ABSTRACT

HUANG, YUMING. A Community Detection Method for Force Chain Characterization in Three Dimensional Granular Packings. (Under the direction of Karen E. Daniels.)

This thesis reports studies of a community detection method which extracts force chains in three-dimensional granular packings, and characterizes the influence of varying the confining pressure and interparticle friction coefficient. Using the molecular dynamics software LAMMPS, we generate 3D granular packings by simulating particles slowly poured into a container and we extract the particles’ positions and contact forces. The simulations are performed over a wide range of pressure $P$ and friction coefficient $\mu$ values. To partition the data into force chain communities, we use a community detection method called modularity maximization, building on recent techniques developed for two-dimensional packings. The size and shape of these communities depends on a resolution parameter $\gamma$, and we find that the method used to select the optimal $\gamma$ in 2D does not extend to 3D. Therefore, we develop a new quantity, the hull ratio, to characterize the shape of the communities and thereby select the optimal $\gamma$. This method successfully extracts community structures that resemble force chains.

To study the influence of the pressure and the friction coefficient, we use three network properties – size, network force and hull ratio – to characterize the force chain communities. We find that the size and the network force of the communities exhibit an approximately linear relationship with each other, and that the cumulative distribution functions (CDF) are approximately exponential. Through observing changes in the CDFs of size and network force, we observe that $P$ and $\mu$ influence the homogeneity of the packing. When $P$ and $\mu$ are both small, increasing either of them will reduce the gravity-induced inhomogeneity. For high friction particles ($\mu > 0.3$), increasing $P$ makes the system more homogeneous.
below $P = 10^{-5}$ (measured in units of the elastic constant), but less homogeneous above. At these high values ($P > 10^{-5}$), increasing $\mu$ makes system even less homogeneous. By observing the vertical distribution of vertical and horizontal components of the normal contact forces, we see an increase of horizontal force at high $P$ and high $\mu$. This effect is distinct from the Janssen effect due to the periodic boundary conditions at the sidewalls. By comparing the distributions, we find that the change in horizontal force significantly influences the community structure. We observe that the CDF of the hull ratio is $\mu$-sensitive only when $P > 10^{-5}$, while the CDF of the hull ratio becomes steeper with increasing $P$ at all $\mu$ values. Therefore, we identify $P = 10^{-5}$ as a crossover point which roughly corresponds to homogeneous packings. These studies show that community detection methods can extract force chains in 3D granular packings, and that characterizing them with network properties reflects the system’s response to different pressure and friction coefficients.
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A Community Detection Method for Force Chain Characterization in Three Dimensional Granular Packings

by

Yuming Huang

A thesis submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the requirements for the Degree of Master of Science

Physics

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APPROVED BY:

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Keith Weninger              Hong Wang

__________________________
Karen E. Daniels
Chair of Advisory Committee
DEDICATION

To my parents.
BIOGRAPHY

The author was born in a small town but grew up in big cities. He always loves exploring unknown fascinating things.
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I would like to thank my advisor, Karen Daniels for her guidance and much help for my research, and great enthusiasm.

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CHAPTER

1

INTRODUCTION

Force chains in granular system are important structures that provide structural support and transmit acoustic waves. Yet we still don't have a universally accepted method to characterize force chains. The purpose of this thesis is to study the force chain structure of 3D granular packings, by means of combining simulations and a community detection method. The goal has two parts, one is trying to extract force chains from granular packings, the other is to use these force chains to study the influence of friction coefficients and pressure on the packings.

In this chapter, I will first introduce some general properties of granular material. Then, in order to lead to our topic of force chain characterization, I'll discuss contact force, both in theory and experiment aspects. After that, I'll introduce some statistical and topological
research about the force structure, as well as people’s endeavors trying to identify force chains. Then I’ll discuss the applications of network science to granular systems. Finally, I’ll do an overview of my work, including the questions to be answered.

\section{Granular System}

Granular systems, as complex systems, exhibit diverse attributes and phenomena under different circumstances \cite{Jae96}. For example, granular systems can be like solid when it's sand on the beach, because people can step on it like rocks. It looks like liquid when you put the same sand in a hourglass and let the sand flow. It can also be like gas when you shake a container full of granular particles hard enough. The complexity is more than that, a particle system with two sizes will segregate when shaken, and big particles will usually climb towards the top \cite{Ros87}. Jamming happens when system gets higher density and load \cite{Hec10}.

The complexity is reflected by granular particles usually being disordered in position, as well as the contact forces between them. The disorder makes the mesoscale structure of particles very complicated. Some patterns, usually called force chains, are found when visualizing force structure, as Figure 1.1. These are known as important structures for system stability \cite{How99} and acoustic transmission \cite{Owe,Som05}. While some research \cite{Pet05,Zha13,Gen15} has been conducted to study force chain structure, there's no universally accepted definition or quantitative description of it. In this thesis, I’ll follow a recently developed technique Bassett et al. \cite{Bas15} which addresses this problem, and check the influence of pressure and friction coefficient on the properties of force chains.
1.2 Contact Force

1.2.1 Hertzian Contact Model

A widely used and accurate model for the normal contact force between granular particles is the Hertzian contact model \([LL] [JJ87]\). The contact force is proportional to deformation (in real situation) or overlap (in simulations). The equation goes as:

\[ f = \alpha \delta^\beta \]  

(1.1)

where \( f \) is the contact force, \( \alpha \) is a constant depending on specific materials, \( \delta \) is the deformation (experiment) or overlap (simulation), with units of length, and \( \beta \) is a constant depending on geometry (usually \( \beta = 1 \) for disks and \( \beta = 3/2 \) for spheres.) My simulation (Chapter 2) adopts a Hertzian model to calculate the contact force according to the particles’
relative position. The accuracy [Che06] of this model helps my simulation runs in a reliable way and yields realistic data.

1.2.2 Contact Force Measurement

In 2D, where particles are disks on a plane, Majmudar et al. [MB05] use photoelastic disks between two crossed circular polarizers to visualize internal stress and obtain contact force information, as Figure 1.1A. Puckett et al. [Pucb] [PD13] use the same principle to develop techniques to locate and detect interparticle forces accurately, have provided a open-source copy of the code [Puca].

The photoelastic method becomes impractical in 3D, as Figure 1.1 B, because the light pattern is influenced by other particles in between. However, other techniques were invented to tackle this problem. Some measure the normal contact force between a particle and the container walls [Liu95] [Mue98] [Bla01] [Mue02]. These studies apply the carbon paper technique, which is based on the relationship between the normal force and the darkness of the carbon mark created by pressing on carbon paper.

However, the measurement of interparticle forces inside the bulk has been very challenging. Sanfratello et al. [San09] measure the internal force chain structure within a dry assembly of granular particles by MRE (Magnetic Resonance Elastography) technique. This technique measures the displacement amplitude of periodically vibrating nuclei. They send low amplitude mechanical vibration through a 3D packing of NMR sensitive oil-filled pharmaceutical particles. Presuming the vibration amplitude along the force chains is the strongest, they show the force chain structure by imaging the amplitude of displacements.

Many [Bru03] [Zho06] [Saa12] [Bro15] [MP11] use 3D imaging techniques, such as to-mography and confocal microscopy, to scan for positions and shapes of 3D soft particles,
and hence calculate contact forces using contact theory. Brujić [Bru03] takes 3D images of compressed emulsion droplets using a confocal laser scanning microscope. The droplets are submerged in a refractive index-matching fluid, so they can scan a sequence of 2D images at different planes and combine them into 3D images. They calculate contact forces based on the contact areas from processing the images. Using the same method, Zhou et al. [Zho06] measure contact forces between 3D frictionless liquid droplets. They obtain high resolution 3D images of droplet surfaces using confocal fluorescent microscopy, enabled by the fluorescent nanoparticle layer. They also calculate the contact forces between droplets by measuring the size of contact area in the images. Mukhopadhyay et al. [MP11] and Brodu et al. [Bro15] use similar refractive index matching tomography to construct the geometry of packings of deformable hydrogel particles. While Mukhopadhyay et al. [MP11] get the normal force values, Brodu et al. [Bro15] are able to get normal contact forces in vectorial detail (including the directions) using a dedicated algorithm. Saadatfar et al. [Saa12] use X-ray tomography on the packing of soft rubber balls. They measure the internal geometry of the packing and the resolution is enough to tell the shape change and contact areas, and thus calculate contact forces.

Simulations are more practical for getting force data. Another advantage of simulation is that it is much easier to have everything in control and get numerically accurate data. Silbert et al. use LAMMPS (the molecular dynamics program used here) to simulate sphere packings and obtain geometry information at different friction coefficients [Sil02a] [Sil02b]. By comparing the distributions of normal contact forces, their simulation data fit well with experimental data, if smallest forces are not taken into account. This indicates there's still a considerable influence of the limit of resolution in experimental measurements.
1.3 Force Structure and Force Chain

In most situations, the positions and directions of contact forces are disordered in space (see Figure 1.1). Aside from measuring the forces, another problem is how to describe the complex force structure.

1.3.1 Statistical Description

In such a complex system, statistical descriptions of individual forces are a natural way to describe force structure. Silbert et al. [Sil02b] use 3D simulations to measure the distribution of particle-particle and particle-wall contact forces and find an exponential-like decay of the distribution at large forces. They also measure contact angles and contact numbers, and the result shows a weak influence of friction on force distribution, force correlation, contact geometry and contact network. Some other studies [Mue98][Bru03][MB05] also examine the force distribution in granular packings by experiments, and find exponential distributions for forces larger than the average.

Snoeijer et al. [Sno04] proposed a force network ensemble method to study 2D hard disk packings. This method samples all the possible force network configurations by considering constraints of force equilibrium. In this way, they can establish realistic force distributions as compared to MD simulation, and they use this method to study the force network anisotropy under shear.

