Computational Studies of the Protocol-dependent Mechanical Properties of Granular Materials

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Abstract

Computational Studies of the Protocol-dependent Mechanical Properties of Granular Materials

Philip Wang
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Dry granular materials are collections of macroscopic-sized grains that interact via purely repulsive and dissipative contact forces. In this thesis, we describe discrete element method (DEM) simulations to characterize the structural and mechanical properties of jammed packings of spherical particles. Many previous studies have shown that the bulk modulus of jammed sphere packings depends only weakly on the pressure during isotropic compression, whereas the ensemble-averaged shear modulus $\langle G \rangle$ increases as a power-law in pressure $P$ at large pressures. However, the origin of the power-law scaling of the shear modulus with pressure is not well-understood. In particular, why is the power-law exponent for $\langle G \rangle$ versus $P$ close to 0.5 for packings of both frictionless and frictional spherical particles with repulsive linear spring interactions and how does the exponent vary with the form of the repulsive interaction potential?

In the first project, we focus on the mechanical response of jammed packings of $N$ frictionless spherical particles during isotropic compression. We show that $\langle G \rangle$ has two key contributions: 1) continuous variations of the shear modulus as a function of pressure along geometrical families, for which the interparticle contact network does not change and 2) discontinuous jumps during compression that arise from changes in the contact network. We find that the form of the shear modulus $G^f$ for jammed
packings within near-isostatic geometrical families is largely determined by the affine response. We further show that the ensemble-averaged shear modulus, \( \langle G(P) \rangle \), is not simply a sum of two power-laws, but \( \langle G(P) \rangle \sim (P/P_c)^a \), where \( a \approx (\alpha - 2)/(\alpha - 1) \) in the \( P \to 0 \) limit, \( \alpha \) is the exponent that controls the form of the purely repulsive interparticle potential, and \( \langle G(P) \rangle \sim (P/P_c)^b \), where \( b \gtrsim (\alpha - 3/2)/(\alpha - 1) \) above a characteristic pressure that scales as \( P_c \sim N^{-2(\alpha-1)} \).

In the second project, we investigate whether jammming preparation protocol of frictional spherical particles gives rise to differences in their mechanical properties. We find that the average contact number and packing fraction at jamming onset are similar (with relative deviations < 0.5%) for packings generated via isotropic compression and simple shear. In contrast, the average stress anisotropy \( \langle \hat{\Sigma}_{xy} \rangle = 0 \) for packings generated via isotropic compression, whereas \( \langle \hat{\Sigma}_{xy} \rangle > 0 \) for packings generated via simple shear. To investigate the difference in the stress state of jammed packings, we develop two additional packing-generation protocols: 1) we adopt a method of shear to unjam packings that were originally jammed by means of compression, and then re-jam them use simple shear and 2) we adopt a method of decompression to unjam packings that were originally jammed by means of shear, and then re-jam them using isotropic compression. Comparing stress anisotropy distributions of the original jammed packings and the re-jammed packings, we find that there are nonzero stress anisotropy deviations \( \Delta \hat{\Sigma}_{xy} \) between the jammed and re-jammed packings, but the deviations are smaller than the fluctuations in the stress anisotropy obtained by enumerating the force solutions within the null space of the contact networks of the jammed packings. These results emphasize that even though the compression and shear jamming protocols generate jammed packings with the same contact networks, there can be residual differences in the normal and tangential forces at each contact,
and thus differences in the stress anisotropy of the packings.

We conclude the thesis with suggested directions for future research. Topics include studies of geometrical families in packings of frictional, spherical particles, studies of the pressure-dependence of the shear modulus for non-spherical particles, and studies of the mechanical properties of frictional, non-spherical particles.
Computational Studies of the Protocol-dependent Mechanical Properties of Granular Materials

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Chapter 1

Introduction

Granular media, such as powders [1], soy beans, sand piles, icebergs [2], riverbeds [3, 4], as well as asteroid belts [5], are ubiquitous in nature. In practical applications, it is the second-most manipulated materials in the world, just after water [6]. In industrial applications, for instance, understanding mixing and demixing of granular media [7, 8, 9] is critical in many processes involving grains and powders. Many geophysical events such as avalanches [10], landslides, and earthquakes also involve the participation of granular materials. There are also works that explore the potential using granular materials as mechanical logical devices [11, 12, 13, 14]. These aforementioned works strongly suggest the extensive applicability of knowledge in granular materials in both fundamental research and applied fields. Dry granular media are collections of macroscopic grains that interact via repulsive contact forces. Mechanical and structural properties of granular media are governed by the particle shape, surface roughness and the repulsive force law. Over the past two decades, computational tools such as molecular dynamics simulations and Monte Carlo simulations have developed rapidly such that we can now study large scale, complex problems [15, 16]. Yet, many fundamental questions in granular materials remain unexplored.

A fundamentally important question concerning granular media is the jamming
transition, where the liquid-like granular media is compressed quasistatically to form disordered, solid-like state \([17, 18, 19]\). In the limit of zero pressure, frictionless grains \((\mu = 0)\) jammed isostatically at critical packing fraction \(\phi_J\) – the number of constraints equals to the total number of degrees of freedom of the system \([20]\), \(i.e.,\)

\[
CN_{iso}^i = 2d_fN'
\]

where \(C\) is the constraints provided by each contact, \(N_{iso}^i\) is the total number of contacts at isostatic, \(N'\) is the number of nonrattler particles in the system and \(d_f\) is the number of degrees of freedom per particle. In frictionless system, \(d_f\) equals to the spatial dimension of the system and directly corresponds to the translational motion of the grain. This results in four contacts per particle on average \((\langle z \rangle \approx 2d = 4)\) in two dimension system. For frictional grains, in addition to the orthogonal translations, rotational motion should also be considered. In the limit of infinite friction coefficient grains, the frictional system will also remain isostatic with each particle carrying three contacts on average \((\langle z \rangle \approx d + 1 = 3)\) in two dimension system. Whereas for intermediate friction coefficient, jammed packings at zero pressure would posses more contacts than \(N_{iso}^i(\mu \to \infty)\), leading to hyperstatic packings \([21]\). The mechanical properties of jammed packings depend on the contact networks for frictionless grains. For example, anisotropic contact network results in anisotropic stress state \([22]\). This can occur at jamming onset and beyond. In this thesis, I would like to focus on gaining a better understanding of the mechanical properties of frictionless and frictional granular materials.

Understanding force-bearing jammed packings is important in better describing and predicting the mechanical and structural properties of granular material. In the seminal work of O’Hern \([17]\), both bulk modulus and shear modulus, defined as

\[
K \sim dP/d\phi,
\]

\(1.2\)
as a function of $\phi - \phi_c$ has been investigated for frictionless spheres above jamming onset. Power-law scaling of bulk modulus on $\phi - \phi_c$ has been demonstrated to be dependent on the affine contribution by applying an uniform compression field without further performing potential energy minimization (Fig. 1.1). On the other hand, power-law scaling of shear modulus on $\phi - \phi_c$ cannot be solely explained by the affine contribution (Fig. 1.2). This suggests the importance to consider both the affine and nonaffine contribution to shear modulus. In recent studies [23, 24], it is demonstrated that ensemble-averaged shear modulus, $\langle G(P) \rangle$, have finite system size dependence for linear repulsive spring potential frictionless grains. $\langle G(P) \rangle$ exhibited power-law scaling as $P^{1/2}$ at high pressure regime as previously shown [17]. At low pressure, however, $\langle G(P) \rangle$ plateaus. One may attributes the plateau to the definition of shear
modulus, that is, the second derivative of the potential energy that is determined by the repulsive contact law \( G \sim \frac{d^2U}{d\gamma^2} \) – which would result in a constant. However, the system size dependence of the plateauing behavior is still puzzling. The origin of the low pressure behavior and system size dependence was later elucidated by a very recent work from the O’Hern group [25]. Finite system size jammed packing can be gradually compressed following potential energy minimization at each of the successive compression steps while maintaining the same contact network until experiencing rearrangement event. Collection of these states that share the same contact network form a geometrical family (Fig. 1.3, see [26]). Using energy conservation derivation for linear repulsive spring potential of frictionless grains, it is demonstrated that for a single geometrical family [25, 26],

\[
G_f(P) = G_0 - \lambda P, \quad (1.4)
\]
where \( \lambda \equiv \phi^{-1} \frac{d^2 \phi}{d \gamma^2} \) and \( \gamma \) is the strain steps. Eq. 1.4 suggests that \( G_f \) has to decrease with \( P \) in a geometrical family. This also suggests that in general, \( \langle G \rangle = \langle G_f \rangle + \langle G_r \rangle \), where \( G_r \) is the rearrangement contribution. In the absence of rearrangement event at sufficiently low pressure, family contribution dominates and leads to the seemingly plateauing of \( \langle G \rangle \). In high pressure regime, rearrangement contribution that raises shear modulus by forming more contacts competes with family contribution that decreases with pressure. Yet, the general form of \( G_f \) is not well-understood. In this thesis, we would like to further investigate the general form of \( G_f \) and to understand how \( G_f \) depends on the exponent that dictates the repulsive force law.

In the original jamming phase diagram (Fig. 1.4 (a)), the boundaries separating jammed states from the unjammed states made no suggestion on how one can access
Figure 1.4: (a) Original jamming phase diagram for athermal packings. $\tau$ is the shear stress and $\phi$ is the packing fraction. The boundary separating jammed and unjammed is the yield stress line. Increasing shear stress or decreasing packing fraction both leads to unjammed states. (b) Revised jamming phase diagram including both the shear jammed states (SJ) and fragile states (F). Jamming is possible for $\phi < \phi_J$ provided sufficient shear stress magnitude.
CHAPTER 1. INTRODUCTION

the jammed states by using a jamming protocol other than isotropic compression. It was previously understood that shearing a finite system size jammed state at yielding stress causes the packing to unjam. This original picture was later revised by the concept of shear jamming [27], demonstrated experimentally, of which one can visit solid-like states through shear for systems having $\phi < \phi_J$ (Fig. 1.4 (b)). This pioneering work raises the question of whether the shear jammed states are unique and can only be access by shear jamming protocol. Jammed frictionless grains at isostatic can be fully described by $\phi$ and $\vec{r}$, where $\vec{r}$ is the position of grains, to extract useful mechanical properties (stress tensor) and structural information (contact network). Frictional grains having intermediate friction coefficients, on the other hand, is typically hyperstatic. What is special about hyperstatic packings is that the set of equations of motion is underdetermined, leading to infinite number of force solutions, or no solution. This introduces difficulty in defining a jammed packing with $\phi$ and $\vec{r}$. The protocol, or history, of how to obtain the jammed packing becomes important for frictional grains. When attempting to explain phase-transition of granular material from equilibrium statistical mechanics point of view, the fact that energy conservation and equipartitioning do not hold make the task nontrivial. The probability of visiting each of the unique jammed states is not equally likely and it can depends on the jamming protocol. Prior attempts on formulating a statistical mechanics picture includes Edwards ensemble [28], force network ensemble [29, 30, 31], and stress ensemble [32, 33]. Despite a recent work from the O’Hern group suggests that one can access the same state through isotropic compression protocol and simple shear protocol for frictionless grains [26], a universal picture that is applicable to frictional particles remains unclear. To establish better understanding of shear modulus for frictional grains, it is essential to first understand how jammed states are sampled.
using different protocols.

This thesis addresses two important open questions related to granular materials. First, what is the shear modulus of granular packings for $\phi > \phi_J$ for frictionless grains? Second, how does frictional jammed packings depend on packing generation protocols?

In Chapter 2, we studied the shear response of overcompressed frictionless granular materials. We demonstrated that $G_f(P)$ carries the form of affine shear modulus at low pressure. Whereas at high pressure it is the combined contribution of geometrical family and rearrangements that result in $\langle G \rangle$.

In Chapter 3, we studied the jamming protocol dependence of frictional packings using the Cundall-Strack contact model. We demonstrated that simple shear jamming protocol results in more sliding contacts by using a novel rejamming protocol to rejam originally compression jammed packings. On the other hand, isotropic compression jamming protocol do not lead to qualitative difference in stick-slide distribution of tangential contacts through rejamming of originally sheared jammed packings.
Chapter 2
Shear Response

2.1 Introduction

Granular materials, such as collections of grains, bubbles, or other macroscopic particles, interact via highly dissipative forces, which cause these materials to come to rest unless they are continuously driven, e.g. by gravity, shear, or other applied deformations [34]. Further, granular materials transition from fluid- to solid-like states with a nonzero static shear modulus when they are compressed to sufficiently large packing fractions [17]. Despite numerous experimental [35], theoretical [36], and simulation studies [37] of the jamming transition in granular media, there are numerous open questions concerning the structural properties and mechanical response of jammed granular packings.

A simple model for jamming in granular materials is one where we consider frictionless, spherical particles that interact via the pairwise, purely repulsive, finite-ranged (“soft particle”) potential [38, 39]:

\[
U(r_{ij}) = \frac{\epsilon}{\alpha} \left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^\alpha \Theta \left(1 - \frac{r_{ij}}{\sigma_{ij}}\right),
\]

(2.1)

where \(r_{ij}\) is the separation between the centers of particles \(i\) and \(j\), \(\sigma_{ij} = (\sigma_i + \sigma_j)/2\) is the average diameter of particles \(i\) and \(j\), \(\Theta(\cdot)\) is the Heaviside step function that
Figure 2.1: Snapshots of $N = 32$ jammed disk packings with repulsive linear spring interactions ($\alpha = 2$ in Eq. 2.1) undergoing isotropic compression before and after a point change where a new contact is added to the contact network (indicated by thin blue lines). In (a), we show an isostatic packing at $P = 10^{-7}$ with $N_c = N_c^0 = 59$ contacts. (b) The packing in (a) has been compressed to $P = 4.60 \times 10^{-6}$ without any changes in the contact network. The vectors indicate the displacements of the particle centers relative to the packing in (a) after multiplying by 100. (c) The packing in (c) has been compressed to $P = 4.65 \times 10^{-6}$, which results in the addition of one contact, $N_c = N_c^0 + 1$, indicated by the thick black line. The shaded particles indicate rattlers.

Prevents particles from interacting if they are not in contact, $\epsilon$ is the characteristic energy scale, and $\alpha$ is the power-law scaling exponent of the interaction. For this interaction potential, the onset of jamming in a system with periodic boundary conditions occurs when the number of interparticle contacts $N_c$ first reaches the isostatic value $[40]$, $N_c^0 = dN - d + 1$, where $d = 2, 3$ is the spatial dimension and $N$ is the number of non-rattler particles $[41]$. Non-rattler particles are particles that are considered force-bearing and contributes to the force balance of the jammed packing. As the system is further compressed, the pressure increases from zero.

An important feature of the mechanical response of jammed particle packings is the dependence of the shear modulus $G$ and bulk modulus $B$ on the pressure $P$ under isotropic compression. Prior computational studies of jammed packings of spherical particles have shown that the pressure dependence of the bulk modulus is dominated by the affine response, whereas the pressure dependence of the shear modulus has
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significant nonaffine contributions [17]. Affine response typically corresponds to the
response of uniformly deformed packing but do not necessarily in force balance. For
example, an effective medium theory, which assumes only affine motion of the parti-
cles, predicts that the shear modulus scales as $G(P) \sim P^{1/3}$ for jammed packings of
spheres with repulsive Hertzian spring interactions [42] (i.e. $\alpha = 5/2$ in Eq. 2.1 [43]),
whereas experiments and simulations have shown that $G$ increases more strongly
than $P^{1/3}$ for packings of Hertzian spheres [39, 44, 45]. Other studies of sphere pack-
ings with repulsive linear spring interactions have shown that the ensemble-averaged
shear modulus is constant at low pressures, $G(P) \sim P^{1/2}$ at high pressures, and
the crossover pressure that separates the two scaling regimes decreases as $1/N^2$ with
increasing system size [24].

What determines the pressure dependence of the shear modulus as packings of
spherical particles are compressed above jamming onset? We have shown in previous
studies [25] of jammed packings of spherical particles (with $\alpha = 2$) that the pressure
dependence of the shear modulus is controlled by two key contributions: geometrical
families [26] and changes in the interparticle contact network [46]. For isotropic
compression, jammed packings within a given geometrical family are mechanically
stable packings with different pressures that are related to each other via continuous,
quasistatic changes in packing fraction with no changes in the contact network. In
prior studies [25], we found that the shear modulus $G^f$ within each geometrical family
decreases with increasing pressure when the interparticle contact network does not
change during compression. In these previous studies, we assumed that (for repulsive
linear spring interactions) $G^f$ varies continuously as $G^f(P)/G_0^f = 1 - P/P_0^f$, where
$G_0^f = G^f(0)$ and $P_0^f$ is the pressure at which $G^f = 0$. In the present work, we
will revisit this assumption and more accurately determine the dependence of $G^f$ on
CHAPTER 2. SHEAR RESPONSE

pressure.

