THE ANALYSIS OF PARTICLE SYSTEMS USING COMPUTER SIMULATIONS

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ABSTRACT

In this paper, we present a simple method of measuring the isothermal pressure of a system of particles. These systems include the ideal gas, the excluded volume principle, and hard spheres under gravity, which is an important characteristic of granular systems. We chose a method using a Monte Carlo simulation to model the particles' movement. We found that the results of our program reflected theoretical predictions and also mirrored those obtained by running Molecular Dynamics simulations. As a result, we conclude that our program provides a simple but accurate model for the behavior of various particle systems including a granular system under the influence of gravity.

INTRODUCTION

Simulations, by their very nature, are a method of exploring the seemingly infinite complexities of reality at a more practical level. Today's fastest mainframe computers are capable of modeling the individual microscopic collisions of many atoms in a system. These simulations are used to obtain the properties of the system by tracking the individual particles. In classical physics, reality is governed by determinism, yet when observing the overall macroscopic properties of such systems, the general motion of a system of particles may be modeled by random movements. By modeling the behavior of particles with a probabilistic system, the macroscopic properties of a system can be predicted very accurately.

Granular systems are homogeneous mixtures (possibly made up of air, soil, cement, detergents or large masses during earthquakes) that exhibit fluidic behavior [1]. When simulating a granular system a conventional modeling method used in a Molecular Dynamics (MD) simulation, is one that keeps track of the momentum of the individual atoms within a system [2]. We can use these simulations to measure the pressure, or force per unit area, on walls in a system. The microscopic approach in such an MD simulation would be very complex and time consuming because the pressure would be determined from the momentum transferred to the wall by each atom.

We have developed an alternate approach that utilizes a computer program to carry out Monte Carlo simulations. This approach employs a random-walk method to simulate particle motion, resulting in a more probabilistic system then a deterministic one. These particles move among points of a lattice structure. When the spaces between these points

are made small enough, their motions adequately mimic the dynamics of a continuous system. Building off the foundation of a simple ideal gas model, we made provisions to take into account the excluded volume of the gas particles and then the effects of gravity on such particles. The combination of all these factors results in a granular system model.

Our objective has been to develop an accurate, but simple model of a granular system. Our model can be extended to encompass other systems and used as an alternate method to predict the behavior of granular particles in general. Research has already been done utilizing Newtonian Mechanics to analyze particle systems in a computer model. Our approach, though, is from the standpoint of probabilities based on the random motion of particles within the system. The output of our simulation can then be compared to a more complex Molecular Dynamic simulation, evaluating the accuracy of our output as well as the comparative difference in computational time and complexity.

THEORY

Pressure is a macroscopic measurement of the microscopic transfer of energy between particles on a volumetric basis. As such,

$$P = -\frac{\partial F}{\partial V},$$

(1)

where P is the pressure, F is the free energy, and V is the volume of the system. Using the equation for free energy,

$$F = -TS,$$

(2)

where T is temperature and S is entropy, we can substitute in the following expression for entropy,

$$S = k \ln \omega.$$

(3)

In equation (3) ω equals the number of states and k is the Boltzmann constant. For a single ideal gas particle $\omega = LH = V$ where L = length, H = height and V is the two-dimensional volume. In a system with N particles, the total entropy is given by

$$S = k \ln \omega^N.$$

(4)

The free energy can also be expressed as

$$F = -kT \ln Z$$

(5)

where Z is the grand partition function.

According to thermodynamics, the partition function is related to the probability of a particle being in a certain state. For the computer model, it is only necessary to predict a particle's state when it is in contact with the wall when determining the pressure. The discrete partition function,

$$Z = \sum e^{\frac{-U}{kT}},$$

(6)

gives the probability of finding a particle at the wall multiplied by the number of ways to find it at the wall. The summation of these probabilities gives the total probability of finding a particle at the wall.

For the equilibrium system being modeled, the kinetic and potential energies will affect Z independently. This leads to the following expression for pressure,

$$P = NkT \frac{\partial(\ln Z)}{\partial V},$$

(7)

where N is the number of particles in the system.

Since the velocity is independent of the volume, we can only concentrate on the spatial portion of Z. Using this fact, and some algebra, we obtain

$$P = \frac{NkT}{V}$$

(8)

Using the following definition of lattice density,

$$\phi = \frac{N}{V},$$

(9)

we obtain the following equation,

$$P = \phi kT.$$

(10)

We can also calculate the pressure of a system that follows the excluded volume principle. In the excluded volume principle, particles cannot occupy the same space; therefore, we can calculate Ω, the number of possible ways of placing N particles in a volume V:

$$\Omega = \frac{V!}{(V - N)!\, N!}.$$

(11)

Substituting Ω into the entropy equation, we get

$$S = k \ln \Omega .$$ (12)

Using Sterling's approximation, $\ln A! = A \ln A - A,$ the equation becomes

$$S = -kV[\phi \ln \phi + (1 - \phi) \ln(1 - \phi)]$$ (13)

We now need the following thermodynamic definition of the probability of finding a particle at the wall,

$$p(N_w) = \frac{\lambda^{N_w}}{Z} \Omega .$$ (14)

To determine pressure using our computer simulation, a value λ is used to represent the probability of finding a particle at the wall (when taking discrete snapshots of the wall):

$$\lambda = e^{\frac{-U}{kT}}$$ (15)

where U represents the potential energy of the system. Lambda takes into account the probable velocity of the particles. A high lambda value would correspond to higher particle velocities while a lower lambda value would correspond to lower particle velocities.