However, the statistics of individual forces does not describe how particles with strong forces connected, i.e. shape and property of the force chains, which are discussed next. In this thesis, we will address the characterization of these mesoscale structures in granular packings.
1.3.2 Force Chain Identification

Force chains are the chain-like structures in a compressed particle system that provide structural support and transmit acoustic waves. Their study may influence our understanding of granular system stability, such as in the context of sandpiles. Force chains can be seen as the connection between individual pairwise interactions, and bulk properties of the system. In order to describe the force structure, many researchers tried to continually develop the idea of force chain, which is a well-known phenomenon that lacks a commonly accepted definition.

Some groups [Pet05][Zha13][Gen15] studied methods to identify individual force chains in 2D granular systems. Some [Pet05][Zha13] choose to describe the rules for how particles in a force chain should be connected and create an automated process for that. First, they set a force threshold to exclude unimportant particles, then decided how forces on the force chains should be aligned. Therefore, they use force orientations to determine the alignment and hence whether a particle is in a force chain. Some studies [Sil02b][Ost06][Kon12] use the force cutoff idea to extract the force chains for further analysis. This method is based on some artificial choice, such as setting force threshold and determining the angle for alignment. Setting a threshold will possibly filter out some weak forces which could be essential in a stable force structure, because a linear chain of particles with strong forces cannot be stable without small supporting forces from the side [Rad98]. This kind of method assumes some phenomenological features of force chains, without digging into the intrinsic characteristics.

Gendelman et al. [Gen15] propose a formalism to solve for the forces in a packing when external forces and orientations of contacts are known. They represent the packing by a matrix, where contact forces are eigenvectors. They describe force chains as large forces...
that provide a rigid tenuous network. They defined an operator to determine the force chains. This idea of tenuous network is similar to our idea of ellipsoidal sparseness and hull ratio introduced in Chapter 3.

1.4 Networks

Granular systems can also be described by networks. In fact, a lot of real-world systems can be represented as networks, such as the internet, human society, and neural networks [New10]. The common character of these systems is that they are composed of individual parts and these parts are linked in some way. In the language of network science, these individual parts are called nodes and the links are called edges. In the internet, computers and other devices are the components and the data transportation between them are the links. In human society, people can be regarded as components of the network, and their relationships are the links. In neural networks, neurons in the brain are components and electrical connections between them are a physical network. In granular systems, especially in granular packings which we care about, grains are the individual parts and the contact forces between grains are regraded as links.

Granular networks are different from networks such as internet and social networks, in that topological information is not enough to fully describe granular networks. Granular networks are classified as spatially embedded networks [Bar11], where nodes and edges have geographical constraints. For example, one particle can only have contact forces with limited number of neighboring particles.

Network science has been used to characterize granular systems for various purposes [WT10][WT12][Kon12][Her11][Nav10][Nav14][Bas12][Bas15]. Walker et al. [WT10] address 2D quasistatic packings from DEM simulations as complex contact networks. They studied
statistics of network properties: degree, clustering coefficient, betweenness centrality, subgraph centrality and network bi-partivity and L-expansion networks, as the system evolves in response to deformation (external loads). They [WT12] also build a taxonomy of granular rheology by identifying groups of particles with similar properties.

Kondic et al. [Kon12] use a topological invariant called the zeroth Betti number $B_0$ [Kac04] to characterize the force network. In 2D simulated disk packings, they found the force chain networks are strongly influenced by friction and by particle size polydispersity because of the vanishing of crystalline order. They also show the size of connected particle clusters decreases when the jamming transition happens, and when the packing fraction (or pressure) is continually increased.

Herrera et al. [Her11] use the broken-links network to capture the dynamics of the granular flow and track the fracture events. They established a time evolving network and found the fracture caused by shear is reflected as the formation of a giant component in the broken-links network.

Navakas et al. [Nav10][Nav14] analyzed the force network by using a graph community detection method to identify force clusters. In this way, they found clusters with particles that are densely connected by force, and the sizes of those clusters increases with increasing pressure [Nav10]. They also tried several well known community detection methods such as edge betweenness, walktrap, infomap and label propagation [Nav14]. They compared the detection results, but the clusters have a bulk shape which is different from force chains Figure 1.1.

Similarly, Bassett et al. [Bas12][Bas15] treat granular packing as a network and utilize a community detection method. They test a big list of network properties on experimental disk packings [Bas12]. However, here they get bulk shape communities similar to Navakas et
al. [Nav10] [Nav14]. In an effort to identify force chain, different from Navakas et al. [Nav10] [Nav14], they made use of the information of the contact network using a geographic null model [Bas15], and they managed to extract chain-like structures in 2D disk packings (see Figure 1.2). One of the advantages of this method compared to setting thresholds is that some small forces can be included in the force chain communities detected. They also find the network properties distinguish different pressures, the presence of friction, and whether the data is from experiment or numerical simulation. Since my method is based on this approach, related concepts and details of this method will be readdressed in Chapter 3.
Figure 1.2 A. experimental picture. B. detected communities. C. Maximizing Gap-factor to decide resolution. Figure reprinted from [Bas15].
1.5 Overview of This Paper

Following Bassett’s method [Bas15], in this thesis we apply the community detection method to 3D granular packings generated by molecular dynamic simulations. Some criteria that are useful in 2D seem to be less useful in 3D and we adapt the original method in order to improve the results. In order to test whether this method is helpful to study the effect of friction and load pressure, we also take the advantage of extracted force chains to examine the system behavior while changing the friction coefficient of the particles and pressure above the packing.

In Chapter 2, we describe the simulation environment and the specific settings. Each step of operation in the simulation is explained. We also describe and show what raw output data would be like, which is helpful for understanding the data processing in the next chapter.

In Chapter 3, we first introduce some basic knowledge about network science, then we describe in detail about the network analysis technique we used, including the method developed by Bassett et al. [Bas15], and the modifications we made for our 3D packings, especially the concept of hull ratio. We are able to extract force chains from 3D packings.

In Chapter 4, we will look at the influence of pressure $P$ and friction coefficient $\mu$ on the force structure of the packing, using the force chains we detected. We find non-monotonic dependence of network properties on pressure at large friction coefficient and that the dependence on friction coefficient is opposite at low and high pressure. We use how pressure and friction coefficient influence the homogeneity of the packing to explain these observations. We also examine the distribution of the horizontal and vertical components of normal contact forces along $z$ axis, and the influence of $P$ and $\mu$ on hull ratio CDF.
Although measuring forces in 3D granular packings has been challenging, researchers have been successful in measuring them in different ways [Bru03][MP11][Saa12][Bro15], as we introduced in section 1.2.2. Having those 3D force data available, we are motivated to develop our analysis method and adapt it to 3D situation. We take advantage of computer simulations to generate data as it enables us to get high precision data on both forces and positions. In order to mimic pouring granular particles into a container, we use the molecular dynamics simulation software LAMMPS [LAMa] to generate packings of hard particles. We extract contact force and particle position data and use it to study force chains. Details of the simulations are included below.
2.1 LAMMPS

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is an open-source software based on a fast parallel algorithm [Pli95] for molecular dynamics (a computer simulation of atoms that numerically solves Newton’s equations of motion). It is maintained by Sandia National Labs. LAMMPS runs from an input script with output that is highly customizable and features many different functions. LAMMPS is widely used by researchers for various topics [Hat12], for example, granular flow [Sil01] and phase change of a thin gold film [SM07]. I utilize LAMMPS for a few features [LAMa] that are useful for my work. LAMMPS runs on a single core or in parallel, so I can either speed up the simulations using a 8-core server or I can avoid complexity introduced by parallel computing by using just a single core.

Another advantage is that, although LAMMPS is a molecular dynamics software, it supports many particle model types, including granular materials. I also have some inter-particle interactions to choose from, including Hertzian and Hookean models for granular materials. Here I use the Hertzian contact model because one of its main predictions (the hemispherical pressure distribution in the contact area) has been verified for hard materials [Che06], and Hertzian model is suitable for polydisperse systems [LAMc]. I can assign names for operations and objects and call them, which makes it possible to set up complex environments and operations. LAMMPS also has many built-in quantities, like translational and rotational kinetic energy, helpful for evaluating the system.
2.2 Simulation Settings

The simulations were set to run on the HPC (High Performance Computing) service at NCSU. For each specific friction and pressure setting, the simulation runs 20 times with different random initial conditions (for details about pouring particles, see section 2.2.2) to get different packings. I average the results, and I also look at variations between the runs.

2.2.1 Model Settings

LAMMPS offers several unit styles to choose from [LAMd], which determine the units for all input and output quantities. For convenience, we use the style $lj$ where all quantities are unitless. In style $lj$, LAMMPS sets the fundamental values of three quantities (mass, distance, energy) to be 1. The actual values of these quantities are expressed as multiples of the fundamental values. Here, we set the diameter of small particles to be 1 (see Table 2.1), which means it is equal to the unit length, therefore the dimension of the simulation box can be regarded as multiples of small particle diameter. For another example, the units of pressure, which are used in both pressure and elastic constants, are $\text{energy/distance}^3$. If we want to convert the units of pressure into physical ones, we just specify the unit of energy and distance we want to use. If the unit of energy is joule and the unit of distance is meter (which makes the diameter of small particles 1 meter), then the unit of pressure (or elastic constants) is Pascals. The specific settings we used are listed in Table 2.1.
2.2. SIMULATION SETTINGS

Here, I give some notes on the choice of some parameters. For the choice of elastic constant $K_n$, if my unit for energy is joule and for length is centimeter (the unit can be in any order of magnitude without loss of generality), then the elastic constant $K_n$ will correspond to a Young’s modulus of $2 \times 10^5 \text{J/cm}^3 = 2 \times 10^5 \text{J/m}^3 = 2 \times 10^{11} \text{Pa}$. This value is close to $Si_3N_4$ (280 - 310 GPa) and Ruby ($Al_2O_3$, 215 - 413 GPa), and harder than glass ($SiO_2$, 50 - 90 GPa).

