AN INTERACTIVE JAVA PROGRAM FOR PLACING HARD DISCS IN A TWO DIMENSIONAL BOX

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Abstract

Java is a powerful programming language which enables students to rapidly build GUI (Graphic User Interface) interfaces. An interesting application area of Java programming is Monte Carlo modeling of materials. In developing interactive modules for modeling projects, students will enhance their skill set in Java programming and also learn about different behaviors of materials. In this note we discuss an application of Java in the investigation of packing in two dimensional fluids.

Introduction

Engineering, mathematics and science students need to develop the ability to abstract and model nature. One important application area is Monte Carlo[1-2] computer simulation of materials. Students will have to combine knowledge from a variety of areas in order to be able to construct reasonable models. They will need to master concepts from algorithm development, chemistry, computer programming, graphics, and statistics. Such a model was developed in an independent study project at Manhattan College.

In a previous publication in this journal Lasky and Bishop[3] presented a Monte Carlo simulation of two dimensional hard discs. In that article the pair correlation function [4], g(r), was computed. This function measures the relative number of particles at a distance from the center of a reference particle and, hence, indicates the ordering present. In this note we show how the same problem can be modeled using a different Monte Carlo approach. We also demonstrate the power of Java for building interactive simulation programs. The Java code is available by writing to the authors.

Method

The current Monte Carlo simulation method consists in placing non-overlapping discs with a diameter of 1.0, into a two dimensional box. The side length of this box, L, is set when the user inputs the total number of discs, N, and system density, ρ, to be studied;

$$L = (N / \rho)^{1/2} \qquad (1)$$

Two random numbers, each between 0 and L, are used to determine the center of each disc. As the disc center coordinates are generated, they are tested against previously placed discs. All centers must be at least one unit apart so that there is no overlapping of discs. The Java program allows for up to 100,000 placement attempts before terminating. If all N discs have been successfully placed, one complete configuration has been generated. The pair correlation function is then computed. The details of this computation are contained in Lasky and Bishop[3]. The user also decides upon the total number of configurations to generate. As is well known, the average values of computed quantities are improved in accuracy as more configurations are used. Each configuration in this model is an independent sample. Figure 1 presents a typical user interaction screen. In this case the user has decided to generate 400 configurations. In each of these the software will attempt to place 100 discs in a box whose dimensions are determined by the input density, 2.

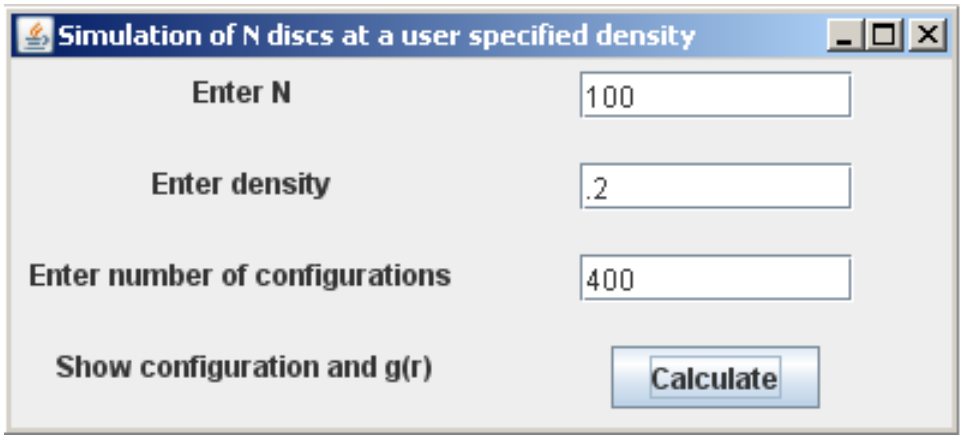

Figure 1: A typical user GUI screen for data entry.

