Computer Simulation of Granular Materials

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Granular materials (or powders) are a special class of matter. They’re not solid, liquid, or gas, yet they behave like any of these states under the proper conditions: they assume a solid state when they reach a certain volume fraction of their constituent particles (the so-called jammed state), can flow like liquid at lower volume fractions or when sheared, or even exhibit the properties of a gas in a highly fluidized bed or when their container is strongly shaken. Jamming occurs when an amorphous collection of particles spontaneously develops rigidity and supports weight like a solid instead of flowing like a liquid. The transition takes place without static spatial ordering but is accompanied by long-range dynamical correlations arising from the collective motion of groups of particles.

The science of granular matter has a long history, with the original classical contributions made by Faraday and Osborne Reynolds. More recently, the topic has attracted condensed-matter physicists and other scientists, as well as engineers, who study complex systems and consider granular matter as a model of more complex materials. As such, granular materials have typically been studied either at the structural (grain) scale or as a continuous medium that exhibits bulk properties. The goal in such studies has always been to bridge the two views, to explain the relationships between such materials’ structures and properties on behaviors.

To fully understand and characterize granular packing at either the macro- or microscale, we must have an accurate picture of their structure. To this end, we aim to obtain detailed information about the shapes, positions, and contact points of all the grains in a packing. However, this ambitious goal presents a considerable technical challenge that John D. Bernal and later David Scott undertook by first measuring the geometrical structure of a packing of grains and then calculating their coordination numbers (that is, the number of particles that each grain touches in the packing). They analyzed the simplest granular packing consisting of mono-sized spheres, which can realistically model such systems as powders. Although Bernal and Scott pioneered this field, their manual grain-by-grain approach is limited to small populations (less than 1,000) and, hence, very limited.

Predicting the physical properties of random packing of spherical particles from their structures isn’t easy. The difficulty is due to the disorder or randomness in the structure. For random close packing (RCP) of spheres, the volume fraction, $\phi_{\text{RCP}} \simeq 0.64$, is a reproducible quantity in experiment, which has raised the hope of describing such a material mathematically. Deriving analytical results, however, is very challenging for packings that contain more than three particles. Although the statistical mechanics approach can provide the global properties of a system of particles, when attempting to solve a given problem in a granular packing with realistic parameters (such as friction between the particles, grain deformation, and so on), the approach might not yield exact analytical results. As a result, computer simulations and experiments remain the only feasible and practical means of probing such systems for detailed quantitative analysis. In this article, I describe some of the most prominent simulation and analysis techniques in detail. I also provide a brief account of experiments and their results in granular dynamics.

Simulation Methods

We can simulate a granular packing by either creating all the system’s possible states—via Monte Carlo (MC) simulation—or by calculating the forces that each particle experiences in the packing and then integrating the equation of motion to obtain the new positions of the particles via the molecular dynamics (MD) simulation approach. Let’s review the most prominent simulation techniques used in the field of granular matter, which are often classified as either sequential or concurrent.
In sequential methods, the system has a small seed of fixed particles as its starting configuration. Then, in several steps, the simulation algorithm adds particles according to a placement rule. In 2D, a surface coverage ratio of 0.547 results from the addition of random disks to a substrate such that the disks don’t overlap. In 3D, a volume fraction of 0.385 can be achieved for spherical particles. A major setback here is that the addition of new spheres becomes increasingly difficult as their number increases.

Charles Bennett developed a mathematically well-defined sequential method for preparing hard-sphere packings on a computer. His algorithm generates a suitable 3D seed cluster on which spheres are added one by one; each next sphere is placed in hard contact with three spheres below it. We can achieve volume fractions between 0.60 and 0.63 and an average coordination number of 6.0 by using this algorithm.

Einar Hinrichsen and his colleagues used a random sequential addition (RSA) algorithm, combined with a growth method, to generate a packing of 2D disks in a plane. Each step divides the plane according to the Voronoi-Dirichile division of space. In this division, random Poisson points are distributed in the plane, and a convex hull process constructs a polygon around each point such that every point within the polygon is closer to its Poisson point than to any other Poisson point. The RSA algorithm then moves each disk in its Voronoi polygon to the center of the largest inscribed circle in the polygon and then increases the disk radius until the first two disks make contact. This process is repeated until no disk can be grown further in size. We can obtain a volume fraction of 0.772 and an average coordination number of 3.0 by using this method in 2D.

In concurrent methods, the entire set of particles is present from the start of the simulation. Various simulation methods use the concurrent technique, the most prominent of which are MD, overlap elimination, energy minimization, and the contact network.