The choice of $K_t = 2/7K_n$ is to make the periods of tangential and normal oscillation equal [Shä96], which makes collisions in simulation similar to experiment. The friction coefficient $\mu$ ranges from 0 to 3, spaced at logarithmic intervals. This range contains extreme conditions as well as common materials, so we can see how systems behave with very low and very high $\mu$. The pressure is bounded to make sure particles are not pushed outside the lower face due to high pressure given timestep=0.001. The magnitude of pressure in units of elastic constant $K_n$ is just below that reported in a recent paper [Owe], which ranges from $2.7 \times 10^{-4}K_n$ to $5.9 \times 10^{-3}K_n$.

2.2.2 Operation

We can see a simple illustration of the operations in Figure 2.1. First, I pour bi-disperse particles into the container through a sieve (random position), without forming a heap. In LAMMPS, I define a volume at the top of the container and generate particles at random positions within it, then let the particles drop. This method mimics pouring particles through a sieve to prevent the formation of a conical heap [Sil02a]. The pouring rate is very slow so as to make the packing as dense as possible. The pouring rate is controlled by setting the fraction of the insertion volume occupied by generated particles for each pouring attempt [LAMb]. The larger the volume fraction, the more particles generated, and
thus the faster the pouring rate. The insertion region generates particles until a set number is reached.

Figure 2.1 A simple illustration of the simulation: first generate a packing of bidisperse particles, then add a slab on top and apply pressure, then add more pressure on it. The lower row shows that the output information is basically the force network (forces less than 5 is not drawn for clarity).
Table 2.1 Settings of the model

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>atom style</td>
<td>sphere</td>
<td>attributes include diameter, mass and angular velocity, as well as coordinates, velocities, atom IDs and types</td>
</tr>
<tr>
<td>boundary condition</td>
<td>side walls are periodic, lower face is non-periodic</td>
<td>lower face has fixed position, particles lost if outside the lower face</td>
</tr>
<tr>
<td>dimension of simulation box</td>
<td>15×15×26</td>
<td>length×width×height</td>
</tr>
<tr>
<td>pairwise interaction</td>
<td>Hertzian model</td>
<td>see following 3 rows</td>
</tr>
<tr>
<td>elastic constant for normal contact, $K_n$</td>
<td>200000 [Sil02a]</td>
<td></td>
</tr>
<tr>
<td>elastic constant for tangential contact, $K_t$</td>
<td>$2/7 K_n$ [Shä96]</td>
<td></td>
</tr>
<tr>
<td>friction coefficient, $\mu$</td>
<td>0, 0.01, 0.03, 0.1, 0.3, 1, 3</td>
<td></td>
</tr>
<tr>
<td>timestep</td>
<td>0.001</td>
<td></td>
</tr>
<tr>
<td>gravity</td>
<td>1 force/mass</td>
<td>default for granular system</td>
</tr>
<tr>
<td>bi-disperse particles diameters</td>
<td>1 and 1.4</td>
<td>the diameter of small particles is equal to the unit length</td>
</tr>
<tr>
<td>particles quantities</td>
<td>1500 particles of each size</td>
<td></td>
</tr>
<tr>
<td>pressure</td>
<td>$0, 10^{-6}K_n, 3 \times 10^{-6}K_n, 10^{-5}K_n, 3 \times 10^{-5}K_n, 10^{-4}K_n$</td>
<td>in the unit of elastic constant for normal contact $K_n$</td>
</tr>
</tbody>
</table>
2.2. SIMULATION SETTINGS

As shown in Figure 2.2, I tested different insertion volume fractions to see how it influences the average number of neighbors. We can see that below an insertion volume fraction of 0.02, I get relatively high and consistent average number of neighbors. For all results presented, I set the pouring rate at an insertion volume fraction of 0.005, which generates about only one particle at each attempt. Since the average number of neighbors decreases with increasing friction coefficient [Sil02b], pouring at such a slow rate can keep the average number of neighbors constant and produces similar configurations, even if I use high $\mu$. Thus, I can study the influence of different $\mu$ under similar initial conditions.

Second, after all the particles are settled at the bottom of the container, I let the kinetic

Figure 2.2 Influence of the insertion volume fraction (related to the pouring rate) on the average number of neighbors. Higher volume fraction means higher pouring rate, and higher average number of neighbors generally means higher packing density.
energy per particle dissipate until it is less than $10^{-8} mg d$ [Sil02a]. Then, I output the position and force information (see section 2.2.3) as the data for $P = 0$.

Third, in order to change the pressure setting of the system, I generate a slab whose size is $15 \times 15 \times 2$, just above the top of the packing. The slab is defined by assembling small particles into an FCC lattice (see the blue slab in Figure 2.1). Then, I apply lowest pressure ($10^{-6} K_n$, see Table 2.1) on the slab to generate the same pressure on the packing, noting that the slab does not have other forces (including gravity) acting on it. After the kinetic energy of the system has dissipated, I increase the pressure value to the second lowest pressure ($3 \times 10^{-6} K_n$, see Table 2.1), then iterate this process and output data at each step until the highest pressure is reached. Thus in a single simulation I can get results at all pressure settings.

### 2.2.3 Output Data

The output data consists of two parts. The first contains local pairwise quantities. This includes atom IDs for each pair of interacting particles, the normal force vector between them, and the tangential force vector between them. The second contains information about each particle: ID, position vector, and the diameter of the particle. Examples of them are shown in Table 2.2 and Table 2.3. Table 2.2 shows a list of neighbors of particles, where the first column is the index of each row. The second and the third columns (corresponding to $c_2[1]$ and $c_2[2]$) are the ids of particles. The three columns corresponding to $c_3[1]$, $c_3[2]$ and $c_3[3]$ are the x, y and z components of normal contact force vectors. The last three columns corresponding to $c_3[4]$, $c_3[5]$ and $c_3[6]$ are the x, y and z components of tangential contact force vectors. Note that in row 4, the force values are all 0. This is because particles are treated as neighbors when they are closer than a specified distance which is a
little longer than the force cutoff. In our case, particle 65 and particle 108 are neighbors but not in contact. Table 2.3 shows a list of all the particles, where the first column shows the ids of particles, the middle three columns corresponding to \( x, y \) and \( z \) are the position vectors of the particles, and the last column shows the particle diameters.

Table 2.2 Sample data from the output file for pairwise information

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
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<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>1 46 65 -14.4408 -1.73337 2.9603 0.648219 1.08313 -1.5457</td>
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<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 46 145 22.2426 -2.69027 -14.592 0.788377 1.31765 -1.8813</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3 65 47 -10.8768 -2.21656 -2.22983 -0.715678 0.569354 2.925</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 65 108 0 0 0 0 0 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5 65 166 -0.0681029 -7.65785 -46.7409 -1.15332 0.917766 4.71273</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6 47 16 -12.9036 -6.82698 2.41374 -0.273674 -0.527492 3.32648</td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

Table 2.3 Sample data from the output file for particle information

| ITEM: ATOMS id x y z diameter |
|------------------------------|-----------------|-----------------|----------------|----------------|
| 46 1.05262 0.251098 0.648406 1.4 |
| 65 2.21797 0.391439 0.411366 1 |
| 47 3.36883 0.62608 0.646522 1.4 |
| 17 7.04078 0.296019 0.619274 1.4 |
| 32 11.4542 0.333379 0.629475 1.4 |
| 157 14.0718 0.487367 0.6318 1.4 |

After removing header lines, I can treat output files as column vectors to import them into MATLAB. To convert the raw data into the format for the community detection code [Ind], I assemble information for particle index and pairwise force into weighted adjacency matrices (will be introduced in Chapter 3).
CHAPTER

3

NETWORK ANALYSIS

3.1 Communities in Networks

Many real-world complex systems can be described as networks [For09], including social networks, neural systems and granular packing. By describing these systems as networks, we treat them as assemblies of nodes and edges. For example, each person in a social network is a node and the relationship or intimacy between two persons is the edge connecting these two nodes. In the granular packings that we are interested in, each particle is considered as a node and the edge encodes the normal contact force between them (see Figure 3.1).

Typically there are community structures in a network. In a social network, people in
the same interest group may interact more often, for example they might join the same event or mention each other very often, and they can be identified as being in the same community. Similarly, in granular packing, particles with strong contact forces may be considered as being in the same community. Since the force chain structure is the main structure that bears the load of the system [How99], the particles in a force chain have strong contact forces with each other, which we can see from the photoelastic picture in Fig 1.1. Therefore, if we detect the community structure in the granular network and those communities follow force chains, we will be able to extract force chains. That is one of the goals of this thesis.
In order to perform community detection (a type of clustering), we use published techniques [Bas15] to find closely connected particles. First of all, we represent the particle network as a weighted adjacency matrix $W$, with each edge weighted by the normal contact force (see Figure 3.1). Note that we record both normal contact forces and tangential contact forces, but only include normal contact forces in determining the communities. $W$ is a $N \times N$ matrix where $N$ is the number of particles. If particle $i$ and particle $j$ are in contact with a normal contact force equal to $f_{ij}$, the element $W_{ij}$ is $f_{ij}/\bar{f}$. In the network perspective, $W_{ij}$ is the weight of the edge between node $i$ and node $j$.