Geometrical families begin and end at “point” and “jump changes” in the contact network [46, 47]. Point changes involve the addition or removal of a single interparticle contact (or multiple contacts when a rattler is added or removed from the contact network) without significant particle motion. Point changes give rise to a discontinuous jump in the shear modulus for power-law exponent $\alpha = 2$ in Eq. 2.1, but not for $\alpha > 2$. In contrast, jump changes correspond to mechanical instabilities [48, 49] with multiple simultaneous changes in the contact network and a discontinuous jump in the shear modulus across the jump change for any $\alpha$. At low pressures, where there are very few changes in the contact network, the geometrical family contribution dominates the ensemble-averaged shear modulus, and thus $\langle G \rangle \sim G_f^0$ for sphere packings with repulsive linear spring interactions in the $P \rightarrow 0$ limit. At finite pressure, both geometrical families and changes in the contact network contribute to the pressure dependence of the ensemble-averaged shear modulus.

In this thesis, we generalize the description of the pressure dependence of the shear modulus for packings of spherical particles compressed above jamming onset to systems with purely repulsive interactions and $\alpha \geq 2$, which includes jammed packings of Hertzian spheres. In particular, we characterize the pressure dependence of the shear modulus for geometrical families for near-isostatic packings and decompose the ensemble-averaged shear modulus into contributions from geometrical families and from point and jump changes in the contact network for $\alpha \geq 2$.

We find several important results. First, we decompose the shear modulus for each geometrical family $G^f$ into the affine $G^f_a$ and non-affine $G^f_n$ contributions [50, 49, 51], where $G^f = G^f_a - G^f_n$. The affine contribution considers the linear response of the jammed packing to an ideal simple shear deformation without relaxation, whereas
the non-affine contribution includes particle motion from minimization of the total potential energy. We show that the affine shear modulus for jammed packings within near-isostatic geometrical families obeys

\[ \frac{G^f_a}{G_{a0}(\alpha)} = \left( \frac{P}{P_0(\alpha)} \right)^{\frac{\alpha-2}{\alpha-1}} - \frac{P}{P_0(\alpha)}, \]  

(2.2)

where \( G_{a0}(\alpha) \) provides a scale for the shear modulus and \( P_0(\alpha) \) is the pressure at which \( G^f_a = 0 \). The affine shear modulus \( G^f_a \) includes two terms: a positive contribution that scales with pressure as \( (P/P_0(\alpha))^{(\alpha-2)/(\alpha-1)} \) and a term that decreases linearly with \( P \) and is independent of the exponent \( \alpha \).

We next characterize the form for the shear modulus \( G^f \) of near-isostatic geometrical families close to point and jump changes in the contact network. We show that when geometrical families persist to large pressures, the non-affine particle motion becomes large, which causes \( G^f_a \) to deviate from the form in Eq. 2.2. As shown previously for packings of spherical particles with repulsive linear spring interactions [25], we find that both geometrical families and changes in the contact network determine the scaling of the ensemble-averaged shear modulus at finite pressure for all \( \alpha \geq 2 \). The ensemble-averaged shear modulus scales as \( \langle G(P) \rangle \sim P^a \), where \( a \sim (\alpha - 2)/(\alpha - 1) \) at low pressures below a characteristic pressure \( P_c \sim 1/N^{2(\alpha-1)} \), and \( \langle G(P) \rangle \sim P^b \), where \( b \gtrsim (\alpha - 3/2)/(\alpha - 1) \) for \( P > P_c \). Specifically, for Hertzian spheres, we find that \( \langle G(P) \rangle \sim P^{1/3} \) for \( P < P_c \) and \( \langle G(P) \rangle \sim P^{2/3} \) for \( P > P_c \), which is consistent with prior experimental [42] and simulation results [39, 17].

The remainder of this article is organized as follows. In Sec. 2.2, we describe the numerical methods used in this study, including the quasistatic, isotropic compression protocol used to generate the jammed packings and the calculations of the pressure, shear stress, and shear modulus for the jammed packings. The key results are presented in Sec. 2.3. We first describe the calculations of the shear modulus as
Figure 2.2: (a) Shear modulus $G^{(1)}$ versus pressure $P$ (black points) for isostatic packings with $N = 32$ disks within 50 geometrical families that maintain their inter-particle contact networks for purely repulsive linear ($\alpha = 2$) spring interactions. The blue lines give the affine contribution $G^{(1)}_a$ (Eq. 2.2) for each geometrical family. Blue open circles (red crosses) at the end of $G^{(1)}$ indicate that the packing experienced a point (jump) change at that particular pressure. In this panel, we do not show packings with $G^{(1)} < 0$. (b) $(G^{(1)}/G_0)(P/P_0)^{-1/2}$ for isostatic geometrical families plotted versus $P/P_0$ for disk packings with repulsive linear ($\alpha = 2$) spring interactions, for several system sizes: $N = 32$ (black upper triangles), 64 (blue circles), 128 (red diamonds), 256 (green downward triangles), and 512 (magenta asterisks). The dashed line is Eq. 2.4 for $\alpha = 2$ and the solid lines are fits to Eq. 2.4. In the inset, we show $\Delta G^{(1)} = G^{(1)}(P/P_0) - G^{(1)}(0)$ (black upward triangles), $\Delta G^{(1)}_n = G^{(1)}_n(P/P_0) - G^{(1)}_n(0)$ (red dots), and $\Delta G^{(1)}_a = G^{(1)}_a(P/P_0) - G^{(1)}_a(0)$ (blue exes) with best fits to Eq. 2.2 (black, red, and blue solid lines, respectively) for an example $N = 32$ packing with $\alpha = 2$. (c) $G^{(1)}$ versus $P$ for the packings in (a) plotted on linear scales (with $G^{(1)} < 0$). The blue lines indicate best fits to Eq. 2.4 for each geometrical family.
a function of pressure for packings in the first and second geometrical families. We determine analytically the affine contribution to the shear modulus within a given geometrical family and compare the affine shear modulus to the total shear modulus obtained from numerical simulations of sphere packings undergoing quasistatic, isotropic compression. We calculate the ensemble-averaged shear modulus $\langle G \rangle$ as a function of pressure and show how the scaling of $\langle G \rangle$ with pressure varies with the power-law exponent $\alpha$. For each $\alpha$, we decompose $\langle G(P) \rangle$ into contributions from geometrical families and changes in the contact network and show that both contributions are important at finite pressure in the large-system limit. In Sec. 2.4, we summarize our conclusions and suggest future research directions. We also include four appendices to provide additional technical details that supplement the main text. In Appendix 2.5.1, we include a derivation of the decomposition of the shear modulus into the affine and non-affine terms and provide explicit expressions to calculate the non-affine term [49, 51]. In Appendix 2.5.2, we provide a derivation of the pressure dependence of the affine contribution to the shear modulus of near-isostatic geometrical families. In Appendix 2.5.3, we calculate the shear modulus for near-isostatic geometrical families as a function of pressure for jammed disk packings with $\alpha = 3$ and for sphere packings with $\alpha = 2$ and $5/2$. In Appendix 2.5.4, we show that since the isostatic geometrical family contribution to the shear modulus includes a strongly negative contribution, the shear modulus can become negative for jammed packings generated at fixed shear strain [52].

2.2 Methods

We investigate the mechanical properties of isotropically compressed jammed packings of bidisperse disks in 2D and spheres in 3D, containing $N/2$ large and $N/2$ small
particles, each with the same mass $m$, and diameter ratio $\sigma_l/\sigma_s = 1.4$. The particles are confined within a square/cubic box with side lengths, $L_x = L_y = 1$ in 2D or $L_x = L_y = L_z = 1$ in 3D, and periodic boundary conditions in all directions. We consider pairwise, purely repulsive, finite-ranged interactions between particles of the form in Eq. 2.1, for which the potential energy scales as a power-law in the overlap between pairs of particles with exponent $\alpha$. Pair forces are calculated using $\vec{f}_{ij} = -dU(r_{ij})/dr_{ij}\hat{r}_{ij}$, where $\hat{r}_{ij} = \vec{r}_{ij}/r_{ij}$ is the unit vector pointing from the center of particle $j$ to the center of particle $i$. Results are presented below for $\alpha = 2$ (linear springs), $5/2$ (Hertzian springs), and 3. The pressure, shear stress, and shear modulus are expressed in units of $\epsilon/\sigma_s^d$ and forces are expressed in units of $\epsilon/\sigma_s$ below.

We calculate the stress tensor $\hat{\Sigma}$ for each mechanically stable packing using the virial expression [53]:

$$\hat{\Sigma}_{\beta\delta} = L^{-d} \sum_{i>j} f_{ij\beta} r_{ij\delta},$$

(2.3)

where $\beta, \delta = x, y, \text{or } z$, $f_{ij\beta}$ is the $\beta$-component of the interparticle force $\vec{f}_{ij}$ on particle $i$ due to particle $j$, and $r_{ij\delta}$ is the $\delta$-component of the separation vector $\vec{r}_{ij}$. Note that we exclude rattler particles when calculating $\hat{\Sigma}_{\beta\delta}$. We define the shear stress as $\Sigma = -\hat{\Sigma}_{xy}$ and the pressure as $P = \hat{\Sigma}_{\beta\beta}/d$. To calculate the shear modulus $G$ numerically for each packing, we apply a series of small affine simple shear strain steps, $x'_i = x_i + d\gamma y_i$, to the jammed packing in combination with Lees-Edwards boundary conditions, where $d\gamma = 10^{-9}$ is the shear strain increment, and minimize the total potential energy $U = \sum_{i>j} U(r_{ij})$ using the FIRE algorithm [54] after each applied shear strain. We then measure the static shear modulus $G = d\Sigma/d\gamma$ in the $\gamma \to 0$ limit.

Below, we will characterize the shear modulus as a function of pressure from the onset of jamming near $P = 0$ to systems that are significantly compressed with
overlaps \( \langle r_{ij} - \sigma_{ij} \rangle / \sigma_{ij} \approx 1\% \). To initialize the system, we randomly place particles in the simulation cell at rest and with no overlaps at packing fraction \( \phi < 0.01 \). We increase the packing fraction in small increments \( d\phi \) by increasing the particle diameters uniformly, and following each compression step, we minimize the total potential energy \( U \). Energy minimization is terminated when \( (\sum_i \tilde{f}_i/N)^2 < 10^{-32} \), where \( \tilde{f}_i = \sum_j \tilde{f}_{ij} \). Note that energy minimization can terminate when all of the pair forces \( f_{ij} \) are near zero (i.e. the system is unjammed) or when the system achieves force balance with nonzero pair forces. After each compression step, we measure the pressure \( P \) and compare it to a target pressure \( P_t \). If \( P < P_t \), we compress the system by \( d\phi \) and minimize the total potential energy. If \( P > P_t \), we return to the system with the lower pressure, reduce the packing fraction increment from \( d\phi \) to \( d\phi / 2 \), and compress the system again, and repeat the process. This process is terminated when the pressure satisfies \( P_t < P < (1 + \zeta)P_t \), where \( \zeta = 10^{-7} \).

We sample more than 1000 jammed packings logarithmically in pressure, spanning from isostatic packings at \( P = 10^{-7} \) to compressed states with \( P = 10^{-2} \) for \( \alpha = 2 \). To generate packings of spherical particles interacting via Eq. 2.1 with \( \alpha = 5/2 \) and 3, we initialized the system with isostatic packings generated using \( \alpha = 2 \) and then performed the compression protocol plus energy minimization using the appropriate \( \alpha \). Using the initialization, we have verified that the isostatic contact networks are the same for all \( \alpha \) that we studied. For \( \alpha = 5/2 \) and 3, the pressures that we sample vary from \( P = 10^{-10} \) to \( 10^{-2} \).

### 2.3 Results

The results concerning the mechanical properties of jammed packings of spherical particles with finite-ranged, purely repulsive interactions are presented in three sec-
Figure 2.3: (a) Shear modulus $G^{(1)}$ versus pressure $P$ (black points) for isostatic packings with $N = 32$ disks within 50 geometrical families that maintain their interparticle contact networks for Hertzian ($\alpha = 5/2$) spring interactions. The blue lines give the affine contribution $G^{(1)}_a$ (Eq. 2.2) for each geometrical family. Blue open circles (red crosses) at the end of each $G^{(1)}$ indicate that the packing experienced a point (jump) change at that particular pressure. We do not show packings with $G^{(1)} < 0$.  (b) $(G^{(1)}/G_0)(P/P_0)^{-2/3}$ for isostatic geometrical families plotted versus $P/P_0$ for disk packings with Hertzian ($\alpha = 5/2$) spring interactions, for several system sizes: $N = 32$ (black upper triangles), 64 (blue circles), 128 (red diamonds), 256 (green downward triangles), and 512 (magenta asterisks). The dashed line is Eq. 2.4 for $\alpha = 5/2$ and the solid lines are fits to Eq. 2.4 for $\alpha = 5/2$. In the inset, we show $G^{(1)}$ (black upward triangles), $G^{(1)}_n$ (red dots), and $G^{(1)}_a$ (blue exes) with best fits to Eq. 2.2 (black, red, and blue solid lines, respectively) for an example $N = 32$ packing with $\alpha = 5/2$.  (c) $G^{(1)}$ versus $P$ for the packings in (a) plotted on a linear scale (and including packings with $G^{(1)} < 0$). The blue lines indicate best fits to Eq. 2.4 for each geometrical family.
tions below. In Sec. 2.3.1, we investigate the shear modulus $G^{(1)}$ for jammed packings of spherical particles that occur in the first, isostatic geometrical families (for power-law exponents $\alpha = 2, 5/2, \text{and} 3$ and several system sizes) and determine how $G^{(1)}$ varies with pressure prior to the first change in the interparticle contact network. (Choose $f = 1$ in Eq. 2.2.) We show that for small pressures, the shear modulus of the first geometrical family, $G^{(1)} \sim G^{(1)}_a$, is given by the affine contribution to the shear modulus. For near isostatic geometrical families that persist to higher pressures, the non-affine contribution plays an important role in determining the behavior of $G^{(1)}(P)$ even though the contact network does not change. In Sec. 2.3.2, we calculate the pressure-dependent shear modulus of jammed packings that belong to the second geometrical family, i.e. packings that have undergone a change in the contact network and now belong to a different geometrical family than the isostatic one that occurs in the $P \to 0$ limit. In Sec. 2.3.3, we determine the ensemble-averaged shear modulus $\langle G \rangle$ and find a master curve for $\langle G(P) \rangle$ as a function of system size. To better understand the pressure dependence, we decompose $\langle G \rangle = \langle G^f \rangle + \langle G^r \rangle$ into contributions from geometrical families $G^f$ and changes in the contact network $G^r$. We show that in the large-system limit both contributions are important for determining the ensemble-averaged shear modulus $\langle G \rangle$ at finite pressure.

2.3.1 Isostatic Geometrical Families

Isotropically compressed jammed packings occur as geometrical families as a function of pressure. Specifically, if we consider a packing at jamming onset with $P = 0$, it will possess packing fraction $\phi_J$, non-rattler particle positions $\vec{R} = \{x_1, x_2, \ldots, x_N, y_1, y_2, \ldots, y_N\}$ in 2D or $\vec{R} = \{x_1, x_2, \ldots, x_N, y_1, y_2, \ldots, y_N, z_1, z_2, \ldots, z_N\}$ in 3D, and a contact network with an isostatic number of contacts, $N_c = N_c^0$. If we compress the jammed system by $d\phi$ (and minimize the total potential energy), the particle positions will
change continuously with $d\phi$ to $\vec{R}'$, the pressure will become nonzero, and as long as $d\phi$ is sufficiently small, the interparticle contact network will not change. At a given pressure $P^*$, which is different for each isostatic contact network, the contact network will undergo a point change or a jump change [47]. In Fig. 2.1, we show the contact network for an isostatic jammed packing (with $N = 32$ and $\alpha = 2$) near the onset of jamming (with $P = 10^{-7}$) and immediately before (with $P = 4.60 \times 10^{-6}$) and after (with $P = 4.65 \times 10^{-6}$) a point change. After the point change, the jammed packing has one extra interparticle contact and $N_c = N^0_c + 1$. This behavior is similar for isotropically compressed packings with larger system sizes, except $P^*$ decreases with increasing system size.

The shear modulus $G^{(1)}$ of isostatic geometrical families can be decomposed into the affine $G_a^{(1)}$ and non-affine contributions $G_n^{(1)}$ [49, 51]: $G^{(1)} = G_a^{(1)} - G_n^{(1)}$. (See Appendix 2.5.1.) The affine contribution $G_a^{(1)}$ considers the linear response of the jammed packing to an ideal simple shear deformation without relaxation, whereas the non-affine contribution $G_n^{(1)}$ includes particle motion from minimization of the total potential energy after the applied simple shear strain. In Fig. 2.2 (a), we show the shear modulus $G^{(1)}$ versus pressure $P$ (on logarithmic scales) for isostatic disk packings within each of 50 different geometrical families generated using $N = 32$ and $\alpha = 2$. We find that for each geometrical family, $G^{(1)}$ tends to a constant in the $P \to 0$ limit, and decreases with increasing pressure. Note that the curves in Fig. 2.2 (a) for $G^{(1)}(P)$ end at different pressures $P^*$ where a point or jump change in the contact network occurs. (We find similar results for jammed sphere packings in 3D with $\alpha = 2$ in Appendix 2.5.3.)

