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Geometry and Statistics of Jammed Granular Matter

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GEOMETRY AND STATISTICS OF JAMMED GRANULAR MATTER

by

MARK R. KANNER

A dissertation submitted to the Graduate Faculty in Physics in partial fulfillment of the requirements for the degree of Doctor of Philosophy
The City College of the City University of New York

2015
This manuscript has been read and accepted for the Graduate Faculty in Physics in satisfaction of the dissertation requirement for the degree of Doctor of Philosophy

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THE CITY COLLEGE OF THE CITY UNIVERSITY OF NEW YORK
Abstract

Geometry and Statistics of Jammed Granular Matter

by

Mark R. Kanner

Adviser: Mark D. Shattuck

We use simulations of soft bidisperse disks to determine the properties of jammed packings and investigate the statistical mechanics of these systems. We have created a novel method for the classification of structural subunits of a packing and to calculate relevant physical quantities. The classification scheme is based on a 20 type decomposition of the Delaunay triangles extracted from the centers of the particles. Subunit frequencies are determined from geometrical properties and used to calculate the important macroscopic system quantities coordination number, packing fraction, and pressure. These relationships suggest that microscopic particle geometry plays an important role in observed macroscopic behavior. In addition, we investigate the contact network evolution during elastic perturbation. We predict the fraction of time a contact will be broken from the the inter-particle potential before perturbation. We explore the energy regions, below particle rearrangement, where our prediction is valid and discuss a physical mechanism for this behavior based on the exchange of potential and kinetic energy between particles.
Acknowledgements

I’d like to thank Mark Shattuck for his time and mentorship. Working with such an accomplished scientist was an honor, and I really grew from the experience. I’d also like to sincerely thank Corey S. O’Hern not only for his insight and guidance, but also for welcoming me into a productive collaboration with him at his lab. I’m deeply indebted to all my classmates and labmates at CUNY, the Levich Institute and at Yale, but especially Aline Hubard, ZhuSong Li, Carl Schreck, Thibault Bertrand, Manuel Mai and Kai Zhang. We all had many productive conversations, and lots of good times too! My family and friends have been incredibly understanding and patient, and I’m thankful for that. I’d also like to thank Christine for being so encouraging and supportive. The help and guidance I received made this project possible, so thanks again to everyone involved!
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Introduction

Why Study Granular Matter?

Granular materials have tremendous technological importance and numerous applications to natural systems. They also represent a serious challenge to statistical physics as an extreme example of a system far from equilibrium. A host of industrial products are principally composed of granular materials, and an even greater amount require the manipulation and processing of grains in their creation[1]. For example, plastics for injection molding and chemical compounds for pharmaceutical products all require pre-processing as granular materials. Industrial engineers have created many clever techniques and protocols to control the confounding behavior observed during granular processing[2], but a general theoretical underpinning for these phenomena is currently lacking.

What is Granular Matter?

Granular matter is composed of macroscopic particles that are large enough that thermal effects on their motion are negligible. For particles larger than about a micron, the energy for one particle to be lifted over another in a gravitational field is significantly greater than the thermal energy fluctuations. For example, the thermal energy for a $D = 1$ mm glass sphere at room temperature $T = 300$ K is $k_b T =$
$4 \times 10^{-21}$ J, but the gravitation energy $mgD \simeq 1.3 \times 10^{-8}$ J, where $k_B$ is the Boltzmann constant, $m$ is the mass, and $g$ is the gravitational constant. This expansive definition of granular matter includes many different materials. As such many natural and industrial materials are granular from powders, soils, sand, rocks[3], the rings of Saturn, to organelles inside a cell[4].

**Why is Granular Matter Interesting?**

The simple definition of a dry granular material, a collection of macroscopic particles interacting through contact forces, belies the complex and non-intuitive phenomenon that are observed. For example, in a rotating drum filled with grains both solid-like and fluid-like behaviors are observed[5]. In the drum, the surface flows like a fluid, but the rest is frozen in solid-body rotation. Tapping a collection of grains causes strongly hysteretic evolution in the packing fraction of the material. The packing fraction is the fraction of the total space taken up by the particles. For example, if grains are loosely poured into a container, then tapping will cause densification. As the strength of the tapping is increased, further densification occurs. However, if the amplitude is subsequently reduced the density will not decrease, but will continue to increase to a maximum density at zero amplitude. However, on repeated cycles of increased and decreased amplitude the density change is repeatable with increased amplitude causing lower density and decrease amplitude causing higher densities[6]. Also grains flowing through a small opening, exit at constant rate irrespective of the pressure placed on them by grains above[7]. This collection of unique phenomenon describe
observations at the macroscopic scale, but there are also microscopic peculiarities that give rise to interesting behavior.

There are two main features that contribute to the unique behavior observed in granular materials. First, interactions between particles are inelastic, and as such granular systems are highly dissipitive. Any perturbed particles will quickly lose their energy due to collisions and inter-particle friction, and they will wind-up in a static state. Constant energy injection is required to achieve steady-state dynamics. Such systems are in a non-equilibrium steady-state. Second the separation of scales between grain motion and collective motions is often small. This is in contrast to ordinary gases, liquids, and solids, in which the molecule size is generally many orders of magnitude less than the macroscopic structural features like waves.

Many successful theories from statistical and fluid mechanics appear to be applicable to granular systems, but fail to describe important observed features of granular behavior. The Navier-Stokes equations are used with great success describing fluid flows, but they fail to predict the constant flow rate with varying overburden of grains through a small opening, as well as, the tendency for grains to jam when flowing through a hopper[8]. Solid granular systems have the requisite quantities of a cannonical ensemble macrostate, but as we will further discuss in this document microstates of the ensemble are non-equiprobable[9]. Since granular systems seem so similar to ordinary systems, the last few decades have seen a significant attempt to borrow standard theories from fluid mechanics, solid mechanics and statistical
mechanics to account for granular phenomena[10]. Much work is still being done to connect microscopic observed variables such as the contact network to macroscopic properties like stress[11].

What are Granular Solids?

While granular materials can exist in both fluid-like and solid-like states, this work is primarily concerned with granular solids that are static or at most undergoing only small perturbations. These materials are collections of particles being compressed by either gravity or repulsive inter-particle contact forces. Most examples that come easily to mind: sand at the beach, a pile of rocks or even a collection of pills in a bottle all depend on several parameters like, shape, radii distribution, friction, and elasticity. In a typical reductionist approach, we select simplified parameters from these attributes that apply broadly across many systems. Many different asymmetrical and irregular grain shapes exist but even within groups of symmetrically shaped objects there are a number of different shapes, spheres, ellipsoidal particles, dimers etc [12]. Many granular solids are composed of poly-disperse disks where radii vary according to a specific distribution, but bi-disperse particles with a diameter ratio of 1:1.4 are typically studied as a proxy. The two sizes prevent the crystallization observed with mono-disperse particles, but are simpler than poly-disperse systems. Elastic constants like the Young’s modulus $E$ measure a material response to deformation, and materials like steel, rock and diamond are considered hard since they have a large $E$. The language of granular material simulation is slightly different.
Typically, hard particles refer to grains that are infinitely hard $E \rightarrow \infty$, and can not deform at all and “soft” particles refer to grains that can deform or overlap by some amount typically much less than the radii of the particle. By this definition simulated soft particles can have a hardmesses equivalent to steel ball bearings or marshmallows. In this work, we exclusively consider soft (in the simulated granular materials sense) 2D disks with bi-disperse particle radii.

**What is Jamming?**

We create granular solids by a processes known as jamming. Starting from a dilute state of point particles the density is increased by growing the particle diameter to compress the system. At low densities particles can move freely in space, hindered only by collisions and their ensuing inter-particle forces. For an increasingly compressed system there is less free space for the particles to rearrange, and finally instead of the loose, liquid like macroscopic state observed at lower densities the grains form a solid where, unless the particles are very soft, further compression fails to change the density significantly and only serves to increase inter-particle forces. Below the jamming threshold particles can always be moved to locations where there are no overlaping particles. The jamming threshold is defined by the point where growing the particle diameters any further will result in particle overlaps which cannot be removed by particle motion.

During compression, but before the density reaches the jamming threshold, the number of contacts per particle, $z$, is essentially zero since any contacting particles can
simply rearrange so that they are not in contact. As the density increases however, there is no room for rearrangement, and at a critical density, $\phi_j$ a contact network will appear and the material will become mechanically stable. For a system to be mechanically stable, there must be force and torque balance on every particle in the network and all small perturbations in the particle positions will cause a restoring force due to an increase in elastic potential energy from increased particle overlaps. For local stability in frictionless two-dimensional (2D) disks, this requires at least three contacts per particle, not all on the same side, but for global stability four contacts are needed. This can be seen by equating the number of degrees of freedom in a packing $dN$ where $d$ is the dimension of the particles and $N$ is the number of particles, with the number of constraints or force imposed by contacts, which for frictionless particle is one per contact, $Nc$. Then $Nc = 2N$ in 2D, and the number of contacts per particle $z = 2Nc/N = 4$, since each contact is between two particles. This simple argument needs to be corrected for the boundary conditions and the method of jamming. For example, in periodic boundary conditions the number of degrees of freedom $dN - d$ is reduced by $d$ due to translation invariance. For compression by diameter increase, the particle diameter is also a degree of freedom, so the total number of degrees of freedom is $dN - d + 1$. Then $z = 2d + (1 - d)/N$ or $z = 4 - 1/N$ for 2D, which reduces to the simple result of $z = 4$ for large systems.