One of the popular methods of community detection is modularity maximization, developed by Newman [New04]. Using modularity maximization, we can determine communities with high internal edge weights, which are regarded as high quality community structures. Recently, this method was successfully applied to 2D disk packings for force chain extraction, with a little modification [Bas15]. We will follow this method and see how it works in 3D. Modularity $Q$ is defined as:

$$Q = \sum_{i,j} [W_{ij} - \gamma P_{ij}]\delta(c_i, c_j)$$  \hspace{1cm} (3.1)$$

where $\gamma$ is a resolution parameter. $c_i$ and $c_j$ are community assignments for particle $i$ and $j$. If $c_i = c_j$ (particle $i$ and particle $j$ are assigned in the same community), then $\delta(c_i, c_j) = 1$, and vice versa. $P_{ij}$ is the expected weight of an edge of a specific null model.

The widely used NG null model [NG04] [New04] assumes all nodes can connect to each
other, which makes the null model:

\[
P_{ij}^{NG} = \frac{k_i k_j}{2m}
\]

(3.2)

where \(k_i\) is the weighted degree of node \(i\), i.e. the sum of all the edges linked to node \(i\), and \(m = \frac{1}{2} \sum_{i,j} W_{ij}\) which is a normalization factor. Since it assumes all the nodes can be connected to each other, the NG null model is the expected weight of edge between node \(i\) and \(j\) if all the nodes are randomly linked.

Prior use of the NG null model [Bas12] [Nav10] on 2D disk packings led to "compact" or "bulk-like" community structures. For granular packings, it is unlikely that a particle can be in contact with more than a few particles, therefore the assumption of NG null model cannot be met. If we include physical constraints in the null model, we have the recent geographical null model [Bas15] that produces force-chain-like communities:

\[
P_{ij} = \bar{f} B_{ij}
\]

(3.3)

Since \(W_{ij}\) is already normalized, here \(\bar{f} = 1\). \(B_{ij}\) is the element in binary adjacency matrix, which corresponds to weighted adjacency matrix; specifically:

\[
B_{ij} = \begin{cases} 
1, & W_{ij} \neq 0, \\
0, & W_{ij} = 0.
\end{cases}
\]

(3.4)

\(B_{ij}\) indicates whether two particles are in contact. If two particles \(i\) and \(j\) are in contact, \(B_{ij} = 1\), otherwise \(B_{ij} = 0\). There can be an edge between two particles only if they are in contact, which is an important constraint on the network structure. Thus we use \(P_{ij}\) as our null model for modularity maximization.

Modularity maximization gives us a high quality community assignment. However, it is
3.2. MODULARITY MAXIMIZATION

a NP-complete problem and will take too long to find the global maximum of \( Q \) if there are too many particles. Here we use a greedy heuristic algorithm code [Ind] designed for community detection to find an approximate maximum of \( Q \) within a reasonable time. Instead of going through all possible combinations, this type of method tries to find a better combination during each trial. The disadvantage of this method is that we can not guarantee a global optimized result, and in extreme situations it can give a very bad result (although this is not likely to happen on real world data). Therefore, we will discuss the stability of this optimization method in Appendix A. Finally, we perform \( Q \) maximization at different resolution parameters \( \gamma \) ranging from 0.01 to 3.

Figure 3.2 shows the result of community assignments after optimizing \( Q \) at different \( \gamma \) values. The color of each community is given according to the strength: its contribution to the modularity \( Q \). We can see that we get some clusters of particles. Some of them look like force chains, especially when \( \gamma > 1 \). To briefly explain why \( \gamma \) has such effect, we can first look at the picture of \( \gamma = 0.4 \) in Figure 3.2, where most particles are in the same community (note that I use "most" not "all" because communities with only one particle are not shown in the picture, but they are definitely minorities). When \( \gamma \) is very small, recall Equation 3.1, and we can see that \( \gamma P_{ij} \) will be small. If \( \gamma \) is small enough that \( W_{ij} - \gamma P_{ij} \) is always positive, then including all the particles in the same community will make all \( \delta(c_i, c_j) \) be 1 instead of 0 and obviously lead to maximal \( Q \). When \( \gamma \) gets larger, null model \( P_{ij} \) will have more influence. In our case, the actual contact geometry will more heavily influence the community detection result, especially the number and the shape of communities. Figure 3.3 shows that the number of communities detected will grow as the resolution parameter \( \gamma \) gets higher, when \( \gamma \) is in range of 0.01 to 3.

It's worth noting that for a special case where \( \gamma = 1 \), which is the default setting, contact
Figure 3.2 Demonstration of community detection results by modularity maximization, with different \( \gamma \) settings. Color represents the contribution of each community to the modularity. Only communities with more than 1 particles are drawn. Here friction coefficient \( \mu = 0.3 \), pressure \( P = 10^{-4} K_n \).
forces between particles ($W_{ij}$) are directly compared with the average contact force ($P_{ij}$) in the system. Those contact forces which are larger than the average contact force are more preferable to be included in communities (force chains in our sense). This choice of $\gamma = 1$ is similar to the common choice when using the threshold method to filter out small forces to find force chains, where the threshold is often set as the average contact force.

To briefly see how the result matches our intuition of force chains, in Figure 3.4 we compare some of the communities with the plot of the actual force network. In Figure 3.4A, we see that these communities exhibit some chain-like shape. We can see more clearly at high $\gamma$ in Figure 3.4B, some clusters grow along some strong "force-chain". However, since

![Figure 3.3 Number of communities detected at different resolution parameter $\gamma$. Friction coefficient $\mu = 0.3$ and pressure $P = 10^{-4} K_n$.](image)
3.3. **LOOKING FOR CHAIN-LIKE STRUCTURES**

Although modularity maximization gives us communities of particles, a different resolution parameter $\gamma$ will give the clusters different shapes, as shown in Figure 3.2. When $\gamma$ is small

---

**Figure 3.4** Overlap of community detection results and actual force network. I filter out many communities by setting the range of size (number of particles of a community), to make the picture clearer. Friction coefficient $\mu = 0.3$ and pressure $P = 10^{-4} K_n$. A. communities from $\gamma = 1.1$, size (number of particles of a community) from 165 to 300, B. communities from $\gamma = 3$, size > 10. Only forces larger than 100 are plotted.

in Figure 3.4B only communities with more than 10 particles are shown, most communities are too small to be called "force chains", therefore $\gamma = 3$ may not be appropriate to be used for force chain extraction. But how do we decide which $\gamma$ to choose? In the next subsection, we try to find criteria to judge how much a community resembles a force chain to help with that question.

### 3.3 Looking for Chain-like Structures

Although modularity maximization gives us communities of particles, a different resolution parameter $\gamma$ will give the clusters different shapes, as shown in Figure 3.2. When $\gamma$ is small...
3.3. LOOKING FOR CHAIN-LIKE STRUCTURES

(about 0.1), all the particles tend to be in the same community, forming a big bulk; when $\gamma$ is around 1, we can see some branched communities; when $\gamma$ is large (about 3), we only get small communities and their shapes are simple, for example, like rods. Since our objective is to extract force chain structures, we need to decide which value of $\gamma$ gives us the best result that resembles force chain structure. I tested the following three methods.

3.3.1 Gap-Factor

The gap-factor (defined in [Bas15]) quantifies the difference between the topological distance (representing the least number of edges between two particles) and the physical distance (linear distance between two particles) of particles in each community; the larger the gap-factor, the larger the difference. The gap-factor is given by:

$$g_c = 1 - \frac{r_c S_c}{S_{max}}$$

(3.5)

where $r_c$ is the Pearson correlation between topological distances and physical distances of all possible pairs of nodes in a community $c$. $S_c$ is the size of community $c$, or rather, the number of nodes (particles) in community $c$. $S_{max}$ is the size of the largest community. Then, the systematic gap-factor $g$ is calculated by averaging $g_c$ of all communities weighted by the size of each community.

This is based on the idea that the topological distance between particles and the physical distance between particles are the same for a straight rod-shape cluster, so are they similar for a compact bulk-shape cluster (Figure 3.5). For these kind of clusters, the gap-factor is small. On the contrary, for a branched cluster, which is what a force-chain typically looks like, has a large gap-factor. If we calculate the gap-factor at different $\gamma$, and find the maximum point, we can choose the corresponding $\gamma$ to be used for further analysis.
3.3. **LOOKING FOR CHAIN-LIKE STRUCTURES**

**CHAPTER 3. NETWORK ANALYSIS**

![Diagram of Gap-factor](image)

Figure 3.5 Schematic illustration of Gap-factor. $L_t$ is hop (topological) distance and $L_p$ is physical distance. Figure reprinted from [Bas15].

The application of gap-factor on 2D packings is successful [Bas15], and their $g$ vs $\gamma$ plot indicates that the maximum is at about $\gamma = 0.9$ (see Figure 1.2). The idea may still make sense for my 3D packing, so I tried this quantity as my first candidate. The result is shown in Figure 3.6. There is a maximum, but not very distinctive, around $\gamma = 1$, and it's also a little noisy, even though the plots have good statistics by averaging 20 simulations.
Figure 3.6 Gap-factor vs. resolution parameter $\gamma$ under different pressures. Error bars indicate the standard deviation of the average value over 20 simulations. Friction coefficient $\mu = 0.3$
3.3.2 Ellipsoidal Sparseness

Since gap-factor does not work as well on our 3D data, I need to find some other quantity to show how the shape of the communities changes while \( \gamma \) changes. I decide to describe force chains in a different way. From either 2D or 3D pictures, a desirable force chain is branched and therefore sparse. A community that looks like a bulk or a small rod is not sparse in space. To describe sparseness of a community, I define ellipsoidal sparseness as:

\[
\rho_c = \frac{V_{\text{particles}}}{V_{\text{ellipsoid}}}
\]

where \( V_{\text{particles}} \) is the total volume of particles in the community and \( V_{\text{ellipsoid}} \) is the volume of the bounding ellipsoid [Mos] of the centers of particles in this community. A sparse community (i.e. like force-chain) has a minimal value of \( \rho_c \). An illustration of bounding ellipsoids in a system is shown in Figure 3.7. In Figure 3.7B We can see some large overlaps between ellipsoids.