We first compare $G^{(1)}(P)$ (black points in Fig. 2.2 (a)) to the affine contribution to the shear modulus $G_a^{(1)}(P)$ (blue lines in Fig. 2.2 (a)), where $G_a^{(1)}(P)/G_{a0}(2) =$
1 − \( P/P_0(2) \) is derived and the expressions for \( G_{a0}(2) \) and \( P_0(2) \) are given in Appendix 2.5.2. On this scale, we do not see large deviations from \( G^{(1)} \sim G_{a}^{(1)} \). The probability distributions for the coefficients \( P_0(2) \) and \( G_{a0}(2) \) for several system sizes are shown in Fig. 2.4 (a) and Fig. 2.5 (a). We find that the average values \( \langle P_0(2) \rangle \sim N^{-2} \) and \( \langle G_{a0}(2) \rangle \sim N^{-1} \) tend to zero in the large-system limit as shown in the insets to Fig. 2.4 (a) and Fig. 2.5 (a).

To investigate \( G^{(1)}(P) \) for jammed packings of repulsive Hertzian disks, we start with an isostatic disk packing generated using repulsive linear spring interactions at the lowest pressure we considered, change the interaction potential from \( \alpha = 2 \) to \( 5/2 \), and minimize the total potential energy. (See the description of the packing-generation protocol in Sec. 2.2.) We verified that each lowest-pressure, isostatic packing for repulsive linear spring interactions gives rise to an isostatic packing for repulsive Hertzian spring interactions. We then repeat (for repulsive Hertzian spring interactions) the same isotropic compression protocol used to generate isostatic geometrical families for systems with \( \alpha = 2 \). We show the shear modulus \( G^{(1)}(P) \) for the isostatic geometrical families for disks with \( \alpha = 5/2 \) (on logarithmic scales) in Fig. 2.3 (a). In contrast to the results for repulsive linear spring interactions, \( G^{(1)} \to 0 \) in the \( P \to 0 \) limit. As we found for \( \alpha = 2 \), \( G^{(1)} \) also decreases at sufficiently large pressures and we do not find significant deviations from \( G^{(1)} \sim G_{a}^{(1)} \) on logarithmic scales. (Similar results for sphere packings in 3D with \( \alpha = 5/2 \) are shown in Fig. 2.15 (a) in Appendix 2.5.3.)

Using Eq. 2.2, we predict \( G_{a}^{(1)}/G_{a0}(3) = (P/P_0(3))^{1/2} \) for jammed packings of spherical particles with \( \alpha = 3 \) in isostatic geometrical families. We show \( G^{(1)}(P) \) for packings with \( \alpha = 3 \) in Fig. 2.16 (a) in Appendix 2.5.3. Thus, from Eq. 2.2, \( G^{(1)}(P) \) tends to zero in the \( P \to 0 \) limit for all \( \alpha > 2 \) and after a characteristic
pressure that depends on the power-law exponent \( \alpha \) and system size \( N \), \( G^{(1)}(P) \) decreases linearly with increasing pressure for all \( \alpha \). The \( -P/P_0(\alpha) \) term in \( G^{(1)}_\alpha \) can give rise to unstable packings with \( G^{(1)} < 0 \) at finite pressures [55, 52, 56], but our results emphasize that all jammed packings possess \( G^{(1)} > 0 \) at sufficiently low pressures. (See Appendix 2.5.4 for statistics of \( G^{(1)} < 0 \) as a function of pressure and system size for several \( \alpha \) values.)

With a more detailed analysis, we can quantify deviations in \( G^{(1)} \) from \( G^{(1)}_\alpha \) by multiplying both sides of Eq. 2.2 by \( (P/P_0(\alpha))^{-(\alpha-3/2)/(\alpha-1)} \) to yield the symmetric form:

\[
\frac{G^{(1)}}{G_0(\alpha)} \left( \frac{P}{P_0(\alpha)} \right)^{-\frac{\alpha-3/2}{\alpha-1}} = \left( \frac{P}{P_0(\alpha)} \right)^{-\frac{1}{2(\alpha-1)}} - \left( \frac{P}{P_0(\alpha)} \right)^{\frac{1}{2(\alpha-1)}}.
\]

For \( P \gg P_0(\alpha) \), the term on the right hand side of Eq. 2.4 with the positive exponent will dominate, whereas for \( P \ll P_0(\alpha) \), the term with the negative exponent will dominate. In Fig. 2.2 (b) and Fig. 2.3 (b), we plot \( (G^{(1)}/G_0(\alpha))(P/P_0(\alpha))^{-(\alpha-3/2)/(\alpha-1)} \) versus \( P/P_0(\alpha) \) for packings in isostatic geometrical families with \( \alpha = 2 \) and 5/2. The data for \( G^{(1)} \) shows reasonable collapse onto a master curve (especially at low pressures) for the shear modulus for \( \alpha = 2 \) and 5/2 for all isostatic packings that we generated.

In Fig. 2.2 (b) and Fig. 2.3 (b), we show that \( G^{(1)} \) deviates from the dimensionless affine scaling form in Eq. 2.4 at large \( P/P_0 \) for some of the packings with \( \alpha = 2 \) and 5/2. In the insets to Fig. 2.2 (b) and Fig. 2.3 (b), we show that the deviations of \( G^{(1)} \) from the scaling form are caused by the growing non-affine contribution to the shear modulus as the pressure increases. These results are the same for \( G^{(1)} \) for all packings that possess deviations at large \( P/P_0 \) in Fig. 2.2 (b) and Fig. 2.3 (b). Since the non-affine motion is increasing toward the end of the isostatic geometrical families, it is likely that it is correlated with a mechanical instability [49, 51].
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To better capture the shear modulus for isostatic geometrical families $G^{(1)}(P)$ over the full range of pressure, we consider the empirical form:

$$\frac{G^{(1)}}{G_0(\alpha)} = \left(\frac{P}{P_0(\alpha)}\right)^{\frac{\alpha-2}{\alpha-1}} - \frac{P}{P_0(\alpha)} \left(\frac{P_0(\alpha) - P_1(\alpha)}{P - P_1(\alpha)}\right)^\kappa,$$

where $G^{(1)}(P_0(\alpha)) = 0$ and $P_1(\alpha) > P_0(\alpha)$ is the pressure at which $G^{(1)}$ has an apparent power-law divergence to $-\infty$ with exponent $0 < \kappa < 1$. In Fig. 2.2 (c) and Fig. 2.3 (c), we show $G^{(1)}(P)$ for $\alpha = 2$ and 5/2 on a linear scale and include $G^{(1)} < 0$. $G^{(1)}(P)$ decreases roughly linearly with pressure for $P_0 < P \ll P_1$, but then decreases much faster as the pressure approaches $P_1$ for several of the geometrical families. The fits of $G^{(1)}(P)$ to Eq. 2.4 in Fig. 2.2 (c) and 2.3 (c) show that it provides a good description of $G^{(1)}(P)$ over the full range of pressure. The probability distributions for $P_1(\alpha)$ for several system sizes and $\alpha = 2$ and 5/2 are provided in Fig. 2.6. For some geometrical families, for example, for those where point changes occur at low pressures, $G^{(1)}(P)$ does not deviate significantly from the affine form in Eq. 2.4 and $P_1$ is much greater than the pressure range we consider. When we do not include the $P_1$ values for these geometrical families in the average, we find that $\langle P_1 \rangle \sim \langle P_0 \rangle \sim N^{-2(\alpha-1)}$.

2.3.2 Shear Modulus for the Second Geometrical Family

In the previous section, we focused on the pressure-dependent shear modulus $G^{(1)}$ of isostatic geometrical families with $N_0^c$ contacts, prior to the first change in the contact network. In this section, we show preliminary studies of the shear modulus $G^{(2)}$ of the second geometrical family after the packing undergoes a point or jump change in the contact network at $P^*$. (See Figs. 2.7 and 2.8.) We find that when isostatic geometrical families undergo changes in the contact network during isotropic compression, $\approx 75\%$ undergo point changes to a second geometrical family and $\approx 25\%$
undergo jump changes to a second geometrical family for packings with repulsive linear and Hertzian spring interactions. These fractions do not depend strongly on system size. After point changes, nearly all of the packings in the second geometrical families possess $N_c^0 + 1$ contacts. (Note that some point changes correspond to rattler particles that join the contact network, and these point changes cannot be described as an isostatic system that gains a single contact.) For packings (with both $\alpha = 2$ and $5/2$ interactions) that undergo jump changes, $\approx 60\%$ of the packings in the second geometrical families possess $N_c^0$ contacts and most of the remaining fraction possess $N_c^0 + 1$ contacts. These results also do not depend strongly on system size.

In Fig. 2.7, we show the shear modulus $G^{(i)}$ (for the first and second geometrical families) as a function of pressure for a series of disk packings during isotropic compression. At $P^*$, the disk packing (with $\alpha = 2$ in (a) and $\alpha = 5/2$ in (b)) undergoes a point change and the isostatic geometrical family transitions to a second geometrical family with $N_c^0 + 1$ contacts. As pointed out in our previous studies [47], $G^{(i)}$ is discontinuous across a point change for $\alpha = 2$, but it is continuous across a point change for $\alpha > 2$. For $\alpha = 2$, we find that $G^{(2)}$ for most of the second geometrical families after a point change obey the same scaling form in Eq. 2.4 for isostatic geometrical families, and the characteristic pressure $P_0 \sim N^{-2}$ and shear modulus $G_0 \sim N^{-1}$ for the second geometrical families tend to zero in the large-system limit. (See Fig. 2.9 (a).) As we found for the first geometrical families in Fig. 2.2 (b), deviations from Eq. 2.4 can occur at large pressures $P > P_0$ when $G^{(2)}$ has a significant non-affine contribution. (See the inset to Fig. 2.9 (a).)

The shear moduli for the second geometrical families, $G^{(2)}$, for packings with $\alpha = 5/2$ after a point change possess deviations from the scaling form in Eq. 2.4 both at small pressures near the first point change and at large pressures near the second
change in the contact network, as shown in Fig. 2.9 (b). For the first geometrical family, there is an important characteristic pressure $P_0$ that determines when $G^{(1)} = 0$. (For the first geometrical families that persist to large pressures, we also identify a characteristic pressure $P_1 > P^*$, which likely signals an instability of the contact network.) For the second geometrical family following a point change with $\alpha > 2$, there is another characteristic pressure, $P^*$, indicating the pressure at which the point change from the first to second geometrical family occurs. For highly nonlinear interactions with $\alpha > 2$, the presence of multiple characteristic pressures causes $G^{(2)}$ to deviate from the affine form in Eq. 2.4. The inset to Fig. 2.9 (b) shows that the deviation of $G^{(2)}$ from the affine scaling form at small pressures is also caused by non-affine particle motion. The deviations of $G^{(2)}$ from the affine scaling form at large pressures following point changes for $\alpha = 5/2$ are similar to those found for $G^{(1)}$ near the end of the first geometrical family.

As shown in Fig. 2.8, the shear modulus $G^{(i)}$ is discontinuous when the system undergoes a jump change for packings with all $\alpha$. If an isostatic geometrical family undergoes a jump change to a second geometrical family, $G^{(2)}$ obeys Eq. 2.4 for packings with $\alpha = 2$ and $5/2$ over a wide range of pressure. (See Fig. 2.9 (c).) Again, there can be deviations in $G^{(2)}$ from the affine scaling form when the second geometrical family persists to large pressures. In future studies, we will investigate the general form of the shear modulus $G^{(i)}(P)$ for the third, fourth, and higher-order geometrical families at elevated pressures.

### 2.3.3 Ensemble-averaged Shear Modulus

In this section, we investigate the pressure dependence of the ensemble-averaged shear modulus $\langle G \rangle$, which is often studied to mimic the large-system limit. As shown in the previous section, jump changes in the contact network give rise to discontinuities
in the shear modulus for packings with all \( \alpha \). In contrast, the shear modulus is continuous across point changes for \( \alpha > 2 \), but it is discontinuous for \( \alpha = 2 \). The shear modulus for a single initial condition \( \lambda \) at \( P = 0 \) undergoing isotropic compression can be written as \( G^\lambda = G^{f,\lambda} + G^{r,\lambda} \), where \( G^{f,\lambda} \) describes the shear modulus along continuous geometrical families and \( G^{r,\lambda} \) includes discontinuities in the shear modulus from point and jump changes. (See Fig. 2.10.) \( G^{r,\lambda} \) for \( \alpha = 2 \) includes discontinuities in the shear modulus from both point and jump changes, whereas \( G^{r,\lambda} \) includes changes in the shear modulus from jump changes only for \( \alpha > 2 \). The ensemble-averaged shear modulus, \( \langle G \rangle \), is obtained by averaging over initial conditions \( \lambda \).

In Fig. 2.11, we show \( \langle G \rangle \), \( |\langle G^f \rangle| \), and \( \langle G^r \rangle \) for \( N = 128 \) disk packings with \( \alpha = 2 \) and \( 5/2 \). At small pressures, \( \langle G \rangle \sim \langle G^f \rangle \) since changes in the contact network are rare. In the \( P \to 0 \) limit, \( \langle G \rangle \) is a constant for packings with \( \alpha = 2 \) and \( \langle G \rangle \sim P^{1/3} \) for packings with \( \alpha = 5/2 \), consistent with the results in Sec. 2.3.1. For packings with \( \alpha = 2 \) and \( 5/2 \), as the pressure increases, \( \langle G^f \rangle \) decreases toward zero and at a characteristic pressure, \( \langle G \rangle \approx \langle G^r \rangle \). As the pressure continues to increase, \( \langle G^f \rangle < 0 \) (since the negative contribution to \( G^f \) dominates at large pressures), which causes the cusp in \( |\langle G^f \rangle| \) in Fig. 2.11. At large pressures, both \( \langle G^f \rangle \) and \( \langle G^r \rangle \) contribute to \( \langle G \rangle \), and \( \langle G \rangle < \langle G^r \rangle \).

In contrast to the affine scaling behavior found for the shear modulus \( G^{(1)} \) of isostatic geometrical families, the pressure dependence of the ensemble-averaged shear modulus \( \langle G \rangle \) is not simply the sum (or difference) of two power-laws in pressure [25], \( \langle G \rangle \sim AP^a + BP^b \) with exponents \( a \) and \( b \). (See Figs. 2.12 and 2.13.) To illustrate this, we consider the dimensionless, symmetric form for \( \langle G \rangle \):

\[
\frac{\langle G \rangle}{G_c} \left( \frac{P}{P_c} \right)^{(a-b)/2} = \left( \frac{P}{P_c} \right)^{(a-b)/2} + \left( \frac{P}{P_c} \right)^{- (a-b)/2},
\]

where \( G_c = \langle G \rangle (P_c)/2 \). Eq. 2.5 is dominated by the \( P^{(a-b)/2} \) term for \( P < P_c \) and
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by the $P^{-(a-b)/2}$ term for $P > P_c$. In Figs. 2.12 (a) and 2.13 (a), we plot Eq. 2.5 as dashed lines for packings with $\alpha = 2$ and $5/2$ and compare it to the simulation results for $\frac{\langle G \rangle}{G_c(\alpha)} \left( \frac{P}{P_c(\alpha)} \right)^{-(a+b)/2}$ for $a \sim (\alpha - 2)/(\alpha - 1)$ and $b \sim (\alpha - 3/2)/(\alpha - 1)$. For packings with both $\alpha = 2$ and $5/2$, the simulation data transitions between the two limiting power-law behaviors ($P/P_c(\alpha)$)$^{-(a-b)/2}$ and ($P/P_c(\alpha)$)$^{-(a-b)/2}$ much more abruptly than the sum of the two power-laws, $(P/P_c(\alpha))^{(a-b)/2} + (P/P_c(\alpha))^{-(a-b)/2}$. To capture this feature in the simulation data, we fit the simulation data for $\langle G \rangle$ to the $p$-norm of the right-hand side of Eq. 2.5, i.e.

$$\frac{\langle G \rangle}{G_c(\alpha)} \left( \frac{P}{P_c(\alpha)} \right)^{-(a+b)/2} = \left[ \left( \frac{P}{P_c} \right)^{p(a-b)/2} + \left( \frac{P}{P_c} \right)^{-p(a-b)/2} \right]^{1/p},$$

(2.6)

with $p \sim 2.5$ ($\sim 2.15$) for packings with $N = 32$ to 512 and $\alpha = 2$ ($\alpha = 5/2$). The $p$-norm generates polynomials with powers between $(a - b)/2$ and $-(a - b)/2$ to capture the kink-like feature in the simulation data. Fits to Eq. 2.6 allow us to collapse $\langle G \rangle(P)$ for all of the system sizes studied, as shown in Figs. 2.12 (b) and 2.13 (b). In the insets, we display the exponent $a \sim (\alpha - 2)/(\alpha - 1)$ that controls the low-pressure behavior of $\langle G \rangle$. The exponent $b \gtrsim (\alpha - 3/2)/(\alpha - 1)$ controls the large-pressure behavior. We also find that $P_c \sim N^{-2(\alpha-1)}$ and $G_c \sim N^{-2(\alpha-3/2)}$, which is the same system-size dependence as that for $P_0$ and $G_0$ for isostatic geometrical families.

