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CONTACT CHANGES OF SHEARED SYSTEMS

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In this chapter, we investigate contact changes in amorphous, athermal, frictionless particle packings under small shear deformations by means of numerical simulations. We focus on the first contact change, as this is where one expects the first significant deviation from strictly linear response. We will establish a scaling relation between the mean strain at which the first contact change happens and the system size and pressure, and find that this strain can accurately be predicted from linear response. We will investigate the effect of a single contact change on the elastic response, and will show that, although strict linear response is no longer valid after a single contact change, the response is still effectively linear in the thermodynamic limit. We discuss the underlying microscopic mechanism for contact changes, and reveal subtle correlations between particle motions and overlap, as well as between subsequent contact changes. Finally, we discuss our findings in the light of several recent related studies of contact changes.
2.1 Introduction

The focus of this chapter is on the first contact change in systems under shear deformation. Earlier work on sheared systems has mostly focused on plasticity \([52, 67–71]\), continuous shear \([38, 41, 42, 72]\) or on the linear response limit \([21, 34, 73–75]\) while earlier work on contact changes has focused on vibrations \([76–78]\) or hard particle systems \([79, 80]\). We instead focus on soft particle systems, as they are descriptive for a wider range of experimentally relevant systems, and focus on experimentally relevant simple shear deformations.

The outline of this chapter is as follows. In § 2.2, we will describe the preparation and deformation of our systems. We focus on the strain at which the first contact change happens in §§ 2.3 and 2.4, and investigate multiple contact changes and the behavior in the thermodynamic limit in § 2.5. Finally, we compare our results to earlier work in § 2.6.

2.2 Method & protocols

For our simulations, we use the standard frictionless soft sphere model \([13, 21]\), which is a simplified version of the viscous model for foam bubbles introduced by Durian \([22]\). We will shear quasi-statically, so only the elastic interactions between particles are taken into account - there is no inertia, nor is there viscous damping. We will focus on so-called \(\varepsilon^+_\text{all}\) packings \([28]\) that have a positive bulk and shear modulus, as well as zero residual shear stress. This is not guaranteed for a square unit cell \([28, 34, 81]\), and we therefore allow the shape of the cell to change.

In this section, we will describe the precise implementation of the periodic boundaries, the particle interactions and the energy minimization algorithms. Finally, we will describe how we apply a simple shear deformation and how we find individual contact changes.

**Boundary conditions.** We use periodic boundaries, as this removes the need to model wall-particle interactions. Instead, particles just interact with their neighbors, which may be periodic copies of particles on the other side of the unit cell.

In a periodic system, each particle has periodic copies at

\[
\vec{r} = \vec{r}_i + n_x \cdot \vec{L}_x + n_y \cdot \vec{L}_y,
\]  

(2.1)
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\[
\begin{align*}
L^2 &= L_{xx} \cdot L_{yy} , \\
\alpha &= L_{yx} / L \\
\delta &= \frac{L_{yy} - L}{L} = \sqrt{L_{yy}/L_{xx} - 1} .
\end{align*}
\]

Traditionally, the unit cell is square, i.e., \( \vec{L}_x = (L, 0) \) and \( \vec{L}_y = (0, L) \), and consequently \( \alpha = \delta = 0 [3, 13, 21] \), but this leads to systems that are...
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stable to compression but potentially unstable to shear [28, 34, 81, 82]. In contrast, here we require that the energy is also at a minimum with respect to these degrees of freedom, which guarantees that the shear modulus is positive and that the residual shear stresses are zero [28, 34], as one expects for a physical system at rest. We keep $L_{xy} = 0$ fixed, which fixes the global rotational degree of freedom.

Particles and their interactions. Our system consists of circular particles with repulsive harmonic interactions. We use a bi-disperse mixture, with $N/2$ small particles with $R_s = 1$ and $N/2$ large particles with radius $R_l = 1.4$, to prevent crystallization [3, 21, 137].

The interaction between particles is determined by their overlap

$$\delta_{ij} = \begin{cases} 
R_i + R_j - |\vec{r}_{ij}| & \text{if } |\vec{r}_{ij}| < R_i + R_j, \\
0 & \text{otherwise.}
\end{cases} \quad (2.5)$$

where $|\vec{r}_{ij}|$ is the distance between particles $i$ and $j$ (Fig. 1.3(a)). Because of the periodic boundaries, this distance is not uniquely defined. The physically relevant value is the minimum distance, so we will define the distance as

$$|\vec{r}_{ij}| \equiv \min_{n_x, n_y} \left| \vec{r}_i - \vec{r}_j + [n_x \cdot \vec{L}_x] + [n_y \cdot \vec{L}_y] \right|, \quad (2.6)$$

where $\vec{r}_i$ and $\vec{r}_j$ are the canonical particle positions. $n_{x,ij} (n_{y,ij})$ is 0 if the closest copy of $j$ to $i$ is the canonical copy, +1 if it is across the right (top) boundary and −1 if it is across the left (bottom) boundary. Contact forces have magnitude $f_{ij} = k\delta_{ij}$, where $k = 1$ is the spring constant, and correspond to the harmonic potential

$$U_{ij} = \frac{k}{2} \delta_{ij}^2, \quad (2.7)$$

Energy, enthalpy and stresses. From the particle interactions, we can now define the macroscopic state variables. First, we have the internal energy, which is given by the sum of all inter-particle potentials,

$$U = \sum_{i,j} U_{ij} = \sum_{i,j} \frac{k}{2} \delta_{ij}^2, \quad (2.8)$$
where the sum runs over all particle pairs.

The enthalpy is then given by

\[ H = U + P_\text{ext} L^2 , \]  

(2.9)

where \( P_\text{ext} \) represents the external pressure on the system.

Finally, we have the boundary stresses: the simple shear stress

\[ \sigma_{yx} = \sigma_{xy} , \]  

(2.10)

the deviatoric (pure shear) stress

\[ \tau = \frac{1}{2} (\sigma_{xx} - \sigma_{yy}) , \]  

(2.11)

and the volumetric stress or internal pressure

\[ P_\text{int} = \frac{1}{2} (\sigma_{xx} + \sigma_{yy}) . \]  

(2.12)

These are computed using the Born-Huang approximation [83, 84]:

\[ \sigma_{ab} = \frac{1}{2L^2} \sum_{i,j} \left[ (\vec{r}_{ij} \cdot \hat{a}) (\vec{f}_{ij} \cdot \hat{b}) \right] \]  

(2.13)

where \( a, b \in \{x, y\} \) and the sum is over all particle pairs \( i, j \).

Units. The small particle radius \( R_s \) and the spring constant \( k \) set all units in our system. The length scale is given by the small particle radius \( R_s \), the stress scale is given by the spring constant \( k \) and energy is measured in units of \( kR_s^2 \).

Preparing a packing. We will now focus on creating a stable packing of particles. Starting with \( N \) randomly positioned particles and a predefined external pressure \( P_\text{ext} \) between \( 10^{-7} \) and \( 10^{-2} \), we minimize the enthalpy until we end up in a stable state, where the forces on particles and boundaries add up to zero.