To calculate the overall sparseness of the packing, I calculate the average \( \rho_c \) weighted by the number of particles in communities. To avoid generating extremely small ellipsoids, I only include communities with more than 8 particles when calculating the overall value. A set of results are shown in Figure 3.8.

The plot of ellipsoidal sparseness shows some success of this kind of idea. The minimal point is between \( \gamma = 1 \) and \( \gamma = 1.5 \). However we can see some noise at large \( \gamma \). The problem might be because I only use the center of each particle in a community to find bounding ellipsoids. For small communities, the bounding ellipsoid calculated can be significantly smaller than particles’ volume. In addition, a bounding ellipsoid does not describe the exact space that a community occupies, as shown in Figure 3.7.
3.3. LOOKING FOR CHAIN-LIKE STRUCTURES

CHAPTER 3. NETWORK ANALYSIS

Figure 3.7 A. examples of bounding ellipsoids. Communities are from $\gamma = 3$ from Figure 3.2. Only communities with more than 8 particles and the corresponding ellipsoids are plotted. B. The assembly of all (except communities with less than 3 particles) bounding ellipsoids in a granular packing. Resolution parameter $\gamma = 1.1$, friction coefficient $\mu = 0.3$, and pressure $P = 10^{-4} K_n$. 

3.3. **LOOKING FOR CHAIN-LIKE STRUCTURES**  

**CHAPTER 3. NETWORK ANALYSIS**

Figure 3.8 Ellipsoidal Sparseness $\rho$ vs. resolution parameter $\gamma$ under different pressures. Error bars indicate the standard deviation of the average value over 20 simulations. Friction coefficient $\mu = 0.3$. 

"[Diagram of Figure 3.8 with labels and annotations]

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3.3. **LOOKING FOR CHAIN-LIKE STRUCTURES**

3.3.3 **Hull Ratio**

Trying to improve on ellipsoidal sparseness, I next used the convex hull (i.e. smallest convex region containing the community) of the community to replace the bounding ellipsoid in the equation, as demonstrated in Figure 3.9. Since the volume of all the particles in a community is just the volume of the compact hull, I call the new quantity the hull ratio which is defined as:

\[ H_c = \frac{V_{\text{particles}}}{V_{\text{convex hull}}} \]  

(3.7)

Here I want to find the convex hull of the particles in a community (to include the size of particles), and not only the convex hull of the center of the particles. To do this, I sample points on the surface of all the spheres using the particle position and diameter. Then I use the `boundary` function, a built-in function in MATLAB 2014b, to find the convex hull for these points. When I sample the surface of one sphere with a 7 x 7 matrix of points, they will sufficiently describe the shape of spheres and convex hull while not using substantial computing time. Figure 3.9 shows the convex hulls calculated with this accuracy.

Similarly, to find the overall hull ratio \( H \), I calculate the average of \( H_c \) weighted by the number of particles in each community, excluding communities which have only one particle. As with \( \rho_c \), the hull ratio \( H \) is minimized when calculated with optimal \( \gamma \). Figure 3.10 shows the result for different pressures. We can see that the minimum value of \( H \) is very clear and relatively consistent for different pressures. Otherwise, the minimum \( H \) is at about \( \gamma = 1.1 \) under each pressure, which is close to the result found by using the gap-factor in 2D [Bas15]. Therefore, we decide to use the hull ratio to find the optimal \( \gamma \).
Figure 3.9 Demonstration of the convex hull. Communities are from $\gamma = 3$ from Figure 3.2. Friction coefficient $\mu = 0.3$, and pressure $P = 10^{-4} K_n$. To help with observation, only communities with more than 10 particles and the corresponding convex hulls are plotted. We can see 5 communities in this picture.
Figure 3.10 Hull ratio $H$ vs. resolution parameter $\gamma$ under different pressures. Error bars indicate the standard error of the average value over 20 simulations. Friction coefficient $\mu = 0.3$. 
3.4 Properties of the Force Chain Network

Beyond the hull ratio, we also use the network quantities size $S$ and network force $\sigma$ as diagnostics for communities, following the same characterization methods in Bassett’s paper [Bas15]. The size $S_c$ (of a community $c$) is the number of particles in the community. The network force $\sigma_c$ is the contribution to modularity $Q$ from a community $c$, defined as:

$$\sigma_c = \sum_{i,j \in C} [W_{ij} - \gamma P_{ij}]$$

(3.8)

where $C$ is the set of nodes in the community; $\sigma_c$ is the sum of the normal contact forces in a community minus the corresponding edges (forces) in a null model, hence the term network force. Communities containing more and larger edges (contact forces) have higher network force, and vice versa. $S_c$ and $\sigma_c$ measure the importance of a community in different ways. It may help to identify important force chains among the supporting structures, as well as characterizing the whole system. We will examine the cumulative distribution function of these quantities in Chapter 4.
4.1 Community Assignment

In prior work on force chain detection in 2D [Bas15], community detection results change for different resolution parameter $\gamma$ and pressure $P$, and also according to whether there is friction. This indicates the force chain structures can be different under different settings. Motivated by their figures, we look at some visualizations under different $\gamma$ and $P$. We also show the corresponding average hull ratio: the ratio between particle volume and convex hull of the communities. By comparing community detection results with the hull ratio vs. resolution parameter plots, we can have a basic understanding of how well hull ratio describes community shape and how the resolution parameter influences community
assignments.

Figure 4.1 shows an example of community detection results and corresponding hull ratio at different resolution parameters $\gamma$. In the picture, only communities with more than one particle are shown. Pictures on the right side (larger $\gamma$) have more single-particle communities than the left side (smaller $\gamma$), indicated by the blank space. Color on each particle is decided by value of network force $\sigma_c$ (see Equation 3.8) of the community that the particle belongs to, so all the particles in the same community have the same color.

However, having similar color does not necessarily mean particles are in the same community (see Figure 4.2). Red communities have higher $\sigma_c$ and blue ones have lower $\sigma_c$. Higher $\sigma_c$ means there are more edges and nodes in the community, and the edges tend to have high weight, so it's safe to say those red bulks (communities) are single communities as long as particles are in contact. In contrary, lower $\sigma_c$ means fewer edges and nodes in a community, and weaker edges, so all those blue particles are not in a single community even though they look like a single pile, and most of them are in communities with only 2 or 3 particles.

Since it is hard to observe community shape from 3D results in Figure 4.1 B, especially for complex situations such as at $\gamma = 1$ and $\gamma = 1.2$ where there are a lot of communities twisted together. It will be helpful to look at some visualizations of extracted communities. In Figure 4.3, we see two examples of mid-size communities at $\gamma = 1.1$. They exhibit the chain-like structure that we are looking for, and they are sparse and have low hull ratio (see Equation 3.7) according to our criteria. Nevertheless, in Figure 4.4, we also have some communities under same $\gamma$, $P$ and $\mu$, which are too small to be called "force-chains". These results shows the effectiveness of community detection method in extracting force chain structures.
Figure 4.1 Community detection results and hull ratio at different resolution parameter $\gamma$. (A) hull ratio $H$ vs. $\gamma$ under different pressures when $\mu = 0.3$. (B) Community detection results from selected pressures and $\gamma$ ($0.4, 0.8, 1, 1.2, 3$). For clarity, communities containing only 1 particle are hidden. Color represents network force $\sigma_c$ of each community, so same color of particles does not necessarily mean they are in the same community.
4.1. COMMUNITY ASSIGNMENT  

Figure 4.2 Examples explaining about red particles and blue particles. The two pictures on the left are from Figure 4.1, which are colored by $\sigma_c$. Pressure $P = 0$ and friction coefficient $\mu = 0.3$. The two pictures on the right are the same community result, and the only difference is that each community is colored randomly, making it easier to differentiate communities. The goal of this figure is to show that red particles are in the same big community, while blue particles are not in the same community, and they are in very small communities.
4.1. COMMUNITY ASSIGNMENT

CHAPTER 4. RESULTS

Figure 4.3 Examples of two medium-size communities. A. a community containing about 100 particles. B. a community containing about 150 particles. Resolution parameter \( \gamma = 1.1 \), friction coefficient \( \mu = 0.3 \), and pressure \( P = 10^{-4} K_n \).

Figure 4.4 Examples of some small-size communities. Those communities have 4 or 5 particles. Resolution parameter \( \gamma = 1.1 \), friction coefficient \( \mu = 0.3 \), and pressure \( P = 10^{-4} K_n \). Community color is related to the vertical position.
We need to decide a $\gamma$ value to use before we analyze the effect of different $P$ and $\mu$. When we compare the community result (Figure 4.1 B) with $H$ vs $\gamma$ curves (Figure 4.1 A), we can see that hull ratio effectively distinguishes between different community morphologies. At high hull ratio, the communities are either too big or too small, while at lowest hull ratio, we find some medium size communities. Since the minimum points are at slightly different $\gamma$, ranging from 0.9 to 1.3, when applying different $P$, I decide to choose $\gamma = 1.1$ as the optimal value that produces most chain-like structures (this choice is also supported by Figure 4.3), and use it for the following analysis.

4.2 Community Size $S_c$ and Network Force $\sigma_c$

4.2.1 Influence of $\mu$ on Community Size and Network Force

We first examine the influence of friction coefficient on the community size $S_c$ (the number of particles in a community) and network force $\sigma_c$ (see Equation 3.8) properties of the force chain structure. First, we set $P = 10^{-4}K_n$ and show community assignments and cumulative distribution figures. Then, we show complete cumulative distribution figures under all pressure settings.