At the jamming point a granular material becomes solid-like since any additional compression just serves to increase particle overlap. Hence this material is quite solid
under further isotropic compression. Exerting a force tangentially to the surface (i.e. shear) of a granular solid is another matter, however. Since granular solids are held together through repulsive forces, shear will cause grains to move and slide[13].

**How Do Jammed Granular Solids Differ?**

In the micro-canonical ensemble of statistical mechanics, the state of a system depends on the number of particles, \( N \), the volume, \( V \), and the energy, \( E \). Mechanically stable packings can be described by the same ensemble variables (\( N \), \( V \), and \( E \)). While the similarities are promising, two important differences exist that prevent a direct translation. First, in ordinary thermodynamic systems, all microstates are equally probable. Microstates are states with the same \( N \pm \Delta N/2 \) particles, \( V \pm \Delta V/2 \) volume, and \( E \pm \Delta E/2 \) energy for arbitrarily small \( \Delta N \), \( \Delta V \), and \( \Delta E \). However, for mechanically-stable jammed granular-solids microstate probabilities differ by many orders of magnitude[9]. Second, the only equilibrium state for the jammed granular-solid is kinetic and elastic energy equal to zero. The velocities of grains must be zero in equilibrium due to dissipation, and therefore the kinetic energy is zero. The elastic potential energy must be zero since at jamming there are no particle overlaps. These differences demonstrate that further study into a different framework is needed to relate microscopic and macroscopic thermodynamic properties like velocities and temperature or positions and entropy. For an ideal gas or an elastic solid, we know the set of variables that tie macroscopic quantities like temperature, pressure and volume and microscopic quantities like velocity and position together. The broad aim of my
The project is to find relationships between the geometrical structure of a granular solid, and observed macroscopic quantities such as packing fraction, pressure, and contact number. To investigate whether neighbors, both contact and non-contact neighbors can determine system properties, and if so, which ones? The simplified computational systems we will consider are composed of 2D disks with a diameter ratio of 1:1.4.

In chapter 1, we will discuss the details of the simulation methods used to create jammed packings. In chapter 2 we will introduce a novel classification scheme to describe the Delauny triangles formed by the particles centers in bidisperse jammed packings. All triangles can be classified into 20 types based on composition and contact type. In chapter 3 we will examine the contact statistics of “thermalize” elastic networks of jammed particles. In this study, the particles are elastic, with no dissipation, but differs from an ordinary solid because the interaction is a purely repulsive contact potential. In chapter 5 we provide overal conclusions from these studies, and finally in chapter 6 we suggest future directions.
Chapter 1

Methods

1.1 Simulations of Granular Solids

The systems we investigate are simulations of 2D frictionless circular grains or disks. We simulate jammed structures for system sizes in the range $N = 8$ to 2500 particles. The simulated systems have periodic boundary conditions at constant volume. To represent a medium composed of repulsive grains, we will use the total potential for particle $i$,

$$V_i = \sum_j V_{ij}, \quad (1.1)$$

and total potential for the system

$$V = \sum_{ij} V_{ij}, \quad (1.2)$$

where

$$V_{ij}(\vec{r}_k) = \frac{\epsilon}{2} (1 - \frac{|\vec{r}_{ij}|}{\sigma_{ij}})^2 \Theta (1 - \frac{|\vec{r}_{ij}|}{\sigma_{ij}}), \quad (1.3)$$

is a repulsive linear-spring interaction between particles $i$ and $j$, which is zero if the particles are not in contact. $\vec{r}_k$ is the position of particle $k$, $\vec{r}_{ij} = \vec{r}_j - \vec{r}_i$ is the vector pointing from the center of particle $i$ to the center of particle $j$, $\sigma_{ij}$ is the
average particle diameter for particle $i$ and $j$, and $\epsilon$ is the energy scale. $\Theta(x)$, the Heaviside function, forces the potential to be zero if the particles are not overlapped. This potential produces a linear inter-particle force $\vec{F}_i$, which is proportional to the overlap. The force on particle $i$ is

$$\vec{F}_i = -\nabla V_i = -K_{ij} \vec{\delta}_{ij} \Theta(|\vec{\delta}_{ij}|),$$

(1.4)

where the spring constant, $K_{ij} = \epsilon/\sigma_{ij}^2$, and

$$\vec{\delta}_{ij} = (1 - |\vec{r}_{ij}|/\sigma_{ij})\hat{r}_{ij}$$

(1.5)

is the overlap vector pointing in a direction from the center of particle $i$ to the center of particle $j$. The process of creating a jammed packing is equivalent to finding the particle positions and diameters for which the potential (1.2) is zero and also a minima (see below). We use either molecular dynamics or conjugate gradient to find the zero-minima. To find minima using molecular dynamics we solve Newton’s law,

$$m_i \vec{a}_i = \sum_j \vec{F}_i - B\vec{v}_i,$$

(1.6)

where $m_i$ is the mass and $a_i$ is the acceleration of particle $i$. The force on the right-hand-side is given by (1.4) with an additional drag term proportional to the velocity of particle $i$, $\vec{v}_i$ with a linear damping coefficient $B$. The damping insures that the
Figure 1.1: A jammed N=16 2D disk particle packing in periodic boundary conditions. A jammed packing is mechanically stable but just at the point where there are no particle overlaps and any change in the particle diameters or position will cause overlaps. Theoretically, the potential is both zero and a minimum, so there is no overlap, the forces are zero, and any perturbation will tend to bring the system back to the minimum.

The system ends up in a minimum. If the damping is large enough the system will basically follow a steepest descent path down the potential energy function. To solve Newton’s Law, we use the second-order velocity Verlet integration scheme[14]. We can also use the conjugate gradient technique to find zero-minima directly from the total potential (1.2). The conjugate gradient technique is a standard numeric technique to find the minima of functions.

Creating a jammed packing of soft particles like the one shown in Fig. 1.1 can be done in four basic steps: 1) system initialization, 2) system compression (e.g., by particle diameter growth), 3) system relaxation (i.e., potential minimization), and 4)
threshold detection. The idea is to create a system whose potential energy is both minimum and nearly zero, i.e., non-zero but smaller than $\epsilon$, where $\epsilon$ is small. This situation is depicted in Fig. 1.2. The upper graphs show schematic potential energies as a function of the particle positions and particle diameter all on one axis. The lower images show the corresponding particle positions and diameter at the blue dot in the graph above. The system on the right is overcompressed. It is a minimum but the potential energy and therefore the pressure is non-zero. The system on the right is under compressed. The particle could move of the diameters could be increased without causing overlaps. The center system is jammed. The potential is zero and it is a minimum.

1. Initialize system: Place $N$ particles in a box of fixed area $A$ uniformly distributed at random. Set the diameter of the particles to the largest value such that no particle will overlap. For particles with different diameters $\sigma_i$ only the particle size ratios $\Gamma_i$ are important. We use the smallest particle diameter $\sigma_0$ to form the ratios, $\Gamma_i = \sigma_i / \sigma_0$. Then the particle diameters are all determined by the value of $\sigma_0$. That is $\sigma_i = \sigma_0 \Gamma_i$. The minimum ratio of an interparticle spacing to the average size ratio $r_{ij} / \Gamma_{ij}$ determines the maximum value for $\sigma_0$ for which no particles will overlap. The initial density,

$$
\phi = \frac{\pi \sigma_0^2}{4A} \sum_{i=1}^{N} \Gamma_i^2. 
$$  \hfill (1.7)
Figure 1.2: Sketch of system potential energies (top). The blue dot represents the current particle positions and diameters (bottom) near jamming. The figure on the left is over compressed. It is at a minimum but it is above jamming. The system on the right is under compressed leading to degenerate minima. It is below the jamming threshold since the particle diameters could be increased without overlap. The system in the middle is just right. It is a single minimum. Its energy is zero, but any increase in particle diameter or change in particle position will lead to overlap.
2. *System compression:* If the system is at zero energy i.e., there are no particle overlaps, as it will be after initialization, compress it by increasing $\sigma_0$ and enlarging the particles, while holding the volume of the space they are in constant.

3. *System relaxation:* Allow the particles to rearrange themselves via molecular dynamics simulation with damping or conjugate gradient until they are at their lowest potential energy.

4. *Threshold detection:* To jam the system while maintaining (nearly) zero pressure we create packings with small overlaps, usually on the order of $\delta \approx 10^{-8}$). This leads to energy on the order of $\epsilon \approx \delta^2 \approx 10^{-16}$. If the system energy is zero after relaxation it must be compressed further and we go back to step (2). If the energy is above $\epsilon$ it must be decompressed and we reduce $\sigma_0$ and then go back to step (2). If the energy is between zero and $\epsilon$ we have a jammed packing and we stop.