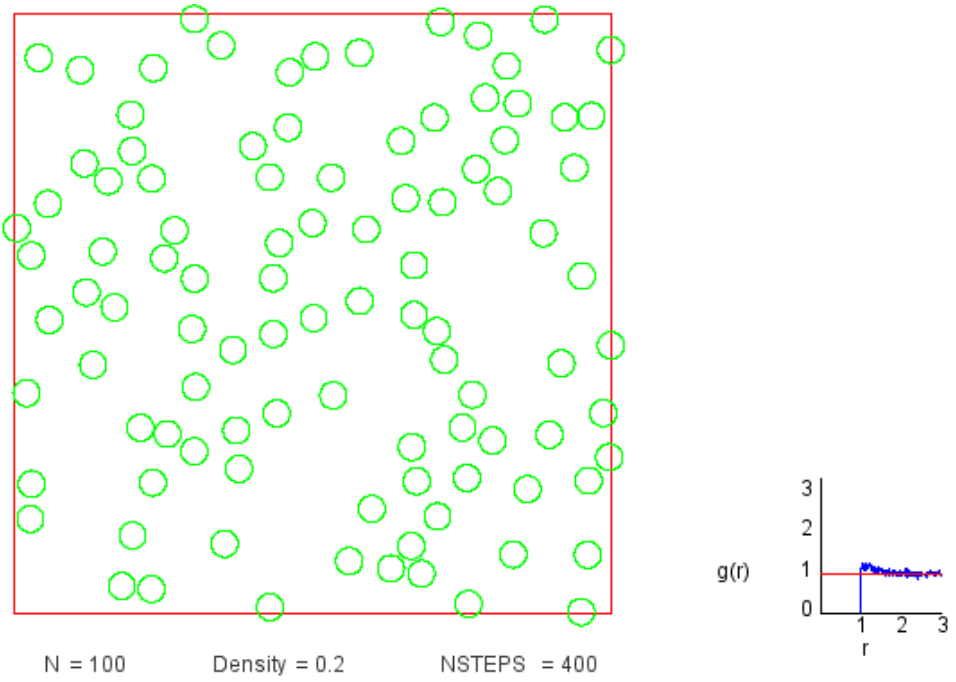

Figure 2: The output screen at a density of 0.2.

Figure 2 illustrates the output frame obtained when the user presses the calculate button. The discs have been drawn explicitly by using the general equations of a circle with radius, ra, and center (xc,yc) to generate points on the circumference,

$$x = xc + ra * \cos(\theta); \quad y = yc + ra * \sin(\theta) \; ; \quad 0 \leq \theta \leq 2\pi \qquad (2)$$

and then connecting them with the Java drawLine method. The world system coordinates have been scaled to those in the screen system [5]. In our case, all distances are scaled according to L and, thus, the rendered images appear to change with density.

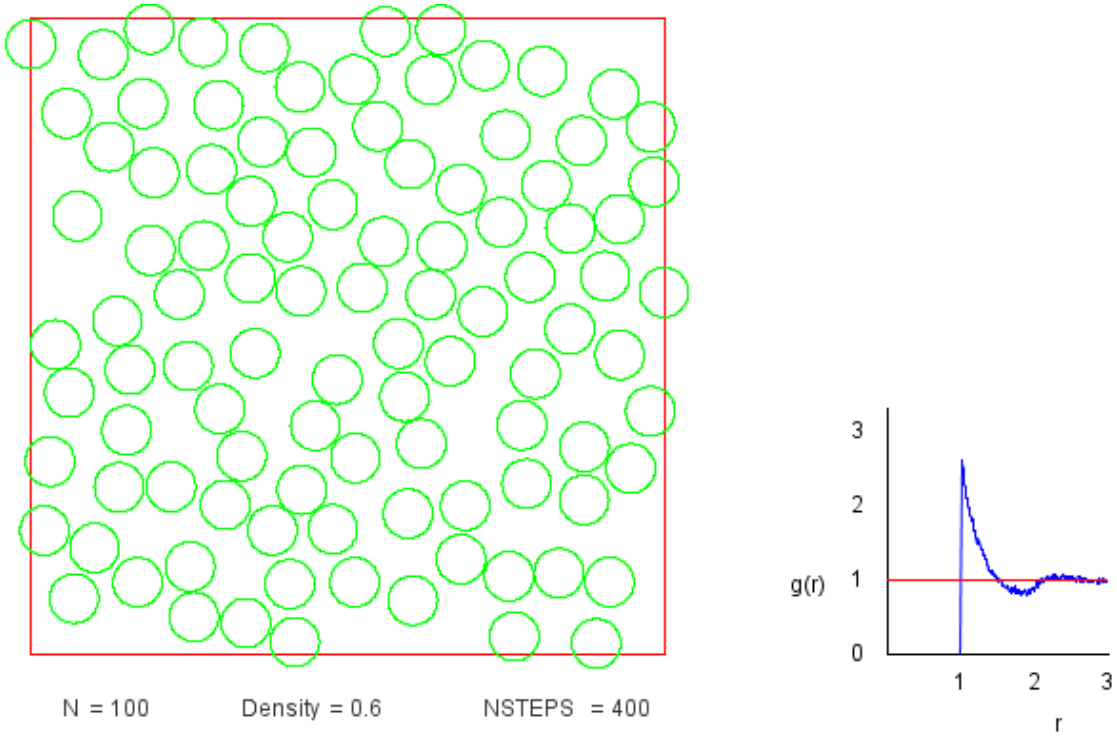

Figure 3: The output screen at a density of 0.6.

In Figure 2 one easily sees the large regions of free space in the box; the system is at a low density. Moreover, the pair correlation function reveals the lack of ordering; it contains only a small, first peak and no subsequent peaks. This mirrors the behavior of a dilute gas in which g(r) has a value of 0.0, due to the non-overlapping condition, until r = 1.0. It then jumps up to and remains, at the value of 1.0 thereafter, since the fluid is uniform.

Figure 3 presents the output screen at a density of 0.6. It is clear that the discs are much more closely packed. Also g(r) now has a sharp first peak and a secondary peak has begun to appear. It becomes more and more difficult to place particles in the box at higher and higher densities because the "free" space is distributed in many regions of the box.

Conclusion

We have developed interactive Java software to investigate two dimensional hard disc systems by a Monte Carlo technique. Our code allows the user to select the number of particles, the system density and the number of configurations. The output screen displays the last configuration alongside the pair correlation function. The configuration snapshots help a student to visualize the structure of materials. The interactive and graphics capabilities of Java are very useful in code development, especially for interactive programs.

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