The substitution of equation (2) into equation (1) gives the following expression,

$$P = -T \frac{\partial S}{\partial V} .$$ (16)

Substituting equation (13) for S gives the pressure equation using the excluded volume principle

$$P = kT \ln(1 - \phi) .$$ (17)

For our discrete model of the system, the pressure is given by

$$P = kT \frac{\Delta \ln Z}{\Delta V} .$$ (18)

The average number of particles at the wall is defined as

$$<N_w> = \lambda \frac{\Delta \ln Z}{\Delta \lambda} .$$ (19)

As a result, by substituting equation (19) into equation (18), we obtain

$$P = \frac{kT <N_w> \Delta\lambda}{\lambda L}.$$ (20)

The density at the wall is defined as

$$\rho_w = \frac{<N_w>}{L}.$$ (21)

The expression for pressure then becomes,

$$P = \frac{kt\rho_w \Delta\lambda}{\lambda}.$$ (22)

Adding this up for all possible values of λ we obtain the following expression for the total pressure of the system:

$$P = \int_0^1 \rho_w \frac{kT}{\lambda} d\lambda.$$ (23)

The computer uses a discrete model with equation (23) to compute the pressure at the wall. We then compare this pressure to the expressions given by equations (10) and (17).

METHODS

Our experimental design is based on the Monte Carlo method. This method is used frequently in numerous disciplines to model occurring phenomena. Instead of looking at a system upon the basis of differential equations which describe every aspect of the system, the Monte Carlo method employs probabilistic particle motions which are governed by a random number generator. This method models the discrete behavior of the system from an overall standpoint, and achieves the desired purpose in a much less cumbersome manner [4]. In particular the Monte Carlo method has had a successful record in modeling other forms of particle transport and interactions. Included among these are electron transport chains used in the treatment of cancer as well as photon interactions in the atmosphere. Therefore it seems reasonable to use such a method when modeling the behavior of particle systems, and likely to produce valid results [5].

In order to simulate an actual granular system, we utilize a 2-D lattice system (100x100 for the ideal gas and 50x50 for the excluded volume and the gravity simulations). We begin by simulating an ideal gas system allowing multiple particles to occupy the same lattice point at once. Next, excluded volume characteristics are applied to the system, restricting one particle per lattice point. Finally, to construct the granular system, a

gravitational bias is added to the system. The particles then undergo a random walk for a specific amount of iterations. The procedure for finding the density over a given period of iterations is done by taking the sum of the number of particles at the wall divided by the total number of completed iterations and the length of the wall.

When dealing with wall collisions, only one wall is considered. The right wall is where the density is measure, while the left wall is considered to have an infinite potential, and thus particles remain motionless when selected to move against it. When the particle is right next to the collision wall, our probability density function, λ, is used to take into account the particle's velocity and to determine the probability of observing the particle colliding with the wall. The values of λ take into account the overall temperature and thus the average velocity of the particles in the system. Low values of λ correspond to the higher overall velocity of the particles. This also complements the Maxwell Boltzmann Distribution since $\lambda = \exp(-U/kT)$, where the value of kT corresponds to the average of $<v^2>$ for the particles. So a higher value of λ would correspond to a lower value of kT. This would result in the majority of the particles moving at lower velocities. The program takes this parameter into account by generating a random number that must be less than the value of λ in order for the particle to be seen colliding with the wall. Consequently, at high values of lambda particles will be more likely to visibly collide with the wall and thus the overall pressure will be higher.

The program starts out by defining the dimensions of the lattice space. The probability function lambda is then inputted allowing for a single λ simulation or a sequence through all possible λ values (0-1). Last, it chooses between running an ideal gas, excluded volume, or granular system simulation. After inputting these values, we start the program by placing the particles randomly on unique positions within the lattice. The mechanism by which the initial position of the particles is determined involves a selection of a random number between 0 and 1. There are two arrays and one matrix present, the arrays define the x and y positions of the particle, while the matrix indicates whether or not a particle is present in the lattice, (0 for not occupied and 1 for occupied). The number of the particles in the system is calculated as well by multiplying the density of the system times its length and height.

The program then moves each of the particles according to a random number generator from 0 to 1. Each of the .25 intervals corresponds to a different direction (left, right, up, down). Because the left wall is considered to be impenetrable, the program ensures that the particle in x coordinate 1 does not move left. When moving right, the program tests whether the x coordinate is one step away from the wall position, H(the maximum x position). If it is, it introduces another test to see whether the value is less than lambda in which case the particle is permitted to hit the wall by moving to H. When moving up and down particles at the top or bottom are permitted to wrap around to the opposite side. This procedure is used for the ideal gas system and excluded volume system. In the excluded volume case, the program tests each position to ensure that the space is not occupied if a particle moves there. If the position is occupied then it stays in its current position.