For $\alpha = 2$, the scaling exponents in the low- and high-pressure limits are $a \sim 0$ and $b \sim 0.60$, and for $\alpha = 5/2$, the scaling exponents in the low- and high-pressure limits are $a \sim 0.36$ and $b \sim 0.70$ [57]. We find similar behavior for $\langle G \rangle$ for jammed sphere packings in 3D for $\alpha = 2$ and $5/2$. In the large-$\alpha$ limit, we predict that the scaling exponents in the low- and high-pressure limits will both approach 1.
2.4 Conclusions and Future Directions

The mechanical response of jammed packings of purely repulsive spherical particles to isotropic compression is complex \[45, 58\]. For example, several studies have shown that effective medium theory, which assumes an affine response to applied deformation, does not accurately predict the behavior of the shear modulus of jammed sphere packings as a function of pressure \[39, 44\]. In addition, simulations of the "soft particle" model \[17\], which assumes purely repulsive, finite-ranged interactions between spherical particles that scale as a power-law in their overlap with exponent \(\alpha\), have suggested that the ensemble-averaged shear modulus scales with pressure as \(\langle G \rangle \sim P^{(\alpha - 3/2)/(\alpha - 1)}\). However, the origin of the scaling exponent \((\alpha - 3/2)/(\alpha - 1)\) for the ensemble-averaged shear modulus is not well-understood.

In a recent study, we showed that there are two important contributions to the shear modulus in jammed packings of spherical particles undergoing isotropic compression \[25\]: continuous variations in the shear modulus from geometrical families, for which the interparticle contact network does not change, and discontinuous jumps in the shear modulus from changes in the contact network. In the present work, we show explicitly for \(\alpha = 2, 5/2,\) and 3 that the form of the shear modulus versus pressure for the first, isostatic geometrical family can be approximated by the affine shear response, i.e. \(G^{(1)} / G_0(\alpha) = (P/P_0(\alpha))^{(\alpha - 2)/\alpha - 1} - P/P_0(\alpha)\). However, we observe deviations of \(G^{(1)}\) from the affine form when near-isostatic geometrical families persist to large pressures \(P > P_0(\alpha)\).

For each initial configuration at \(P \sim 0\) that we isotropically compress, we can decompose the shear modulus \(G = G_f + G_r\) into contributions from geometrical families \(G_f\) and from discontinuities arising from point and jump changes in the contact network \(G_r\). We show that the ensemble-averaged shear modulus \(\langle G \rangle \sim \langle G_f \rangle\) at
low pressures since changes in the contact network are rare. At larger pressures, the geometrical family contribution is dominated by the $-P$ term (or other negative higher-order terms in $P$), $\langle G^f \rangle < 0$, and $\langle G \rangle < \langle G^r \rangle$. We find that both $\langle G^f \rangle$ and $\langle G^r \rangle$ are important for determining $\langle G \rangle$ at finite pressure in the large-system limit. Further, we show that the pressure dependence of $\langle G \rangle$ is not simply a sum of two power-laws over the full range of pressure, but $\langle G \rangle \sim P^{(\alpha-2)/(\alpha-1)}$ in the $P \to 0$ limit, $\langle G \rangle \sim P^b$ at large pressures, where $b \gtrsim (\alpha - 3/2)/(\alpha - 1)$, and the characteristic pressure that separates these scaling regimes, $P_c \sim N^{1/[2(\alpha-1)]}$, tends to zero in the large-system limit.

This work suggests several new areas for future research. First, we investigated the pressure-dependence of the shear modulus for the first, isostatic geometrical family and provided preliminary results for the shear modulus of the second geometrical family with $N^0_c + 1$ contacts. However, we do not yet know the pressure dependence of the shear modulus for higher-order geometrical families that occur at higher pressures. The answer to this question is crucial for developing a theoretical description for the mechanical response of jammed packings undergoing isotropic compression, since the ensemble-averaged shear modulus depends on the pressure dependence of $G^f$. Second, numerical simulations suggest that the ensemble-averaged shear modulus for packings of frictional spherical particles has similar pressure dependence as that for packings of frictionless spherical particles, scaling roughly as $\langle G \rangle \sim P^{(\alpha-3/2)/(\alpha-1)}$ at large pressures [59]. However, the separate contributions to the shear modulus from geometrical families and changes in the contact network have not yet been studied for packings of frictional spherical particles. Third, several computational studies have shown that $\langle G \rangle \sim P^n$ at large pressures for jammed packings of non-spherical particles [60, 61] with $\alpha = 2$, where $0.5 < \eta < 1$. These results suggest
that the scaling exponent for $\langle G(P) \rangle$ at large pressures depends on both the particle shape [62] (e.g. aspect ratio $A$) and $\alpha$. It will be interesting to determine $\eta(A, \alpha)$ to understand how the rotational degrees of freedom affect the mechanical response of jammed packings of nonspherical particles. Further, for packings of non-spherical particles undergoing isotropic compression, there have not been detailed studies of the separate contributions to $\langle G \rangle$ from geometrical families and from changes in the contact network.

2.5 Appendix

2.5.1 Affine and Nonaffine Contribution to $G^{(1)}$

In this Appendix, we derive expressions for the affine and non-affine contributions [49, 51] to the shear modulus $G^{(i)}$ of near-isostatic geometrical families. (We consider 2D systems here, but a similar derivation holds for 3D systems.) When we apply an affine simple shear deformation, the particle positions are transformed to $(x'_i, y'_i) = (x^0_i + \gamma y^0_i, y^0_i)$ consistent with Lees-Edwards periodic boundary conditions, where $(x^0_i, y^0_i)$ are the particle positions in the undeformed, reference jammed packing. After each simple shear strain increment $\gamma$, we minimize the total potential energy $U$ at constant packing fraction. Thus, after relaxation, the positions of the particles can be written as the sum of an affine term plus a nonaffine term caused by energy minimization:

$$\left( x'_i, y'_i \right) = \left( x^0_i + \gamma y^0_i + x^n_i, y^0_i + y^n_i \right). \quad (2.7)$$

For each reference jammed packing, we can write the total potential energy as a function of the shear strain and non-affine particle positions, $r^n_{i\beta}$, where $i = 1, 2, \ldots, N$ indicates the particle index and $\beta = x, y$ indicates the Cartesian component of $\vec{r}$. We assume that the jammed disk packing is at a potential energy minimum after each
shear strain increment and the total force on each particle remains zero. Thus,
\[ f_{i\beta} = - \left( \frac{\partial U}{\partial r_{i\beta}} \right)_\gamma = - \left( \frac{\partial U}{\partial r^n_{i\beta}} \right)_\gamma = 0, \]  
(2.8)
where \((.)_\gamma\) indicates that the derivatives are evaluated at a fixed shear strain \(\gamma\). We can then take the derivative of Eq. 2.8 with respect to \(\gamma\),
\[ - \frac{df_{i\beta}}{d\gamma} = \left( \frac{\partial^2 U}{\partial r^n_{i\beta} \partial \gamma} \right) + \left( \frac{\partial^2 U}{\partial r^n_{i\beta} \partial r^n_{j\beta}} \right) \frac{dr^n_{j\beta}}{d\gamma} \]  
\[ = \left( \frac{\partial^2 U}{\partial r^n_{i\beta} \partial \gamma} \right) + \left( \frac{\partial^2 U}{\partial r^n_{i\beta} \partial r^n_{j\beta}} \right) \frac{dr^n_{j\beta}}{d\gamma} = 0. \]  
(2.9)
The shear stress \(\Sigma\) is related to the total derivative of the potential energy with respect to \(\gamma\):
\[ \Sigma L^d = \frac{dU}{d\gamma} = \frac{\partial U}{\partial r^n_{i\beta}} \frac{dr^n_{i\beta}}{d\gamma} + \frac{\partial U}{\partial \gamma}. \]  
(2.10)
Note that for a given reference configuration at fixed strain \(\gamma\), taking derivatives with respect to \(r_{i\beta}\) is equivalent to taking derivatives with respect to \(r^n_{i\beta}\).

Using Eq. 2.9, we can solve for the derivative, \(dr^n_{i\beta}/d\gamma\):
\[ \frac{dr^n_{i\beta}}{d\gamma} = -M^{-1}_{ij} \Xi_{j\beta}, \]  
(2.11)
where
\[ \Xi_{i\beta} = \frac{\partial^2 U}{\partial r^n_{i\beta} \partial r^n_{j\beta}} \]  
(2.12)
and the Hessian matrix \(M_{ij}\) is defined by the second derivatives of the total potential energy \(U\) with respect to the particle coordinates,
\[ M_{ij} = \frac{\partial^2 U}{\partial r_{i\beta} \partial r_{j\beta}}. \]  
(2.13)
Using Eq. 2.10, we can calculate the shear modulus $GL^d = d\Sigma/d\gamma$,

$$GL^d = \frac{d}{d\gamma} \left( \frac{\partial U}{\partial \gamma} + \frac{\partial U}{\partial r_{ij}^n} \frac{dr_{ij}^n}{d\gamma} \right)$$

(2.14)

$$= \frac{\partial^2 U}{\partial \gamma^2} + \frac{\partial^2 U}{\partial r_{ij}^n \partial r_{ij}^n} \frac{dr_{ij}^n}{d\gamma}$$

(2.15)

$$= \frac{\partial^2 U}{\partial \gamma^2} - \Xi_{ij\beta} M_{ij}^{-1} \Xi_{ij\beta}.$$  

(2.16)

Thus, we find that the shear modulus $G = G^a - G^n$, where $G^a = L^{-d} \partial^2 U / \partial \gamma^2$ is the affine contribution and $G^n = L^{-d} \Xi_{ij\beta} M_{ij}^{-1} \Xi_{ij\beta}$ is the non-affine contribution.

In particular, the shear modulus for each geometrical family can be decomposed as $G_f^f = G_{f_a}^f - G_{f_n}^f$.

### 2.5.2 $G_{f_a}^f (P)$ Derivation

In this Appendix, we calculate the pressure dependence of the affine contribution to the shear modulus $G_{f_a}^f$ for geometrical families of near-isostatic jammed packings of spherical particles. We consider packings near jamming onset and apply an affine simple shear deformation to their particle coordinates, $(x_i', y_i', z_i') = (x_i^0 + \gamma y_i^0, y_i^0, z_i^0)$ in 3D or $(x_i', y_i') = (x_i^0 + \gamma y_i^0, y_i^0)$ in 2D, where $(x_i^0, y_i^0, z_i^0)$ in 3D and $(x_i^0, y_i^0)$ in 2D are the particle positions in the original jammed packing, consistent with Lees-Edwards boundary conditions for simple shear strain $\gamma$. The affine contribution is obtained by calculating $G_{f_a}^f = \partial \Sigma / \partial \gamma$, where the shear stress is given by

$$\Sigma = \epsilon L^{-d} \sum_{i>j} \left( -\frac{x_{ij} y_{ij}}{\sigma_{ij} r_{ij}} \right) \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)^{\alpha-1} \Theta \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right).$$

In Eq. 2.17, $x_{ij}$ and $y_{ij}$ are the $x$- and $y$-separations between the centers of particles $i$ and $j$. Thus, for the affine contribution, $G_{f_a}^f = L^{-d} \partial^2 U / \partial \gamma^2$, we obtain

$$G_{f_a}^f = L^{-d} \epsilon \sum_{i>j} \left[ \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)^{\alpha-1} \frac{y_{ij}^4}{\sigma_{ij} r_{ij}^3} + (\alpha - 1) \frac{x_{ij}^2 y_{ij}^2}{\sigma_{ij}^2 r_{ij}^5} \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)^{-2} \right] \Theta \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right).$$

(2.17)
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To determine $G_f^a$ as a function of pressure, we write the pressure

$$P = \frac{\epsilon}{dL^d} \sum_{i>j} \frac{r_{ij}}{\sigma_{ij}} \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)^{\alpha-1} \Theta \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)$$

in terms of the particle separations. If we define

$$\overline{P}_{ij} = \epsilon \frac{r_{ij}}{\sigma_{ij}} \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)^{\alpha-1} \Theta \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)$$

(2.18)

and assume that $\overline{P}_{ij}$ scales linearly with pressure for all $i, j$ pairs,

$$\overline{P}_{ij} = dL^d \chi_{ij} P,$$  (2.19)

where $\chi_{ij}$ is independent of pressure, we can use Eqs. 2.18 and 2.19 to express $G_f^a$ in Eq. 2.17 as a function of pressure. (We have verified numerically for packings with $\alpha = 2$ and $5/2$ that $\chi_{ij}$ is nearly independent of pressure for near-isostatic geometrical families. Deviations only occur near the end of geometrical families.) We find that the affine contribution to the shear modulus for near-isostatic geometrical families is given by

$$G_f^a = L^{-d} \left( dL^d \right)^{\alpha-2} \sum_{i>j} (\alpha - 1) \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{\alpha-2} \frac{x_{ij}^2 y_{ij}^2}{\sigma_{ij}^2 r_{ij}^2} \chi_{ij}^{\alpha-2} \theta \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right) + dP \sum_{i>j} \frac{y_{ij}^4}{r_{ij}^4} \chi_{ij} \theta \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right).$$  (2.20)

We can express Eq. 2.20 in dimensionless form,

$$\frac{G_f^a}{G_{a0}(\alpha)} = \left( \frac{P}{P_0(\alpha)} \right)^{\alpha-2} - \frac{P}{P_0(\alpha)},$$  (2.21)

if we define $G_{a0}(\alpha) = f(\alpha)^{\alpha-1} g^{2-\alpha}$ and $P_0 = (f(\alpha)/g)^{\alpha-1}$, where $f(\alpha) = L^{-d} \left( dL^d \right)^{\alpha-2} \sum_{i>j} (\alpha - 1) \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{\alpha-2} \frac{x_{ij}^2 y_{ij}^2}{\sigma_{ij}^2 r_{ij}^2} \chi_{ij}^{\alpha-2} \theta \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)$ and $g = d \sum_{i>j} \frac{y_{ij}^4}{r_{ij}^4} \chi_{ij} \theta \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)$. Both $f(\alpha)$ and $g$ are roughly independent of pressure and $g$ does not depend on the power-law exponent $\alpha$. In Eq. 2.21, $G_f^a = 0$ when $P = P_0(\alpha)$. For repulsive linear spring interactions, $G_f^a / G_{a0}(2) = 1 - P/P_0(2)$ and for repulsive Hertzian spring interactions, $G_f^a / G_{a0}(5/2) = (P/P_0(5/2))^{1/3} - P/P_0(5/2)$, as discussed in Sec. 2.3.
2.5.3 \( G^{(1)} \) for 2D, \( \alpha = 3 \) System and 3D, \( \alpha = 2 \) and 5/2 System

In this Appendix, we provide the results for the shear modulus for isostatic geometrical families for 2D jammed packings of purely repulsive disks with \( \alpha = 3 \) and 3D jammed packings of purely repulsive spheres with \( \alpha = 2 \) and 5/2. In Fig. 2.14 and Fig. 2.15, we show that \( G^{(1)} \sim G_a^{(1)} \) for sphere packings with \( \alpha = 2 \) and 5/2. \( G^{(1)} \) for \( \alpha = 2 \) is constant and \( G^{(1)} \) for \( \alpha = 5/2 \) scales as \( P^{1/3} \) in the \( P \to 0 \) limit and \( G^{(1)} \) begins decreasing at larger pressures. In Fig. 2.16, we also show that \( G^{(1)} \) for jammed disk packings with \( \alpha = 3 \) is well-approximated by Eq. 2.2, scaling as \( P^{1/2} \) in the \( P \to 0 \) limit and then decreasing at larger pressures. (Note that for many of the geometrical families for \( \alpha = 3 \), a change in the contact network occurs before the \( -P \) term begins contributing significantly to \( G^{(1)} \).)