We start by placing \( N/2 \) small particles with \( R_s = 1 \) and \( N/2 \) large particles with radius \( R_l = 1.4 \) at random positions \( \vec{r}_i^* \) within a square box of size

\[ L_{\text{init}}^2 = \phi_{\text{init}} \left( \frac{N}{2} \pi R_s^2 + \frac{N}{2} \pi R_l^2 \right) , \]  

(2.14)
Contact changes of sheared systems

where \( \phi_{\text{init}} \equiv 0.8 \) is chosen to be far below the jamming density \( \phi_J \approx 0.84 \). We use a combination of the Conjugate Gradient method [85] and the Fast Inertial Relaxation Engine (FIRE) [86] algorithms. The latter is much faster, but becomes unstable when the overlaps between particles are large. We therefore first use the Conjugate Gradient method to resolve the largest overlaps. We keep the boundaries fixed, and minimize the energy until

\[
|\Delta U| \leq 10^{-2} \cdot U . \tag{2.15}
\]

After the large overlaps are resolved, we can safely switch to the FIRE algorithm. We now also allow the boundaries (i.e., \( L_{xx}, L_{yy}, \) and \( L_{yx} \)) to deform. We relax the system until we reach a state where

\[
|\Delta H| \leq 10^{-17} \cdot H , \text{ and} \\
|\sigma_{yx}| \leq 10^{-15} . \tag{2.16}
\]

The resulting state has positive shear moduli, vanishingly small shear stresses, and a pressure given by the target pressure \( P_{\text{ext}} \).

Simple shear. We are interested in the response to an applied simple shear deformation. We do this by moving the boundaries into a new state

\[
\begin{align*}
\vec{L}_x(\gamma) &= \vec{L}_x(0) , \\
\vec{L}_y(\gamma) &= \vec{L}_y(0) + \gamma L \cdot \hat{x} ,
\end{align*} \tag{2.17}
\]

i.e., we change \( \alpha \to \alpha + \gamma \), while keeping \( L^2 \) and \( \delta \) constant. The system is now no longer in an enthalpy minimum, so we relax the system, using the FIRE algorithm, but keeping boundaries in the new deformed state. We relax the system until

\[
|\Delta H| < 10^{-13} \cdot H , \tag{2.18}
\]

where we sacrifice a small error in the particle positions for simulation speed. This is accurate enough to detect contact changes and to determine the behavior of stress and energy at the contact change. We find the details of the relaxation requirement do not influence the detection of contact changes, and the relative error in \( \sigma_{xy} \) is typically less than \( 10^{-6} \). An example of the resulting particle displacement is shown in Fig. 2.2.
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The corresponding stress and enthalpy response is shown in Figs. 2.3(c) and 2.3(d).

To detect contact changes, we apply a strain, relax the system, and compare the new overlaps of each particle pair \( i, j \) to the initial state, until we detect a change in the contact network (\( \delta_{ij} = 0 \leftrightarrow \delta_{ij} > 0 \) for any pair \( i, j \)). We then use the bisection method to find the contact change strain: we move back to the last state before the contact change, and test a strain between the last known state before and the first state after the contact change. Specifically, we initially apply a strain

\[
\gamma = 10^{-9} \cdot 10^\zeta
\]

where we increase \( \zeta = 0, 1, \ldots \) until we find that the contact network changed. We then bisect \( \zeta \) until we have determined the strain at the contact change \( \gamma_* \) up to \( \Delta \gamma / \gamma_* < 10^{-6} \), as shown in Figs. 2.3(a) and 2.3(b).

Treatment of rattlers. Rattlers are always a special case in simulations: because they are free to move, their behavior is ill-defined. In our simulations, we encounter rattlers in two distinct ways: first, a particle with three contacts can become a rattle. Because of force balance, all three contacts go to

![Figure 2.2: Particle trajectories in response to a simple shear strain \( \gamma = 9.8 \times 10^{-6} \), for the \( N = 256 \) particle system at \( P = 10^{-6} \). Lines indicate displacements (magnified \( \times 5000 \)), color indicates displacement parallel to the applied shear. The unit cell is slightly non-square and marked as a gray box.](image-url)
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**Figure 2.3:** Convergence to the first contact change for the system shown in Fig. 2.2 \((N = 256, P = 10^{-6})\). (a) Contact change detection algorithm. Red △ indicate states without a contact change \((γ < γ_*)\), blue ▽ states have had at least one contact change \((γ > γ_*)\). We rapidly scan shear space until we find a state with a changed contact network (step 4). We then bisect the strain space to determine \(γ_*\). (b) The bisection algorithm continues until \(Δγ/γ_* < 10^{-6}\). (c) The stress response before the first contact change (red pluses) is linear as a function of \(γ\). After the contact change (blue crosses) the response changes drastically. (d) The enthalpy change during deformation. Because of the linear stress response, the enthalpy change is quadratic in \(γ\).

zero overlap together. This is detected correctly in our simulations, and the event is recorded as a single event in which three contacts are lost (Fig. 2.4).

The case of a rattler becoming part of the load-bearing network is different. Before the rattler gains three contacts, it’s fully free to move, and we can therefore not determine the strain at which it becomes part of the network again accurately — if another algorithm had been used, the path of the particle and therefore also the joining strain could be different. We will therefore not include these contact making events in our analysis of the first contact change.

One might worry that this biases the mean strain and the statistics of breaking or closing a contact. Indeed, we find that, in our simulations, contact changes in which a rattler annihilates happen at a relatively small strain (typically 50 – 80% of the mean strain). At the same time, these events
Figure 2.4: (a) Zoom-in of a packing where particle $r$ becomes a rattler after the first contact change ($N = 22, P = 1.5 \cdot 10^{-5}$). Neighboring particles $A$, $B$ and $C$ are indicated. (b) Overlap of $r$ with the neighboring particles $A$, $B$ and $C$ as a function of strain $\gamma$. Symbols are our results from simulations, while the lines indicate predictions using linear response. The simulation finds $\gamma^\text{DNS}_*= 2.45 \cdot 10^{-5}$, while linear response predicts $\gamma^\text{LR}_*= 2.41 \cdot 10^{-5}$.

are rare: We find they are most prevalent in large systems at intermediate pressures, but even there they only make up a few percent of the events. We find that the overall effect on the mean strain is also limited to a few percent, while we measure changes in the mean strain over multiple orders of magnitude. The probability of the first contact being a contact making event decreases somewhat, as 5–15% of making events involve a rattler re-joining the contact network. Because we are interested in the scaling behavior, we are comfortable ignoring these events.