In Figure 4.5, sample community assignments are shown for all the $\mu$ values we used, while keeping $P = 10^{-4}K_n$ and using the optimal resolution parameter $\gamma = 1.1$. The three figures in the first row ($\mu = 0, 0.01, 0.03$) look similar to each other, and they all have small communities. The last two ($\mu = 1, 3$) look similar and they have a single big community on top and weak communities in the bottom. Similarly, Silbert et al. [Sil10] reported that the packing fraction and coordination number (the average number of contacting neighbors per particle) decrease gradually as $\mu$ increases from 0, saturating when $\mu$ is larger than 1.
This saturation is also reflected in the cumulative distribution figures below.

Figure 4.6 are plots of the cumulative distribution of community size $S_c$ (the number of particles in a community) and the network force $\sigma_c$ (see Equation 3.8) at different $\mu$, with only the y axis in logarithmic scale. It shows the fraction of communities above a certain community size $S_c$. We notice that these two plots are similar, and we find an approximately linear relationship between $S_c$ and $\sigma_c$ in Figure 4.7. In Figure 4.6, we see that plots at $\mu = 0, 0.01$ and $0.03$ are almost in superposition, so are those at $\mu = 1$ and $3$, which corresponds with our observation in Figure 4.5.

When we look at $S_c$ distributions, we see that most communities are small, with only about 10% of communities having more than 1 particle. For medium and large communities ($S_c > 100$), the distribution is approximately exponential at high $\mu$ (1 and 3). Similar exponential distribution for large forces (not $S_c$ or $\sigma_c$) is found in many studies [Sil02b][Mue98][Bru03][MB05] of granular packings. By observing the curves in the small-$S_c$ ($< 100$) regime, we see the number of small and median communities increases with $\mu$. By observing the tails of the plots, we see more big ($> 300$) communities as $\mu$ increases.

When we look at the $\sigma_c$ distributions, we still see that $\sigma_c$ distributes exponentially when $\sigma_c$ is relatively large ($> 10^5 K_n$) and at high $\mu$ (1 and 3). Also, the maximum value of $\sigma_c$ increases notably as $\mu$ increases. This is obvious when looking at $\mu = 1$ and $3$ in Figure 4.5. A big red community form at the top of the packing, and red means the community has high value of $\sigma_c$. As will be discussed in section 4.2.3, this is related to higher $\mu$ changing the tangential forces and horizontal force transmission. Further plots and analysis supporting this are shown in section 4.2.3.

In Figure 4.8 and Figure 4.9, we plot the cumulative distribution function (CDF) of the size $S_c$ and the network force $\sigma_c$ against $\mu$, where each subplot has different pressure.
Figure 4.5 Community assignments at different $\mu$. Resolution parameter $\gamma = 1.1$ and pressure $P = 10^{-4} K_n$. Color indicates the network force of the community. Color scale within each example is from zero (dark blue) to the max network force value (red)
4.2. COMMUNITY SIZE $S_c$ AND NETWORK FORCE $\sigma_c$

Figure 4.6 Cumulative distribution of community size $S_c$ and network force $\sigma_c$ at different $\mu$. Pressure $= 10^{-4} K_n$. Resolution parameter $\gamma = 1.1$. Only Y axes are in logarithmic scale. $Pr(\text{Size} > S_c)$ is the fraction of communities whose community size is above a certain value $S_c$. $Pr(\text{network force} > \sigma_c)$ is the fraction of communities whose network force is above a certain value $\sigma_c$. 

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Figure 4.7 Scatter plot of Network Force \( \sigma_C \) vs. Community Size \( S_C \). Pressure \( P = 10^{-4} K_n \). Friction coefficient \( \mu = 0.3 \). Resolution parameter \( \gamma = 1.1 \). Data is from 1 simulation.
4.2. COMMUNITY SIZE $S_C$ AND NETWORK FORCE $\sigma_C$

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$P$ setting, as indicated. We again describe the CDF of $S_c$ and $\sigma_c$ together here, since they show very similar trends. When we compare the trends of both CDF plots against $\mu$, different pressures (subplots) show different trends at low vs. high $P$. At low pressure ($P = 0, 10^{-6}K_n, 3 \times 10^{-6}K_n$), as $\mu$ increases, the distribution of $S_c$ and $\sigma_c$ get narrower, indicating there are fewer large-size communities. Interestingly, at relatively high pressure $P = 3 \times 10^{-5}K_n$ and $10^{-4}K_n$ (and $P = 10^{-5}K_n$ for $\sigma_c$ only), the distribution get broader as $\mu$ increases, which is opposite to the trend at low pressure.

To interpret this change of trend, I describe the homogeneity of the system to simplify observations of changes in the size distribution. In [ZM05], they similarly describe the packing to be more homogeneous when the force distribution get narrower. In our case, a more homogeneous system means it has fewer large communities and more medium-size community and has a narrower distribution of $S_c$ and $\sigma_c$. At high $\mu$, the directions of forces are more diverse, instead of mostly pointing downward. This makes system more homogeneous at low pressure (where the main effect is only gravity). However, this generates a big single community on the top at high pressure, which makes the system less homogeneous. These can be seen clearly in Figure 4.5, where the last row shows big red communities on the top of packings. In section 4.2.3, we will verify our explanation.

We can compare the CDFs when $P = 0$ (where there is only gravity), with the conclusion from a study of the geometry of frictionless and frictional sphere packing under gravity [Sil02a]. They found as the friction coefficient was increased, the coordination number (average number of contacts per particle) decreased smoothly. That means each particle has fewer supports. From our CDFs, we can see that as $\mu$ increases, the largest communities (formed by pressure gradient caused by gravity, which will be illustrated in section 4.2.3) tend to break down into medium or small ones. This mean that there are fewer supporting
4.2. COMMUNITY SIZE $S_c$ AND NETWORK FORCE $\sigma_c$

forces between particles at the bottom, which is consistent with [Sil02a]. However, in another paper [Sil02b] they found that local contact geometry, which is represented by distribution of contact angles, has a weak dependence on friction. While our CDFs for $S_c$ and $\sigma_c$ show a clear dependence on $\mu$ except when $P = 10^{-5} K_n$ (note it is a crossover of the trend in Figure ?? and Figure 4.9). Since $S_c$ and $\sigma_c$ are the properties of communities (force chains), they represent how closely particles are connected in the packing. We can conclude that for different friction coefficients, contact geometry will remain similar but the strength of connections between particles can change a lot.

4.2.2 Influence of $P$ on Community Size and Network Force

We can examine the influence of pressure on the community size $S_c$ (the number of particles in a community) and network force $\sigma_c$ (see Equation 3.8) properties of the force chain structure. First we set $\mu = 0.3$ (a common value for granular materials) and look at some community assignments pictures and cumulative distribution figures. Then we show cumulative distribution figures under all $\mu$.

Figure 4.1B shows sample community assignments at different $P$. If we look at the middle column (where $\gamma = 1$), when $P = 0$, the bottom part of the packing tends to form a big community, because there are higher forces in the bottom, due to gravity. When $P$ is larger, the communities seem to be more homogeneous. Statements from Makse et al. [Mak00] support this observation, where they report a more homogeneous spatial distribution of contact forces as pressure increases. Zhang et al. [ZM05] also report that the force distribution is more homogeneous as pressure increases. Similar and clearer conclusions can be obtained even when we look at $\gamma = 3$. At $\gamma = 3$, when $P = 0$, the non-single-particle communities gather in the bottom; when $P$ is larger, the non-single-particle
4.2. COMMUNITY SIZE $S_c$ AND NETWORK FORCE $\sigma_c$

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Figure 4.8 Cumulative distribution of size $S_c$ against $\mu$, where each subplot is at different pressure $P$. Resolution parameter $\gamma = 1.1$. Data is from all 20 simulations.
4.2. COMMUNITY SIZE $S_C$ AND NETWORK FORCE $\sigma_C$

Figure 4.9 Cumulative distribution of network force $\sigma_c$ against $\mu$, where each subplot is at different pressure $P$. Resolution parameter $\gamma = 1.1$. Data is from all 20 simulations.
4.2. COMMUNITY SIZE $S_C$ AND NETWORK FORCE $\sigma_C$

Communities distribute more evenly. We can even see the tendency at $P = 10^{-4} K_n$ that more non-single-particle communities form in the top of the packing.

Figure 4.10 shows plots of cumulative distribution of community size $S_c$ and network force $\sigma_c$ at different $P$, with only y axis in logarithmic scale. We put them together since they are similar. When we look at the $S_c$ distributions, we see approximately exponential distribution at all pressures when $S_c > 100$ (for large communities). For $S_c < 100$, the number of small size communities decreases monotonically with pressure. This may be because larger $P$ makes the force distribution more homogeneous, which will result in less "lonely" particles, hence less communities with one or very few particles. This is consistent with observation from Zhang et al. [ZM05], that the number of particles with zero coordination number decreases as pressure increases.

When we look at network force $\sigma_c$ distributions, we still see approximate exponential distributions at all pressures. By observing the curves in small $\sigma_c$ region, we see that higher pressure leads to fewer small network force communities. That's simply because higher pressure generates higher normal contact forces, a key contributor to the network force calculation.

Both plots show trends only when $S_c$ or $\sigma_c$ is small. For large $S_c$ or $\sigma_c$, it is difficult to determine whether there is a trend or just statistical fluctuations. However, we will later see (Figure 4.11 and Figure 4.12) that CDFs of $S_c$ and $\sigma_c$ strongly depend on pressure when $\mu < 0.3$. The statistical analysis accounting for statistical fluctuation is in Appendix A.