Finally, we added a component to our program that attempts to simulate the effects of gravity on a particle system. At a basic level, the gravity function calculates a variable probability of moving vertically on the basis of the particle's height in the lattice. The gravity function calculates a random number and then uses this random number to determine whether or not the particle will move left, right or remain in the same position. However, the function checks to ensure that no other particle is located in the same location in order to preserve the principle of excluded volume. Adding to the program, the gravity function then determines independently of the horizontal motion whether or not the particle will move up or down. Based on the height of the particle, the probability of moving up or down changes due to gravity. The algorithm to determine whether or not the particle moves up or down is as follows: If the random number is less than $.5+.5(y/H)$, the particle moves down. As a result, the higher the particle goes, the greater the probability that the particle will move down. For example, at the top of the lattice, the probability of the particle moving down will be one, whereas at the bottom of the lattice, the probability of moving up will be approximately one half. Due to the multiplication by .5, the algorithm maximizes at the top and does not allow the deciding comparison to be greater than one. After factoring in the effect of gravity, the function again checks to ensure that no particle exists above or below the particle. After the particles are moved vertically in the lattice, the function calculates the density and returns the density at each height level of the lattice. As a result, the gravity function combines excluded volume with the effects of gravity in order to return the density of particles at the bottom of the lattice.

Our use of FORTRAN is justified because of the relative ease with which it performs large calculations. The program itself, after its invention in the 1950s by an IBM team, was recognized for its ability to simplify calculations while not requiring the user to have an extensive background in computer programming. It quickly caught on in the scientific community, and was used in controlling nuclear reactors along with other great engineering feats. Its two major versions include FORTRAN 77 and FORTRAN 90, the latter of which is employed in this program. [6]

RESULTS AND ANALYSIS

The results we obtained from our computer simulations paralleled our theoretical predictions. The graph of lambda versus the density at the wall for an ideal gas system resulted in ten linear series of points (Figure 1). The lines that represent the higher densities have steeper slopes. λ itself is a constant that regulates the probability that a particle visibly appear to strike the wall based on its kinetic energy. In the case of our program, we use a randomly generated number to model the particles' behavior. It represents the kinetic energy of an individual particle and thus determines whether it will be seen striking the wall. As explained earlier, if we were to take snapshots of the system using time-lapse photography, faster particles would be seen at the wall much less frequently than slower-moving particles, which would appear to be at the wall for extended time intervals. Therefore this number provides a way to designate how different particles will interact with the wall. If the number is less than λ, the particle is allowed to strike the wall. Otherwise, it does not move. As λ increases, the probability that the random number will be less than λ increases, and so, the ρw will increase as well.