1.2 *Shear*

The packing-generation methods discussed to this point in the chapter employed periodic boundary conditions in square cells with side length $L$. An illustration of periodic boundary conditions for a 2D mechanically stable packing of bidisperse disks with $N = 6$ is provided in Fig. 1.2. Eight image cells surround the central cell to specify the interparticle interactions near the boundaries. (In 3D, 26 image cells surround the central cell.) We see that disk 5 interacts with disks 3, 4, and 6 in the central
cell. In contrast, disk 6 interacts with disk 5 in the central cell, 2′ is the lower image, 4″ in the right image, and 1″″ in the lower right image. (Note that if the diameter of one of the particles is larger than half of the box size, \( \sigma > L/2 \), it can interact with more than one image of the same particle.) To maintain continuous evolution of the particle trajectories, the particles may move out of the central cell during the packing-generation process, but this does not affect the interparticle separations and forces.

These systems can also be used to study the linear and nonlinear response of static packings to applied simple shear strain. To implement simple shear, an affine shear is applied to all particles \( i \) in the central cell,

\[
x'_i = x_i + \Delta \gamma y_i,
\]

where \( \Delta \gamma \) is the strain increment, \( x \) is the shear flow direction, and \( y \) is the shear gradient direction, coupled with simple shear-periodic ([15],[16]) boundary conditions. Shear periodic boundary conditions are illustrated in Fig. 1.3 for two-dimensional systems. The top/bottom row of image cells is shifted to the right/left by \( \Delta \gamma L \). We identify the particles in the main or image cells that contact each of the particles in the main cell and, following the application of shear strain, relax the system using energy minimization at fixed locations of the image cells. This is followed by the application of successive shear strain increments and energy minimization to a prescribed total shear strain \( \gamma \).
Figure 1.3: Illustration of the implementation of simple shear in Lees-Edwards boundary conditions for a packing of bidisperse disks. The image cells above and below in the central cell in the shear-gradient direction are also shifted by $\pm L \Delta \gamma$ in the shear flow direction.

Simple shear deformation can also be implemented by shifting top and bottom rigid boundaries by $\pm \Delta \gamma L$ in the shear flow direction and applying periodic boundary conditions in the directions perpendicular to the shear gradient direction with or without affine distortions in the bulk, as shown in Fig. 1.4. After each movement of the boundaries, the system can be relaxed using energy minimization. Boundary-driven shear allows one to model the interactions between the sheared material and the container and set up strongly nonlinear velocity profiles [17].
1.3 Vibrations

In simulations of elastic jammed granular materials vibrations can be induced by spatially perturbing the particles. Each particle is given a small initial velocity $\vec{v}_n$ and the system is allowed to evolve according to Newton’s Laws, with the resulting integrals being solved by a second order Verlet integration [14]. This initial velocity gives the system kinetic energies $E = 1/2 \sum_n v_n^2$ in the range of $10^{-15} < E < 10^{-4}$. The mass of all particles and the energy scale, $\epsilon$, are one. To achieve an energy $E$ we impart a random gaussian velocity with standard deviation $\sigma = \sqrt{2E/N}$. The protocol for vibration is three step:

1. Create a mechanically stable packing of $N$ particles. The systems we study are slightly above jamming, with $\Delta \phi \approx -10^{-8}$.

2. Raise the energy of the system by $E$ distributed randomly to each of the particles.
3. Allow the system to evolve

From these three steps we create many vibration periods for many systems and observed contact breaking. From [18], systems in which no contact breaking occurs are called Iso-coordinated solids (ICS). In systems with more energy, particles break contacts and are called Hypo-coordinated solids (HCS). If more energy is added in addition to contact breaking large scale particle rearrangements also occur.
Chapter 2

Triangle Decomposition

2.1 Introduction

In this chapter, we use simulations of 2D bidisperse disks to determine the properties of jammed packings and investigate the statistical mechanics of these systems. We explain a novel method for classifying structural subunits of a packing and use the structures to calculate relevant physical quantities. The classification scheme is based on a 20 type decomposition of the Delaunay triangles extracted from the centers of the particles in the packing. We find that the distribution of each type has a universal form, independent of total number of particles $N$ in the packing for $N=8-10,000$, and that the parameters describing this form saturate as $N$ is increased beyond $N=20$. We measure the distribution of the particle connections, the area distributions of the different structures, and nearest neighbor distributions. We explore the extent to which the nearest-neighbor distributions can predict the properties of the entire packing.

A microcanonical ensemble is defined as the complete set of states a mechanical system in equilibrium can have with identical values for energy, number of particles and system volume; $E$, $N$ and $V$ respectively [19]. Each unique value of energy,
number of particles and volume is defined as a macrostate. For a system such as an ideal gas, a microstate is a unique assortment of the positions and velocities and many microstates compose each macrostate. The power in an ensemble picture is being able to easily relate measurable macroscopic quantities like volume and energy to microscopic quantities like positions and velocities. For athermal granular systems particle velocities are often irrelevant, because the system is in equilibrium and all velocities are zero, or the system is deforming slowly enough that the velocities are arbitrarily small and the system is rate-independent. However we can investigate geometrical relationships in the positions. From 1.1, we can see there are a limited number of neighbor interactions, since only a few particles can fit around a given particle.

We developed a method to geometrically group particles together, to express the microstate of the system in terms of the groups, and to find properties of the resulting structures. Having microstructures to count enables us to investigate new statistical relationships and help to identify which measurable quantities are significant.

### 2.2 Triangulation

It is nice if the geometric sub-units tile all space and Delaunay triangles satisfy this requirement. A Delaunay triangulation can be created on a set of points by drawing circumcircles on groups of three points in such a way that no circumscribed circle encloses another point Fig. 2.1. After selecting the correct points on each circumscribed circle connect
2.3 Triangle Classification

The triangle decomposition consists of Delaunay triangles with their vertices in the center of the particles of the system. This configuration tiles space and groups particles together in threes. Since each particle is 360 degrees around and the triangle
Figure 2.2: The 20 types of triangles that tile all space for an N=32 packing. The rows are differentiated by contact number, with the top row having three, the second row having two, etc. The columns are differentiated by particle composition, with the leftmost column being all small particles (SSS), the second to left being two small particles and a big one (SSB) and so on. (see text for more details).
vertices must fill all the possible angular space the number of triangles in a packing is twice the number of particles. For a 2D bi-disperse system of soft particles, we define twenty types of triangles as classified by the particle composition and the triangle edge type. Figure 2.2 shows a 32 particle packing with the decomposition overlaid on the left and the 20 individual triangle types on the right. On the right of the figure, the triangle types are displayed in columns representing the composition (i.e., the number of particles small and big). The first column (reds) is composed of all small (SSS) particles, and the second column (greens) is two small particles and a big particle (SSB), the third column (blues) is one small particle and two big particles (SBB) and the forth column (yellows) is all big particles (BBB). The rows represent the number of contacts in each triangle. Each side of the triangle connects one particle to another. Some of the connected particles are touching and are contacts. In the top row, each triangle side is a contact for a total of 3 contacts. In the second row two sides are contacts and one is not a contact for a total of 2 contacts. However, for the second column (SSB) and second row (2 contacts) there are two distinct ways to distribute the contacts. In the type 6 triangle the missing contact is between the small and large particles, but in type 7 the missing contact is between the two smalls. The same situation occurs for the pairs 7 and 8, 12 and 13, 14 and 15. In the fourth row there are no contacts and so like row 1 there is only one way to distribute them per composition. Each triangle is color coded and numbered based on its particle type and contact number attributes.
A major challenge relating microscopic and macroscopic quantities for athermal granular systems is selecting which microscopic variables to consider. Our aim is to start with geometrical interactions, specifically voronoi neighbors in the form of delaunay triangles, and catalog their properties.

With our decomposition outlined we will use the statistical properties from this targeted set of subsystem definitions and constraints to determine connections between microscopic and macroscopic quantities. Specifically we relate mean subsystem probabilities to the average number of contacts per particle, $z$.