2.5.4 Negative \( G \) Statistics

In this Appendix, we quantify the frequency with which disk packings generated using the strain-controlled energy minimization method possess negative shear moduli. (We have verified that all packings generated via isotropic compression, even those with negative shear moduli, possess positive bulk moduli.) The shear modulus for the first geometrical family, \( G^{(1)} > 0 \) in the \( P \to 0 \) limit, but it decreases with increasing pressure. Thus, the shear modulus can become negative if a point or jump change in the contact network does not occur abruptly after the start of the first geometrical family. In Fig. 2.17, we show the distribution \( p(P_-) \) of the pressure \( P_- \) at which the isostatic geometrical family first becomes negative. We find that \( \langle P_- \rangle \sim P_0 \) and thus \( \langle P_- \rangle \) tends to zero in the large-system limit. \( \langle P_- \rangle \sim N^{-2} \) and \( \sim N^{-3} \) for packings with \( \alpha = 2 \) and 5/2, respectively. After a jump change and after a point change for \( \alpha = 2 \), the shear modulus for the second geometrical family \( G^{(2)} \) jumps discontinuously to
either a positive or negative value, depending on the value of $G^{(1)}$ at the end of the first geometrical family and the magnitude and sign of the discontinuous jump in the shear modulus. As the pressure increases, the upward jumps in the shear modulus become larger than the continuous decreases in the shear modulus along geometrical families, and thus the shear modulus remains positive. In Fig. 2.18, we show the fraction of disk packings $F(P)$ at each pressure with a negative shear modulus. The maximum fraction of packings with negative shear moduli is $\approx 0.4$ and occurs at $P_{\text{max}}/P_c \approx 1$. Thus, $P_{\text{max}} \sim N^{-2}$ and $\sim N^{-3}$ for $\alpha = 2$ and $5/2$, respectively.
Figure 2.4: Probability distributions of the characteristic pressure $P_0(\alpha)$ for (a) $\alpha = 2$ and (b) $5/2$ for $N = 32$ (black upward triangles), 128 (blue circles), 512 (red diamonds). ($P_0(\alpha)$ was obtained using a best fit of the data for $G^{(1)}$ to Eq. 2.4.) The insets to (a) and (b) display $\langle P_0 \rangle$ (averaged over geometrical families) versus system size $N$ for $\alpha = 2$ and $5/2$, respectively. The dashed lines have slopes equal to $-2$ and $-3$ in the insets to (a) and (b).
Figure 2.5: Probability distributions of the characteristic shear modulus $G_{a0}(\alpha)$ for (a) $\alpha = 2$ and (b) $5/2$ for $N = 32$ (black upward triangles), 128 (blue circles), 512 (red diamonds). ($G_{a0}(\alpha)$ was obtained using a best fit of the data for $G^{(1)}$ to Eq. 2.4.) The insets to (a) and (b) display $\langle G_{a0} \rangle$ (averaged over geometrical families) versus system size $N$ for $\alpha = 2$ and $5/2$, respectively. The dashed lines have slopes equal to $-1$ and $-2$ in the insets to panels (a) and (b).
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Figure 2.6: Probability distributions of the characteristic pressure $P_1(\alpha)$ for (a) $\alpha = 2$ and (b) $5/2$ for $N = 32$ (black upward triangles), 128 (blue circles), 512 (red diamonds). (See Eq. 2.4 for the definition of $P_1(\alpha)$.) The insets to (a) and (b) display $\langle P_1 \rangle$ (averaged over geometrical families) versus system size $N$ for $\alpha = 2$ and $5/2$, respectively. The dashed lines have slopes equal to $-2$ and $-3$ in the insets to panels (a) and (b).
Figure 2.7: Shear modulus $G^{(i)}$ of a series of $N = 32$ disk packings with repulsive (a) linear and (b) Hertzian spring interactions as the system undergoes a point change during isotropic compression (at $P \approx 1.29 \times 10^{-5}$ for $\alpha = 2$ and $P = 1.37 \times 10^{-6}$ for $\alpha = 5/2$ indicated by vertical dashed lines) from the isostatic (black upward triangles) geometrical family with $N^0_c$ contacts to the second geometrical family (blue circles) with $N^0_c + 1$ contacts.
Figure 2.8: Shear modulus $G^{(i)}$ of a series of $N = 32$ disk packings with repulsive (a) linear and (b) Hertzian spring interactions as the system undergoes a jump change during isotropic compression (at $P \approx 1.23 \times 10^{-4}$ for $\alpha = 2$ and $P = 4.57 \times 10^{-6}$ for $\alpha = 5/2$ indicated by vertical dashed lines) from the isostatic (black upward triangles) geometrical family with $N_c^0$ contacts to a second geometrical family (blue circles) with $N_c^0 + 1$ contacts.
Figure 2.9: (a) \( (G^{(2)}/G_0)(P/P_0)^{-1/2} \) versus \( P/P_0 \) for packings with \( \alpha = 2 \) in the second geometrical family following a point or jump change in the contact network. \( (G^{(2)}/G_0)(P/P_0)^{-2/3} \) is plotted versus \( P/P_0 \) for packings with \( \alpha = 5/2 \) in the second geometrical family following (b) a point change or (c) a jump change in the contact network. In (a)-(c), several system sizes are shown: \( N = 32 \) (black upper triangles), 64 (blue circles), 128 (red diamonds), 256 (green downward triangles), and 512 (magenta asterisks). The dashed lines in (a)-(c) give Eq. 2.4 for \( \alpha = 2 \) in (a) and \( 5/2 \) in (b) and (c). In the insets to panels (a)-(c), we show \( \Delta G^{(1)} = G^{(1)}(P/P_0) - G^{(1)}(0) \) or \( G^{(1)}(P/P_0) \) (black upward triangles), \( \Delta G^{(1)}_n = G^{(1)}_n(P/P_0) - G^{(1)}_n(0) \) or \( G^{(1)}_n(P/P_0) \) (red dots), and \( \Delta G^{(1)}_a = G^{(1)}_a(P/P_0) - G^{(1)}_a(0) \) or \( G^{(1)}_a(P/P_0) \) (blue exes) with best fits to Eq. 2.2 (black, red, and blue solid lines, respectively) for an example \( N = 32 \) packing with \( \alpha = 2 \) (inset to (a)) and \( 5/2 \) (insets to (b) and (c)).
Figure 2.10: Shear modulus $G^\lambda$ for initial condition $\lambda$ at $P = 0$ undergoing isotropic compression as a function of pressure $P$ for an $N = 32$ packing with repulsive (a) linear (black upward triangles) and (b) Hertzian spring interactions (blue circles). $G^\lambda = G^{f,\lambda} + G^{r,\lambda}$ can be decomposed into the contributions from the continuous geometrical families $G^{f,\lambda}$ and discontinuities $G^{r,\lambda}$ caused by point and jump changes in the contact network.
Figure 2.11: Ensemble-averaged shear modulus $\langle G \rangle$ (black upward triangles) as a function of pressure $P$ for $N = 128$ packings with (a) $\alpha = 2$ and (b) $5/2$ decomposed into contributions from geometrical families $|\langle G^f \rangle|$ (blue circles) and changes in the contact network $\langle G^r \rangle$ (red diamonds). In (a), the dashed line has slope equal to $1/2$ and in (b), the dashed and dotted lines have slopes equal to $1/3$ and $2/3$, respectively.
Figure 2.12: (a) Ensemble-averaged shear modulus $\langle (G_0/G_c)(P/P_c)^{-\alpha}\rangle^{1/2}$ versus $P/P_c$ for jammed disk packings with $\alpha = 2$ and system sizes $N = 32$ (black upward triangles), 64 (blue circles), 128 (red diamonds), 256 (green downward triangles), and 512 (magenta asterisks). The dashed lines have slopes equal to $-1/4$ and $1/4$. The dotted line gives Eq. 2.5. (b) $\langle G_0/G_c \rangle$ plotted versus $(P/P_c)^{1/2}$ for the same data in (a). The solid lines in (a) and (b) are fits to Eq. 2.6 with $p = 2.5$ for system sizes $N = 32$ to 512. The upper left inset shows $P_c$ (black asterisks) and $G_c$ (blue circles) versus $N$. The dotted and dashed lines have slopes equal to $-1$ and $-2$, respectively. The lower right inset gives the exponents $a$ (black upper triangles) and $b$ (blue diamonds), used in fits to Eq. 2.6 versus $N$. The horizontal dotted and dashed lines indicate $a = 0$ and $b = 0.5$, respectively.
Figure 2.13: (a) Ensemble-averaged shear modulus $\langle G \rangle / G_c (P/P_c)^{(a+b)/2}$ versus $P/P_c$ for jammed disk packings with $\alpha = 5/2$ and system sizes $N = 32$ (black upward triangles), 64 (blue circles), 128 (red diamonds), 256 (green downward triangles), and 512 (magenta asterisks). The dashed lines have slopes equal to $-1/6$ and $1/6$. The dotted line gives Eq. 2.5. (b) $\langle G \rangle / G_c$ plotted versus $(P/P_c)^{(a+b)/2}$ for the same data in (a). The solid lines in (a) and (b) are fits to Eq. 2.6 with $p = 2-15$ for system sizes $N = 32$ to 512. The upper left inset shows $P_c$ (black asterisks) and $G_c$ (blue circles) versus $N$. The dotted and dashed lines have slopes equal to $-2$ and $-3$, respectively. The lower right inset gives the exponents, $a$ (black upper triangles) and $b$ (blue diamonds), used in fits to Eq. 2.6 versus $N$. The horizontal dotted and dashed lines indicate $a = 1/3$ and $b = 2/3$, respectively.
Figure 2.14: (a) Shear modulus $G^{(1)}$ within isostatic geometrical families versus pressure $P$ for individual $N = 64$ sphere packings in 3D with $\alpha = 2$ repulsive interactions. The solid blue lines are fits to Eq. 2.2. (b) $(G^{(1)}/G_0)(P/P_0)^{-1/2}$ plotted versus $P/P_0$ for the data in (a) and isostatic geometrical families with $G^{(1)} < 0$. The dashed line gives Eq. 2.4 for $\alpha = 2$, and the solid black lines are fits to Eq. 2.4.
Figure 2.15: Shear modulus $G^{(1)}$ within isostatic geometrical families versus pressure $P$ for individual $N = 64$ sphere packings with $\alpha = 5/2$ repulsive interactions. The solid blue lines are fits to Eq. 2.2. The dashed line in (a) has slope equal to $1/3$. (b) $(G^{(1)}/G_0)(P/P_0)^{-2/3}$ plotted versus $P/P_0$ for the data in (a) and isostatic geometrical families with $G^{(1)} < 0$. The dashed line gives Eq. 2.4 for $\alpha = 5/2$, and the solid black lines are fits to Eq. 2.4.
Figure 2.16: Shear modulus $G^{(1)}$ within isostatic geometrical families versus pressure $P$ for individual $N = 32$ jammed disk packings with repulsive interactions with power-law exponent $\alpha = 3$ in Eq. 2.1. The dashed line has slope equal to $1/2$. The solid blue lines are fits to Eq. 2.2 for each of the 50 geometrical families. (b) $(G^{(1)}/G_0)(P/P_0)^{-3/4}$ plotted versus $P/P_0$ for the data in (a) and isostatic geometrical families with $G^{(1)} < 0$. The dashed line gives Eq. 2.4 for $\alpha = 3$, and the solid black lines are fits to Eq. 2.4.
Figure 2.17: The probability distribution $p(P_-)$ of the pressure $P_-$ at which the shear modulus for the isostatic geometrical family first becomes negative $G^{(1)} < 0$ for disk packings with (a) $\alpha = 2$ and (b) $5/2$ and system sizes $N = 32$ (black upward triangles), 64 (blue circles), 128 (red diamonds), 256 (green downward triangles), and 512 (magenta asterisks).
Figure 2.18: Fraction of packings $F(P)$ at each pressure that possess a negative shear modulus for disk packings with (a) $\alpha = 2$ and (b) $5/2$ and system sizes $N = 32$ (black upward triangles), 64 (blue circles), 128 (red diamonds), 256 (green downward triangles), and 512 (magenta asterisks).
Chapter 3

Jamming Protocols

3.1 Introduction

Granular materials, which are collections of macroscopic-sized grains, can exist in fluidized states when the applied stress exceeds the yield stress or in solid-like, or jammed, states when the applied stress is below the yield stress [17, 39]. Many recent studies [63, 64, 65, 66, 67, 68] have shown that the structural and mechanical properties of jammed granular packings depend on the protocol that was used to generate them. For example, when granular packings are generated via simple or pure shear, the force chain networks appear more heterogeneous and anisotropic. In contrast, for granular packings generated via isotropic compression, the force distribution is more uniform [69, 27, 70, 71, 72]. This protocol dependence for the structural and mechanical properties of jammed packings makes it difficult to accurately calculate, and even properly define, their statistical averages.

An important question to address when considering how to calculate statistical averages of a system’s structural and mechanical properties is to determine which states are to be included in the statistical ensemble. For jammed granular packings, the relevant set of states is the collection of mechanically stable (MS) packings [73, 74] with force and torque balance on every grain. In addition, the average properties of
the ensemble of MS packings depend on the probabilities with which each MS packing occurs, and the probabilities can vary strongly with the packing-generation protocol.

We recently investigated how the mechanical properties of granular systems composed of bidisperse frictionless disks interacting via pairwise, purely repulsive central forces \[26\] depend on the packing-generation protocol. In this case, the relevant ensemble of jammed states is the collection of isostatic MS packings \[26, 75, 76, 21\] with \(N_c = 2N' - 1\) interparticle contacts, where \(N' = N - N_r\), \(N\) is the number of disks, and \(N_r\) is the number of rattler disks with less than 3 contacts. We compared MS packings of frictionless disks generated via simple or pure shear (i.e. shear jammed packings) and those generated via isotropic compression (i.e. compression jammed packings). We found that compression jammed packings can possess either positive or negative stress anisotropy \(\hat{\Sigma}_{xy} = -\Sigma_{xy}/P\), where \(\Sigma_{xy}\) is the shear stress and \(P\) is the pressure of the MS packing. In contrast, shear jammed MS packings possess only \(\hat{\Sigma}_{xy} > 0\) and these packings are identical to the MS packings generated via isotropic compression with \(\hat{\Sigma}_{xy} > 0\). Thus, the ensemble of jammed packings generated via shear and isotropic compression is the same, but shear (in one direction) selects jammed packings with only one sign of the stress anisotropy.

In this thesis, we will investigate a similar question of whether exploring configuration space through shear versus through compression samples the same set of MS packings, except we consider the case of jammed packings of dry, frictional disks. A key feature of frictional systems is that the forces at each interparticle contact must obey the Coulomb condition \[77, 78\], where \(f^t_{ij} \leq \mu f^n_{ij}\), \(f^n_{ij}\) and \(f^t_{ij}\) are the normal and tangential forces at the contact between particles \(i\) and \(j\), and \(\mu\) is the static friction coefficient. If \(f^t_{ij}\) exceeds \(\mu f^n_{ij}\), the contact will slide to satisfy the Coulomb condition. Further, the number of contacts for MS packings of frictional disks is below
the isostatic value \( z_{iso} = 4 \), and as a result there are many solutions for the normal and tangential forces for each fixed network of interparticle contacts. Thus, one can imagine that different protocols for generating jammed packings of frictional disks can give rise to MS packings with different distributions of sliding contacts, different force solutions for a given contact network, or even different types of contact networks.

We carry out discrete element modeling (DEM) simulations of bidisperse frictional disks in two dimensions (2D) to compare the properties of MS packings at jamming onset generated via simple shear and isotropic compression. We find five significant results: 1) The average packing fraction \( \langle \phi_J(\mu) \rangle \) and contact number \( \langle z_J(\mu) \rangle \) at jamming onset versus friction coefficient \( \mu \) for the ensemble of MS packings generated.
via isotropic compression and simple shear are similar (with deviations < 0.5%). In particular, both shear and compression jammed packings can possess a range of average contact numbers $\langle z_{ij} \rangle$ between 3 and 4, depending on $\mu$. 2) As with frictionless disks, we find that MS packings of frictional disks generated via isotropic compression possess both $\hat{\Sigma}_{xy} > 0$ and $\hat{\Sigma}_{xy} < 0$, whereas MS packings generated via simple shear possess only one sign of the stress anisotropy. 3) For each MS packing generated via simple shear, we can decompress the packing to remove all of the frictional contacts and recompress it to generate an MS packing with particle positions that are nearly identical to those of the original shear jammed MS packing. Similarly, for each MS packing generated via isotropic compression, we can shear it in a given direction to unjam it and remove all of the frictional contacts and shear it back in the opposite direction to generate an MS packing with disk positions that are nearly identical to those of the original compression jammed packing. 4) Even though the disk positions are nearly identical, we find a small, but significant difference between the stress anisotropy of the shear jammed packings and that for the compression rejammed packings. Similarly, we find a smaller, but significant difference in the stress anisotropy between the compression jammed packings and that for the shear rejammed packings. The fluctuations in the stress anisotropy between the originally jammed packings and the re-jammed packings from the DEM simulations are much smaller than the fluctuations obtained by enumerating all normal and tangential forces solutions from the null space for each fixed contact network. 5) We also show that even though we can generate MS packings with nearly identical particle positions via the DEM simulations with our rejamming protocols, the packings can possess very different mobility distributions $P(\xi)$, where $\xi = F_{ij}^t / \mu F_{ij}^n$, and numbers of sliding contacts. We find that deviations in the stress anisotropy can occur for
packings with similar mobility distributions (i.e. between compression jammed and shear re-jammed packings) and for packings with different mobility distributions (i.e. between shear jammed and compression re-jammed packings). There are thus two key distinct contributions to the stress anisotropy: the width of the distribution of stresses from the null space solutions and the distribution of sliding contacts.