Figure 4.11 and Figure 4.12 show the CDFs of $S_c$ and $\sigma_c$ as a function of $P$, where each subplot has different frictional coefficient $\mu$. (These are the same plots as in Figure 4.8 and 4.9, rearranged to give another perspective.) Figure 4.11 and Figure 4.12 are similar to each other. At low $\mu$ ($\mu < 0.1$), both CDFs have low tails as $P$ increases, meaning there are fewer
4.2. COMMUNITY SIZE $S_C$ AND NETWORK FORCE $\sigma_C$

Figure 4.10 Cumulative distribution of community size $S_C$ and network force $\sigma_C$ at different $P$, $\mu = 0.3$. Resolution parameter $\gamma = 1.1$. Only Y axis is in logarithmic scale. $\Pr(\text{Size} > S_C)$ is the fraction of communities whose community size is above a certain value $S_C$. $\Pr(\text{network force} > \sigma_C)$ is the fraction of communities whose network force is above a certain value $\sigma_C$. 
large communities and the system is more homogeneous. When $\mu > 0.1$, the tail decreases until around $P = 10^{-5}K_n$ (especially for $S_c$, $P = 3 \times 10^{-6}K_n$ for $\sigma_c$), then increases as $P$ gets higher, meaning the homogeneity increases then decreases (this is verified in Figure 4.13). By looking at same set of CDF from two aspects (vs. $\mu$ and vs. $P$), we can see $\mu$ and $P$, in our parameter range, have a similar influence on the shape of the CDF plots of $S_c$ and $\sigma_c$. This observations leads us to perform further investigation of combined influence of $\mu$ and $P$ in the next section.

The community size CDFs in Figure 4.11 are comparable with another study utilizing community detection technique [Nav10], where they did not use geometry null model and thus resulted in bulk shape communities. They found that the community size increases as pressure increases, while we generally (except high $\mu$) find more small and medium communities and less big communities as pressure increases. This indicates that choosing a specific null model does make a difference.

These CDFs of $S_c$ and $\sigma_c$ give us similar conclusions with the previous 2D study of force chain [Bas15] using similar technique. They found the community size distribution is exponential, while we found both size and network force have exponential distribution. They found high-pressure force networks exhibit compact communities, and we see large bulk communities at high pressure as well.

### 4.2.3 Combined Influence of $\mu$ and $P$

In order to give a consistent interpretation for all of the trends shown in CDF plots, we plot the average spatial distribution of community size $S_c$ and network force $\sigma_c$ at different depths. This turns out to give enough information to support the trend we observed in CDF plots. To further explain the results in terms of force configuration, we show the vertical
4.2. COMMUNITY SIZE $S_C$ AND NETWORK FORCE $\sigma_C$

Figure 4.11 Cumulative distribution of size $S_C$ against $P$, where each subplot is at different pressure $\mu$. Resolution parameter $\gamma = 1.1$. Data is from all 20 simulations.
4.2. COMMUNITY SIZE $S_C$ AND NETWORK FORCE $\sigma_C$

Figure 4.12 Cumulative distribution of network force $\sigma_C$ against $P$, where each subplot is at different pressure $\mu$. Resolution parameter $\gamma = 1.1$. Data is from all 20 simulations.
4.2. COMMUNITY SIZE $S_c$ AND NETWORK FORCE $\sigma_c$

and horizontal force distribution at different depths.

Figure 4.13 shows the distribution of average community size $S_c$ and the distribution of average network force $\sigma_c$ along the z axis. To calculate this, in each depth interval I find the $S_c$ and $\sigma_c$ of the community that each particle belongs to, and average them respectively. The similarity of distributions of $S_c$ and $\sigma_c$ is consistent with the similarity between CDF plots of $S_c$ and $\sigma_c$. Therefore, we’ll analyze distributions of $S_c$ as an example.

The size distribution along z axis (depth) is clearly divided into 3 regimes: negative slope, almost vertical slope and positive slope distribution. Each is colored separately. A negative slope distribution (colored red) means the average size in the bottom is larger than the middle part and the top. An almost vertical distribution (colored yellow) means the average size is roughly the same across different depths, indicating a rather homogeneous system. A positive sloped distribution (colored blue) means the average size is larger in the top than the bottom. This figure explains how the homogeneity of the system is affected by $\mu$ and $P$. For example, if we look at the bottom 3 rows, it is easy to conclude that, when $\mu > 0.1$, as pressure gets higher, the homogeneity increases until about $P = 10^{-5} K_n$ then decreases, which verifies the conclusion I made from observing Figure 4.8. Furthermore, these two kind of gradients from low and high pressures distinguish the corresponding CDF plots in Figure 4.11, and therefore we know they are inhomogeneous by different mechanisms. In the red regime, we also use color gradient to show the relative difference in slope, and we see a monotonic trend as we change $\mu$ and $P$. The yellow area is where the system is the most homogeneous and the transition of trend happens, and it corresponds to the $P = 10^{-5} K_n$ crossover point we identify in this section and we will see again in next section.

Figure 4.14 shows the distribution of horizontal forces and vertical forces along the z
Figure 4.13 Distributions of average size $S_c$ and network force $\sigma_c$ along z axis (depth), at all $\mu$ and $P$ settings. Plots are divided into three regimes and colored according to whether it’s negative sloped, vertical or positive sloped. Resolution parameter $\gamma = 1.1$. Each plot is averaged over 20 simulations. All axes are kept the same for comparison.
axis (depth), at all $\mu$ and $P$. To calculate this, for each depth, I sum up the forces between all particle pairs positioned in the depth interval. The vertical force is defined as the absolute value of $z$ component of the normal contact force vector. The horizontal force is defined as the absolute value of the combination of $x$ and $y$ component of the normal contact force vector.

This figure helps to explain the effect of both friction coefficient and pressure, in terms of how forces distribute in the packings. At high pressure, as friction coefficient $\mu$ gets higher, a change happens: horizontal forces in the top region (corresponding to high $z$ value) tend to get larger than horizontal forces in the bottom, also larger than vertical forces. This explains why the big community forms on the top. In the small pressure regime, the horizontal and vertical forces are consistent with each other, and reflect the effect of the gravity. As pressure increases, the distribution of vertical forces and horizontal forces start to deviate from each other. Also, both vertical and horizontal force distributions get more homogeneous.

The force distribution along $z$ axis can be compared with the Janssen effect [Jan95] (translation [Spe06]). The Janssen effect describes that the pressure in the bottom of a granular packing in a container saturates when the packing is high enough. This is caused by force chains connecting horizontally to the walls, which support the upper part of the packing. In our setup, we use periodic boundary conditions, which means there is no wall to support the upper part. As expected, we see the gradient of force distribution induced by gravity, when pressure is small (see Figure 4.14). However, we still observe a rise of horizontal forces in the upper part at high $P$ and $\mu$.

Note that the most homogeneous community distributions (yellow) in Figure 4.13 do not completely correspond with the most homogeneous force distributions in Figure 4.14.
4.3 Hull Ratio vs. $\mu$ and $P$

The hull ratio $H_c$ (see Equation 3.7) is an important network property of a community, which measures the ratio between particle volume and convex hull volume. In this section we examine the influence of friction coefficient $\mu$ and pressure $P$ on the cumulative distribution of hull ratio. We show the complete cumulative distribution figures over all $\mu$ and $P$ settings from two perspectives.

Figure 4.15 shows the CDF of the hull ratio $H_c$ as a function of $\mu$, where each subplot has different pressure $P$. We notice that most (about 90% to 95%) communities have zero $H_c$. This is because we assign those communities to zero hull ratio, and they are excluded from calculation of the overall hull ratio. If we ignore single particle communities, about half of communities have $H_c \sim 1$, and those communities correspond with small communities. We can see that only when $P$ is large enough ($> 10^{-5} K_n$, which is the crossover we identify from Figure 4.8 and Figure 4.9), the CDF curves are $\mu$ sensitive. If we just look at large pressure ($> 10^{-5} K_n$) situations, by observing the slope of the curves, we can see the number of communities with non-zero hull ratio tend to increase with $\mu$. This means larger $\mu$ tends to generate more strong connections between particles, in another word, chain-like communities.
4.3. HULL RATIO VS. $\mu$ AND $P$

CHAPTER 4. RESULTS

Figure 4.14 Distribution of vertical and horizontal contact forces along $z$ axis (depth), at all $\mu$ and $P$ settings. Resolution parameter $\gamma = 1.1$. Each plot is averaged over 20 simulations. All axes are kept the same for comparison.
Figure 4.15 Cumulative distribution of hull ratio $H_c$ against $\mu$, where each subplot is at different pressure $P$. Resolution parameter $\gamma = 1.1$. Data is from all 20 simulations.
Figure 4.16 shows the CDF of the hull ratio $H_c$ against $P$, where each subplot has a different friction coefficient $\mu$. The slopes of the CDF plots monotonically increase with pressure. Note that the CDFs of hull ratio do not depend on $\mu$, which is different from what we observed for size and network force. The reason for this difference is that the CDFs of size and network force mainly depend on the existence of the large communities, while hull ratio is not primarily affected by largest communities, since largest communities are bulk-shape and do not have lower hull ratio values than medium communities. As Figure 4.17 shows, large and medium communities have similar low $H_c$ values and $H_c$ and $S_c$ do not have linear correlation. In fact, the hull ratio CDFs are strongly controlled by the number of single/double-particle communities, because those communities have highest and constant hull ratio values. Since higher $P$ enhances the link between particles, and thus decreases the number of single/double-particle communities effectively, we can see the consistent trend in Figure 4.16.