The graph of λ versus ρw for an excluded volume system also produces expected results (Figure 2). This is a system in which only one particle can occupy a single space at any given instant, more accurately modeling a real system where particles have a finite volume and do interact with one another. In this case, the lines are not linear, but reach an asymptote as the spaces at the wall are filled and no new particles can enter. In the ideal gas system, potentially all of the particles in the system can be at the wall, because multiple particles can occupy a single space. However, this is not possible in the excluded volume system, and thus the lines curve toward an asymptote as the spaces at the wall are filled.
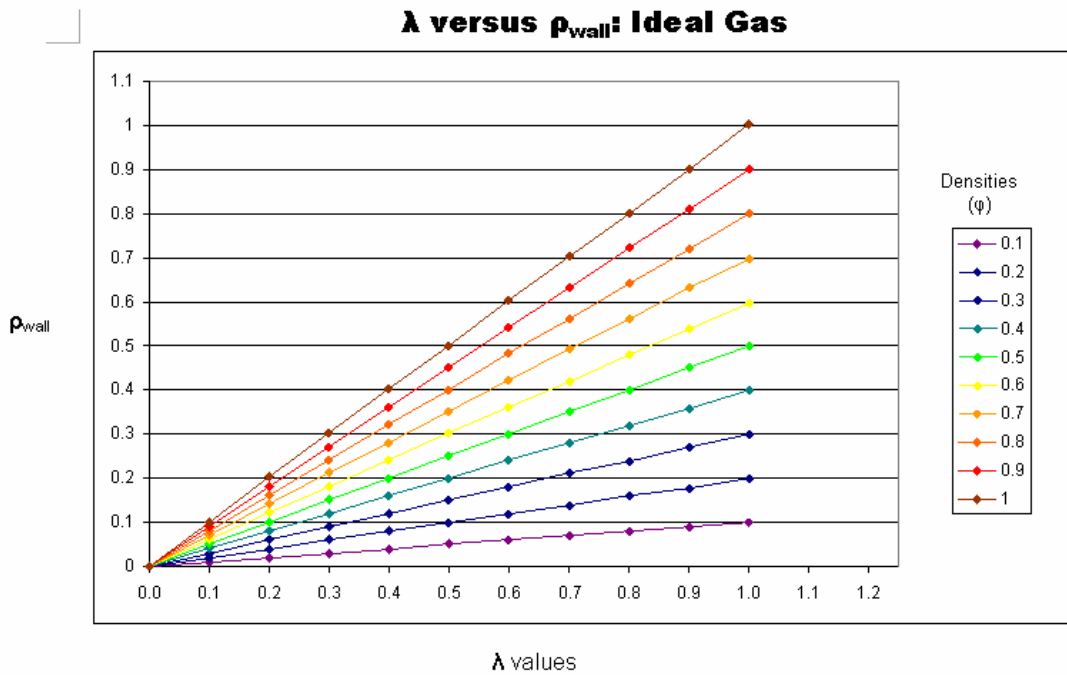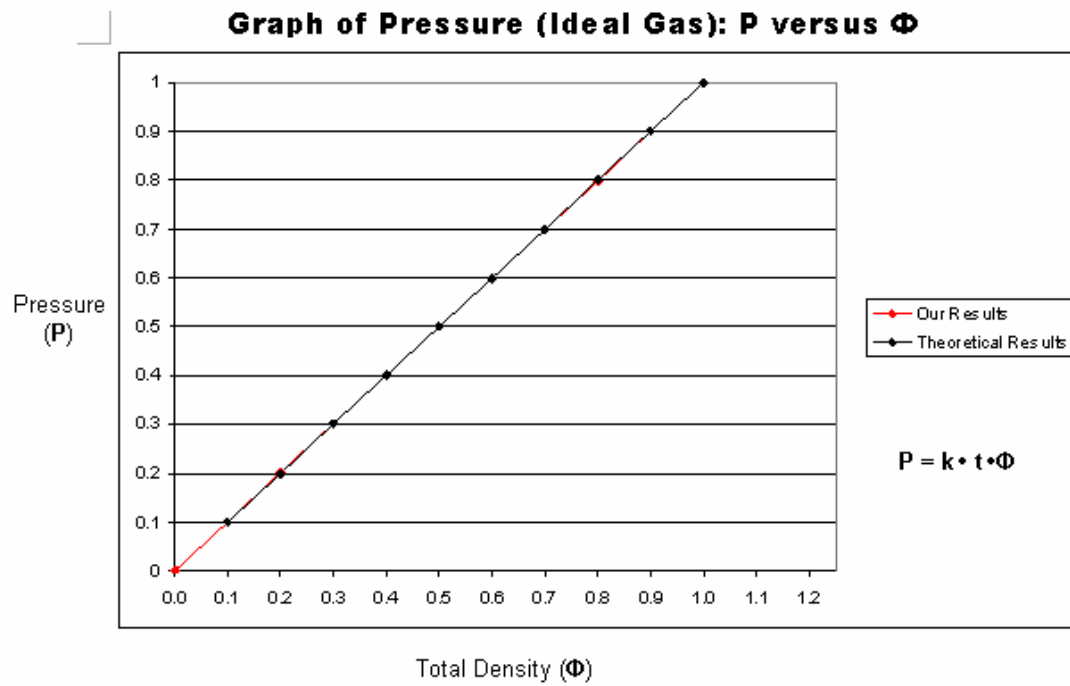