### 2.4 Calculation of the Triangle Probabilities

Once the 20 types of triangles in the decomposition are identified, it is necessary to determine their probabilities. Intuitively it's reasonable to assume that the triangles aren't equi-probable, but which triangles are the most common, the least? An approximation describing the frequencies of each column in Fig. 2.2 or composition (SSS, SSB, SBB, BBB) based on the size ratio of small to big particles and the average number of contacts per particle is described by Dodds in [20]. The thinking is that larger particles will have more space for particles around them and proportionally more triangles, but otherwise the distribution is random. So the two key factors are the size of the particles and the proportional number of particles there are in the packing. The probability of a small particle taking part in a triangle is the number of small neighbors (both contact and non-contact voronoi neighbors, which Dodds
Figure 2.3: Terms of the expansion in equation 2.2 where each term is the probability of obtaining the triangle shown below it.

counts as the same thing) over the total number of neighbors possible. We call this quantity $Z_S$. $Z_B$ is the probability of a big particle taking part in a triangle. $Z_S$ can be written as

$$Z_S = \frac{C_S}{6N}$$  \hspace{1cm} (2.1)

where $C_S$ is the total number of small neighbors in the packing and the $6N$ in the denominator comes from $C = 3N_{Tri} = 6N$, where $C$ is the total number of neighbors and there are three neighbors per triangle and two triangles per particle. In Dodds’ approximation the frequencies for each composition are proportional to the terms corresponding to the triangles composition in the expression:

$$(Z_S + Z_B)^3$$  \hspace{1cm} (2.2)

where $Z_S$ is the probability of a small particle being involved in a contact and $Z_B$ is the probability of a large particle being involved. $c_S = \frac{C_S}{N_S}$ and $c_B = \frac{C_B}{N_B}$ are the average number of connections on a small and big particle, regardless of whether the
connection is a contact or not. We measure $c_S = 5.5691$ and $c_B = 6.4309$ from 7981 $N = 256$ packings with $n_S = n_B = 1/2$. Notice that $Z_S = 2.7845$, $Z_B = 3.2155$, and $Z_S + Z_B = 6.0000$. We can write $n_{S(B)} = N_{S(B)}/N$, where $N_{S(B)}$ is the total number of small (big) particles and $c_{S(B)} = C_{S(B)}/N_{S(B)}$, where $C_{S(B)}$ is the total number of connection on a small (big) particle. Then $Z_S + Z_B = n_S c_S + n_B c_B = (C_S + C_B)/N$, and $(C_S + C_B)$ is the total number of triangle sides, which is 3 times the number of triangles. As mentioned earlier the total number of triangles is $2N$ because each triangle contains 180 degrees of disk angle. Therefore $(C_S + C_B)/N = 3(2N)/N = 6$. So $Z_S = 6 - Z_B = C_S/N = 6 - C_B/N$. $C_S$ and $C_B$ can also be calculated from the assumption that the average number of connections on a particle is determined from the size of the angle formed by the triangle vertex on a particle. If the average angle taken by a triangle is $\theta$ then the average number of connections is

$$C_S/N_S = 2\pi/\theta = 1/\alpha, \tag{2.3}$$

where $\alpha$ is the fraction of the circle taken by a triangle. Therefore if we assume the particles are randomly distributed then the average fraction taken by a triangle on a small particle,

$$\alpha_S = \alpha_{SSB}Z_B^2 + 2\alpha_{SSS}Z_S^2 + \alpha_{BSS}Z_S^2 \tag{2.4}$$

which is just the angle taken up by each combination of particle type weighted by the particle type probability. The middle term in equation 2.4 has a two in front of
it since the neighboring particles in the triangle can be configured as small big or big small to get the same result. From geometric considerations

\[ \alpha_{SBB} = \frac{1}{2\pi} \cos^{-1} \left( \frac{1 + 2\Gamma - \Gamma^2}{(1 + \Gamma)^2} \right) \approx \frac{1}{6} + \frac{\Gamma - 1}{2\sqrt{3\pi}}. \]  
(2.5)

is the fraction of the small particle taken by the small vertex of a (SBB) triangle,

\[ \alpha_{SSB} = \frac{1}{2\pi} \cos^{-1} \left( \frac{1}{1 + \Gamma} \right) \approx \frac{1}{6} + \frac{\Gamma - 1}{4\sqrt{3\pi}}, \]  
(2.6)

is the fraction of the small particle taken by the small vertex of a (SSB) triangle,

\[ \alpha_{SSS} = \frac{1}{2\pi} \cos^{-1} \left( \frac{1}{2} \right) = \frac{1}{6}, \]  
(2.7)

is the fraction of the small particle taken by the small vertex of a (SSS) triangle, and \( \Gamma = \sigma_L/\sigma_S \). For the big particle,

\[ \alpha_B = \alpha_{BBB}Z_B^2 + 2\alpha_{BBS}Z_BZ_S + \alpha_{BSS}Z_S^2 \]  
(2.8)

where

\[ \alpha_{BBB} = \alpha_{SSS} = 1/6, \]  
(2.9)
is the fraction of the big particle taken by the big vertex of a (BBB) triangle,

\[ \alpha_{BBS} = \frac{1 - 2\alpha_{SBB}}{4}, \]  

(2.10)

is the fraction of the big particle taken by the big vertex of a (BBS) triangle, and

\[ \alpha_{BSS} = \frac{1 - 4\alpha_{SSB}}{2}, \]  

(2.11)

is the fraction of the big particle taken by the big vertex of a (BSS) triangle. The relation between the big and small \( \alpha \)'s is due the fact that the BSS triangle and the SSB triangle are the same, we only need different angles. The \( \alpha \) equation also assume that all sides of the triangles are contacts. This is clearly wrong as seen in Fig. 2.2 not all triangles are from the first row. Finally combining (2.3) and (2.4) and using \( Z_S = n_{SCS} = C_S/N \) we have,

\[ \frac{Z_S(\alpha_{SBB}Z_B^2 + 2\alpha_{SSB}Z_SZ_B + \alpha_{SSS}Z_S^2)}{(Z_B + Z_S)^2} = n_S, \]  

(2.12)

and

\[ \frac{Z_B(\alpha_{BBB}Z_B^2 + 2\alpha_{BBS}Z_SZ_B + \alpha_{SSS}Z_S^2)}{(Z_B + Z_S)^2} = n_B. \]  

(2.13)

These two equation could be solved simultaneously for \( Z_S \) and \( Z_B \), however, we know
\[ Z_B = 6 - Z_L \] therefore,

\[ \frac{Z_S(\alpha_{SBB}(6 - Z_S)^2 + 2\alpha_{SSB}Z_S(6 - Z_S) + \alpha_{SSS}Z_S^2)}{36} = n_S. \tag{2.14} \]

This equation can be solved analytically using Mathematica. There are two complex and one real solution. However, the equation contains hundreds of term so we solved it numerically and found \( Z_S^c = 2.7251 \). This can be compared to the measured value \( Z_S^a = 2.7845 \) a difference of 2%. Now we can compare the distribution of triangle compositions three ways: 1) from the measure triangles, 2) from (2.2) using the measured value of \( Z_S^a \), and 3) from (2.2) using the calculated value of \( Z_S^c \). From (2.2), the terms of \((Z_S + Z_B)^3\) are proportional to the frequencies of the corresponding triangle composition. To normalize we divide each term by \((Z_S + Z_B)^3\) so, for example, the probability of getting SSB (i.e., column 2 in Fig. 2.2) is

\[ P_{21} = P_{SSB} = \frac{3!}{s!b!} z_S^s(1 - z_S)^b, \tag{2.15} \]

where \( s \) is the number of small and \( b \) is the number of big particles in the triangle. A graph of the probabilities of the four types are shown in Fig. 2.4. The calculated probability compare well with the measured probabilities. Using (2.15) with the measured value of \( z_S = Z_S/6 = 0.4641 \) is a little closer to the direct measurement with a mean absolute deviation of 0.0026 or about 1%, but the full calculation using
Figure 2.4: Comparison of measured and calculated triangle composition probabilities. The probability is shown three ways: 1) directly measured from the \( N = 256 \) particle system (blue line). 2) from (2.15) using the measured \( z_S = 0.4641 \) (green circles). 3) from (2.15) using the calculated \( z_S = 0.4542 \) (red +).

(2.15) with the calculated value of \( z_S = 0.4542 \) also compares well with a mean absolute deviation of 0.0071 or about 3%. This confirms that the spatial distribution of the particles is basically random and the error associated with the assumption that all triangle sides are contacts is small. This allows us to calculate an upper bound on the density of a random packing of particles. Assuming that for the densest random packing all triangle sides do have contact then we can calculate the total area of all of the triangles. The assumption is that only the first row triangle types 1–4 are in the packing and the fraction of each type is give by (2.15) using the calculated \( z_S \). The first row triangles have areas measured in small particle diameters of, \( A_1 = \sqrt{3}/4 \), \( A_2 = \sqrt{\Gamma(2 + \Gamma)/4} \), \( A_3 = (1 + \Gamma)\sqrt{(5\Gamma + 1)(3\Gamma - 1)/16} \), and \( A_4 = \Gamma^2\sqrt{3}/4 \). Thus
the density is
\[ \phi = \frac{\pi (n_S + n_B \Gamma^2)}{8 \sum_{i=1}^{4} A_i P_i} = 0.8722. \] (2.16)

