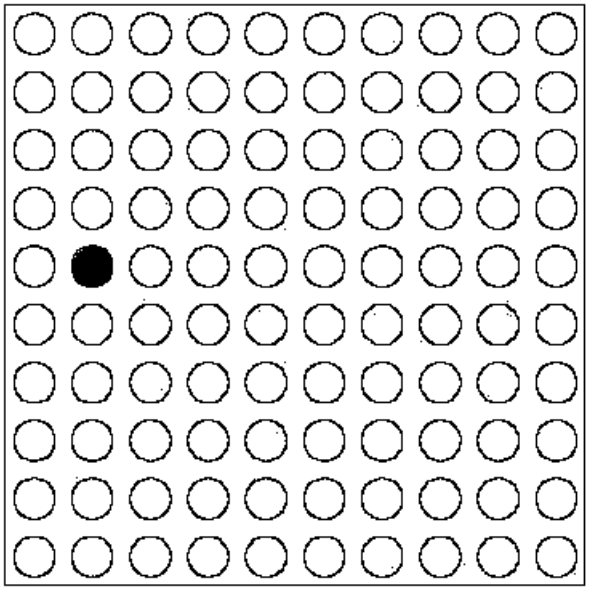

Figure 2a Initial Configuration.

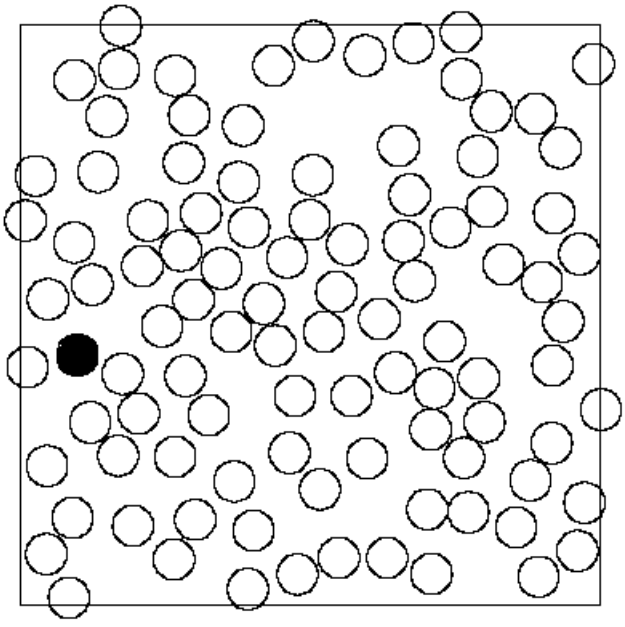

Figure 2b Configuration after 50 MC steps.

Since the successive positions of the particles are not independent, it will take many MC steps to converge from the arbitrary initial state to a representative equilibrated state. Only the equilibrated steps are employed in the final calculations. Hence, some number of steps must be discarded before the runs are continued to obtain equilibrated steps. Even after the equilibrated regime is reached there is still serial correlation between each step in the MC process. We have addressed this problem by computing the pair correlation at fixed intervals which encompass many MC steps. Thus, the pair correlation function is computed by averaging over both the appropriate number of particles and the number of equilibrated samples. The details of the pair correlation function calculations are contained in the earlier paper by Lasky and Bishop [1].

Results

The simulation has been developed by using the gnu C compiler on a PC with the Linux operating system. Production runs were generated for 12,000,000 MC steps and 2,000,000 steps were discarded. The sampling interval was set at 2,000 steps so that there were 5,000 equilibrated samples to average over. The equation of state has been obtained by finding the value of the pair correlation function at contact. This is determined by fitting a line to the first peaks of the pair correlation functions and then extrapolating to the appropriate contact value, as illustrated in Havlicek and Bishop [3]. Once the contact value has been determined, the equation of state is found from Eq. 3. The Z values for all the systems studied are contained in Table I. Zsp are the theoretical values predicted by the scaled particle theory [5]:

$$Zsp = 1 / (1 - \eta)^2 \qquad (4)$$

Here η is the packing fraction, which in two dimensions is related to the number density by

$$\eta = \rho (\pi/4) \sigma^2 \qquad (5)$$

Another theoretical equation is Henderson's [13] modification of the scaled particle theory.

$$Zh = (1 + \eta^2/8) / (1 - \eta)^2 \qquad (6)$$

Also listed in the table are Zkr which are the values found by Kolafa and Rottner [14] for N = 4,000, 9,000, 16,000 and 50,000 starting from a square lattice and using molecular dynamics methods. Also shown are Zel from Erpenbeck and Luban [15] with N=1512 or 5822 employing a mixture of molecular dynamics and MC simulation methods. Zmc100 and Zmc400 are our new MC results when N=100 and 400 starting from a square initial configuration and Zmc100t are the results for N=100 when the starting lattice is triangular (see Figures 1a and 1b).

In all cases the data are consistent with each other within 1%. Since typically a 400 particle simulation required, as expected for the $O(N^2)$ algorithm employed here, about sixteen times the computer time needed for the corresponding 100 particle one, unless one wants extremely high accuracy, the smaller particle system should be adequate for simple simulations at lower densities. Also our new data are in agreement with the theoretical predictions for the equation of state.