Figure 1. λ vs. ρ_{wall} for an Ideal Gas System
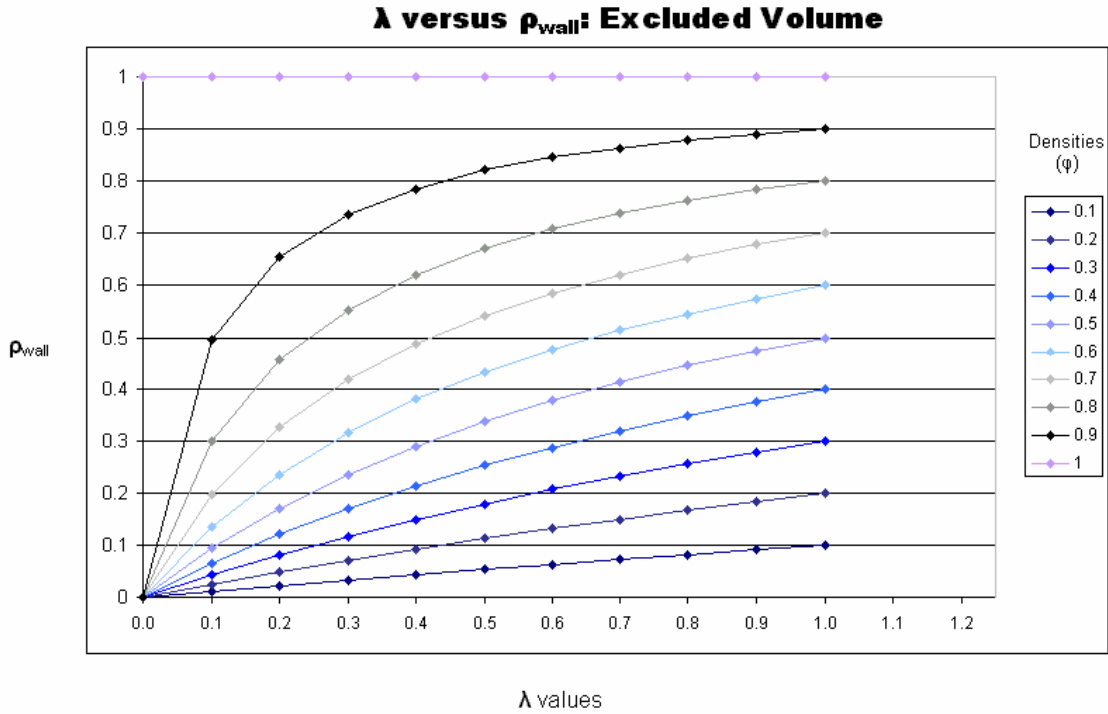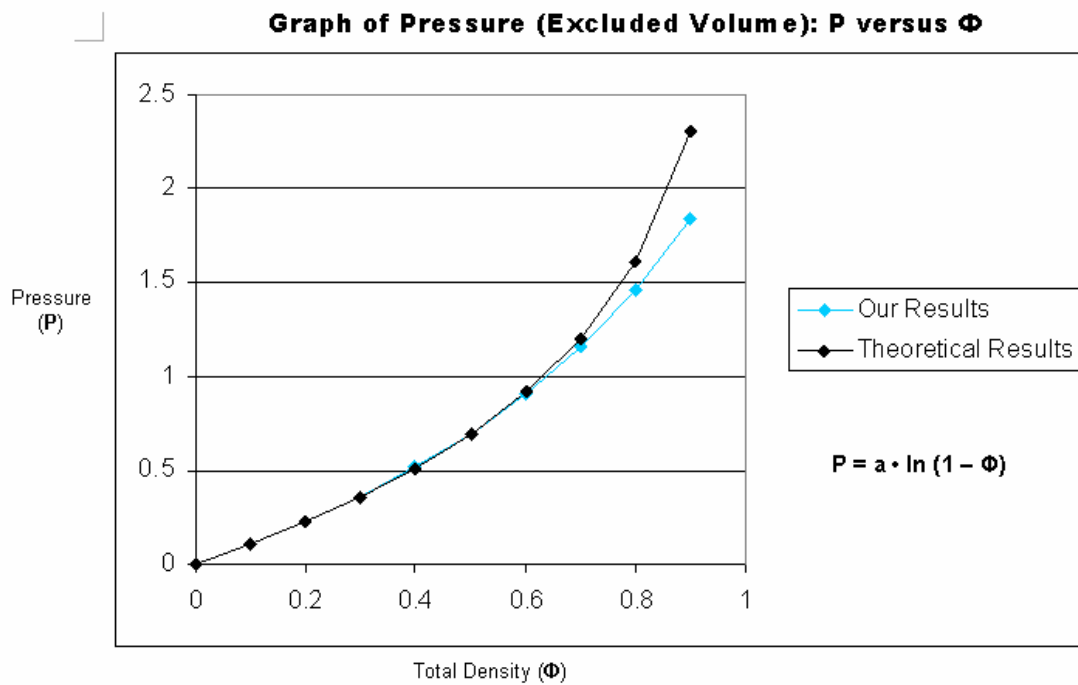
Figure 2. λ vs. ρ_{wall} for an Excluded Volume System

To obtain a graph of the P vs ϕ, all the equations for the ρ_w vs λ curves were calculated. These equations representing ρ_w vs λ were subsequently integrated with respect to lambda in equation 23 in order to calculate the pressure at the wall. This yields the equation of P as a function of Φ, the total system density. The actual formula for this equation is $P = kT\Phi$, where k is a constant and T is temperature. However, in our program kT is set equal to *1*. Each line in the ideal movement graph represents a different system density, and so each line yields one value for P. When this process is repeated for every system density from *0* to *1*, all of the generated P values from each integral are plotted as a graph of P with respect to Φ. For the ideal gas, the graph is a straight line, as the pressure at the wall may steadily increase ad infinitum. This is because there is no limit to the number of particles that can be found at the wall (Figure 3).

The process by which pressure was calculated for an excluded volume system is basically the same as it was for an ideal gas. However, since the graphs for the excluded volume movement were not linear, the pressure equations are at a higher power than they were for ideal movement. The equation for pressure is still equation 23. However, the theoretical value for excluded volume is *P=kTln(1- Φ)*, where *kT* is once again set to equal *1* for the purposes of simplifying our program. When the system densities are substituted into their respective pressure equations and a graph is formed, the graph increases toward an asymptote (Figure 4). Obviously, this is due to the growing lack of space at the wall as it is gradually filled by particles. Therefore, pressure will max out once the spaces are filled.