Simulation range. As we will study changes in individual contacts, and in particular probe the strain at which the first contact change takes place, we anticipate that we need to study finite size effects, i.e. the role of the number of particles $N$ in tandem with the role of the pressure $P$. Moreover, we anticipate that many quantities will rescale with $N^2 P$ [28, 33, 65]. We have therefore prepared various ensembles — groups of sheared systems with the same number of particles and pressure. Most ensembles contain 100
systems; some larger ensembles contain up to 5000 systems. The following ensembles were prepared:

- To characterize the behavior at the first contact change, we created a set of ensembles having \( N \) and \( P \) on a log-spaced grid, with \( N = 16, 32, \ldots, 1024 \) and \( P = 10^{-7}, 10^{-6.5}, \ldots 10^{-2} \), and a set at intermediate \( N = 22, 45, \ldots 724 \) for \( P = 10^{-2} \) and \( 10^{-7} \). These are sheared until we find at least one contact change.

- To characterize the effects of multiple contact changes (§ 2.5.2), we sheared the ensembles at \( N = 16, P = 10^{-6}, N = 1024, P = 10^{-6} \) and \( N = 1024, P = 10^{-2} \) up to 25 contact changes.

- To investigate anisotropy, ensembles with \( N = 16, 256, 1024 \) particles at \( P = 10^{-3} \) and \( N = 16, P = 10^{-6} \) were sheared in the inverse direction.

### 2.3 Numerical results

In this section, we will first discuss at which strain \( \gamma^* \) the first contact change occurs, the relative prevalence of making or breaking a contact, and the anisotropy in the type of events. We will then discuss the distribution of \( \gamma^* \) within an ensemble at fixed \( N \) and \( P \), and will discuss how the ensemble average \( \gamma_{cc} = \langle \gamma^* \rangle \) scales with \( N \) and \( P \).

#### 2.3.1 The first contact change

For each packing in an \((N, P)\) ensemble, we determine the strain of the first contact change \( \gamma^* \), as described in § 2.2. Within a single ensemble, typically consisting of 100 realizations, we find that \( \gamma^* \) can vary over three orders of magnitude. In Fig. 2.5(a) we show the cumulative distribution function (CDF) of \( \gamma^* \) for \( N = 256 \) ensembles at various pressures. We observe two important properties: First, the typical scale of the strain \( \gamma^* \) increases with pressure \( P \). Second, we find that, although the distributions are wide, their shape is mostly independent of \( P \). In § 2.3.2, we will take a detailed look at these distributions and their scaling.
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**Figure 2.5:** (a) Cumulative distribution functions (CDF) $\Pr(\gamma^* < \gamma)$ of the contact change strain $\gamma^*$ for ensembles with $N = 256$ particles at various pressures. The horizontal shift between curves shows that the characteristic strain increases with $P$. (b) Stacked probabilities for the first contact change being a break event (blue striped), a make event (red striped), a make event involving rattlers (red) or a mixed event, where contacts are both broken and created (black), again for $N = 256$ ensembles. A small amount of new contacts involve a rattler becoming part of the contact network. At low pressures, all contact changes involve a contact being broken. The probability of the contact change being a new contact increases with pressure, up to 40% at $P = 10^{-2}$. Both mixed events and new contacts involving a rattler are very rare.

**Figure 2.6:** Radial distribution function $\rho(\theta)$ of the contact orientation for making (blue) and breaking (red) events, for $N = 256, P = 10^{-3}$. New contacts are created along $\theta = 3\pi/4$, while contacts are broken along $\theta = \pi/4$. 

Making and breaking. In Fig. 2.5(b), we show a stacked probability graph of the different contact change types. We distinguish events where one or more contacts are broken (break), events where one or more contacts are created (make) and events where contacts are both broken and created (mixed). Within the make class, we can distinguish events where a particle which originally was a rattler now becomes part of the contact network (make (rattler)).

At low pressures, we find that the vast majority of events consists of contacts being broken. This probability decreases with increasing pressure, to 59% at \( P = 10^{-2} \). At this pressure, we find that 38% of events create a new contact. In § 2.4.4, we will show how these probabilities vary as a function of \( N^2 P \).

Of all make events, 5 – 15% involve rattlers. This is consistent between ensembles, with no clear dependence on either \( N \) or \( P \). Finally, the number of mixed events increases with pressure, but is < 5%, independent of \( N \).

In the following sections, we will focus on the simple make and break cases; we will not include make (rattler) or mixed events. We remove the first because the behavior of rattlers creating new contacts is ill-defined, as discussed in § 2.2. Mixed events are not included because of their relative scarcity.

Anisotropy in bond direction. When we shear our system, we expect anisotropy to build up [87]. We measure the anisotropy by measuring the contact orientation \( \theta \) for each contact that is created or broken. \( \theta \) characterizes the direction for the connection vector \( \vec{r}_{ij} \) between the two particles, and is \( \pi \)-periodic.

A simple shear deformation along the \( x \) (\( \theta = 0 \)) axis compresses the system along \( \theta \approx \frac{3}{4} \pi \) and extends it along \( \theta \approx \frac{1}{4} \pi \). We therefore expect breaking contacts to cluster around \( \theta \approx \frac{1}{4} \pi \), while new contacts should cluster around \( \theta \approx \frac{3}{4} \pi \).

In Fig. 2.6 we show the resulting radial distribution function \( \rho(\theta) \) for broken and created contacts. We indeed observe the majority of making events have \( \frac{1}{2} \pi \leq \theta < \pi \), while the majority of breaking events have \( 0 \leq \theta < \frac{1}{2} \pi \). This shows that anisotropy is relevant already at the first contact change.
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|        | $\gamma \uparrow \text{bk}$ | $\gamma \uparrow \text{mk}$ | total | Pr($\gamma \uparrow \text{bk} | \cdot$) |
|--------|-------------------------------|-------------------------------|-------|---------------------------|
| $\gamma \downarrow \text{bk}$ | 412                           | 239                           | 651   | 0.63                       |
| $\gamma \downarrow \text{mk}$ | 198                           | 129                           | 327   | 0.61                       |
| total  | 610                           | 368                           | 978   |                            |

Table 2.1: Relative prevalence of making and breaking under forward and backward shear strain for $N = 256$, $P = 10^{-3}$.

*Anisotropy in making and breaking.* Finally, we investigated whether the type of contact change and the direction of shear are correlated: If we break a contact when we shear a packing in the forwards direction, are we more likely to *make* a contact when we shear in the *backwards* direction, and vice versa? To test this, we have determined the prevalence for making and breaking under forward ($\gamma \uparrow$) and backward ($\gamma \downarrow$) shear for an ensemble of 978 packings at $N = 256$ and $P = 10^{-3}$. In Table 2.1, we show counts of the four possible combinations of making and breaking under forward and backward shear. Our data supports the notion that the type of contact changes in one shear direction is uncorrelated to the type in the other direction. For example, $\Pr(\gamma \uparrow \text{bk} | \gamma \downarrow \text{bk}) \approx \Pr(\gamma \uparrow \text{bk} | \gamma \downarrow \text{mk}) \approx 0.62$.