Figure 3.2: Average (a) contact number $\langle z_J \rangle$ and (b) packing fraction $\langle \phi_J \rangle$ at jamming onset for MS packings generated via simple shear (filled triangles; dotted lines) and isotropic compression (open triangles; solid lines) plotted versus the static friction coefficient $\mu$ for $N = 128$ bidisperse frictional disks. The averages were calculated over more than 50 independent MS packings at each $\mu$. 
CHAPTER 3. JAMMING PROTOCOLS

The remainder of the article is organized as follows. The Methods section (Sec. 3.2) introduces the Cundall-Strack model [79] for static friction between disks, the definitions of the stress tensor, shear stress, and stress anisotropy, and the details of the isotropic compression and simple shear packing generation protocols. In addition, we describe the protocols to decompress and then recompress shear-jammed packings and shear unjam and then shear jam compression-jammed packings. The Results section (Sec. 3.3) describes our findings for the average packing fraction and contact number at jamming onset versus the static friction coefficient for MS packings generated via both protocols. In addition, we show the stress anisotropy and mobility distributions for each protocol that we use to generate MS packings. In the Conclusion and Future Directions section (Sec. 3.4), we summarize our results and describe promising future research directions, e.g. enumerating the force solutions for the null space of contact networks generated via isotropic compression and shear. In addition, we include three Appendices. In Appendix A, we include calculations of the distribution of normal stress differences in shear and compression jammed packings. In Appendix B, we provide the exact form of the jammed packing fraction versus shear strain for two bidisperse hard disks to motivate the parabolic form for geometrical families. In Appendix C, we provide a sensitivity analysis for how the numerical parameters in the packing-generation protocols affect the extent to which shear and compression jammed packings can be unjammed and then re-jammed to reach the same particle positions and stress anisotropy of the original jammed packing.

3.2 Methods

We perform DEM simulations of frictional disks in 2D. We consider bidisperse mixtures of disks with \( N/2 \) large disks and \( N/2 \) small disks, each with the same mass.
$m$, and diameter ratio $\sigma_i/\sigma_s = 1.4$ \cite{80}. The MS packings are generated inside a square box with side length $L$ and periodic boundary conditions in both directions. The disks interact via pair forces in the normal (along the vector $\hat{r}_{ij}$ from the center of disk $j$ to that of disk $i$) and the tangential $\hat{t}_{ij}$ directions (with $\hat{t}_{ij} \cdot \hat{r}_{ij} = 0$). We employ a repulsive linear spring potential for forces in the normal direction:

$$U_n(r_{ij}) = \frac{K\sigma_{ij}}{2} \left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^2 \theta \left(1 - \frac{r_{ij}}{\sigma_{ij}}\right),$$

(3.1)

where $r_{ij}$ is the separation between disk centers, $\sigma_{ij} = (\sigma_i + \sigma_j)/2$, $\sigma_i$ is the diameter of disk $i$, $K$ is the spring constant in the normal direction, and $\theta(.)$ is the Heaviside step function that sets the interaction potential to zero when disks $i$ and $j$ are not in contact.

We implement the Cundall-Strack model \cite{79} for the tangential frictional forces. When disks $i$ and $j$ are in contact, $f_t^{ij} = K_t\vec{u}_t^{ij}$, where $K_t = K/3$ is the spring constant for the tangential forces and $\vec{u}_t^{ij}$ is the relative tangential displacement. $\vec{u}_t^{ij}$ is obtained by integrating the relative tangential velocity \cite{81,82}, while disks $i$ and $j$ are in contact:

$$\frac{d\vec{u}_t^{ij}}{dt} = \vec{v}_t^{ij} - \frac{(\vec{u}_t^{ij} \cdot \vec{v}_{ij})\vec{r}_{ij}}{r_{ij}^2},$$

(3.2)

where $\vec{v}_t^{ij} = \vec{v}_i - \vec{v}_j$, $\vec{v}_t^{ij} = \vec{v}_t^{ij} - \vec{v}_{n}^{ij} - \frac{1}{2}(\vec{\omega}_i + \vec{\omega}_j) \times \vec{r}_{ij}$, $\vec{v}_n^{ij} = (\vec{u}_t^{ij} \cdot \hat{r}_{ij})\hat{r}_{ij}$, and $\vec{\omega}_i$ is the angular velocity of disk $i$. $\vec{u}_t^{ij}$ is set to zero when the pair of disks $i$ and $j$ is no longer in contact. We implement the Coulomb criterion, $f_{t}^{ij} \leq \mu f_{n}^{ij}$, by resetting $|\vec{u}_t^{ij}| = u_t^{ij} = \mu f_{n}^{ij}/K_t$ if $f_{t}^{ij}$ exceeds $\mu f_{n}^{ij}$. The total potential energy is $U = U_n + U_t$, where $U_n = \sum_{i>j} U_n(r_{ij})$ and $U_t = \sum_{i>j} K_t(u_t^{ij})^2/2$.

We characterize the stress of the MS packings using the virial expression for the stress tensor \cite{26}:

$$\Sigma_{ij\delta} = \frac{1}{A} \sum_{i>j} f_{ij\beta}r_{ij\delta},$$

(3.3)
where $\beta, \delta = x, y, A = L^2$ is the area of the simulation box, $f_{ij}^{\beta}$ is the $\beta$-component of the interparticle force $\vec{f}_{ij}$ on disk $i$ due to disk $j$, and $r_{ij}^{\delta}$ is the $\delta$-component of the separation vector $\vec{r}_{ij}$. We define the stress anisotropy as $\hat{\Sigma}_{xy} = -\Sigma_{xy}/P$, the normal stress difference as $\hat{\Sigma}_N = (\Sigma_{yy} - \Sigma_{xx})/2P$, and the pressure as $P = (\Sigma_{xx} + \Sigma_{yy})/2$. We measure length, energy, and stress below in units of $\sigma_s, K\sigma_s$, and $K/\sigma_s$, respectively.

We employ two main protocols to generate MS packings: 1) isotropic compression at fixed shear strain $\gamma$ and 2) simple shear at fixed packing fraction $\phi$. (See Fig. 3.1.) For protocol 1 (isotropic compression), we first randomly place the disks in the simulation cell without overlaps. We then increase the diameters of the disks according to $\sigma'_i = \sigma_i (1 + d\phi/\phi)$ where $d\phi < 10^{-4}$ is the initial increment in the packing fraction. After each small change in packing fraction, we minimize the total potential energy $U$ by adding viscous damping forces proportional to each disk’s velocity $\vec{v}_i$. Energy minimization is terminated when $K_{\text{max}} < 10^{-20}$, where $K_{\text{max}}$ is the maximum kinetic energy of one of the disks.

If $U/N < U_{\text{tol}}$ after minimization, we increase the packing fraction again by $d\phi$ and then minimize the total potential energy. To eliminate overlaps, we typically set $U_{\text{tol}} = 10^{-16}$, which means that the typical disk overlap is $< 10^{-8}$. If after minimization, $U/N > 2U_{\text{tol}}$, the growth step is too large and we return to the uncompressed packing of the previous step with $U/N < U_{\text{tol}}$. Instead, we increase the packing fraction by $d\phi/2$, and minimize the total potential energy. We repeat this process until the total potential energy satisfies $U_{\text{tol}} < U/N < 2U_{\text{tol}}$, at which we assume that the packing has reached jamming onset at packing fraction $\phi_J$. This compression protocol ensures that the system approaches jamming onset from below.

For protocol 2, we first prepare the system below jamming onset at $\phi_t < \phi_J$ (using protocol 1). We then apply successive simple shear strain increments $d\gamma$ by
shifting the disk positions, $x_i' = x_i + d\gamma y_i$, and implementing Lees-Edwards boundary conditions, which are consistent with the applied affine shear strain. The initial shear strain increment is $d\gamma = 10^{-4}$. After an applied shear strain increment, we minimize the total potential energy. Energy minimization is again terminated when $K_{\text{max}} < 10^{-20}$. If $U/N < U_{\text{tol}}$ after minimization, we increment the shear strain again by $d\gamma$ and minimize the total potential energy. If after minimization, $U/N > 2U_{\text{tol}}$, the shear strain step is too large and we return to the packing at the previous strain step with $U/N < U_{\text{tol}}$. Instead, we increment the shear strain by $d\gamma/2$, and minimize the total potential energy. We repeat this process until the total potential energy satisfies $U_{\text{tol}} < U/N < 2U_{\text{tol}}$, at which we assume that the packing has reached jamming onset at total shear strain $\gamma_J$.

Energy minimization is carried out by integrating Newton’s equations of motion for the translational and rotational degrees of freedom of each disk in the presence of static friction and viscous dissipation. For the translational degrees of freedom, we have

$$m \frac{d^2 \vec{r}_i}{dt^2} = \vec{f}_i^n + \vec{f}_i^t + \vec{f}_i^d,$$

where $\vec{f}_i^n = \sum_j \vec{f}_{ij}^n$, $\vec{f}_{ij}^n = -dU/n/d\vec{r}_{ij}$, $\vec{f}_i^t = \sum_j \vec{F}_{ij}^t$, $\vec{F}_{ij}^t = -b^n v_i$, $b^n$ is the damping coefficient, and the sums over $j$ include disks that are in contact with disk $i$. For the rotational degrees of freedom, we have

$$I_i \frac{d\vec{\omega}_i}{dt} = \vec{\tau}_i - b^t \vec{\omega}_i,$$

where $I_i = m\sigma_i^2/8$ is the moment of inertia for disk $i$, $b^t$ is the rotational damping coefficient, and

$$\vec{\tau}_i = \frac{1}{2} \sum_j \vec{r}_{ij} \times \vec{F}_{ij}^t$$

is the torque on disk $i$. We chose $b^n$ and $b^t$ so that the dynamics for the translational and rotational degrees of freedom are in the overdamped limit.
CHAPTER 3. JAMMING PROTOCOLS

After generating MS packings using these two protocols, we measure the contact number \( z = N_c/N' \), where \( N_c \) is the total number of contacts in the system, shear stress anisotropy, and normal stress difference of the MS packings. For these measurements, we recursively remove rattler disks with fewer than three contacts for frictionless disks or fewer than two contacts for frictional disks.

3.3 Results

In this section, we first describe our results for the average contact number and packing fraction of MS packings generated via isotropic compression and simple shear. We then explain why the distribution of the shear stress anisotropy differs for compression and shear jammed packings. We also develop a protocol where we unjam shear jammed packings and then re-jam them via isotropic compression and a protocol where we unjam compression jammed packings and then re-jam them via applied shear strain. We then compare the contact network and stress anisotropy of the original jammed packings and the re-jammed packings, and show that the disk positions of the re-jammed packings are nearly identical to those for the original jammed packings. We find small differences in the stress state of the original jammed packings and the re-jammed ones, but these differences are smaller than the fluctuations obtained by enumerating all of the normal and tangential force solutions for a given jammed packing consistent with force and torque balance.

3.3.1 Packing Fraction and Contact Number

In Fig. 3.2, we show (for \( N = 128 \)) that the contact number \( \langle z_J \rangle \) and packing fraction \( \langle \phi_J \rangle \) at jamming onset are similar for compression and shear jammed packings over the full range of friction coefficients \( \mu \). (The relative deviations are less than 0.5%). The data for \( \langle z_J \rangle \) and \( \langle \phi_J \rangle \) for the isotropic compression protocol in Fig. 3.2 (a) and
Figure 3.3: Average total shear strain $\langle \gamma_J \rangle$ required to jam a collection of disks with (a) $N = 32$ as a function of packing fraction $\phi$ for several friction coefficients, $\mu = 0$ (black triangles), 0.1 (blue circles), and 1.0 (red squares) and for (b) $\mu = 0.1$ and several system sizes, $N = 16$ (black triangles), 32 (blue circles), 64 (red squares), and 128 (green stars). The vertical dashed line indicates $\langle \phi_J \rangle$ for compression jammed packings with $\mu = 0.1$ and $N = 64$. 
(b) were generated at shear strain $\gamma = 0$. We find the same results when compression jammed packings are generated at different values of $\gamma$. For both protocols, we find that $z \approx 4$ in the small-$\mu$ limit and $z \approx 3$ in the large-$\mu$ limit, as found previously in numerical studies of frictional disks [65]. The average packing fraction $\langle \phi_J \rangle \approx 0.835$ in the small-$\mu$ limit and $\approx 0.765$ in the large-$\mu$ limit. The crossover between the low- and high-friction behavior in the contact number and packing fraction again occurs near $\mu_c \approx 0.1$ for both protocols. This crossover value of $\mu$ is similar to that found previously in compression jammed frictional disk packings [65, 75].

The average packing fraction at jamming onset is slightly smaller for shear jammed packings compared to that for compression jammed packings. This small difference in packing fraction stems from differences in the compression and shear jamming protocols. For each initial condition $i$, we generate a compression jammed packing with $\phi_J^i$. Then, for each $i$, we generate a series of unjammed configurations with $\phi_J^i \alpha < \phi_J^i$ and shear them until they jam at $\gamma_J$. To obtain $\langle \phi_J \rangle$ for the shear jamming protocol, we average $\phi_J^i$ over $i$ and $\alpha$ for all systems that jammed. This protocol for generating shear jammed packings is thus biased towards finding MS packings with packing fractions lower than those found for isotropic compression. Despite this, the packing fraction at jamming onset $\langle \phi_J(\mu) \rangle$ for the two protocols differs by less than 0.5% over the full range of $\mu$.

Prior results for isotropically compressed packings of spheres in three spatial dimensions [65] have shown that $\langle z_J(\mu) \rangle$ and $\langle \phi_J(\mu) \rangle$ show qualitatively the same behavior as the results for shear and compression jammed disk packings in Fig. 3.2. For packings of frictional spheres, $\langle z_J(\mu) \rangle$ varies between 4 and 6, and $\langle \phi_J(\mu) \rangle$ varies between 0.55 and 0.64, with a transition from frictional to frictionless behavior around $\mu_c \sim 0.1$. 
In Fig. 3.3, we show the average shear strain $\langle \gamma_J \rangle$ required to find a jammed packing starting from an initially unjammed packing using the shear jamming protocol as a function of packing fraction. In panel (a), we plot $\langle \gamma_J \rangle$ versus $\phi$ for several friction coefficients. The average strain increases with decreasing packing fraction and the range of packing fractions over which a shear jammed packing can be obtained shifts to lower values with increasing friction coefficient. In panel (b), we show $\langle \gamma_J \rangle$ versus $\phi$ at $\mu = 0.1$ and several system sizes. We find that the slope $d\langle \gamma_J \rangle/d\langle \phi_J \rangle$ increases with increasing system size. For the $\mu = 0.1$ data in panel (b), we expect $\langle \gamma_J \rangle$ to become vertical near $\phi \approx 0.82$, which is $\langle \phi_J(\mu) \rangle$ for compression jammed packings, in the large-system limit. The system-size dependence of $\langle \gamma_J \rangle$ is similar to that found for packings of frictionless disks [63]. Thus, we predict that the range of packing fraction over which shear jamming occurs to shrink with increasing system size. In particular, we expect shear jamming to occur over a narrow range of packing fraction near $\langle \phi_J(\mu) \rangle$ obtained from isotropic compression in the large-system limit.

### 3.3.2 Stress Anisotropy of Compression and Shear Jammed Packings

In previous studies, we showed that a significant difference between shear and compression jammed packings of frictionless disks is that shear jammed packings possess a non-zero average shear stress anisotropy $\langle \hat{\Sigma}_{xy} \rangle > 0$, whereas compression jammed packings possess $\langle \hat{\Sigma}_{xy} \rangle = 0$. We find similar behavior for MS packings of frictional disks. In Fig. 3.4, we show the distribution of shear stress anisotropy $P(\hat{\Sigma}_{xy})$ for packings with three friction coefficients $\mu = 0, 0.1, \text{and } 1.0$ using the isotropic compression and shear jamming protocols. For the isotropic compression protocol, $P(\hat{\Sigma}_{xy})$ is a Gaussian distribution with zero mean, whereas $\hat{\Sigma}_{xy} > 0$ for packings generated via simple shear (in a single direction). The stress anisotropy distributions $P(\hat{\Sigma}_{xy})$ for
Figure 3.4: Probability distributions of the shear stress anisotropy $\hat{\Sigma}_{xy}$ for packings generated via isotropic compression (open symbols) and simple shear (filled symbols). For both packing-generation protocols, we show distributions for $N = 64$ and friction coefficients $\mu = 0$ (triangles), 0.1 (circles), and 1.0 (squares). The distributions were obtained from more than $10^3$ independently generated jammed packings. The dashed line is a Gaussian distribution with zero mean and standard deviation $\Delta \sim 0.1$ and the solid lines are Weibull distributions with scale and shape parameters $\lambda \sim 0.17$ and $k \sim 3.0$, $\lambda \sim 0.21$ and $k \sim 3.5$, and $\lambda \sim 0.27$ and $k \sim 3.9$ from left to right.
simple shear are Weibull distributions with shape and scale factors that depend on \( \mu \) [4]. In Fig. 3.5, we show the corresponding averages of the shear stress anisotropy distributions. We find that \(<\hat{\Sigma}_{xy}> = 0\) for all \( \mu \) for packings generated using isotropic compression. In contrast, for packings generated via simple shear, \(<\hat{\Sigma}_{xy}> \approx 0.13\) [83] for \( \mu \rightarrow 0 \) and \(<\hat{\Sigma}_{xy}> \) increases with \( \mu \) until reaching \(<\hat{\Sigma}_{xy}> \approx 0.25\) in the large-\( \mu \) limit.