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**Figure 3. Pressure versus Total Density for an Ideal Gas System**

Figure 4. Pressure versus Total Density for an Excluded Volume System

Comparing our results to a Molecular Dynamics (MD) simulation, we found that our random walk method, a relatively simple program which moves particles on the sole basis of probability, exhibits similar results. Our program is efficient in measuring particle behavior as it draws similar results to the MD simulation while using only a fraction of its system resources and running time. This can be seen by comparing two snapshots of the simulation with just the excluded volume in effect. Figure 5 is a snapshot of the full blown MD simulation, Figure 6 is the snapshot produced by our Monte Carlo simulations. As you can see, the snapshots are indistinguishable. Both were produced using a visual basic program which we constructed to create a visual representation of the particle movements

The MD simulation is 300 pages long, and takes into account the laws of physics, including Newton's laws of motion and particle interactions. It uses actual formulas in place of estimations and probability. It also treats particles not as point particles, but as actual particles with volume and mass. The particles operate on a continuous system, unlimited by a lattice framework of coordinate points. Needless to say, this program is much more complex, as it factors in many more parameters in its calculations creating the most accurate simulation possible.
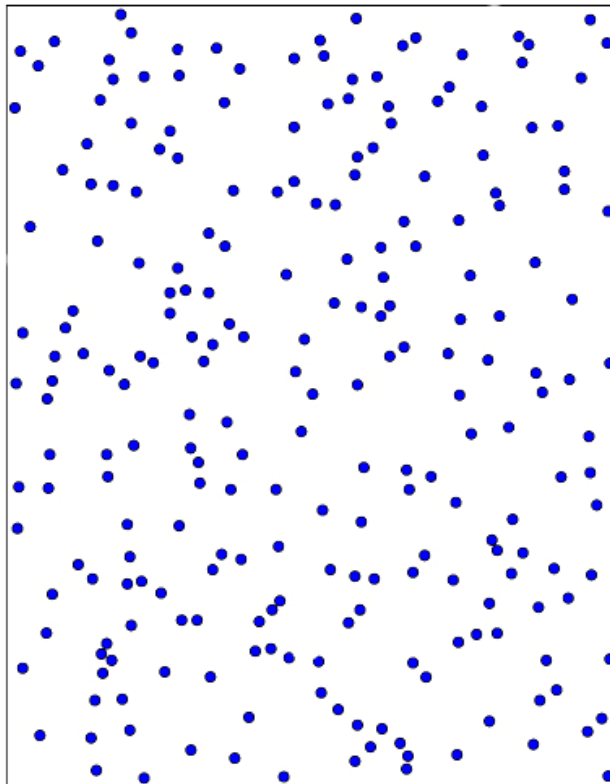

Figure 5. Snapshot of particles with the excluded volume principle created with a complex MD simulation.
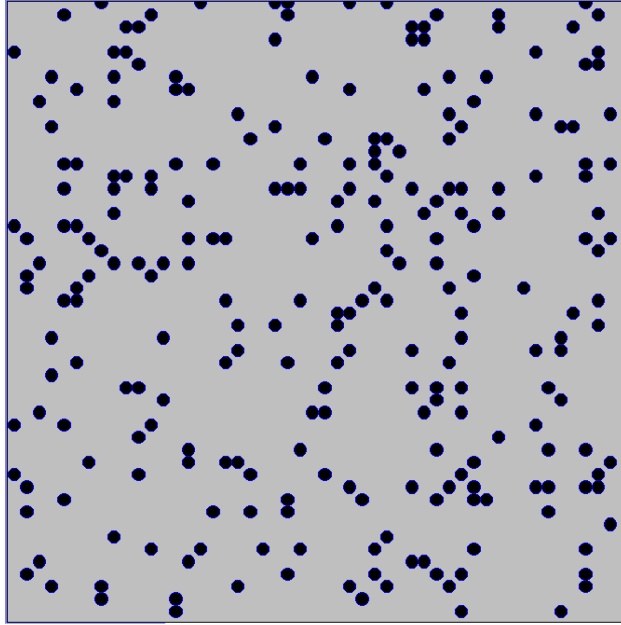
Figure 6. Snapshot of particles with the excluded volume principle created with our Monte Carlo Simulation.