More formally, we calculated the Pearson’s chi-square statistic,

$$
\chi^2 = \sum \frac{(O - E)^2}{E}
$$

(2.20)

where the sum runs over all four observations $O$, and $E$ is the expected number of observations in the case of independence, e.g.,

$$
O_{\text{bk,bk}} = 412 ,
$$

(2.21)

$$
E_{\text{bk,bk}} = 978 \cdot \Pr(\gamma \uparrow \text{bk}) \cdot \Pr(\gamma \downarrow \text{bk}) = 406.0 ,
$$

(2.22)

and find $\chi^2 = 0.689$. The cutoff typically used for significant deviations ($p = 0.05$, 1 degree of freedom) is $\chi^2 > \chi^2_{0.05} = 3.841$. We find $\chi^2 \ll \chi^2_{0.05}$, supporting our observation of independence.

#### 2.3.2 Strain Distributions

We will now take a more detailed look at the distribution of the strain at the first contact change, to show that contact changes can essentially be
described as a Poisson process. For large systems, the shape of the CDF closely resembles that of an exponential distribution, whose CDF is given by

\[
\Pr(\gamma_* \leq \gamma) = \begin{cases} 
1 - e^{-\gamma/\beta} & (\gamma \geq 0), \\
0 & (\gamma < 0), 
\end{cases}
\]

(2.23)

where \(\beta\) is the mean of the distribution. To emphasize the resemblance between our numerical distributions and the exponential distribution, we show complementary CDFs (tail distributions) of \(\gamma_*\), rescaled by the ensemble mean \(\langle \gamma_* \rangle\), i.e. \(\Pr(\gamma_* \geq k \cdot \langle \gamma_* \rangle)\). For an exponential distribution, the CCDF is thus given by

\[
\Pr(\gamma_* > k \cdot \langle \gamma_* \rangle) = e^{-k} \quad (k \geq 0),
\]

(2.24)
In Fig. 2.7(a) we plot the rescaled CCDFs for an exponential distribution (dotted black curve) and for our simulation data (colored curves), and we find our data indeed closely corresponds to an exponential distribution.

As a formal means of checking conformance to an exponential distribution, we used the Anderson-Darling test [88, §1.3.5.14], with which we test the hypothesis "these values of $\gamma_*$ were drawn from an exponential distribution". We use a 5% confidence interval, i.e., there is a 5% probability we reject the hypothesis for samples that were drawn from an exponential distribution.

In Fig. 2.7(b), we graphically show the results of the test. For $N = 256$, we observe the distributions at $P \geq 10^{-5}$ are indistinguishable from an exponential distribution. This is consistent with a Poisson process, where contact changes are independent of each other.

Nevertheless, we observe deviations for small systems and low pressures. This is not surprising: it seems unlikely for contact changes to be independent of each other if there are only a limited number of contacts. The boundary between rejection and non-rejection corresponds to the transition to extended systems for $N^2 P \log_{10}(N)^{-0.7} > 1$ [28, 34], indicated with a blue curve (§ 2.3.3).

Note that the $N^2 P \log_{10}(N)^{-0.7} < 1$ region also includes many ensembles where the hypothesis is not rejected. This does not, however, imply the data set has been drawn from an exponential distribution; it merely indicates the data is indistinguishable from a set drawn from an exponential distribution. In these cases, we are dealing with small sample sizes ($\leq 100$ samples), which makes it hard to distinguish the measured distribution from that of an exponential distribution.

For larger sample sizes, this explanation is no longer satisfactory, and taking the underlying distribution to be exponential is a more reasonable interpretation. We observe that large ensembles where the hypothesis was not rejected all have $N^2 P \log_{10}(N)^{-0.7} \gg 1$. We conclude that the transition to extended systems also governs where the distribution of $\gamma_{cc}$ is well-described by an exponential distribution and, therefore, where the contact breaking is a Poisson process.

We can now inspect what kind of distribution describes small systems at low pressures. In Fig. 2.8(a), we show rescaled CCDFs for $N = 16$ systems at various pressures, and notice clear deviations from exponential. The most significant deviation is at low $k$, where we find $\Pr(\gamma_* > k \cdot \langle \gamma_* \rangle)$ is
As an alternative to an exponential distribution, we fit a Weibull distribution to our data. Whereas the exponential distribution describes the amount of strain before failure if the failure rate $h$ (number of events per unit strain) is constant, the Weibull distribution describes the strain before failure if the failure rate depends on the applied strain as $h \sim \gamma^{c-1}$. The CDF of the distribution is given by

$$\Pr(\gamma_s \leq \gamma) = \begin{cases} 1 - e^{(-\gamma/\lambda)^c} & (\gamma \geq 0), \\ 0 & (\gamma < 0), \end{cases} \quad (2.25)$$

where $\lambda$ determines the scale, and $c$ the shape of the distribution. The mean is given by $\langle \gamma_s \rangle = \lambda \Gamma(1 + 1/c)$ [89], where $\Gamma$ is the gamma function. The
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The rescaled complementary distribution is thus given by

\[ \Pr(\gamma > k \cdot \langle \gamma \rangle) = e^{\left(-k/\Gamma(1+1/c)\right)^c} \quad (k \geq 0). \]  

(2.26)

Using maximum likelihood estimation, we fit our data to a Weibull distribution, and find \( c \approx 1.2 \) for \( P \leq 10^{-3} \). In Fig. 2.8(a), we find this gives a much better fit to the data than an exponential distribution. To interpret this, when \( c > 1 \), the distribution is skewed to higher values of \( k \), as the failure rate \( h \sim k^{c-1} \) increases with \( k \). We find relatively few values at low \( k \) and relatively many values at high \( k \) — hence events at small strain are suppressed.

### 2.3.3 Scaling

We now discuss the variation of the mean contact change strain \( \gamma_{cc} = \langle \gamma_+ \rangle \) with \( N \) and \( P \). Even when the distributions are not purely exponential, their mean is well-defined. We have also seen that \( \gamma_{cc} \) depends on \( P \). What kind of scaling for \( \gamma_{cc} \) with \( N \) and \( P \) should we expect?

In Fig. 2.9, we show \( \gamma_{cc} \) as function of both pressure and system size. The data suggests that there are two regimes: one where \( \gamma_{cc} \) depends solely on pressure and not on packing size, and a second regime where \( \gamma_{cc} \)
Figure 2.10: Excess number of contacts $N_{\text{exc}} = N\Delta z/2$ as a function of $N^2P$ (blue curve, based on [28, 33, 34]). Arrows indicate volumetric strains corresponding to a single contact change.

depends on both. We observe $\gamma_{cc}$ increases with pressure in both regimes, but decreases with increasing packing size in the second regime. This is not unexpected: contacts are easier to break if the confining pressure is small, and if there are more contacts, you are more likely to encounter a single weak contact.

In the following subsections, we will introduce two closely related scaling arguments, which both lead to the same prediction for the relation between $\gamma_s$ and $N$ and $P$: a direct argument for compressive strain and a stress-based argument for shear strain. We will then compare the predicted scalings to our computational data.