Now we will extend Dodds’ idea to include the non-contact triangle sides. We can write the number of contact and non-contact sides in a particular triangle as a fraction of the mean number of Voronoi neighbors \( c_S \) and \( c_B \), which we calculated above then we use a weighted average for \( Z_S \), written as

\[ \frac{s\bar{Z}_S + s\hat{Z}_S}{Z_S + \hat{Z}_S} \] (2.17)

where \( s \) is the number of contacting sides around the small particles in a triangle and \( \hat{s} \) is the number of non-contacting sides around the small particles in a triangle, \( c_S \) is the mean fraction of contacting neighbors, and \( \hat{c}_S \) is the mean fraction of non-contacting neighbors. Combining a similar equation for \( Z_B \) and (2.2)

\[ P_{s\hat{s}b\hat{b}} = 2^k \frac{3!}{s!\hat{s}!b!\hat{b}!} \left( \frac{s\bar{Z}_S + s\hat{Z}_S}{Z_S + \hat{Z}_S} \right)^s \left( \frac{b\bar{Z}_B + b\hat{Z}_B}{Z_B + \hat{Z}_B} \right)^b, \] (2.18)

where \( s = (s + \hat{s})/2 \) the total number of small neighbors and \( b = (\hat{b} + \hat{b})/2 \) the total number of big neighbors. \( k \) is an integer value related to the overcounting contacting and non contacting sides. Equation (2.18) is normalized by dividing by all allowed
values of \((\bar{s}, \hat{s}, \bar{b}, \hat{b})\). For example the unnormalized probability of a type 1 triangle is

\[
P_1 = P_{6,0,0,0} = 2^{-3} \left( \frac{6\bar{Z}_S}{\bar{Z}_S + \hat{Z}_S} \right)^3.
\]  

(2.19)

\(P_1\) is unnormalized. After normalization the \(p_1 = P_1 / \sum P_i = 0.0147\). The measured value is 0.0123. Figure 2.5 shows a comparison between (2.18) and the measured triangle probabilities.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{triangle_probabilities.png}
\caption{Comparison of measured and theoretical triangle probabilities.}
\end{figure}

\section{Static Probabilities}

The outlined technique for calculating triangle probabilities applies to a broad range of system sizes. Figure 2.5 shows that for any \(N > 100\) triangle probabilities remain
Figure 2.6: Mean triangle probability for a variety of system sizes. The most probable triangle is $T=9$, with a value of $p_9=0.156$. The four triangles with zero contacts are amongst the least probable. For $N > 100$ the values remain constant and a number of mean triangle probabilities are equivalent.

constant and for $N > 20$ the changes are relatively small. This feature decouples the probabilities from system size and allows $N$ to become arbitrary over some minimal amount.

In addition to granular systems subject to simple shear with Lees-Edwards boundary conditions show static triangle probabilities. This system in 2.7 has $N=16$ particles, which is below the threshold for probabilities irrespective of system size and accounts for the difference in probabilities between the measured values of $P_t$. 
2.6 Decomposition Distributions

While thus far we have investigated mean triangle values, we will now look at how triangles are distributed across different packings. Figure 2.8 shows the distributions. We show in figure 2.6 that triangle probability distributions are $\Gamma$ distributed. This allows for a complete probabilistic description of packing subunit types in terms of $N$, $N_T$ and the shape and scale parameter $k$ and $\theta$ respectively of the gamma distribution. From 2.6 we see that the shape parameter is not coupled to system size and the scale parameter increases nearly linearly with $N$, yielding the relations for a specific triangle type $T$.  

Figure 2.7: Sorted triangle probabilities for a static $N=16$ case, and for the same system undergoing simple shear over a a strain of 2 with Lees Edwards boundary conditions
Figure 2.8: Measured distribution of a canonical set of triangle types for an $N=256$ system. The x-axis is the number of triangles of the specified type found in a packing, and the y-axis is the probability of finding that amount. For the types symmetrically distributed, the peak of each curve would be the mean value.

Figure 2.9: For a canonical set of triangles, the shape parameter $k$ increases nearly linearly with $N$ and the scale parameter $\theta$ is constant over a range of $N$. 
Figure 2.10: This figure shows that for a 256 particle packing, a Γ distribution can be fit to the pdf of triangle numbers per type, $N_T$. The dots are the results from data, and the lines are the fit. A variety of system sizes for $N_9$ are shown.

\[ k(N) = k_T N \quad (2.20) \]

and

\[ \theta(N) = \theta_T. \quad (2.21) \]

The gamma distribution of triangle types is also robust over the range of studied system sizes fig 5 shows this for $T=9$.

Using the pdf of the Γ distribution it is possible to write an analytical expression for
the probability of the number of triangles, $N_T$ in terms of the number of particles, $N$.

$$p(N, N_T) = \left(\frac{N_T}{\theta_T}\right)^{k_T N - 1} \frac{\theta_T}{\theta_T} \frac{1}{\Gamma(k_T N)} e^{-\frac{N}{\theta_T}}$$  \hspace{1cm} (2.22)

### 2.6.1 Contact Number per Particle

A monte-carlo type approach to local particle behavior is the granocentric model [21]. This model uses statistics of local particle interactions from contacts and nearest neighbors to determine contact number and local volume. The first version of the model places particles sampled from a chosen distribution around a central particle until the total solid angle of the central particle is taken up. With a full set of particles around the central particle, contacts are added randomly via a tuneable parameter. The aggregate statistics of many many central particles are then collected to yield the average number of contacts. The triangle decomposition should provide similar results for these values.

We use the more computation friendly but equivalent granocentric protocol from [22]. It consists of six steps:

1. Place a central particle.

2. Add a particle selected from a bi-disperse distribution around the central particle if the angle subtended on the central particle is less than a threshold, $\Omega^*$.

   (See Fig. 2.11.)

3. Give the newly added particle a contact with the central particle with proba-
4. If the particle isn’t a contact move it a distance $\delta$ away where delta is the average distance between the edges of non-contacting particles.

5. If the new total angle filled is above $\Omega^*$ keep the particle half the time and exit.

6. Repeat starting at the second step.

The model contains three adjustable parameters, the first is the threshold angle above which the central particle is considered surrounded, $\Omega^*$. The particle will be considered surrounded if the following inequality is true

$$\Omega > (2\pi - \Omega^*)$$

To reduce oversampling small particles, if a particle is picked and $\Omega$ is above the
threshold then half the time the particle is kept and half it is not. For our comparison we used the value $\Omega^* = 0.59$. As $\Omega^*$ is a tuneable parameter it was selected by qualitative means to fit the measured data. Once a set of surrounding particles has been selected, contacts are added randomly with probability $p$. No consideration is given to a potential force balance. Given that the central particles neighbors compose a voroni cell, in a real packing a particles voronoi neighbors each have some probability of being a contact. We measured this value from our data set, and $p = 0.3176$. To obtain the final parameter, $\delta$ we measured the distance between particle edges for our $N=256$ system and used inversion sampling to obtain $\delta$ values. We found $\delta=0.19205$ A concise method of predicting measured microscopic quantities in a jammed granular system is obtainable using the triangle decomposition. To find the average number of force bearing neighbors a particle we group together triangles in pairs based on the total number of contacts they contain. Picking two triangles selects an angular distance equivalent to a particle. If the triangular subunits in a packing are isotropic and only constrained by subunit probability, then any two triangles should have an equivalent contact probability as a particle. It is possible then to find the average number of contacts per particle by multiplying the probabilities of the pairs of triangles that sum up to a particular average number of contacts per particle for
instance to calculate $p(3)$

$$p_c(3) = p_1p_{17} + p_1p_{18} \cdots + p_2p_{17} + p_2p_{18} \cdots + p_5p_{11} + p_5p_{12} \cdots + p_{10}p_{16}$$

(2.24)

Where all triangle pairs that together have three contacts have been chosen. This includes first row triangles paired with fourth row triangles and second row triangles paired with third row triangles. To generalize this technique for all possible contact numbers we create a 20 by 20 companion matrix, $C_c$, that consists of ones and zeros to select the appropriate triangle pairs while taking the inner product of the triangle probability vectors $p_t$ a 1 by 20 vector of the mean triangle probabilities. This relationship can be written as equation 2.25. In fig. 6 we compare the mean contact number probabilities per particle to the measured values, and the companion matrixes for $C_0$, $C_1$ and $C_2$ have been summed together as they all represent non-mechanically stable particles. We write this matrix as $C_0$.

$$p_c = p_tC_c p_t^T$$

(2.25)

A comparison of the number of contacts per particle between the granocentric model as described in 2.6.1, the measured value, and the triangle probabilities (measured) shows a reasonable agreement.
Figure 2.12: A comparison of measured mean number of contacts per particle for an N=256 particle system and the theoretical prediction based on the technique described in eq. 2.25.
2.6.2 Packing Fraction

The packing fraction is the area of the particles divided by the total area. For 2-D bi-disperse systems this is

\[ \phi = \frac{\sum B \pi R^2_B + \sum S \pi R^2_S}{V} \]  (2.26)

where the B and S subscripts denote the big and small particle radii respectively, N is the number of particles, R is the particle radii and V is the volume of the total enclosed space. At jamming the packing fraction, \( \phi_j \), of a 2-D bi-disperse system is approximately 0.84. Packing fraction is a macroscopic quantity of particular significance due to the different mechanical properties granular systems exhibit at different packing fractions. At \( \phi = \phi_j \) the system becomes jammed and the particles can’t rearrange without an input of energy. We found area distributions are distributed by row from figure 2.2.

Figure 2.13 shows the pdf for the four different rows from figure 2.2. The vertical line is \( A_1 \), a delta function which is characteristic of \( T=1,2,3,4 \). \( A_5 \) in the second row has a bimodal distribution, \( A_{11} \) and \( A_{17} \) both have a peak at the second local maximum of the bimodal \( A_5 \) distribution and a long decreasing tail at larger areas.