In order to compare the two programs, we graphed density versus vertical position plots indicating the densities in increments based on height (Figures 7, 8). We also have snap shots of both systems created by the Visual Basic program. Figure 9 is a snapshot of the particles created with the complex program, Figure 10 is a snapshot of the Monte Carlo system. Both graphs indicated that the density increases exponentially towards the bottom of the container. The two graphs are very similar. Indeed, it is even that, the two data sets differ only in miniscule detail.
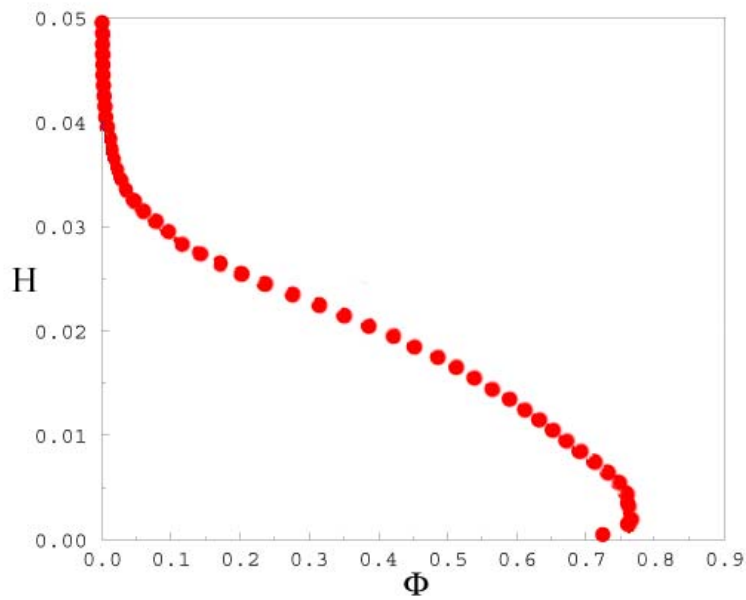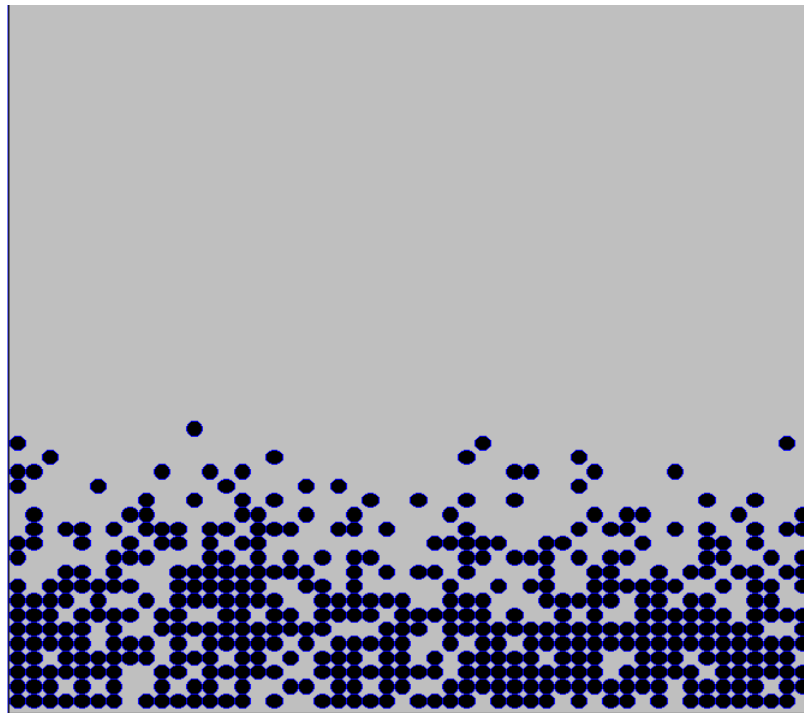
Figure 7. Total Density versus vertical position using the complex MD simulation program
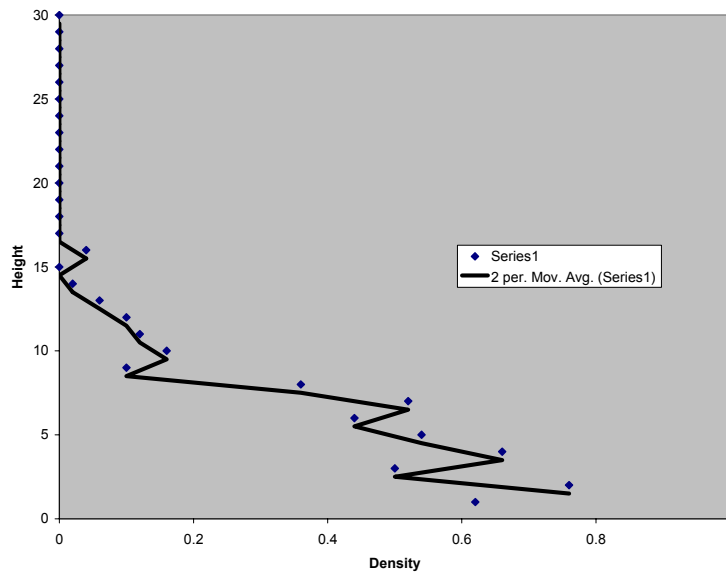
Figure 8. Total Density versus vertical position as produced by our Monte Carlo Simulation Program
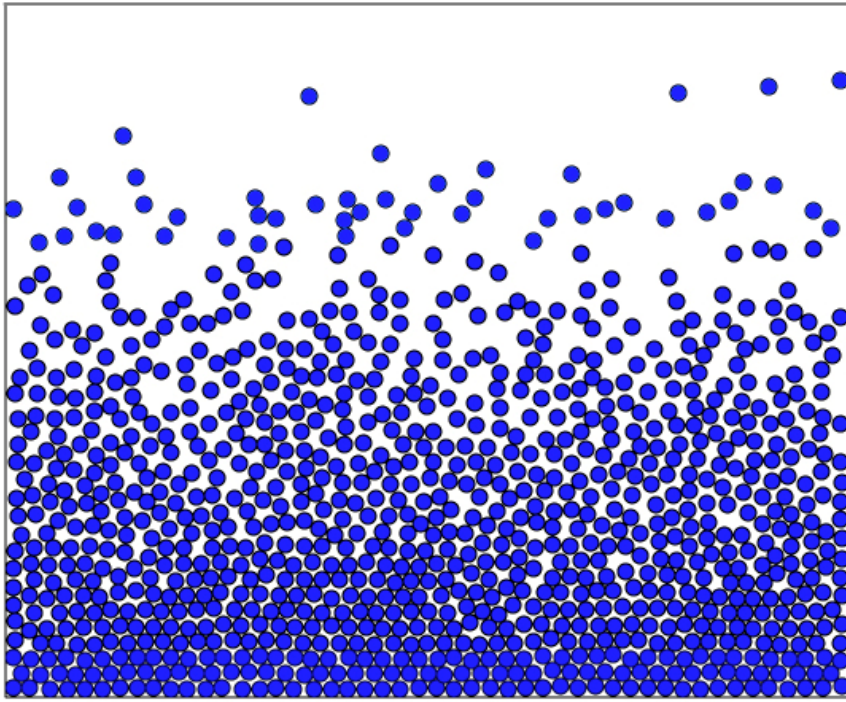
Figure 9. Snapshot of a gravity simulation produced by a complex MD simulation

Figure 10. Snapshot of a gravity simulation produced by our Monte Carlo simulation.