Compression. We start with a compressional argument, based on estimating the strain scale for making and breaking a contact under compression. There is a clear relationship between compression and the number of contacts: we gain contacts if we compress the system and we lose contacts if we expand the system. The scaling that relates the excess contact number $N_{\text{exc}} = \Delta z/2$ to $N$ and $P$ is well-known from earlier work [28, 33, 34], and is shown in Fig. 2.10. There are two branches: a plateau $N_{\text{exc}} \sim 1$ at low
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pressures and a square root pressure dependence $N_{\text{exc}} \sim \sqrt{N^2P}$ at higher pressures.

How far do we need to expand or compress a system at given $N$ and $P$ to induce a contact change? In the high-pressure regime, we can take the derivative $\pm \frac{\partial}{\partial P} \left( \sqrt{N^2P} \right) \sim \pm N/\sqrt{P}$, which gives us the number of contacts changed due to unit pressure change. Its inverse, $\delta P \sim \pm \sqrt{P}/N$, then gives us the pressure change needed for a single contact change. The compressional strain is the pressure change divided by the bulk modulus $K$: $\varepsilon_{cc} \sim \pm \delta P/K$. As $K$ is independent of $N$ and $P$ [21], we simply find $\varepsilon_{cc} \sim \pm \sqrt{P}/N$.

In the low-pressure finite size regime, the number of contacts is independent of pressure. Can we then still determine the pressure change required for a contact change? We can, because the plateau has a finite length. On the one hand, the plateau ends at $P = 0$, as we unjam our system and lose all contacts. On the other hand, the plateau ends when we enter the large system size regime at $N^2P \sim 1$ and gain one new contact.

The scales for making and breaking a contact are thus no longer the same in the finite size regime: To break a contact, we unjam the system by reducing the pressure with $\delta P \sim P$, and we find $\varepsilon_{bk} \sim -P$. To create a contact, we increase pressure up to the beginning of the large system regime, at $P_{\text{target}} = 1/N^2$. As we are initially in the small system regime, the current pressure $P \ll 1/N^2$ and can be neglected, and the pressure change $\delta P = P_{\text{target}} - P \approx -1/N^2$. We thus need to apply a strain $\varepsilon_{mk} \sim -1/N^2$. The contact *change* strain will be given by the minimum of the absolute making and breaking strains. As $P \ll 1/N^2$, we thus expect $\varepsilon_{cc} \sim P$.

Summarized, this argument leads to these characteristic strains for contact changes under compression:

$$
\varepsilon \sim \begin{cases} 
\varepsilon_{bk} & \varepsilon_{mk} & \varepsilon_{cc} \\
-P & 1/N^2 & P \\
-\sqrt{P}/N & \sqrt{P}/N & \sqrt{P}/N 
\end{cases} \text{ for } N^2P \ll 1, \\
\text{for } N^2P \gg 1.
$$

As we will see, arguments based on shear, as well as our numerical results, find the same scaling for these strains.

**Shear.** We can also formulate an argument for the scaling of $\gamma_{cc}$ under *shear* from dimensional analysis. Other than taking $\gamma_{cc}$ constant, there is no clear
strain scale, so we will construct the argument using stress instead. We will start by determining the mean contact change stress in an ensemble, $\sigma_{cc} = \langle \sigma_* \rangle$.

There are three stress scales in the system: the confining pressure $P$, the bulk modulus $K$ and the shear modulus $G$. As we are describing shear, it seems unlikely that $K$ is relevant. If the mean stress $\sigma_{cc}$ would scale with $G$, we would end up with a constant strain, and we have already seen that $\gamma_{cc}$ is not constant. This suggests that the only relevant stress scale is the confining pressure $P$, so we will take $\sigma_{cc} \sim P$.

The stress scale will also depend on the system size. Say we have a packing with $N$ particles, which has a contact change at $\sigma = \sigma_{cc}$. If we duplicate this system, we will have $2N$ particles, and two contact changes will have happened at the same stress $\sigma_{cc}$, so we expect that $\sigma_{cc} \sim 1/N$.

Combining these two scalings suggests the following scaling:

$$\sigma_{cc} \sim P/N,$$  \hspace{1cm} (2.28)

which is not strongly inconsistent with our data (Fig. 2.11). Next, we determine the strain scale $\gamma_{cc}$ via the shear modulus $G = \sigma/\gamma$. From earlier

---

**Figure 2.11**: $\sigma_{cc} = \langle \sigma_* \rangle$ as a function of $P/N$. Colors and symbols indicate system size. The data supports an overall scaling $\sigma_{cc} \sim P/N$, but the lack of a good collapse suggests this does not describe the entire behavior.
2.3. Numerical results

Figure 2.12: (a) Scaling of the strain at first contact change $\gamma_{cc}$ as function of $N$ and $P$. Symbols and colors indicate packing sizes. Lines indicate power law functions with exponent 1 (lower branch) and 0.5 (upper branch). (b) Log corrections improve the collapse.

work [22, 33, 34], we know $G$ scales as

$$G \sim \begin{cases} \sqrt{P} & \text{for } N^2 P \gg 1, \\ 1/N & \text{for } N^2 P \ll 1, \end{cases}$$

(2.29)

which, combined with the stress scaling we derived, suggests the following scaling for $\gamma_{cc}$:

$$\gamma_{cc} \sim \sigma_{cc}/G \sim \begin{cases} (P/N)/\sqrt{P} & \sim \sqrt{P}/N \quad \text{for } N^2 P \gg 1, \\ (P/N)/(1/N) & \sim P \quad \text{for } N^2 P \ll 1. \end{cases}$$

(2.30)

This argument does not distinguish between making and breaking contacts. The choice of $P$ as stress scale is consistent with the breaking of contacts, as the overlap $\delta \sim P$. When we compare the scaling to the compressional argument (Eq. (2.27)), we find it is indeed consistent with the breaking case, but not with the making case. Nonetheless, the argument is still consistent with the overall scaling, because the behavior is dominated by breaking contacts.
**Contact changes of sheared systems**

Numerical results. We can now compare our numerical results to the scaling relationship predicted by the arguments given above. We will initially not distinguish between the making and breaking of contacts because making events become exceedingly rare at low $P$, leading to poor statistics. In § 2.4.3, we will use linear response to take a more detailed look at the different types of events, including the difference between the making and breaking of contacts.

The suggested scaling in Eq. (2.30) implies that plotting $N^2 \gamma_{cc}$ as a function of $N^2 P$ should collapse all numerical data:

$$N^2 \gamma_{cc} \sim \begin{cases} \sqrt{N^2 P} = (N^2 P)^{0.5} & \text{for } N^2 P \gg 1, \\ N^2 P = (N^2 P)^1 & \text{for } N^2 P \ll 1. \end{cases} \quad (2.31)$$

We have plotted our numerical results in Fig. 2.12(a) and get a good (but not great) collapse. We retrieve the expected scaling behavior from Eq. (2.31), but we still find a minor dependence on system size. It has been suggested that the upper critical dimension for jamming is two, which implies logarithmic corrections in system size [28]. Using the form suggested in [28], we find a very good collapse (Fig. 2.12(b)). Consistently with what was recently found for the contact number and for the elastic moduli [28], also contact making and breaking under shear follows finite size scaling, with two distinct scaling regimes.