Static Simulations
We can consider a static granular packing as a random packing of its constituent grains. Static in this context means that the granular packing is in equilibrium under the weight of the grains for the given boundary condition—in other words, all the forces are in balance, and the system is stationary. We can simulate static granular piles by using both the MC and MD methods. Although the MD method is more suitable for the study of time-dependent phenomena, researchers often use the MC method to simulate events that take too long for the MD to reach.

An MC simulation creates a system of \(N\) particles; it generates a particle configuration by successive random particle displacement. The particles interact through a potential. The probability of accepting a configuration of the particles is such that the accepted configurations explore asymptotically the configuration space according to an equilibrium probability density. The newly generated states with a lower energy have a higher probability of being accepted according to the Boltzmann distribution. If there are \(g(E)dE\) states with energy between \(E\) and \(E + dE\), then the Boltzmann distribution predicts a probability distribution for the energy as follows:

\[
p(E)dE = \frac{g(E)e^{-\beta E}}{\int g(E')e^{-\beta E'}dE'}dE , \tag{1}
\]

where \(g(E)\) is the density of states, and the integration is over all the possible states in the configuration space that the granular system can occupy.

The MD method follows one sample of a microcanonical ensemble in time. For a system of \(N\) particles, the method calculates the forces and torques that each particle experiences and then uses them to solve Newton’s equations of motion. The solutions to these equations explore the phase space along a surface of constant energy. MD simulations can use either hard or soft particles to produce a packing, by either increasing the density or through particle growth mechanisms. A simple algorithm responsible for the input to MD simulations places \(N\) points in a cell randomly (with a uniform distribution) with periodic boundary conditions and gives them velocity before growing them in size with time at an equal rate. As the particles grow, the available free space to move becomes smaller and, thus, the particles increasingly collide with each other. The process continues until the rate of collisions diverges (and becomes very large). The packing fraction achieved in this method depends on the constant growth rate, \(a_0\). In 2D, for example, a growth rate of \(a_0 = 10^{-3}\) results in volume fraction \(\Phi = 0.895\), whereas \(a_0 = 10^3\) results in \(\Phi = 0.852\). For spheres in 3D, a growth rate of \(a_0 = 1.0\) yields \(\Phi = 0.637\). In 1D, the particles pack with long-range order, whereas in 2D, the packing diversity increases but the packing itself is still well ordered. In 3D, however, the order is replaced with random packing.

Mechanical Contraction
Stephen Williams and Albert Philipse developed a general algorithm for creating RCP for arbitrary particle shapes. Their general idea is
that a random packing is formed by rapidly quenching (cooling) the system to force the particles into permanent positions before they get into a thermodynamically more preferable phase.

Suppose our initial conditions are a cubic cell with periodic boundary conditions in which we create a dilute fluid at equilibrium via the standard MC technique. To ensure a rapid quenching, we must follow two steps and repeat them until we reach a termination condition. In the first step, we reduce a cubic cell’s volume by a small amount and scale the particles’ positions by a factor \( s \). A particle at the corner of the cubic cell will be at the corner of the scaled cubic cell. Thus, for \( sb = b' \), the new volume \( V' = V - \Delta V = (sb)^3 \), where \( b \) is the length of the cubic cell. From this relation, we can easily calculate the scaling factor \( s \).

In the second step, the scaling of the particles’ positions leads to the possibility of their overlapping. If this happens, we move the overlapping particles outside each other in the direction in which to move these particles. We then introduce a speed \( s \) at which the total overlap is changing:

\[
s = \sum_{j=1}^{Z} \delta_j \frac{\partial k}{\partial t},
\]

where a factor \( \delta_j \) is introduced to remove particles that overlap most. The speed \( s \) is only determined by overlapping particles. We then introduce a kinetic energy-type constraint on the velocity of particle \( i \):

\[
a_i^2 + a_j^2 + a_k^2 = 1.
\]

Using the Lagrange multipliers, we can calculate the velocity’s direction as follows:

\[
a_u = \sum_{j=1}^{Z} \delta_j \frac{\partial k^u}{\partial t}.
\]

Having obtained the velocity’s direction and the distance between the particles, we repeat the calculation for all the particles and update their positions at the same time. This process repeats for a large number of steps. If, at the end, all the particles aren’t overlapping, we contract the volume as in the first step. If we still have overlapping particles, the system has reached its densest state, so we determine the volume fraction for the previous non-overlap state. The highest volume fraction we can obtain for random sphere packing by using this method is \( \Phi = 0.631 \).