CONCLUSIONS

In conclusion, our simulations demonstrate that a simple program written using the "random-walk" Monte Carlo method and a lattice framework can model the behavior of various types of particle interactions, including particles in ideal gas, excluded volume, and gravity scenarios. Graphs of λ vs. ρ_w matched the theoretical predictions almost exactly for both the ideal gas (a linear graph) and the excluded volume (a logarithmic curve). The movements of the particles in the simple program which are defined by the "random-walk" method show a strong correlation to the movements of the particles in a Molecular Dynamics simulation which are defined by many parameters including energy, friction, and Newton's Laws of Motion for both the excluded volume and the gravity scenarios.

These results show that granular systems can be simulated accurately through probabilistic means. This validates using a simpler and less time-consuming Monte Carlo-type process over a complex Molecular Dynamics simulation in representing the behavior of granular particles, suggesting further extensions to the description of granular systems in general.

FUTURE DIRECTIONS

Other factors can be added and tested by our particle system simulation. One of these factors is known as the Yukawa Potential, which states that in a system of particles with charge and spherical symmetry, a particle will have a movement bias toward the other particles with the greatest potential energy relative to itself. This potential energy is based on the charge of the particles and the distances between them.

The potential can be quantified by the equation,

$$U = b^2 \frac{e^{-r/R}}{r}$$

where U is the potential energy between two particles, b is a constant representing the coupling strength of the particles, R equals Planck's constant divided by the quantity $2\pi mc$, and r is the distance between two particles. This equation is calculated between one particle and every other particle in the system. The particle for which U is highest is the one that the particle moves toward.

Attempts to program the Yukawa potential into the simulation have led to some changes in the Yukawa formulae due to the need to be able to feasibly perform the many calculations required for the potential to work. The aspect of charge has been removed from the program due to its potential to work. The aspect of charge has been removed from the program due to its excessive complexity, leaving only the distance between particles as the variable in our simulation. The coupling constant and R have been set to 1 for the same reason. A simplified constant λ_1 which equals $e^{-1/r}$ has been created. A random number is

then compared to λ_1. If the number is less than λ_1, it moves randomly, otherwise, it moves toward a bias. λ_1 itself is separated into two constants, λ_x and λ_y where

$$\lambda_x = \lambda \left(\frac{x}{\sqrt{x^2 + y^2}}\right)$$

$$\lambda_y = \lambda \left(\frac{y}{\sqrt{x^2 + y^2}}\right)$$

All of the λ_x's and λ_y's are summed up, and compared to each other. Whichever is the greatest becomes the direction in which the particle moves. If λ_x is negative and greater than λ_y, the particle will move to the left. If it is positive, the particle moves to the right. Similarly, if λ_y is negative and greater than λ_x, the particle moves down. If it is positive, the particle moves up. Thus, the rigorous calculations required to implement the full Yukawa potential have been simplified in order to add yet another testable factor into the particle simulation.

The work we have established here can in the future have direct applications as well. Familiarity of the behavior of particle systems, particularly granular systems, has potential application in fields as diverse as manufacturing and earthquake prediction. Industries involving the handling of granular systems comprise over one trillion dollars each year in the United States economy. Yet research concludes that on average, these industries are only operating at 63% capacity. Industries that involve granular particles include agriculture and the manufacturing of fertilizer, soil, and salt. Accurate models detailing granular behavior would help these companies become more efficient in the handling, processing and packaging of materials. [7]

Pharmaceutical companies also deal extensively with granular particles, such as the powdered form of many drugs before processing. The increased development of pharmaceuticals in the economy today also emphasizes the need for simple, accurate ways of analyzing granular movement. The growing importance of industries that depend on granular analysis will create a need for technology and research in this field. [8]

NASA itself has stepped up its research on granular systems. Granular materials that are found on lunar and Martian soil could potentially be used for research and construction projects [9]. In a separate field of rocket technology, NASA is concerned with fine airborne particles in their rockets. In such an enclosed space, even the smallest particles can accumulate and eventually cause damage to astronaut habitats and water and gas recovery systems [10].

Finally, a highly significant application of granular systems is that it could provide a more complete understanding of natural phenomena such as earthquakes and avalanches. An earthquake is essentially a large granular system, and can be broken down into individual granular models of dirt and debris particles. Eventually, we may be able to predict the action of these particles so accurately that we would foresee not only the time and duration of earthquakes, but information involving fault lines and ground movements

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as well.

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