### 2.4 Linear response

We will now show that many properties of the first contact change can be deduced from the rest state at $\gamma = 0$ using linear response. Instead of using a direct numerical simulation (DNS), we estimate the trajectories of (non-rattler) particles from their linear elastic response: $\vec{x}_i(\gamma) = \vec{x}_i(0) + \vec{u}_i(0) \cdot \gamma$, where $\vec{u}_i(0) = [\partial \vec{x}_i / \partial \gamma](0)$ is calculated directly from the rest state. This strategy not only allows us to obtain the correct strains for the first contact change, but also gives us insight into the microscopic mechanisms. In particular, linear response allows us to probe the closing of contacts in detail, which is difficult in DNS simulations since, at low $N^2 P$, it becomes exceedingly rare for the first contact change to be a contact making event (Figs. 2.5(b) and 2.17(b)).
Why are we allowed to assume that the response remains linear up to the first contact change? In essence, we will show that the nonlinear behavior of jammed packings emerges due to the cumulative effects of many contact changes. In contrast, between contact changes, the stress-strain response is essentially linear (§ 2.4.1). After calculating the linear response for our systems (§ 2.4.2), we will show that it predicts the contact change strains with surprising accuracy (§ 2.4.3): Linear response predicts its own demise! Finally, we investigate the breaking and closing of contacts independently (§ 2.4.4) and find that their characteristic strains scale differently. From these strains, we then accurately predict how often the first contact change is a contact making event in the DNS simulations.

2.4.1 Stress response

First, we will show that the stress-strain response of our systems is essentially linear in the DNS simulations. From the simulations, we find the shear stress $\sigma(\gamma)$ at various strains before the first contact change (Fig. 2.13(a)). We then fit this response with a second-order polynomial $\sigma = G_{\text{fit}} \gamma + \lambda \gamma^2$, and quantify the relative contribution of the quadratic component.

We quantify the contribution by calculating the ratio between the quadratic and linear contributions to $\sigma$ at the contact change strain $\gamma^*_c$:

$$Q = \left| \frac{\lambda \gamma^*_c}{G_{\text{fit}} \gamma^*_c} \right| = \left| \frac{\lambda \gamma^*_c}{G_{\text{fit}} \gamma^*_c} \right|. \quad (2.32)$$

For the typical example in Fig. 2.13(a), we find $Q = 0.014$. We also show an extreme example with $Q = 0.267$ in Fig. 2.13(b). In Fig. 2.13(c), we have plotted the CDF of $Q$ for four ensembles. We find the largest deviations from linear response for small systems at high pressure ($N = 16, P = 10^{-2}$), but even there the quadratic term is small compared to the linear term, with $\langle Q \rangle = 1.4 \cdot 10^{-2}$.

In Fig. 2.14(a), we plot $Q$ as function of $N$ and $P$. The most important observation is that $Q$ remains small: in the vast majority of cases, $Q < 10^{-3}$, and the nonlinear case shown in Fig. 2.13(b) is truly exceptional. The two regions where $Q$ appears to be the largest are for small $N$ and large $P$, and for large $N$ and small $P$. The origins for these deviations are different. For large systems at low pressure, the larger deviation is caused by inherent nonlinearities in the system, as indicated by the high median squared
Contact changes of sheared systems

**Figure 2.13**: Stress response for (a) a packing with a typical deviation from linear $Q = 0.014$ and (b) a packing with a very large deviation $Q = 0.267$ (both $N = 16, P = 10^{-2}$). The simulation data (red ×) is fitted with the second-order polynomial (blue solid curves) $\sigma = G^{\text{fit}} \gamma + \lambda \gamma^2$, from which we determine $Q = |\lambda \gamma^* / G^{\text{fit}}|$. The black dotted curves are the linear contribution $\sigma = G^{\text{fit}} \gamma$; the green dash-dotted curves are the linear response predictions $\sigma = G^{\text{LR}} \gamma$. The gray vertical lines indicate the strain at the first contact change $\gamma^*$. (c) CDF of $Q$ for various ensembles. There is no clear trend with either $N$ or $P$. For the curve with largest mean ($N = 16, P = 10^{-2}$), we find that the mean $\langle Q \rangle = 1.4 \cdot 10^{-2}$ and standard deviation $s_Q = 2.8 \cdot 10^{-2}$ are both much smaller than 1 — hence linear response captures the majority of stress-strain curves very well.

Quadratic component $[\lambda^2]_{0.5}$ of the stress-strain relation (Fig. 2.14(b)), where we use the median due to the large influence of outliers on the mean $\langle \lambda^2 \rangle$. Small systems at high pressures exhibit a small quadratic component, but due to the larger strains involved, the deviation from linear response becomes significant in this regime. Nevertheless, the quadratic contribution to the stress is always small compared to the linear contribution, and we therefore expect to be able to predict the response of the system directly from linear response.
2.4. LINEAR RESPONSE

**Figure 2.14:** (a) Mean deviation from linear response at the first contact change for different ensembles. Strains are very well described by linear response for small systems at low pressures. Significant deviations only occur for small systems at high pressures and large systems at low pressures. (b) Median squared quadratic component $[\lambda^2]_{0.5}$. The component is of the order $10^{-2}$ in most cases, but grows to $10^2$ for large systems at low pressure (close to jamming).
2.4.2 Calculating the linear response

In this section we will briefly review how, based on the initial particle positions, box size and box shape, we determine the linear response of the system. Given an applied deformation of the box, we can determine the resulting particle motion, forces and energy cost [21, 24, 28, 30, 34].

The state of the system can be described as a vector

\[
|q\rangle = |q_x, q_b\rangle = \{x_1 \ldots x_N, y_1 \ldots y_N\}, \{L_{xx}, L_{xy}, L_{yx}, L_{yy}\}
\]  

(2.33)

where \((x_i, y_i)\) is the position of particle \(i\) and the four parameters \(L_{ab}\) describe the box size and shape. We only include particles that are part of the load bearing network (non-rattlers).

We then prescribe a displacement \(|\Delta q\rangle\). We determine the energy in the new state \(|q + \Delta q\rangle\) by expanding \(U\) up to second order:

\[
U(|q + \Delta q\rangle) = U(|q\rangle) + \langle J_q | \Delta q \rangle + \frac{1}{2} \langle \Delta q | H_q | \Delta q \rangle + O(\Delta q^3)
\]  

(2.34)

where

\[
\langle J_q \rangle = \langle \frac{\partial U}{\partial x_1}, \ldots, \frac{\partial U}{\partial L_{yy}} \rangle
\]

(2.35)

is the Jacobian and

\[
H_q = \left(\begin{array}{ccc}
\frac{\partial^2 U}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 U}{\partial x_1 \partial L_{yy}} \\
\vdots & \ddots & \vdots \\
\frac{\partial^2 U}{\partial x_N \partial L_{yy}} & \cdots & \frac{\partial^2 U}{\partial L_{yy}^2}
\end{array}\right)
\]

(2.36)

the extended Hessian at state \(|q\rangle\) [24, 34, 90]. Because the initial state is at an energy minimum, the Jacobian term is zero, and the leading contribution to the energy is quadratic and comes from the extended Hessian.