Since the normal stress difference \( \hat{\Sigma}_N \) does not couple to simple shear strain, \( P(\hat{\Sigma}_N) \) is a Gaussian distribution with an average normal stress difference \( \hat{\Sigma}_N = 0 \) for both compression and shear jammed packings for all \( \mu \). (See Appendix A.)

We showed in previous studies [74] that MS packings of frictionless disks occur in geometrical families in the packing fraction \( \phi \) and shear strain \( \gamma \) plane. For frictionless disks, geometrical families are defined as MS packings with the same network of interparticle contacts, with different, but related fabric tensors. The packing fractions of MS packings in the same geometrical family are related via \( \phi = \phi_0 + A(\gamma - \gamma_0)^2 \), where \( A > 0 \) is the curvature in the \( \phi-\gamma \) plane, and \( \phi_0 \) is the minimum value of the packing fraction at strain \( \gamma = \gamma_0 \) [26]. The parameters \( A, \phi_0, \) and \( \gamma_0 \) vary from one geometrical family to another. See Appendix B for motivation for the parabolic form of geometrical families in the \( \phi-\gamma \) plane.

Using a general work-energy relationship for packings undergoing isotropic compression and simple shear, we showed [21] that for packings of frictionless disks, the shear stress anisotropy can be obtained from the dilatancy, \( d\phi_J/d\gamma \):

\[
\hat{\Sigma}_{xy} = -\frac{1}{\phi} \frac{d\phi_J}{d\gamma}.
\]

(3.7)

The isotropic compression protocol can sample packings with alternating signs of \( d\phi_J/d\gamma \) (and thus \( \hat{\Sigma}_{xy} > 0 \) and \( < 0 \)), whereas the shear jamming protocol can only sample packings with \( d\phi_J/d\gamma < 0 \) (and thus \( \hat{\Sigma}_{xy} > 0 \)). We expect similar behavior for packings of frictional disks, however, it is more difficult to identify single geometrical
families. First, Eq. 3.7 does not account for sliding contacts, and thus geometrical families must be defined over sufficiently small strain intervals such that interparticle contacts do not slide. In addition, for each MS packing of frictional disks in a given geometrical family, there is an ensemble of solutions for the normal and tangential forces [77], not a unique solution, as for the normal forces in packings of frictionless disks. The extent to which packings with the same contact networks (and particle positions) can possess different shear stress anisotropies will be discussed in more detail in Sec. 3.3.3 below.

Figure 3.5: Average shear stress anisotropy $\langle \hat{\Sigma}_{xy} \rangle$ at jamming onset for MS packings generated via simple shear (filled triangles) and isotropic compression (open triangles) plotted versus the static friction coefficient $\mu$ for $N = 128$. The error bars indicate the standard deviation in $P(\hat{\Sigma}_{xy})$ for each protocol.
3.3.3 Unjam and Rejam Compression and Shear Jammed Packings

In Sec. 3.3.1, we showed that compression and shear jammed packings have similar contact number $\langle z_J(\mu) \rangle$ and packing fraction $\langle \phi_J(\mu) \rangle$ over the full range of $\mu$. However, in Sec. 3.3.2, we demonstrated that $\langle \hat{\Sigma}_{xy} \rangle = 0$ for compression jammed packings and $\langle \hat{\Sigma}_{xy} \rangle > 0$ for shear jammed packings. Does this significant difference in the stress state of MS packings occur because the packings generated via isotropic compression are fundamentally different from those generated via simple shear?

To address this question, we consider two new protocols—protocol A, where we decompress each shear jammed packing, releasing all of the frictional contacts, and then re-compress each one until each jams, and protocol B, where we shear unjam each compression jammed packing, releasing all of the frictional contacts, and then shear each one until each jams. The goal is to study protocols that allow the system to move away from a given jammed packing in configuration space, removing all of the frictional contacts, and determine to what extent the system can recover the original jammed packing using either compression or shear. We compare the particle positions, shear stress anisotropy, and contact mobility for the original and re-jammed packings. If there is no difference between the original jammed and re-jammed packings, all MS packings can be generated via compression or shear. For protocols A and B, we will focus on systems with $N = 16$ and $\mu = 0.1$, but we find similar results for systems with larger $N$ and different $\mu$.

In Fig. 3.6 (a), we illustrate protocol A. We decompress each shear jammed packing at fixed $\gamma$ by $\Delta \phi \sim 10^{-8}$ that corresponds to the largest overlap, so that none of the particles overlap and all of the tangential displacements are set to zero. We then recompress each packing by $\Delta \phi$ in one step and perform energy minimization.
Figure 3.6: (a) Illustration of protocol $A$ where we first generate a shear jammed packing (solid black lines), then decompress the shear jammed packing by $\Delta \phi$ and recompress it by $\Delta \phi$ to jamming onset (blue dashed line). (b) Probability distribution of the shear stress anisotropy $P(\hat{\Sigma}_{xy})$ for the original shear jammed packings (leftward filled triangles) and those generated using protocol $A$ (open rightward triangles) for systems with $N = 16$ and $\mu = 0.1$. The solid line is a Weibull distribution with scale and shape parameters $\lambda \sim 0.27$ and $k \sim 2.5$, respectively.
Figure 3.7: (a) Illustration of protocol $B$ where we first generate compression jammed packings (solid black lines). The compression jammed packings possess either $d\phi_J/d\gamma < 0$ (left) or $d\phi_J/d\gamma > 0$ (right). For packings with $d\phi_J/d\gamma < 0$, we apply simple shear to the left by $\Delta\gamma$ to unjam them and then rejam them by applying $\Delta\gamma$ to the right (dashed blue lines on the left). For packings with $d\phi_J/d\gamma > 0$, we apply simple shear to the right by $\Delta\gamma$ to unjam them and then rejam them by applying $\Delta\gamma$ to the left (dashed blue lines on the right). (b) Probability distribution of the shear stress anisotropy $P(\hat{\Sigma}_{xy})$ for the original compression jammed packings (leftward filled triangles) and those generated using protocol $B$ (rightward open triangles) for systems with $N = 16$ and $\mu = 0.1$ The solid line is a Gaussian distribution with zero mean and standard deviation $\Delta \sim 0.2$. 
In Table 3.1, we show that out of the original 8925 shear jammed packings, protocol A returned 99% compression rejammed packings with the same contact networks as the original shear jammed packings and only 1% of the compression rejammed packings possessed different contact networks. None of the packings were unjammed after applying protocol A. Even though the memory of the mobility distribution of the original shear jammed configuration is erased using protocol A, we show in Fig. 3.6 (b) that the distributions of the shear stress anisotropy $P(\hat{\Sigma}_{xy})$ are very similar for the original shear jammed and compression rejammed packings. (We do not include the small number of rejammed packings with different contact networks and the unjammed packings in the distributions $P(\hat{\Sigma}_{xy})$.) In particular, both the compression rejammed packings and the original shear jammed packings possess $\hat{\Sigma}_{xy} > 0$, and thus the distributions have nonzero means, $\langle \hat{\Sigma}_{xy} \rangle > 0$. This result implies that there is not a fundamental difference between shear and compression jammed configurations, since the isotropic compression protocol can generate “shear jammed” configurations.

We now consider a related protocol where we shear unjam compression jammed packings and then apply simple shear to rejam them. In Fig. 3.7 (a), we illustrate protocol B. We first generate an ensemble of compression jammed packings. Compression jammed packings can jam on either side of the parabolic geometrical families $\phi_{J}(\gamma)$; roughly half with $d\phi_{J}/d\phi < 0$ and half with $d\phi_{J}/d\phi > 0$. For packings with $d\phi_{J}/d\phi < 0$, we shear by $\Delta \gamma \sim 10^{-8}$ in the negative strain direction to unjam the packing. For packings with $d\phi_{J}/d\phi > 0$, we shear by $\Delta \gamma \sim 10^{-8}$ in the positive strain direction to unjam the packing. In both cases, to unjam the system, we apply simple shear strain in extremely small increments $\delta \gamma = 10^{-12}$, with each followed by energy minimization, until $U/N < U_{\text{tol}}$. Note that for protocol A, it is straightforward to identify the largest particle overlap and then decompress the system until there are no
overlaps and the system becomes unjammed. However, in protocol B, we seek to unjam compression jammed packings by applying simple shear strain, and we do this by applying simple shear strain in small increments to reduce the total potential energy below \( U_{\text{tol}} \). (The sensitivity of our results on \( U_{\text{tol}} \) will be discussed in Appendix C.) After unjamming the packing in protocol B, we reset the tangential displacements at each nascent contact to zero. We then rejam the packings by applying the total accumulated shear strain \( \Delta \gamma \) in a single step in the opposite direction to the original one, which allows the system to return to the same total strain, and perform energy minimization.

In Table 3.1, we show that out of the original 1987 compression jammed packings, protocol B returned 96% shear rejammed packings with the same contact networks as the original compression jammed packings and only 4% shear rejammed packings with different contact networks. None of the packings generated using protocol B were unjammed. As shown in Fig. 3.7 (b), the distribution \( P(\hat{\Sigma}_{xy}) \) of shear stress anisotropies is nearly identical for the original jammed packings and the rejammed packings. In both cases, \( P(\hat{\Sigma}_{xy}) \) is a Gaussian distribution with zero mean. This result emphasizes that isotropic stress distributions can be generated using a shear jamming protocol (when we consider shear jamming in both the positive and negative strain directions).

We now compare directly the structural and mechanical properties of the original shear jammed packings and those generated using protocol A and the original compression jammed packings and those generated using protocol B. We calculate the root-mean-square (rms) deviations in the particle positions,

\[
\Delta r = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} \left( \vec{r}^{A,B}_i - \vec{r}^{S,J,C,J}_i \right)^2},
\]

(3.8)
and shear stress anisotropy,

$$\Delta \hat{\Sigma}_{xy} = \sqrt{\left(\hat{\Sigma}_{xy}^{A,B} - \hat{\Sigma}_{xy}^{SJ,CJ}\right)^2},$$

(3.9)

between the original shear jammed (SJ) packings and the packings generated using protocol A and the original compression jammed (CJ) packings and the packings generated using protocol B. In Fig. 3.8 (a), we show the frequency distribution of the deviations in the particle positions $\Delta r$ for systems with $N = 16$ and $\mu = 0.1$. $\langle \Delta r \rangle \sim 2 \times 10^{-12}$ is extremely small, near numerical precision. Thus, the shear jammed packings and those generated via protocol A have nearly identical disk positions, and the compression jammed packings and those generated via protocol B have nearly identical disk positions.

We perform a similar comparison for the stress anisotropy (for systems with $N = 16$ and $\mu = 0.1$) in Fig. 3.8 (b). Even though the disk positions are nearly identical between the shear jammed and compression re-jammed packings, the typical rms deviations in the stress anisotropy $\langle \Delta \hat{\Sigma}_{xy} \rangle$ is finite. The distribution $\Delta \hat{\Sigma}_{xy}$ for the rms deviations in stress anisotropy between shear jammed packings and compression re-jammed packings has a peak near $10^{-2.5}$ (open triangles). The stress anisotropy fluctuations are nonzero because packings of frictional disks with the same particle positions can have multiple solutions for the tangential forces as shown using the force network ensemble [84]. We find similar results for the differences in the stress anisotropy between the compression jammed packings and the shear re-jammed packings, however, the fluctuations are an order of magnitude smaller with $\langle \Delta \hat{\Sigma}_{xy} \rangle \sim 10^{-3.5}$. In contrast, when $\mu = 0$, we find that $\langle \Delta \hat{\Sigma}_{xy} \rangle \sim 10^{-7}$ (nearly four orders of magnitude smaller) when comparing shear jammed packings and packings generated via protocol A with $\Delta r < 10^{-12}$.

We also compare the distributions of the mobility at each contact $\xi = F_{ij}^t/\mu F_{ij}^n$ for
the shear jammed packings and the compression re-jammed packings, as well as the compression jammed packings and the shear re-jammed packings. In Fig. 3.9 (a), we show that the original shear jammed packings have a significant number of contacts that are near sliding with $\xi \sim 1$ and a smaller fraction with $\xi \sim 10^{-3}$. However, the compression re-jammed packings have essentially no sliding contacts, and instead most contacts possess $\xi \sim 10^{-3}$. Thus, we find that the jamming protocol can have a large effect on the contact mobility distribution. We find that applying successive shear strains for sufficiently large strains (as is done for shear jammed packings) is able to generate many contacts near sliding. To our knowledge, our study is one of the first to show that shear jammed packings possess more contacts near the sliding threshold than compression jammed packings.

In Fig. 3.9 (b), we show $P(\xi)$ for the original compression jammed packings and the shear re-jammed packings. These distributions are similar with a small fraction of sliding contacts and an abundance of contacts with $\xi \sim 10^{-3}$. For $\mu > 10^{-2}$, previous studies have shown that compression jamming does not allow tangential displacements to accumulate so that the tangential forces can approach the sliding threshold [85]. For protocol $B$, where we shear unjam the compression jammed packings, and then shear re-jam them, the applied strain is sufficiently small that the tangential displacements do not accumulate and allow the tangential forces to approach the sliding threshold. This result is consistent with the fact that the stress anisotropy fluctuations between compression jammed and shear re-jammed packings are smaller compared to the stress anisotropy fluctuations between shear jammed and compression re-jammed packings.
Figure 3.8: (a) The frequency distribution $p(\Delta r)$ of the root-mean-square deviations in the positions of the disks between shear jammed packings and those generated using protocol $A$ (triangles) and between compression jammed packings and those generated using protocol $B$ (circles). (b) The frequency distribution $p(\Delta \hat{\Sigma}_{xy})$ of the root-mean-square deviations in the stress anisotropy between shear jammed packings and those generated using protocol $A$ (triangles) and between compression jammed packings and those generated using protocol $B$ (circles). For the data in both panels, $N = 16$ and $\mu = 0.1$. 
Figure 3.9: (a) The frequency distribution of the mobility $p(\xi)$, where $\xi = f_{ij}^s / \mu f_{ij}^n$ for each contact between disks $i$ and $j$, for shear jammed packings (open triangles) and compression re-jammed packings (open circles) with $N = 16$ and $\mu = 0.1$. (b) $p(\xi)$ for compression jammed packings (open triangles) and shear re-jammed packings (open circles) with $N = 16$ and $\mu = 0.1$. The filled symbols indicate the frequency of contacts that slid with $f_{ij}^s = \mu f_{ij}^n$. 
Table 3.1: (first row) Comparison of the contact networks (CN) for the original shear jammed (SJ) packings and compression rejammed packings. (second row) Comparison of the contact networks for the original compression jammed (CJ) packings and shear rejammed packings.

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### 3.4 Conclusion and Future Directions

In this thesis, we used discrete element modeling simulations to compare the structural and mechanical properties of jammed packings of frictional disks generated via isotropic compression versus simple shear. We find that several macroscopic properties, such as the average contact number $\langle z_J \rangle$ and packing fraction $\langle \phi_J \rangle$ at jamming onset, are similar for both packing-generation protocols. For both protocols, $\langle z_J(\mu) \rangle$ varies from 4 to 3 in the low- and high-friction limits with a crossover near $\mu_c \approx 0.1$. $\langle \phi_J(\mu) \rangle$ varies from $\sim 0.835$ to 0.76 in the low- and high-friction limits with a similar crossover value of $\mu_c$.

The average stress state of mechanically stable (MS) packings generated via isotropic compression is different than that for MS packings generated via simple shear. The average stress anisotropy $\langle \hat{\Sigma}_{xy} \rangle > 0$ for MS packings generated via shear, but $\langle \hat{\Sigma}_{xy} \rangle = 0$ for packings generated via isotropic compression. Isotropic compression can sample MS packings with both signs of $\hat{\Sigma}_{xy}$, whereas simple shear (in one direction) samples packings with only one sign of the stress anisotropy.

To investigate in detail the differences in the stress state of MS packings generated via simple shear and isotropic compression, we developed two additional protocols. For protocol A, we decompress shear jammed packings so that the frictional contacts
are removed and then re-compress them to jamming onset. For protocol B, we shear unjam MS packings generated via isotropic compression so that the frictional contacts are removed, and then shear re-jam them. These studies address an important question—to what extent can protocols A and B recover the contact networks and stress states of the original jammed packings. We find that even though protocols A and B can recover the particle positions (and contact networks) of the original jammed packings, the rejammed and original jammed packings have small, but significant differences in the stress anisotropy, e.g. $\Delta \hat{\Sigma}_{xy} \sim 10^{-3.5}-10^{-2.5}$ for systems with $\mu = 0.1$.