In addition, an approximation of the mean packing fraction can be estimated using
Figure 2.13: pdf of all the areas of only small particle triangles where $A_1$ is a delta function, $A_5$ is a bimodal distribution and $A_{11}$ and $A_{17}$ have long tails and a single peak.

Figure 2.14: Plot of triangles in the second row shows a bimodal distribution.
Table 2.1: Table of triangle index, $T$ and measured mean triangle area, $\langle A_T \rangle$ for diameters $\sigma_S=1$ and $\sigma_L=1.4$ calculated from simulation of 7981 256 particle systems.

The average area, $\langle A_T \rangle$, is calculated using Heron’s formula using disk radii for the contact sides and disk radii plus $\delta$ for the non-contact sides. For our $N=256$ system $\langle \phi \rangle=0.837$, and equation 2.27 yields a value of 0.831.

**Statistical Properties of the Delaunay Triangle Decomposition Without Floaters**

In MS packings typically around five percent of particles have fewer than three contacts. Even though these particles don’t contribute to the mechanical stability of the
system, during packing formation they are necessary to obtain the observed structure. In an effort to keep the number of triangles constant from one packing to the next we have included them in our calculations, and investigate the impact their removal would have. Figure 2.15 shows the limited impact excluding floaters has on triangle probabilities. The probabilities vary by only a few percent, and given this we continue to include floaters in our calculations.

![Figure 2.15: Mean triangle probabilities with and without floaters.](image)
2.7 Calculation of Pressure Using the Delaunay Triangle Decomposition

For our 2-D bidisperse system, the stress tensor between particles, $\Gamma$, is given as

$$\Gamma = \sum_{i,j} Tr \left( \vec{d}_{ij} \vec{F}_{ij} \right) = \sum_{i,j} d_{ij} F_{ij} Tr \begin{pmatrix} \cos^2 \theta_{ij} & \cos \theta_{ij} \sin \theta_{ij} \\ \cos \theta_{ij} \sin \theta_{ij} & \sin^2 \theta_{ij} \end{pmatrix} \quad (2.28)$$

where $i$ and $j$ are indexed over all particles, $\theta$ is the angle from the horizontal of the vector from the center of particle $i$ to the center of particle $j$, $d$ is the distance between particle centers and $F$ is the inter-particle force. Equation is equivalent to the internal virial [23] for particles with no overlap, the force between them is zero. The off diagonal elements are small compared compared to the diagonal elements (for our data each off diagonal element is around 0.025). This gives $Tr(...)=1$ and we can write the pressure as

$$\Gamma = \sum_{i,j} d_{ij} F_{ij} \quad (2.29)$$

which is a scalar quantity. One technique we attempted was to coarse grain the pressure by triangle type. If force is distributed in a measurable distribution across particle contacts then triangle type should provide a reasonable coarse grained estimation of $\Gamma$ as

$$\Gamma = \sum_T N_T \Gamma_T \quad (2.30)$$

The distribution of forces on particles in figure 2.16 shows the force pdf on small
particles. Due to the energy scale, small particles are "harder" than large particles as it would take the same amount of force to overlap two small particles as it would two big particles. This attribute enables a distinguishablity between triangles composed of different particle types. For instance if there was no difference in particle hardness and indexing over triangle type $<\Gamma_1>=<\Gamma_2>=<\Gamma_3>=<\Gamma_4>$ but since they are different there will be a unique mean for many triangle types. Averaged over many systems we see that equation 2.30 gives an accurate mean pressure per packing, but as evidenced in figure 2.17 fails to describe the breadth of observed pressures.

### 2.8 Simplified Calculation of Microstate Probability

We define microstates of granular systems as any packing that has unique dynamical matrix eigenvalues.
Our method is to relate triangle frequencies within a particular packing to the probability of that packing occurring. The thinking being that the triangle probabilities would cause certain frequency distributions within a packing to be extremely improbable or even impossible (a bi-disperse packing couldn’t contain all type 20 triangles for instance).

An attempt was made to enumerate microstates in terms of triangle frequencies and nearest neighbors. Qualitatively the statistics of microstate occurrence can be described as the probability a unique set of triangles occurs times the probability that the set has a particular configuration. We investigated the relative influence of each of these two factors.

Figure 2.17: pdf of the forces acting on the small particles of the packing.
Triangle frequency distributions have degenerate states. Figure 2.18 shows an instance where the triangle frequencies are similar, but the packing has unique dynamical matrix eigenvalues and a different packing fraction, $\phi$. Table 2.8 shows results for two small systems that have been completely enumerated and their triangle frequencies compared. As can be seen there are triangle degenerate states that are actually unique even for cases with small numbers of states (the $N=8$ system has $N_s=164$ states and there are three distinct states that all have a similar triangle distribution). This level of degeneracy is too high to yield a quantitative depiction of microstate probabilities purely by triangle frequency distribution.

In addition to measuring triangle frequencies we also began to calculate the multiplicity of a single triangle frequency measurement. If the number of different triangle arrangements could be completely enumerated then we would know the probability that we are observing a particular triangle configuration. To do this we tried to find the number of ways triangles could fit next to each other assuming only like sides could touch. In our packings there are six types of sides: SS-C, SS-NC, SB-C, SB-
Figure 2.18: Two triangle degenerate packings. The packing on the left has $\phi = 0.66$ and the right packing has a $\phi = 0.726$.

NC. BB-C and BB-NC where SS stands for small small, SB small big etc. C and NC represents contact and non-contact respectively. Only similar side types could connect so some triangles would never be found next to each other. Triangles with NC sides have varying side lengths so in a typical reductionist approach we try a first order approximation. We consider the number of configurations of equilateral triangles that are unique under rotation, reflection and translation.

The way our method works is to start with a single triangle and individually add additional triangles to it to grow the figure. As triangles are added, a state emerges and this state is compared to previously measured configurations in order to determine the probability. For one, two and three triangle systems there is only a single state with theoretical probability $p_t = 1$. As seen in figure 2.19 for four triangle systems there are three unique states with probabilities $p_t(N_1) = 0.4$, $p_t(N_2) = 0.4$ and $p_t(N_3) = 0.2$. The range of states possible for a five triangle system are depen-
Figure 2.19: Any side of triangle $A$ can connect with any of the sides of the figure to its right, and there are three possible resulting figures, $N_1$, $N_2$ and $N_3$. $N_1$ is created if the triangle is placed on either of the two sides labeled 1, and since there are five sides total the theoretical probability is $p_t(N_1) = 0.4$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_s$</td>
<td>1</td>
<td>3</td>
<td>4</td>
<td>12</td>
<td>24</td>
<td>66</td>
<td>160</td>
<td>431</td>
<td>954</td>
<td>1776</td>
<td>2608</td>
</tr>
</tbody>
</table>

Table 2.3: The number of triangles, $N$, and the number of states, $N_s$.

dent on the configuration of the four triangle system and with increasing numbers of triangles these relationships increase in complexity. For small systems we make the calculations by hand, but for systems larger than eight triangles we found the number of states by computer simulation. Figure 2.20 and figure 2.21 depict the states and probabilities for seven and eight triangle systems. Table 2.8 lists the number of states for larger system sizes.

As system size increases there is a tiling effect and fewer of the resulting states wind up
Figure 2.20: The image on the left is the 24 distinct states that can be created from 7 triangles. The black number is their theoretical probability, $p_t$, the blue is their probability from simulation, $p_s$, and the green is $\log \sqrt{(p_t - p_s)^2}$. The figure on the right shows how the log of the square root of the sum of the differences decreases with the number of simulation steps. This decrease shows that we can find a number arbitrarily close to the theoretical value with our simulator.

as long strands. The relationship between triangle number and the number of states is exponential, and slope measurements from figure 2.22 yields the final equation for $N_s$.

Equation 2.31 shows us the relationship between the number of states as a function of the number of equilateral triangles.

$$N_s = e^{0.95N-3.5} \quad (2.31)$$

Finding the number of states equilateral triangles can be configured in yields insight into the properties of triangularly tiled systems; namely that the most probable configurations tend to tile space and that the number of available systems increase
Figure 2.21: The 66 unique configurations of eight triangles. The black number is their theoretical probability, the blue is the probability measured by simulation, and the green value is $\log \sqrt{(p_t - p_s)^2}$. 
Figure 2.22: The log of the number of states versus the number of triangles. The slope of this line is 0.95. The small curve observed around N=12,13 comes from unsaturated states.

exponentially. Comparing to our bi-disperse system (which is in itself an idealized system) this first order approximation leaves out the fact that only certain triangle sides can connect with each other. Moreover all of the non-contact sides have complex length distributions. While it seems reasonable to assume that different types of sides would merely change the slope of the exponential increase in system states, the result of changing side lengths is more mysterious and would require a number of arbitrary protocol decisions to be made in terms of non contact side length.
Chapter 3

Contact Statistics During Vibration

We use simulations of bidisperse disks that interact via purely repulsive linear springs to determine properties of contact networks during vibration at various energies and pressures. From a set of initially existing contacts in a mechanically stable reference state the contact probability during vibration can be predicted by measuring the inter-particle potential before vibration. We explore the energy regions below particle rearrangement where our prediction is valid and discuss a physical mechanism for this behavior based on the exchange of potential and kinetic energy between particles.