The number of particles that can be included in static simulations of granular materials is a problem for all the simulation methods described so far. Most experimental systems contain more than \( 10^5 \) particles, and the computation time for simulating such large systems is itself too large.

Tomaso Aste and his colleagues performed an extensive series of experiments on static random packing of equal-sized spheres. They used a series of geometrical and topological tools to deduce the granular material’s properties. Such tools are now widely used in simulations and experimental studies to explore a granular packing’s geometry and topology. Table 1 describes the characteristics of the packings they investigated. The researchers used X-ray computed tomography (CT), which generates a 3D image of the system, to probe the packing’s internal 3D structure. Reconstructing the 3D representative of a sample requires three basic steps:

- Capture images (2D projections) of the sample at several known angles.
- Filter the images (also known as pre-processing) to remove artifacts.
- Back-project the filtered images using some known reconstruction algorithm.

Each of these steps is computationally intensive and requires a huge amount of memory and computer resources.

### Structural Analysis

Next, let’s examine some of the tools used for the basic structural analysis of packings of particles. For the pur-
pose of demonstration, we’ll use some of the experimental datasets (bead-A, bead-B, bead-C, and bead-D in Table 1) that Aste and his colleagues used as model sphere packing systems.

**Radial Distribution Function**

A central quantity in the studies of atomic structures, fluids, and porous media is the radial distribution function (also known as the pair correlation function or the two-point correlation function). This quantity determines the average density within a radial distance relative to any point in the structure.3,14 We can formulate the radial distribution function as follows:

$$g(r) = \frac{1}{V} \int_I I'(x) I'(x + r) dx,$$

where indices $i$ and $j$ represent two arbitrary points (particles) within the structure, $r$ is the distance between (the centers of) the two particles, and $I(x) = 1$ if the spatial coordinate $x$ coincides with a particle within the structure, and zero otherwise. Clearly, $g(r)$ should approach 1 for large $r$, and at very short $r$, it must be zero because two particles can’t occupy the same space. However, for statistically homogeneous media composed of different phases, the two-point correlation function can also be interpreted as the probability of finding the two ends of a line segment with length $r$ within the phase of study.15

The correlation function provides a measure of how the endpoints of the line segments in a particular phase are correlated. For isotropic media, the correlation function attains its maximum value of $\Phi$ (which is the volume fraction of the particular phase for which the correlation function is computed) at $r = 0$, followed by an exponential decay16 to its asymptotic value of $\Phi^2$. Figure 1 displays the correlation function of the bead packs for which Aste and his colleagues performed calculations on the beads’ centers using the following formula:16

$$n_i(r_i) - n_j(r_j) = \int_{r_0}^{r_1} g(r) 4\pi r^2 dr,$$

where $n_i(r)$ is the average number of spheres’ centers within a radial distance $r$ from a given sphere center.

A pronounced peak is seen at $r = d$, which corresponds to the neighbors in contact. Then, the probability of finding neighbors decreases with $r$, reaching a minimum at around $1.4d$. Subsequently, at larger radial distances, the probability increases again, forming two peaks at $r = \sqrt{3}d$ and $r \geq 2d$. Beyond the two peaks, it continues to fluctuate with decreasing amplitudes. The details of the second and third peaks, plotted in Figure 1a, show that the two peaks at $r = \sqrt{3}d$ and $r \geq 2d$ both increase in height with the packing density, with the peak at $r = 2d$ growing faster than the one at $r = \sqrt{3}d$ (see Figure 1b).

**Coordination Number**

One of the most interesting parameters in the literature of granular packs is the average number of spheres in contact with each sphere.2,3 We can deduce an exact computation of the number of touching spheres only from the geometry of granular packings with infinite resolution, where we can identify the contact points with infinite precision. This is achievable, to a good approximation, from the simulation, but in experimental studies, many sources of error prevent an accurate measurement, which is why accurate simulations are so important. In tomography, the main limiting factor is image resolution. X-ray diffraction from the edges of grains also results in unclear grain–grain contacts.

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**Figure 1.** Correlation function. (a) Normalized radial distribution function of the experimental data provided in Table 1; the inset shows the ratio between the value of the peak at $2d$ and $\sqrt{3}d$. (b) The detail of the two peaks, respectively, at $\sqrt{2}d$ and $2d$ vertical lines.
Aste and his colleagues devised a deconvolution method based on the radial distance between the bead centers to determine each sphere’s average number of touching neighbors. This method essentially deconvolutes the contribution of touching neighbors from the contribution of nearest neighbors in images obtained from experiments. We can also base the calculation of the coordination number directly on the geometry of the grains obtained from their tomogram. The latter method is less sensitive to the precision of grain center coordinates and polydispersity than the deconvolution method described earlier, but it has the advantage of giving local information about the coordination number of each bead in the pack. However, its precision is limited by voxel resolution in the CT image. Figure 2 shows the average coordination number of all the samples presented in Table 1.