For a given displacement, the energy cost is thus given by

\[
\Delta U = \frac{1}{2} \langle \Delta q | H_q | \Delta q \rangle ,
\]

(2.37)

and the resulting forces on particles and boundaries are

\[
|f\rangle = H_q |\Delta q\rangle .
\]

(2.38)

Typically, however, we do not know the displacement of each particle. Instead, we wish to calculate the displacement of the particles given a
change in the boundaries, i.e., find a state where, given the new boundaries, the sum of forces on each particle is zero. To find this state, we split the extended Hessian into four parts:

\[
H = \begin{pmatrix} H_{xx} & H_{bx}^T \\ H_{bx} & H_{bb} \end{pmatrix},
\]

where the ordinary Hessian \(H_{xx}\) describes the particle-particle interactions, \(H_{bx}\) the interactions between boundaries and particles, and \(H_{bb}\) those between different boundaries. We can then rewrite Eq. (2.38) as follows:

\[
\begin{pmatrix} |\Delta f_x\rangle \\ |\Delta f_b\rangle \end{pmatrix} = \begin{pmatrix} H_{xx} & H_{bx} \\ H_{bx} & H_{bb} \end{pmatrix} \begin{pmatrix} |\Delta q_x\rangle \\ |\Delta q_b\rangle \end{pmatrix}.
\]

where \(|\Delta q_x\rangle\) and \(|\Delta q_b\rangle\) are the displacements of particles and boundaries, and \(|\Delta f_x\rangle\) and \(|\Delta f_b\rangle\) the corresponding forces. Setting the forces on the particles to zero, we find

\[
|\Delta f_x\rangle = H_{xx} |\Delta q_x\rangle + H_{bx}^T |\Delta q_b\rangle = 0.
\]

Solving for \(|\Delta q_x\rangle\) gives us particle displacements as a function of the deformation of the simulation box

\[
|\Delta q_x\rangle = -H_{xx}^{-1} H_{bx}^T |\Delta q_b\rangle.
\]

Unfortunately, \(H_{xx}^{-1}\) cannot be calculated due to the two zero-energy translational modes. Instead, we choose to use the Moore-Penrose pseudoinverse \(H_{xx}^+\), which fixes the zero-energy translational modes in place [91, §6.4]:

\[
|\Delta q_x\rangle = -H_{xx}^+ H_{bx}^T |\Delta q_b\rangle.
\]

The full displacement vector is then given by

\[
|\Delta q\rangle = \begin{pmatrix} -H_{xx}^+ H_{bx}^T |\Delta q_b\rangle \\ |\Delta q_b\rangle \end{pmatrix}.
\]

To calculate the energy cost and the stress on the boundary, we use Eq. (2.40), and find

\[
|\Delta f_b\rangle = H_{bx} |\Delta q_x\rangle + H_{bb} |\Delta q_b\rangle = (H_{bb} - H_{bx} H_{xx}^+ H_{bx}^T) |\Delta q_b\rangle.
\]
The corresponding stress can be calculated as

$$|\Delta \sigma_b\rangle = \left| \frac{\Delta f_{xx}}{L_{xx}}, \frac{\Delta f_{xy}}{L_{xy}}, \frac{\Delta f_{yx}}{L_{yx}}, \frac{\Delta f_{yy}}{L_{yy}} \right|,$$

but in practice, it is more convenient to calculate the stress by using the Born-Huang approximation (Eq. (2.13)) on the new particle positions $|q'_x\rangle = |q_x\rangle + |\Delta q_x\rangle$. The stress also allows us to determine the elastic modulus corresponding to a given boundary deformation

$$c_q = \frac{\langle \Delta \sigma_b | \Delta q_b \rangle}{\langle \Delta q_b | \Delta q_b \rangle}.$$

For the resulting energy change we use $|\Delta f_x\rangle \equiv 0$ to find

$$\Delta U = \frac{1}{2} \langle \Delta q_b | \Delta f_b \rangle = \frac{1}{2} \langle \Delta q_b | (H_{bb} - H_{bx} H_{xx}^+ H_{bx}^T) | \Delta q_b \rangle.$$

We now have all ingredients in place to calculate, for a given boundary deformation, the particle displacements, stress response and energy change from linear response. In the next section, we will use this to calculate the strain at the first contact change.

### 2.4.3 Contact change strains

In this section, we will describe how we calculate the contact change strains from linear response, and we will compare their values to the results from
direct numerical simulations. First, for each particle pair $i,j$, we determine the contact change strain $\gamma_{ij}$, defined as the strain where the particles, assuming linear trajectories, break contact or make a new contact. By minimizing over all strains, we then calculate (i) the strain at which the first new contact is made $\gamma_{*,mk}^{LR}$, (ii) the strain at which the first contact breaks $\gamma_{*,bk}^{LR}$, and (iii) the strain at the first contact change $\gamma_{*}^{LR}$, which is the minimum of $\gamma_{*,mk}^{LR}$ and $\gamma_{*,bk}^{LR}$. We can then, for each packing, compare these values of the strain to their counterparts obtained by simulation.

Calculating $\gamma_{*}^{LR}$. For each particle pair $i,j$, we determine the velocity

$$\vec{u}_i = \vec{\partial x}_i / \partial \gamma . \tag{2.49}$$

by evaluating Eq. (2.43) with the unit simple shear deformation $|\Delta q_b| = L\hat{L}_{xy}$. The inter-particle velocities are then given by

$$\vec{u}_{ij} = \vec{u}_i - \vec{u}_j - n_{y,ij}L\hat{x} , \tag{2.50}$$

where the last term incorporates the velocity between the copies of the periodic box. Combining these, we can solve

$$|\vec{r}_{ij} + \gamma_{ij}\vec{u}_{ij}| = R_i + R_j \tag{2.51}$$

for $\gamma_{ij}$ to determine when the overlap $\delta_{ij} = 0$. There are, in general, two solutions for $\gamma_{ij}$, but only one of them is physically relevant, as indicated in Fig. 2.15(b) and (c): the physically relevant value is the minimal positive strain.