Mechanically stable granular solids have force and torque balance on all particles. As such the contact network is robust; removing a single contact and the force balance is disrupted for the entire system. During vibration at appropriate energy ranges, contacts break and reform. It is reasonable to guess that the contacts in the solid break randomly, but we will demonstrate that this is not the case.

3.1 Reference State Properties

We define a reference state as a mechanically stable system of elastic particles as in figure 3.1. In this diagram the contact network is overlaid. We chose small systems with $N \leq 16$ to avoid floaters since they aren’t mechanically stable. For soft particles
there is a small overlap between contacting disks, $\delta_c$, where $c$ is an index over all the contacts in a packing. For the systems we investigated the overlaps are typically on the order of $10^{-7}$.

### 3.2 Vibration Protocol

From the reference state we subject this system to a small anisotropic perturbation and let the system evolve. The energy ranges of this perturbation are small enough so that the system doesn’t have any large scale rearrangements, but large enough so that there is contact breaking. For $\langle \delta_c \rangle = 10^{-7}$ energies from $10^{-12} < E < 10^{-5}$ or so are in this range. Some variation exists based on individual system features.
Since the system is entirely elastic the dynamics will continue indefinitely. Figure 3.2 is a 2-D histogram of a particle's center during simulation. The particle spends most of the time near its starting position, but occasionally travels out further. The trajectories of these forays can be seen in the loop-like structures towards the edge of the figure. The clear structure of the particle's motion demonstrates that the sampling rate is high enough to obtain good data.

Upon vibration we measure the time steps where the contact is activated. This quantity can be written as a matrix, where the rows are indexed over each contact from the reference state and the columns are indexed over time steps. This matrix, $M_{ct}$, is depicted in 3.3, where it is readily seen that different contacts are activated with varying frequencies and duration. In the following sections we will investigate
Figure 3.3: Contact matrix $M_{ct}$ measured for an N=12 system that has 21 contacts, each row corresponds to a contact found in the reference state, and each column is an individual time step in the simulation. The red lines represent the contact being activated at the time step and the blue lines represent a time step where the contact isn’t activated.

different statistics, and propose a method to predict their magnitudes based on the reference state of the system.

3.3 Contact Probability

Figure 3.3 shows that the frequency with which contacts are activated varies significantly. We can write the contact probability as $p_c$. Equation 3.1 shows how to
calculate $p_c$ from $M_{ct}$ where $t_{max}$ is the total number of time steps.

$$p_c = \frac{\sum_t M_{ct}}{t_{max}} \quad (3.1)$$

We are interested in finding what quantities from the reference state can be used to determine $p_c$. Figure 3.4 shows a plot of the contact probability vs. the reference state overlap for all particles in an N=12 system. This figure clearly demonstrates that within certain parameters there is a relationship between the two quantities, smaller initial overlaps are related to lower values of $p_c$ during vibration. We wish to describe this behavior, first by using a simplified 1-D model.
3.4 1-D Model

We can use a 1D approximation to model how the contact probability is affected by $\delta_c$. The top row in figure 3.4 shows three particles with the central particle having two contacts. Each contact, $\delta_1$ and $\delta_2$ has the same magnitude of overlap, $\delta_c$. In the second row, the central particle has been given some velocity, $v_c$. At the exact moment of contact breaking, $\delta_2 = 2\delta_c$. This means the central particle needs to be moved a minimum distance of $\delta_c$ to break a contact. We may use energy conservation considerations to find the minimum velocity the particle must be give to break its contact

$$v_{c_{\text{min}}} = \sqrt{\frac{k\delta_c^2}{m}}$$

(3.2)

Once contact breaking occurs, energy in the packing is spread among all vibrational modes and particle velocities are Gaussian. The probability that $v_c < v_{c_{\text{min}}}$ and the particle is in contact is then just

$$p_c(v_c < v_{c_{\text{min}}}) = \int_0^{v_{c_{\text{min}}}} e^{-\frac{mv_c^2}{2kt}} dt = \int_0^{\sqrt{\frac{mv_{c_{\text{min}}}}{2kt}}} e^{-t^2} dt = erf\left(\sqrt{\frac{k\delta_c^2}{T}}\right)$$

(3.3)

3.4.1 2-D Prediction

Our 1-D case, described in the previous section can be generalized to 2-D by using two different features. First, that once contact breaking occurs, energy in the packing is spread among all vibrational modes [25]. Second, that we can use our 1-D
Figure 3.5: A sketch showing the 1D case where the top system of 3 particles is in its static reference state and both contacts have magnitude $\delta_c$. In the bottom set the center particle has velocity $v_c$ and at the point just where the contact 1 is broken $\delta_2 = 2\delta_c$. In the sketch the distance between the non-contacting particles has been exaggerated to demonstrate that contact 1 has been broken.

approximation by looking at velocities along each contact.

From the bottom row in the simple 1-D case illustrated in figure 3.4 we see that just at contact breaking the additional energy stored in the second contact is equal to $\delta_c$.

In 1-D this is easy to visualize, all the contact breaking energy is stored in a single second contact, however for the 2-D case illustrated in figure 3.4.1 the energy from the first contact overlap is now stored in the additional two contacts to the left. The key idea is that regardless of contact interactions on the rest of the particle, $\frac{1}{2}k\delta_c^2$ is the minimum amount of kinetic energy required to break that contact. This energy is then spread to other contacts in the system, all modes of which are excitable. The second method required to generalize the 1-D case is by measuring only the component of a
Figure 3.6: Sketch of a 2D system, where the central particle is given a velocity \( v_c \) along the axis of contact 1.

particle’s velocity along it’s contact. For two particles, \( \vec{v}_i \) and \( \vec{v}_j \), the velocity along their mutual contact is

\[
\vec{v}_c = \left( (\vec{v}_i - \vec{v}_j) \cdot \hat{r}_{ij} \right) \Theta \left( 1 - \frac{\vec{r}_{ij}}{\sigma_{ij}} \right) \tag{3.4}
\]

From these two considerations we can still use equation 2.25 to make a prediction of \( p_c \), assuming that \( v_c \) is the quantity described in equation 3.4. The predictions are shown in figures 3.7 and 3.8, first over a range of energies, and second over two different configurations. Figure 3.7 shows the comparison over a range of energies. As expected at low vibration energy \( p_c \) is 1 for all contacts, and with increasing energy, \( p_c \) decreases. The prediction from equation 2.25 are the lines, where at higher energies the prediction becomes less accurate. Figure 3.8 shows a comparison between measured and theoretical values for two different configurations where there is a good
Figure 3.7: Contact probability vs $E$, where $\delta$ is weighted by the energy stored in the reference state, $U_0$ and the kinetic energy, $K$.

fit between measured value and theory.

### 3.5 Mean Contacts

For vibrated solids, a phase transition from an Iso-coordinated solid (ICS), meaning that there is no to a Hypo-coordinated solid (HCS) was found [18]. This transition describes a drop in the mean number of contacts, $\langle N_c \rangle$, from the number of contacts in the reference state to about half that amount. We wish to use our calculation of $p_c$ to predict this transition. We can use equation 3.1 to write $\langle N_c \rangle$ in terms of $p_c$ via
Figure 3.8: Measured $p_c$ (circles) and theoretical $p_c$ (lines) vs particle overlap for two different configurations, one in black and one in blue.

substitution and then compare our predicted value to the measured value.

$$\langle N_c \rangle = \sum_c \sum_t \frac{M_{ct}}{t_{\text{max}}} = \sum_c p_c$$  \hspace{1cm} (3.5)$$

Figure 3.9 shows this comparison, and for six orders of magnitude our technique predicts the measured value of $\langle N_c \rangle$ quite well. Beyond this range the contact network decouples from the reference state network, and additional techniques are required to predict its behavior.
Figure 3.9: Mean number of contacts vs E.
Chapter 4

Information Entropy in Granular Systems

Shannon entropy is the amount of information in a message received, typically given in bits [26]. Equation 4.1 is the Shannon entropy, where \( p_i \) is the probability of measuring event i.

\[
S = \sum_i p_i \ln p_i
\]  

(4.1)

The form of equation 4.1 is similar to the Gibbs entropy and this is no mere coincidence. There is a deeper relationship between thermodynamic entropy and Shannon entropy, primarily that as heat is added to a system the amount of information needed to describe all the potential microstates of the resulting macrostate increases [27]. This connection yields a novel means of finding the entropy of a thermodynamic system. The idea in [28] is if you had a simulation of an ideal gas at a certain temperature you could write the velocities of the molecules down in a list, compress the list and that set of numbers would be a file of a certain size. If you were to increase the temperature of your simulation and follow the same procedure; writing the velocities of particles and compressing them, the new file size would be larger by an amount proportional to the change in entropy of the system. If this is true, then you should be able to do the reverse; from the size difference of the compressed files it should be
possible to determine the temperature of the system.