From Figure 4.16, we can also draw a similar conclusion as from Figure 4.15: when $\mu$ is higher, the hull ratio CDF is more sensitive to $P$. This is consistent with a conclusion in the previous 2D study about force chain [Bas15], that the geometry of the frictionless packings appear to be less affected by pressure than those that are frictional. It’s more difficult to tell the geometry of a 3D packing than in 2D, since it is difficult to just look at the picture of the packing. However, since the hull ratio $H_c$ represents the degree of branching of a community, we can use it to tell how much the geometry of the packing is changing.
Figure 4.16 Cumulative distribution of hull ratio $H_c$ against $\mu$, where each subplot is at different pressure $P$. Resolution parameter $\gamma = 1.1$. Data is from all 20 simulations.
Figure 4.17 Scatter plot of Hull ratio $H_c$ vs. Community Size $S_c$. Pressure $P = 10^{-4} K_n$. Friction coefficient $\mu = 0.3$. Resolution parameter $\gamma = 1.1$. Data is from 1 simulation.
In this thesis, we have shown that community detection methods can be successfully applied to 3D granular packings. We also find a new quantity, the hull ratio $H$, which characterizes the community shape in 3D. This solves the problem that the original one (gap-factor) does not work well in 3D, and the hull ratio helps us successfully extract ideal force chain structure. All three network properties ($S_c$, $\sigma_c$ and $H_c$) have noticeable dependence on $P$ and $\mu$. We describe the effect of $\mu$ and $P$ on community structures in a similar way.

For our data, we used molecular dynamics software LAMMPS to generate 3D granular packings (described in Chapter 2). We simulate the process of pouring particles slowly into a container. Since we want to study the influence of $P$ and $\mu$ on network properties, we set
a range of μ as particle attributed and run each value separately. To change P, we generate
a slab on the top of the packing and apply different forces onto it. For each specific setting
of P and μ, we have 20 independent runs to improve statistics.

In Chapter 3, we apply community detection methods to our 3D granular packings.
The specific community detection method is call modularity maximization. A geographic
null model is used to include physical constraints, so that we are able to successfully
extract chain-like structures. The resolution parameter γ can change the community sizes
and shapes we find. To find the optimal result for chain-like communities, we need to
determine the value of resolution parameter γ while performing modularity maximization.
We observed that the gap-factor quantity that works well in 2D seems to work less well
3D as means to identify this optimum. Therefore, we create two new measures (ellipsoid
sparseness and hull ratio) to replace it. We observe that the hull ratio outperforms both
the gap-factor and the ellipsoid sparseness. Our hull ratio can differentiate community
shape effectively, and the optimum value does not shift very much with increasing pressure.
Therefore, we decide to use hull ratio to determine the optimal γ.

With this force-chain-extraction method optimized for 3D granular packings, we first
determine (in Chapter 4) that the optimal γ value is 1.1. Then, we use this method under
this particular γ setting as a automated process to find communities as optimal force chain
structure from all of the data. We calculated the size $S_c$, network force $\sigma_c$ and hull ratio
$H_c$ for those communities and find out $S_c$ and $\sigma_c$ partly have approximate exponential
distributions. We find $S_c$ and $\sigma_c$ are in approximately linear relationship, which makes their
plots similar to each other. Through their dependence on μ, I find distributions are similar
when $0 < \mu < 0.03$ and $\mu > 1$, respectively. Through CDFs showing the dependence of P
and μ, we show that P and μ influence the homogeneity of community distribution in the
packing. Specifically, the inhomogeneity induced by the pressure gradient from gravity can be reduced as either $P$ and $\mu$ increases from 0. However, when $\mu$ is high, increasing $P$ makes the system more homogeneous until around $P = 10^{-5} K_n$, after which it returns to being less homogeneous. Another interesting phenomenon is that when $P$ is high ($> 10^{-5} K_n$), increasing $\mu$ makes system less homogeneous, the opposite behavior from when $P$ is low. We identify $P = 10^{-5} K_n$ as a crossover point. These phenomena are supported and explained when we show the distribution of $S_c$ and $\sigma_c$ along z axis (depth), at all $P$ and $\mu$. We find the crossover point corresponds to the parameter-regime where community distribution is homogeneous. We also examine the average force distribution along the z axis, at all $P$ and $\mu$. This shows the increase of horizontal forces in the top of the packing when $P$ and $\mu$ is large, although we do not have sidewalls as in the Janssen effect. The increase of horizontal forces has a significant effect on community structures. We also find that the CDF of the hull ratio $H_c$ is sensitive to $\mu$ only when $P$ is large enough ($> 10^{-5} K_n$), and that the slope of the CDF monotonically increases with pressure at all the $\mu$ value.

There are still many questions left in my work. As an outlook, we can expand our parameter range, i.e. higher $P$ and $\mu$, which could benefit Figures 4.13, in which the range of blue area at higher $P$ is unclear. This would allow for a better understanding of the combined effect of $P$ and $\mu$. We can try to find a more complete description of the distribution of network properties, maybe even statistical explanations. We can include tangential contact forces (friction) in our network analysis and see how the communities differ from the ones from normal contact forces. We can look at what higher resolution parameter can bring us. Although it does not give optimal force chain structure in our standard, it does give information of the structure at different length scales. We can also try to apply this force-chain-detection technique in some quasistatic or even dynamic
situations, and observe the time evolution of force chains and their properties.
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In the appendix we discuss the reliability of our results, from two aspects, optimization stability and statistics of 20 simulations.

### A.1 Optimization Stability

Modularity maximization is a NP-complete problem, that is why we use a greedy heuristic algorithm to find an approximately optimized $Q$ value. We want to test how stable the optimization method is, i.e. how much $Q$ varies, and how much that influences the community structure. In Figure A.1, the relation between average hull ratio and modularity $Q$ is plotted from 100 individual optimization. We see that $Q$ varies in a small range and there is no
A.1. OPTIMIZATION STABILITY

APPENDIX A. OPTIMIZATION AND STATISTICS

Figure A.1 Scatter graph of average hull ratio vs. $Q$. Data is from 100 independent optimization.

obvious correlation between average hull ratio and $Q$. Even if we find the maximum $Q$ value out of 100 optimization, which is considered to correspond to the best community assignment, we can’t guarantee at all that hull ratio is the lowest which is favored. Therefore, we do not get an advantage by doing 100 rather than just 1 optimization.

In Figure A.2, we show the fraction of particles appear commonly in a certain number of largest communities among 70% or 90% of optimization results. For example, on the solid line, point (X:5, Y:0.03958) means that if we consider particles in the 5 largest communities, we find about 4% of particles appear in at least 90% of optimization. on the dashed line, point (X:5, Y:0.2667) means about 26% of particles in largest 5 communities appear in at least 70% of optimization. Point (X:10, Y:0.7036) shows if we want 70% of particles to appear
A.2 Statistics of 20 Simulations

We did 20 individual simulations for each parameter setting. To show that 20 simulations give reliable results, we first look at how the number of simulations affect the choice of resolution parameter $\gamma$. Figure A.3 shows plots of hull ratio $H_c$ vs. resolution parameter $\gamma$ which we use to choose optimal $\gamma$. The difference is that here we show plots from each simulation, while in Chapter 3 we used the average of 20 simulations to pick the optimal $\gamma$.

Figure A.2 Percentage of particles appear in 90% and 70% of 100 optimization. $P = 10^{-5} K_n, \mu=0.3$.

in 70% of optimization, we need to count largest 10 communities. These plots show that we do not get very consistent results from different optimization, although we get similar optimized modularity and overall community structure.
We can see in Figure A.3 that the optimal $\gamma$ in each plot corresponds very well.

In Figure A.4, we show $H_c$ vs. $\gamma$ plots averaged over certain number of simulations samples. In selecting samples, we use bootstrapping method (sampling with replacement) to pretend we have infinite number of simulations. We see that the plot with single simulation (bottom one) is more noisy than others, and as we look upward, the plot gets more smooth as averaging number increases. When we average over 10, 15 and 20 simulations samples, the resulting plots look almost identical. This means 20 simulations are enough for determining optimal $\gamma$.

To see that the CDF plots have enough statistics as well, in Figure A.5, Figure A.6 and Figure A.7, we present how the plots collapse as we increase the number of simulation samples.
Figure A.4 Hull ratio $H_c$ vs. resolution parameter $\gamma$. Each plot is an average from certain number of sample of simulations, ranging from 1 to 20 from bottom plot to top plot. Plots are set offset from each other.
samples to take into account. When we only use 1 sample out of 20 simulations to generate the CDF plot (blue lines) and do this 1000 times, they spread widely and evenly aside the real plot (dashed line). When we use 5 samples, the resulting plots (green lines) have narrower dispersion. And when we use 10 or 20 samples, we get plots (yellow and red lines) very close to the real plot generate by all 20 simulations. This means we can obtain stable CDF plots if we use at least 10 simulations.

Note that the blue lines are shorter than other colors in log-scale plots. That’s because the last point (of the biggest $S_c$ or $\sigma_c$) of CDF is at $Pr = 0$, and it cannot be drawn in log scale. However when we include more than 1 sample, especially when we have 10 or 20 samples, most of the "last points" from single sample are survived and the real last points out of them is not drawn. Nevertheless, this does not influence our conclusion that 20 simulation is enough for stable CDF plots.
A.2. STATISTICS OF 20 SIMULATIONS APPENDIX A. OPTIMIZATION AND STATISTICS

Figure A.5 CDF of size $S_c$ when pressure $P = 10^{-4}K_n$ and friction coefficient $\mu = 0.3$. Dashed line is the actual plot after utilizing data from all 20 simulations. Colored lines are generated by using certain number of bootstrapping samples from 20 simulations. Each colored plot is generated 1000 times to see its variance.
Figure A.6 CDF of network force $\sigma_c$ when pressure $P = 10^{-4} K_n$ and friction coefficient $\mu = 0.3$. Dashed line is the actual plot after utilizing data from all 20 simulations. Colored lines are generated by using certain number of bootstrapping samples from 20 simulations. Each colored plot is generated 1000 times to see its variance.
Figure A.7 CDF of hull ratio $H_c$ when pressure $P = 10^{-4} K_n$ and friction coefficient $\mu = 0.3$. Dashed line is the actual plot after utilizing data from all 20 simulations. Colored lines are generated by using certain number of bootstrapping samples from 20 simulations. Each colored plot is generated 1000 times to see its variance.