**Contact Network Analysis**

Figure 3a shows a network of touching beads within sample bead-E, and Figure 3b shows the contact network of the reconstructed subsection of sample bead-C. We can explore such networks for footprints of anisotropy (the preferred directions that the network of touching spheres eventually forms). Any grain- or large-scale order can introduce correlation in the contact network. A simple way to test the contact network of grain packs for such correlations is by comparing the network with an uncorrelated contact network model.

We can develop a model for a network of uncorrelated contacts based on the fact that the grains touch one another with equal probability at random positions on the grains’ surfaces. If $P$ is the probability of finding a connection within the solid angle $\Omega$, the probability of finding a network of $n$ uncorrelated connected links is $P_n = P^{n-1}$, where $P = \Omega/\pi$. Consequently, the average chain length is

$$\pi = \frac{\sum n P^{n-1}}{\sum P^{n-1}} = \frac{1}{1-P},$$

and we can also derive $\pi^2$ similarly:

$$\pi^2 = \frac{\sum n^2 P^{n-1}}{\sum P^{n-1}} = \frac{1 + P}{(1-P)^2}.$$ (9)

Note that in this model, the chain length is dependent only on $P$ or $\Omega$.

With the position of grain centers and contact points on the bead surfaces, we can then identify the link with touching beads. The search for such links should be done between grains touching in all directions; these directions are based on the discretization of a unit sphere’s surface (see Figure 3c). Each line segment connecting a unit sphere’s center to the points on the surface of the sphere in Figure 3c represents a direction. At any direction, we can do the search at a variety of solid angles—in other words, for a given direction, we form a solid angle from the bead’s center with its central axis aligned with that particular direction. Once we find a link within a solid angle, we’ve found a chain of links with length 2. Repeating this process for all touching grains within that solid angle leads us to finding the chain of touching grains for a given solid angle and direction.

Figure 4a compares the uncorrelated model with sample bead-E. The plots imply a small degree of correlation within bead pack bead-E, which we can best view by choosing the direction on the unit sphere in a particular order. Note that $\theta = 0^\circ, 180^\circ$ is the direction of gravity. The plot indicates a small difference induced by gravity within a packing of hard spheres.

**Dynamics Simulations: Compacting Granular Media**

It’s possible to numerically simulate the flow of granular materials by using disk or spherical particles—specifically, we can apply different contact models between particles to obtain the dynamic interaction between the stress and strain rate. The seminal work of Heinrich Hertz on elastic spheres is one of the earliest contributions to this complex subject. A summary of theo-
retical development for idealized cases appears elsewhere. All the theories pursue a key question: do characteristics of the contact model affect a granular material’s bulk behavior?

Surprisingly, not much has been reported in simulations (or experiments) about this issue. In an attempt to address this question, B.K. Mishra and C.V. Murty compared the results between a linear and a nonlinear contact model applied to a ball mill. They found that if they chose parameters in the linear model by minimizing the difference between the contact forces over the entire duration of impact, the power requirement that the two models predicted for the ball mill would almost be the same.

One of the most widely used grain–grain interaction models is the linear spring-dashpot model with a frictional limit in the tangential direction. Essentially, it solves the equations of motion for the trajectory, spin, and orientation of every particle and the confining system’s boundary. For simulation purposes, the model considers a simple general contact law with a parallel spring and dashpot element. The spring element can be either linear or Hertz nonlinear, and the dampening part can take on a linear or nonlinear form as well. Figure 5 shows the conventionally used spring-dashpot model for approximating the collision of grains.
The normal force $F_n = -K_n \Delta x + C_n \nu_n$ comprises a linear spring to provide the repulsive force, whereas a dashpot dissipates a proportion of the relative kinetic energy. The particles are also allowed to overlap by the stiffness $K_n$ of the spring in the normal direction. We choose the normal dampening coefficient $C_n$ according to the coefficient of restitution. The tangential force is

$$F_t = \min(\mu F_n, K_t \int \nu_i \cdot d_i + C_t \nu_i),$$

where the vector $F_i$ and velocity $\nu_i$ are defined in the plane tangent to the surface at the contact point. The integral represents an incremental spring that stores energy from the relative tangential motion, which is the elastic tangential deformation of the contacting surfaces. Depending on the contact’s history, it’s possible for the spring to load in one direction and simultaneously unload in the orthogonal direction. The total tangential force is restricted by the Coulomb frictional limit at which point the surface contact shears, and the particles begin to slide over each other.