Thinking of entropy in terms of information provides yet another approach to understanding statistical mechanics. In granular statistical mechanics however, the tools are more limited. Without knowing the probability of each microstate we can’t calculate the Fortunately, we do have access to compressed file sizes of granular systems. This chapter investigates using the technique outlined above to determine the entropy of granular systems. We will first show that file size from the simulation of an ideal gas can be used to determine the entropy, then we will use this same technique to find the entropy of a granular system.

4.1 Ideal Gas

To use our technique we first sample the velocity of ideal gas particles having a Boltzmann distribution. Next we calculate the entropy of an ideal gas as given by the Sakur-Tetrode equation

\[
S = kN \ln \left( \left( \frac{V}{N} \right) \left( \frac{U}{N} \right)^{\frac{3}{2}} \right) + \frac{5}{2} kN \left( \frac{5}{3} + \ln \frac{4\pi m}{3h^2} \right)
\]  \hspace{1cm} (4.2)

The plot in figure 4.1 shows a comparison between the internal energy, U and the entropy. Using the thermodynamic relationship in 4.3 the slope of this line is equal to the temperature. This assumption is indeed correct, the simulation was created for temperatures between 25K and 39K and the slope between the first and second point is 25.5, the average temperature the simulation was run at for those two points.
Figure 4.1: Plot of the internal energy vs. the entropy calculated for a simulated ideal gas, of N=128000, m=10^{-24} kg in the temperature range of 25K to 39K. From thermodynamic relationships, the slope of this line is the temperature.

The slope between the second and third points is 26.5, etc.

\[
\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_{V,N} \tag{4.3}
\]

With confirmation that using the Sakur-Tetrode equation is indeed the correct way to determine the entropy of an ideal gas we can next compress the velocity distributions at the same range of temperatures and compare these two quantities. This comparison is possible since each individual macrostate in the ensemble is determined by a unique energy. The entropy of the velocities that make up that macrostate are also unique then. To compress the files we use Huffman encoding. This technique works by
assigning a code to each value in the list, with the most frequently occurring value receiving the shortest code, the second most frequently occurring value taking the second shortest code, etc. [29] When calculating the entropy of our system using the file size we must choose a resolution to consider. Surely if we choose a greater number of digits per particle this would increase the amount of information stored. If we choose too small a resolution we could miss critical system behavior and the velocity distributions would appear nearly uniform. A balance can be struck between the system size and the resolution of the particles that captures the essential shape of a Boltzmann velocity distribution. Setting the number of particles several orders of magnitude larger than the number of significant figures gives a reasonable result. 4.2 Shows the result of a comparison between the entropy calculated using equation 4.2 and the entropy calculated using the file size of a velocity distribution. The slope is constant with a scaling factor $s \approx 0.58$.

### 4.2 File Size of Granular Systems

While Edward’s original approach to the statistical mechanics of granular systems has been described in [10], entropy and temperature measurements are furthered in [30]. This approach describes an ensemble, $\Omega(\Gamma, N, V)$ where $\Gamma$ is as written in equation 2.7, the internal virial of the stress tensor, $N$ is the number of particles and $V$ is the
volume. This ensemble proposes the following granular thermodynamic relationship

$$\alpha = \left( \frac{\partial S}{\partial \Gamma} \right)_{N,V}$$  \hspace{1cm} (4.4)

which is analogous to the familiar thermodynamic relationship described in equation 4.3. $\alpha$ is a temperature like quantity called the angoricity by Edwards. Similar to the cannonical ensemble, different subsections of a granular solid can be equilibrated by $\alpha$[31][30]. It is possible to calculate the entropy of a granular system and test its validity using equation 4.4. If the angoricity can be measured using the technique described in [30] and compared with the angoricity measured from equation 4.4 using
the information entropy, then it is reasonable to assume that this is a sound technique. A strength of the information entropy approach is that while the Gibbs entropy isn’t directly applicable to a granular statistical mechanics, the information entropy is; we are simply counting the information needed to describe the stresses in a packing. The next steps are to extract $\alpha$ from figure 4.3 by measuring the slope and compare it to the angoricity measured by the technique described in [30]
Chapter 5

Conclusions

Our work in this document primarily focuses on finding relationships between measured quantities of jammed granular materials. Quantities such as packing fraction, co-ordination number and stress are known to be indicative of how systems respond to strain and compression. We measured microscopic quantities like contact angle and distance between particles, and enumerated these quantities as a twenty type Delaunay triangle decomposition. Our aim was to relate the decomposition frequencies to measureable system values.

Key findings that microscopic quantities like contact angle and distance between particles in a packing are important indicators of observed quantities. Our supposition that any angular space on a particle in a bidisperse packing is occupied randomly allows the techniques we use to work. Segregated, dilute or compressed systems would surely change measured probabilities.

While there are a number of important quantities we can predict, some quantities are notable by their absence. Equiprobable microstates are a hallmark of statistical mechanics but granular solid microstates have probabilities that are many orders of magnitude different from each other. Variations in decomposition subunits are a promising quantity to investigate; a packing with triangle distributions far from mean
values may have correspondingly rare microstate probabilities. From our studies, it is not trivial to relate the triangle decomposition to microstate probabilities. In addition to measuring static states we also investigated vibrating systems at contact breaking. Vibrations were shown to not be random, and a theory for their occurrence was created. Over many orders of magnitude this model fits well. At higher energies the prediction diverges.
Chapter 6

Future Directions

6.1 Evolution of Triangle Decomposition During Jamming and shear

Apart from our vibrated systems, we have used the triangle decomposition on purely static systems. We wish to study dynamic systems undergoing compression and shear as well. As a packing forms there are no particle contacts, and the Triangle decomposition would consist entirely of non-contact triangles. This state continues from system initialization until just past jamming. At any small compression above jamming the contact network forms and the decomposition will have the subunit frequencies we have described in chapter 2. We wish to study the triangle types as the system compresses and use them to predict triangle probabilities above jamming. Figure 6.1 illustrates the triangle decomposition at three different levels of compression.

The distribution of triangle types evolve as systems are jammed by compression or as they are sheared. We analyze the statistics of the triangle types and identify specific transition events during compression, jamming, and shear.
Figure 6.1: The figure on the left shows a three by three tiling of a dilute $N=16$ particle system with the Delaunay triangle decomposition overlaid. The middle figure shows a percolated system, particles coming into contact with each other, but rearrangements still possible. The final image on the right shows the decomposition for a jammed system.

6.2 Effective potential of a Vibrated Particle

Non-zero interparticle potentials given by equation 1.3 require particle overlap. For a static system, any point a distance greater than a radii away from the center of every particle would have zero potential. Due to vibrated particle motion however, the edges of each particle can be found outside the static particle region. This means that in vibrated systems particles can interact in areas that previously had zero potential. A future goal is to find an expression for the effective potential, $V_{eff}$ as a way to measure time averaged system response for granular solids in the HCS regime.

From figure 6.2 we see two regions, region I is the space around a particle where the particle is always found. In this region the potential will be similar to that in equation 1.3. Region II is the space beyond region I where the particle is only sometimes
Figure 6.2: A time averaged sketch of two vibrating particles next to each other. The edge of a vibrated particle will always be found outside region I and inside region II. The distance between region I and region II is temperature dependent, and with decreasing temperature region I expands and region II contracts until they both rest on the reference state particle edge. In this sketch the particles are slightly overlapping in region II.

found. Outside of region II, the particle is never found. The general expression for the effective potential is

\[
V_{\text{eff}} = \left( \bar{\epsilon} + \frac{\hat{\epsilon}}{2} \right) \Theta(1 - \frac{\hat{r}_{ij}}{\bar{\sigma}_{ij}}) + \bar{\epsilon} f(r_{ij} - \hat{\sigma}_{ij}) \Theta(1 - \frac{\hat{r}_{ij}}{\bar{\sigma}_{ij}}) \Theta(\frac{\hat{r}_{ij}}{\bar{\sigma}_{ij}} - 1) \tag{6.1}
\]

where \( \hat{\sigma}_{ij} \) is the mean width of region I for particle i and j as depicted in figure 6.2 and \( \bar{\sigma}_{ij} \) is the mean width of region II for particle i and j. \( \bar{\epsilon} \) is the vibrational energy scale, i.e. the energy required to press two particles together so that only a linear spring interaction potential remains, this means that \( \bar{\epsilon} \) is a function of temperature. \( \epsilon \) is the total energy scale of the system. The key then is to find the functional form of \( f(r_{ij} - \hat{\sigma}_{ij}) \). This can be measured by looking at histograms of a particle’s distance from it’s reference state position and relating \( f \) to one minus the cdf of this histogram.
Figure 6.3: Histogram of a vibrated particle’s displacement from its reference state. The small bump around \((r - r_0)/r_{\text{max}} = 1\) comes from the particles slowing down at collision. This effect can be more or less pronounced in different particles.

and using this quantity as a weighting function for the regular linear spring potential. Figure 6.2 shows the shape of this distribution, a time averaged distance of the particle from it’s central position. The bump around the maximum value is from particles slowing down at the height of their collisions. This effect can be seen in the center particle histogram in figure 3.2. With \(V_{\text{eff}}\) in hand, it will be possible to determine other time averaged, or bulk system quantities without measuring dynamics.
Bibliography