Figure 3 presents the equation of state, Z, as a function of the density. All the data are in excellent agreement with the Henderson theoretical curve at the higher densities. The Table indicates that there is no significant difference between the square and triangular lattice MC results.

Table I: Equation of State Data.

ρ	Zsp	Zh	Zmc100	Zmc400	Zmc100t	Zkr	Zel
0.0385	1.063	1.064					1.063
0.0577	1.097	1.098					1.097
0.0750	1.129	1.130	1.127		1.126		
0.1000	1.178	1.179					
0.1155	1.210	1.211					1.211
0.1500	1.285	1.287	1.285		1.291		
0.2000	1.407	1.412					
0.2309	1.492	1.498					1.498
0.3000	1.712	1.723	1.736	1.721	1.720		
0.3849	2.054	2.078					2.077
0.4000	2.126	2.152	2.154		2.153	2.151	
0.4500	2.392	2.429				2.428	
0.5000	2.711	2.764	2.773		2.770	2.760	
0.5500	3.099	3.172				3.165	
0.5774	3.348	3.434					3.424
0.6000	3.577	3.676	3.670		3.658	3.664	
0.6415	4.062	4.191					4.172
0.6500	4.174	4.310	4.301	4.301	4.302	4.288	
0.7000	4.933	5.120	5.090		5.093	5.082	
0.7217	5.329	5.543					5.496
0.7500	5.921	6.178	6.073	6.090	6.103	6.113	
0.7698	6.396	6.689					6.607
0.8000	7.239	7.596	7.490		7.475	7.477	

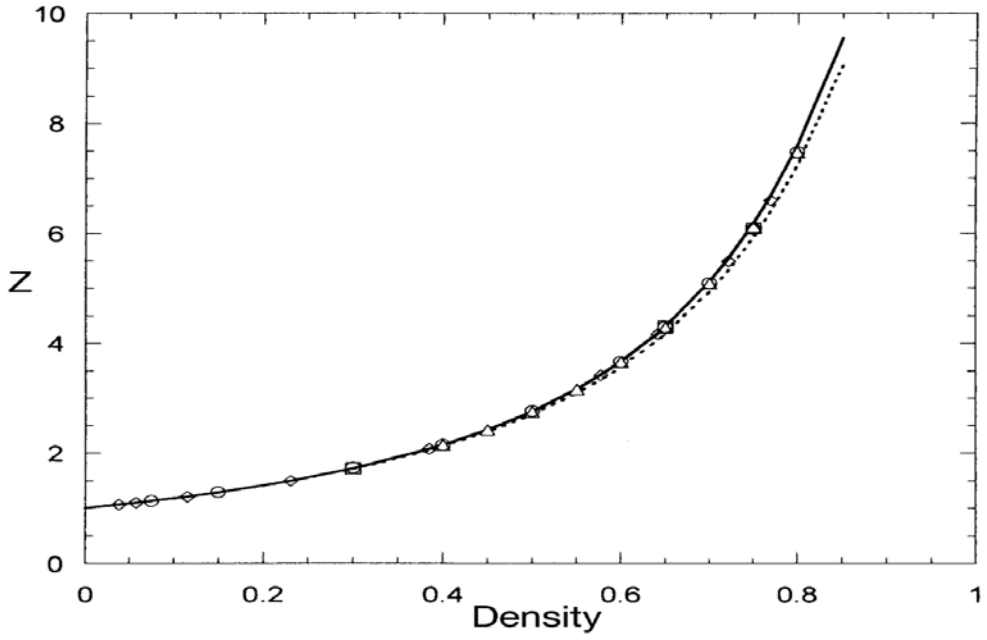

Figure 3: The equation of state, Z, as a function of the density. The solid and dotted lines are the Henderson and scaled particle theoretical predictions, respectively, Eqs. 6 and 4. The up triangles and the diamonds are the Kolafa and Rottner [14] and Erpenbeck and Luban [15] simulation data, respectively. The circles and squares are the current MC data for N = 100 and N = 400, respectively.

Conclusion

We have investigated two dimensional homogenous hard disk systems by Monte Carlo simulations. Numerical tools such as linear least squares line fits have been used to compute the equation of state from the contact pair correlation function. The results are in excellent agreement with other simulations and theories. There is no significant difference between initializing the simulation from the square or triangular lattice. Animations can be used to indicate the nature of the equilibration. Modeling projects such as the one described here provide a clear demonstration of some aspects of the behavior of materials and thus strongly enhance student understanding and intuition.

Appendix: The Manhattan College Undergraduate Research Program

Manhattan College has a long tradition of involving undergraduates in research and was one of the original members of the Oberlin 50. This is a group of undergraduate institutions whose students have produced many PhDs in engineering and science. At Manhattan College, students can elect to take an independent study course for three credits during the academic year. In addition, the College provides grant support to the students for ten weeks of work during the summer. I have personally recruited the students from my junior level course in Systems Programming. Previously published articles in this journal by Manhattan College student co-authors are a very effective recruitment tool. The students have also presented their results at a variety of undergraduate research conferences including the Hudson River Undergraduate Mathematics Conference and the Spuyten Duyvil Undergraduate Mathematics Conference.

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Meena A. Balady is currently a student in the computer science program at Manhattan College.

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