To understand the stress fluctuations of frictional packings with nearly identi-
Figure 3.11: The frequency distribution $p(\sigma_{\hat{\Sigma}_{xy}})$ of the standard deviation of the stress anisotropy from the null space solutions for each of the compression jammed packings. The peak in $p(\sigma_{\hat{\Sigma}_{xy}})$ is $\sigma_{\hat{\Sigma}_{xy}} \approx 10^{-2}$.

cal particle positions, we carried out preliminary studies of the null space solutions for force and torque balance on all grains using the contact networks from the MS packings generated via isotropic compression [86]. For each packing of frictional disks, force and torque balance on all grains can be written as a matrix equation $A_{lm}F_m = 0$, where $A_{lm}$ is a $3N \times 2N_c$ constant matrix determined by the contact network and $F_m$ is a $2N_c \times 1$ vector that stores the to-be-determined normal and tangential force magnitudes $f_{ij}^n$ and $f_{ij}^t$ at each contact. For frictional disk packings, the system is underdetermined with $3N > 2N_c$. Using a least-squares optimization approach [87], we solve for the normal and tangential force magnitudes such that $f_{ij}^n > 0$, and $f_{ij}^t \leq \mu f_{ij}^n$.

The stress anisotropy frequency distribution $p(\hat{\Sigma}_{xy})$ from the null space solutions for an example compression jammed packing (with $N = 16$ and $\mu = 0.1$) is shown in Fig. 3.10. We find that the DEM-generated solutions belong to the set of null
space solutions, but there are many more. In particular, the width of $p(\hat{\Sigma}_{xy})$ from the null space solutions is much larger than the width of the distribution of the stress anisotropy obtained for the given compression jammed packing from protocol $B$. We performed similar calculations of the null space solutions for all compression jammed packings. In Fig. 3.11, we show the frequency distribution of the standard deviations $\sigma_{\hat{\Sigma}_{xy}}$ of stress anisotropy from the null space solutions over all of the compression jammed packings. We find that the width of the fluctuations of the stress anisotropy from the null space solutions for a given packing are comparable to fluctuations of the stress anisotropy over all compression jammed contact networks using DEM. In future studies, we will carry out similar calculations to understand how the fluctuations in the stress anisotropy from the null space scale with system size $N$ and friction coefficient $\mu$. For example, we will investigate over what range of $N$ and $\mu$ are the null space stress anisotropy fluctuations larger than the stress anisotropy fluctuations from varying contact networks. Addressing this question will allow us to predict the differences in the structural and mechanical properties of jammed packings of frictional particles that arise from the packing-generation protocols, such as isotropic compression and both continuous and cyclic pure and simple shear [88].

3.5 Appendix

3.5.1 Normal Stress Difference in Jammed and Rejammed Packings

In this Appendix, we describe the results for the normal stress difference for jammed packings of frictional disks generated via simple shear and isotropic compression. In
Figure 3.12: Probability distribution of the normal stress difference $P(\hat{\Sigma}_N)$ for jammed packings generated via isotropic compression (open symbols) and simple shear (closed symbols) for $N = 64$ and friction coefficients $\mu = 0$ (triangles), 0.1 (circles), and 1.0 (squares). The distributions were obtained from more than $10^3$ independently generated jammed packings. The solid lines are Gaussian distributions with zero mean and standard deviations $\Delta \approx 0.091$, 0.093, and 0.114 for $\mu = 0$, 0.1, and 1.0, respectively.

Fig. 3.12, we show the probability distribution $P(\hat{\Sigma}_N)$ of the normal stress difference for both shear and compression jammed packings with $N = 64$ at $\mu = 0$, 0.1, and 1.0. Simple shear and isotropic compression do not strongly couple to $\hat{\Sigma}_N$ and thus we find that $P(\hat{\Sigma}_N)$ is a Gaussian distribution centered at zero with a width that depends on $\mu$. We also calculated $\Delta \hat{\Sigma}_N$, which is the rms deviation in the normal stress difference between the rejammed and original jammed packings for protocols A and B. In Fig. 3.13, we show that (as for the stress anisotropy), the rms deviation in the normal stress difference $\Delta \hat{\Sigma}_N$ is typically larger between shear jammed packings and compression rejammed packings, compared to that between compression jammed packings and shear rejammed packings.
Figure 3.13: The frequency distribution $p(\Delta \hat{\Sigma}_N)$ of the root-mean-square deviation in the normal stress difference between shear jammed packings and those generated using protocol A (triangles) and between compression jammed packings and those generated using protocol B (circles).
3.5.2 Parabolic Geometrical Families

Geometrical families are collections of jammed packings that share the same interparticle contact network at different values of the packing fraction at jamming onset $\phi_J$ and either pure or simple shear strain $\gamma$. In this Appendix, we present a derivation of the relation between $\phi_J$ and $\gamma$ for a simple example of jammed packings of two hard disks (one small disk with diameter $\sigma_s$ and one large disk with diameter $\sigma_l$) undergoing pure shear strain $\gamma = \ln \left( \frac{L_x}{L_y} \right)$ in a box with side walls with lengths $L_x$ and $L_y$ in the $x$- and $y$-directions. We first express the box lengths $L_x = \sigma_l(1 + \cos \theta)$ and $L_y = \sigma_l(1 + \sin \theta)$ in terms of the angle $\theta$ between the horizontal axis of the box and $\vec{r}_{ij}$ connecting the centers of the disks. See Fig. 3.14 (a). Thus, the pure shear strain satisfies

$$\gamma = \ln \left( \frac{1 + \cos \theta}{1 + \sin \theta} \right).$$  

(3.10)

In addition, we can write the jammed packing fraction as

$$\phi_J = \frac{\phi_1}{(1 + \cos \theta)(1 + \sin \theta)},$$  

(3.11)

where

$$\phi_1 = \frac{\pi(\sigma_s^2 + \sigma_l^2)}{(\sigma_s + \sigma_l)^2}.$$  

(3.12)

Using Eqs. 3.10 and 3.11, we can eliminate the dependence on $\theta$ and write $\phi_J$ in terms of $\gamma$:

$$\phi_J = \phi_1 \left[ \sqrt{2} - 2 \cosh \left( \frac{\gamma}{2} \right) \right]^2.$$  

(3.13)

Eq. 3.13 is similar to a parabola, which can be seen by expanding it in powers of $\gamma - \gamma_0$ about the minimum at $\gamma_0 = 0$ and retaining terms up to $(\gamma - \gamma_0)^2$:

$$\phi_J = \phi_0 + A(\gamma - \gamma_0)^2,$$  

(3.14)

where $\phi_0 = (6 - 4\sqrt{2})\phi_1$ and $A = \left(1 - \frac{\sqrt{2}}{2}\right)\phi_1$. We carried out discrete element method simulations to generate jammed packings at each value of the pure shear...
strain $\gamma$ for two bidisperse hard disks. The DEM results for $\phi_J(\gamma)$ agree with the analytical result as shown in Fig. 3.14. For small systems, a single geometrical family can exist over a wide range of strain. Also, for pure shear in small systems, the parabolic geometrical family is centered on $\gamma = 0$. In contrast, for simple shear of two hard bidisperse disks (in fixed wall boundary conditions), the parabolic geometrical family is not centered on $\gamma = 0$ as shown in Fig. 3.15.

### 3.5.3 Sensitivity of Results on Numerical Parameters of Packing-Generation Protocols

In this Appendix, we investigate how the ability to generate the original jammed packing from the rejamming protocols A and B depends on parameters associated with the packing-generation protocols. When determining the packing fraction at jamming onset, we seek particle configurations for which the total potential per particle $U/N$ is nonzero, but small, i.e. $U_{\text{tol}} < U/N < 2U_{\text{tol}}$ and $U_{\text{tol}} = 10^{-16}$ for the results provided in the main text. To better understand the sensitivity of our results on $U_{\text{tol}}$, we calculate the frequency distribution for rms deviations in the positions between shear jammed packings and compression rejammed packings as a function of $U_{\text{tol}}$. For $U_{\text{tol}} = 10^{-16}$, $p(\Delta r)$ is narrow with a peak near $\Delta r \approx 10^{-12}$ as shown in Fig. 3.16. However, for $U_{\text{tol}} = 10^{-14}$ and $10^{-12}$, $p(\Delta r)$ broadens dramatically, with non-zero probability between $\Delta r = 10^{-11}$ and $10^{-7}$. These results emphasize that it is more difficult to recover the original jammed packing for packings that are over-compressed because over-compressed packings are further from the unjammed state, increasing the likelihood that the system can find a pathway to another jammed configuration during the re-jamming process.

Does the stress anisotropy for shear jammed and compression re-jammed packings (or for compression jammed and shear re-jammed packings) differ for systems at
Figure 3.14: (a) Illustration of a jammed packing of two bidisperse disks $i$ and $j$ in a simulation cell with side lengths $L_x$ and $L_y$ in the $x$- and $y$-directions. $\theta$ gives the angle between the center-to-center separation vector $\vec{r}_{ij}$ and the $x$-axis. (b) The packing fraction at jamming onset $\phi_J$ versus the pure shear strain $\gamma$ for packings of two bidisperse disks obtained from Eq. 3.13 (solid blue line) and DEM simulations (open triangles). The jammed packing fraction $\phi_0$ and pure shear strain $\gamma_0$ at the minimum and the curvature $A$ of the parabola are given in the main text.
Figure 3.15: (a) The packing fraction at jamming onset $\phi_J$ versus the simple shear strain $\gamma$ for packings of two bidisperse disks obtained from DEM simulations (open triangles). We also show a fit to a parabolic form, $\phi_J = \phi_0 + A(\gamma - \gamma_0)^2$, where $\phi_0 \approx 0.49$, $A \approx 0.34$, and $\gamma_0 \approx 1.03$ (solid blue line).
Figure 3.16: Frequency distribution $p(\Delta r)$ of the root-mean-square deviations in the positions of the disks between shear jammed packings and those generated using protocol A for $U_{\text{tol}} = 10^{-16}$ (black triangles), $10^{-14}$ (blue circles), and $10^{-12}$ (red squares), $N=16$ and $\mu=0.1$.

$\mu = 0$? In general, the stress anisotropy distributions are similar for jammed and re-jammed packings, but the precise values of the stress anisotropy can differ for each original jammed packing and its re-jammed counterpart. We find that the average value of the stress anisotropy difference $\langle \Delta \hat{\Sigma}_{xy} \rangle \approx 10^{-5}$ (between shear jammed and compression re-jammed packings) for $\mu = 0.1$, but $\langle \Delta \hat{\Sigma}_{xy} \rangle \approx 10^{-7.5}$ is much lower for $\mu = 0$. (See Fig. 3.17.) In contrast to the results for $\mu > 0$, $\langle \Delta \hat{\Sigma}_{xy} \rangle$ for $\mu = 0$ scales to zero with the degree to which the simulations can maintain force balance.
Figure 3.17: The frequency distribution \( p(\hat{\Delta} \Sigma_{xy}) \) of the root-mean-square deviations in the stress anisotropy between shear jammed packings and those generated using protocol A for \( N = 16 \) and \( \mu = 0 \).
Chapter 4
Conclusion

In this thesis, we presented two numerical studies on dense packings of soft grains on structural and mechanical properties associated with shear protocol and compression protocol. We presented the theoretical prediction of pressure dependent shear modulus for frictionless grains. The theoretical prediction derived from affine approximation has been measured and compared, and we are able to identify the source of deviation in the functional form of shear modulus. In the frictional grains study, we proposed a novel protocol to quantify the distinction between compression jamming protocol and shear jamming protocol of frictional grains. This work suggests that jamming protocol plays an important role in frictional grains.

In Chapter 2, we studied extensively the geometrical family contribution to the total shear modulus, $G(P)$. We also addressed the limitation of effective medium theory when nonaffine motion is dominant [42, 89, 90]. The ensemble averaged total shear modulus, $\langle G \rangle = \langle G_f \rangle + \langle G_r \rangle$, is the sum of the geometrical family contribution, $G_f$, and the rearrangement contribution, $G_r$. Each rearrangement event caused by compression generally leads to an increase in the number of contacts each particle is bearing and result in larger shear modulus. On the other hand, the variation of shear modulus within each geometrical family strongly depends on the force law exponent,
α. We found that the functional form of the affine approximation dominates most of the time during compression along a geometrical family. When the packing is approaching a rearrangement event due to mechanical instability, nonaffine contribution dominates and causes $G$ to decrease much faster than $\sim P$. The rapid decrease in $G$ with $P$ results in deep negative values, a commonly overlooked characteristic in shear modulus statistics. We included these negative values in our $\langle G \rangle$ and showed that the power-law scaling at high pressure regime deviates from the reported value from literature [36]. We have also investigated geometrical families with $N_c^0 + 1$ contacts and found that by distinguishing between point change and jump change, $G(P)$ imminent to forming new contact exhibits different behaviors. For jump changes (hence irreversible), $G(P)$ obeys the form of $G_a$ along the geometrical family until mechanical instability builds up. Whereas for point changes (hence reversible), $G(P)$ only obeys the form of $G_a$ in the “intermediate” section of the geometrical family. This observation is important in constructing analytical expression of $G(P)$ for high pressure geometrical families having more than $N_c^0$ contacts.

In chapter 3, we studied the problem of jamming protocol dependence of frictional grains. It has been shown previously that finite system size frictionless packings do not have jamming protocol dependence, i.e., one can find the same jammed packing $(\phi, \gamma, \vec{x})$ by isotropic compression or by simple shear. We showed that this is not strictly the case for frictional grains. Through a novel packing rejam protocol that enable us to visit packings with identical contact network and negligible particle displacement, we showed that history-dependent tangential forces have jamming protocol dependence. Shear jammed packings, if unjammed then rejammed by isotropic compression, will have fewer sliding contacts. On the other hand, rejam an isotropic compression jammed state by simple shear also result in a shift in mobility distri-
Figure 4.1: \( \langle G \rangle / G_c \) plotted versus \( (P/P_c)^{(a+b)/2} \) for jammed disk packings with \( \alpha = 2 \) and system sizes \( N = 32 \) (black upward triangles), 64 (blue circles), 128 (red diamonds), 256 (green downward triangles), and 512 (magenta asterisks). Only positive \( G \) are considered in the \( \langle G \rangle \) calculation. The upper left inset shows \( P_c \) (black asterisks) and \( G_c \) (blue circles) versus \( N \). The dotted and dashed lines have slopes equal to \(-1\) and \(-2\), respectively. The lower right inset gives the exponents, \( a \) (black upper triangles) and \( b \) (blue diamonds), used in fits to Eq. 2.6 versus \( N \). The horizontal dotted and dashed lines indicate \( a = 0 \) and \( b = 0.5 \), respectively.

These results suggest that frictional grains must be investigated further to understand the jamming protocol dependence.

The studies presented in this thesis raise a series of open questions. With regard to chapter 2, there are several future directions worth exploring. First, what does a geometrical family look like for packings possessing \( N^0_c + n \) contacts, where \( n > 1 \)? Understanding high pressure family is crucial in developing theoretical description of shear response of jammed packings. Second, apart from the power-law scaling of \( \langle G(P) \rangle \), frictional spherical grains have not been studied extensively – specifically regarding geometrical family. Can we still observe point change in frictional system?
CHAPTER 4. CONCLUSION

Our results in frictional system seem to imply that frictional jammed packings are irreversible. Third, what is the particle shape dependence on \( \langle G(P) \rangle \)? Does \( G_f \) always decrease with \( P \) at the respective large \( P \) range of the geometrical family? For example, packings of elongated particles may dilates in a way that it produces interesting behavior \[26\]. Fourth, how do packings accumulates nonaffine contribution through compression \[92, 93\]? Can we arrive at an analytical expression for total \( G \)? Finally, what is the “complete” distribution of \( G(P) \)? By including negative \( G \) in calculating the ensemble averages, we see discrepancy in high pressure power-law exponent of \( \langle G(P) \rangle \). Removing negative samples from the distribution, on the other hand, recovered the same power-law exponent reported in other literature in the large system limit (see lower right inset in Fig. 4.1). With regard to chapter 3, the most interesting question would be to really understand whether simple shear protocol is capable of visiting states that are inaccessible by isotropic compression. Null-space method has been shown to be a useful tool to solve for force-balance solutions \[86, 94\]. Our preliminary work using null-space method samples one possible distribution of force-balance solutions from a given contact network, \( \mu \) and \( \vec{r} \). Is it possible to show that simple shear protocol always samples specific part of the distribution while isotropic compression samples other part? In addition, can we sample the entire distribution through some other protocols such as cyclic shear \[95, 96, 97, 98\]? Another interesting question regarding frictional packings would be to understand the distinction between geometrical frictional models \[75, 99\] versus functional frictional models \[78, 100, 101, 102\] when it comes to jamming protocols. What is the role of stick-slip condition of these models \[103\], again, concerning jamming protocols? It would be interesting to investigate the history dependence of each of these models. Perhaps geometrical frictional models are reversible – opening the door to study point changes
and jump changes in frictional grains. Finally, can we develop a geometrical model that is applicable in high pressure? Relaxing from the hard disks limit of the soft disks model inevitably run into the problem of double counting, or multiple counting, of the normal force contribution [104], leading to the overestimates of normal forces. Solving this problem allows us to study more accurately the pressure dependence of mechanical and structural properties of frictional grains. There are many aspects of granular materials that remain unexplored and worth investigating.
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