Jil Shunying and her colleagues performed extensive spring-dashpot simulations with one linear and two nonlinear dampening choices. They concluded that contact mechanics plays an important role at the binary collision level, both quantitatively and qualitatively, but that the linear contact model is sufficient to qualitatively describe the bulk behavior of granular materials.

Hernan Makse and his colleagues studied nonlinear elastic properties of granular packing by direct measurement of force transmissions in granular matter. Previous studies indicated that for forces greater than the average value, the distribution of intergrain contact forces is exponential. In addition, photelastic visualization experiments and simulations have shown that the contact forces are strongly localized along the force chains that carry most of the applied stress. The existence of force chains and exponential force distributions are thought to be closely related, but Makse and his colleagues concluded that when the stress (pressure) is increased, to the point of increasing significantly the number of contacts from its initial critical value of $Z_c$ ($Z_c = 4$ for frictional and $Z_c = 6$ for frictionless grains). The distribution of forces crosses over to a Gaussian, and the system becomes elastic and homogeneous down to a scale comparable to the grain size. Their simulations also indicate that the crossover is associated with a loss of localization and an ensuing homogenization of the force-bearing stress paths.

Based on the numerical and experimental works mentioned here, it’s safe to make the following general statement about the probability distribution of forces $P(f)$ within a granular pile:

$$P(f) \propto \begin{cases} \left(\frac{f}{\bar{f}}\right)^\alpha & \text{for } f < \bar{f} \\ \exp(-\beta f / \bar{f}) & \text{for } f > \bar{f} \end{cases},$$

where both $\alpha$ and $\beta$ are fitting parameters.

Despite all the numerical efforts and the statistical modeling studies, very few experiments have determined the status of the stress distribution in a pile of compressed granular packing. Previous experiments in 3D assemblies have confined themselves to measurements of the probability distribution of the forces exerted at the boundaries shared with the container, thus reducing the problem’s dimensionality. These measurements provide a quantitative understanding of the inhomogeneity of stress transmission within the bulk. However, these methods don’t have access to the spatial arrangement of the contact force network or other structural features, such as the force chains and arching, which have been postulated as signature of jamming.

In an attempt to understand how stress is distributed in three dimensions in a compressed granular packing, I’ve worked with other researchers on a series of experiments with deformable mono-sized spherical elastic rubble balls. We used X-ray microtomography for 3D imaging at different stages of compression. Using image analysis techniques, it’s possible to track individual grains/contacts and their deformation as the grains move in response to the external load. We can also resolve grain positions, shapes, and contact areas (see Figure 6), which is proportional to the force transmitted between the touching grains. This provides a powerful tool for characterizing non-affine displacements at the microscale and their role in overall mechanical behavior. Study-
ing such systems provides insight into the connection between microscopic organization and the macroscopic response of granular piles.

We can also obtain force distribution within the pile at different stages of compaction. These measurements confirm a broad exponential tail for large forces. They are, however, preliminary and require more extensive experiments and analysis.

Foams and Granular Materials

Such properties of granular materials as geometry, dilatancy, and rheology have closely equivalent counterparts in foams and bubbles. Should we regard a gas bubble as a frictionless, compressible particle? Douglas Durian and others have tried to integrate foam theory with granular and atomic systems by using a single idealized model for all three. Do foams offer any advantages to those interested in exploring generic properties of disordered systems? Perhaps—foams have relatively well-defined and understood local structure and interactions. They don’t have solid friction, although they could have other problematic effects.

For 3D foam systems, the challenge is to see and characterize the foam’s full inner structure, which isn’t immediately visible from outside. Direct measurement of the 3D structure of solid foams is now available from synchrotron imaging and X-ray CT; see Figure 7. This allows the measurement of the microstructure’s complex morphology, which greatly resembles sphere packing, as can be seen in Figure 7.

Static characterization of granular materials is relatively straightforward, although the determination of the local organization of granular packing can be difficult. The connection between the microscopic organization and macroscopic response of the granular pile is still a challenge, both computationally and experimentally.

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References

Figure 7. Direct measurement of the 3D structures. (a) The autocorrelation function of elastic balls system. Note the shift in the peaks as the pressure increases. (b) The distribution of coordination number in the same system. Grains with connectivity two and three belong to the boundary of system.