The first contact change for the entire system is then determined by taking the minimum of the strain over all particle pairs $i,j$:

$$\gamma_{*}^{LR} \equiv \min(\gamma_{ij}) . \tag{2.52}$$

We can also limit ourselves to breaking and making strains to determine the first broken and the first new contact independently:

$$\gamma_{*,bk}^{LR} \equiv \min_{i,j \text{ in contact}} \gamma_{ij} , \tag{2.53}$$

$$\gamma_{*,mk}^{LR} \equiv \min_{i,j \text{ not in contact}} \gamma_{ij} . \tag{2.54}$$

This allows us to study closing events directly, which is difficult in DNS simulations due to their rarity at low pressures.
Comparison with numerical simulations. We now show that linear response accurately predicts the contact change strain. For each individual system, we compare the linear response value $\gamma^{LR}_{*}$ to the corresponding strain $\gamma^{DNS}_{*}$ from the DNS simulation. In Fig. 2.16, we plot PDFs of $\gamma^{LR}_{*}/\gamma^{DNS}_{*}$ to quantify the relative deviation from the simulation. We observe that $\gamma^{LR}_{*}$ is a good predictor for $\gamma^{DNS}_{*}$. First, these distributions are peaked around 1, which shows the mean strain found in linear response matches that of the simulations very well. Second, the standard deviation of the distributions, $s$, is of the order of 5% for small systems and 1% for large systems. At $P = 10^{-2}$, the largest packings have a standard deviation of $7 \times 10^{-3}$, which increases to $5 \times 10^{-2}$ for small systems. The largest standard deviation is obtained for very small systems ($N = 16$) at high $P$ ($10^{-2}$). We find a strong dependency on pressure: for $P = 10^{-6}$, the distributions become very narrow around 1. The standard deviations remains on the order of $10^{-2}$ due to outliers. We conclude that for all parameters considered, the differences between the strains obtained by linear response and direct numerical simulation are small. In addition to determining the right contact change strain, we found that in over 90% of
2.4. LINEAR RESPONSE

In conclusion, linear response provides us with a powerful tool to predict the behavior of packings. It allows us to predict the first contact change correctly, as well as determining microscopic properties unavailable in the DNS simulations. We note in passing that the correct prediction of contact changes suggests that shearing jammed packings might also be implemented in terms of a discrete event simulation, where, instead of slowly stepping through strain space, we immediately jump from contact change to contact change.

Rattlers. In § 2.2, we discussed the effect of rattlers in the DNS simulations. We will now focus on their effect in linear response. The creation of a rattler, i.e., a particle losing all its contacts, is also well-defined in linear response. In Fig. 2.4, we show a packing at the verge of creating a rattler (a), and show the overlap $\delta_{ri}$ of particle $r$ with its neighbors $A$, $B$, and $C$ as a function of strain $\gamma$ (b). In the simulations (symbols), we find the overlaps smoothly go to zero while approaching the contact change strain $\gamma_*$. In linear response, we find a slightly different contact change strain for each contact, but they are within $|\Delta \gamma / \gamma_*| < 10^{-4}$. As in § 2.2, we do not include systems where a rattler becomes part of the contact network in our analysis.

2.4.4 Scaling of ensemble averages obtained in linear response

Now that we have established that we can predict contact changes using linear response, we will study the making and closing strains in detail. Based on Eq. (2.27), we expect three scaling regimes for the contact change strains: for low $N^2P$, $\gamma_{mk} \sim 1/N^2$ and $\gamma_{bk} \sim P$, while for high $N^2P$, both $\gamma_{bk}$ and $\gamma_{mk}$ are expected to scale as $\sqrt{P/N^2}$. As before, these scalings suggest scaling collapse if we plot $N^2\gamma$ as a function of $N^2P$:

$$
N^2\gamma \sim \begin{cases} 
N\sqrt{P} = (N^2P)^{0.5} & \text{for } N^2P \gg 1, \\
N^2P = (N^2P)^1 & \text{for } bk, N^2P \ll 1, \\
1 = (N^2P)^0 & \text{for } mk, N^2P \ll 1.
\end{cases}
$$

In Fig. 2.17(a), we plot our linear response data using this rescaling. As in § 2.3.3, applying log corrections [28] improves the collapse (Fig. 2.17(b)).
For low $N^2P$, we find that the data is well described by the expected power laws, but for high $N^2P$, we find that neither branch cleanly scales as $\gamma \sim \sqrt{P}/N$, even though the branches combined do appear to scale that way. The branches slowly converge, and join around $N^2P \sim 10^{-4}$. We expect that for larger systems, for which $N^2P$ can be large while $P$ remains small, the clean square root scaling will be recovered for both branches.

What do these different scalings imply for properties that we can measure in the DNS simulation, specifically for the contact change strain $\gamma_{cc}$ and the prevalence of making versus breaking events? Starting with the exponential CDFs (Eq. (2.23)) for making and breaking,

$$
\Pr(\gamma_{*,mk} \leq \gamma) = 1 - e^{-\gamma/\beta_{mk}} \quad \gamma \geq 0,
$$

$$
\Pr(\gamma_{*,bk} \leq \gamma) = 1 - e^{-\gamma/\beta_{bk}} \quad \gamma \geq 0,
$$

where $\beta$ is the mean value of the distribution, we can derive the CDF for the minimum of the distributions, assuming $\gamma \geq 0$:

$$
\Pr(\min\{\gamma_{*,mk}, \gamma_{*,bk}\} \leq \gamma) = \Pr(\left[\gamma_{*,mk} \leq \gamma\right] \lor \left[\gamma_{*,bk} \leq \gamma\right])
= 1 - e^{-\gamma/\beta_{mk}} e^{-\gamma/\beta_{bk}}
= 1 - e^{-\gamma/\beta_{cc}},
$$

Figure 2.17: (a) Scaling of ensemble averaged breaking (▽) and making (△) strains $\gamma_{bk}^{LR} = \langle \gamma_*^{LR}, bk \rangle$ and $\gamma_{mk}^{LR} = \langle \gamma_*^{LR}, mk \rangle$ from linear response. (b) As in Fig. 2.12, log corrections significantly improve the quality of the collapse.
2.4. Linear response

so the mean contact change strain becomes

$$\beta_{cc} = \frac{1}{1/\beta_{bk} + 1/\beta_{mk}}. \quad (2.59)$$

We can also derive the probabilities of the first change being a breaking or making event. We will derive $\Pr(mk) = 1 - \Pr(bk)$ rather than $\Pr(bk)$, as the former vanishes for $N^2P \to 0$.

$$\Pr(mk)^{LR} = \int_{0}^{\infty} \Pr([\gamma_{*,mk} = \gamma] \land [\gamma_{*,bk} > \gamma]) \, d\gamma$$

$$= \int_{0}^{\infty} \left[ \frac{1}{\beta_{mk}} e^{-\gamma/\beta_{mk}} \cdot \left[ e^{-\gamma/\beta_{bk}} \right] \right] \, d\gamma$$

$$= -\frac{1/\beta_{mk}}{1/\beta_{mk} + 1/\beta_{bk}} e^{-\gamma(1/\beta_{mk}+1/\beta_{bk})} \bigg|_{0}^{\infty}$$

$$= \frac{1}{1 + \beta_{mk}/\beta_{bk}}. \quad (2.60)$$

For $N^2P \gg 1$, we found that in linear response $\beta_{mk} \sim \beta_{bk} \sim \sqrt{P/N^2}$. This means that breaking and making a contact are equally likely, and the mean strain $\beta_{cc}$ is half that of the individual strains. For $N^2P \ll 1$, the behavior is different. In this regime, $\beta_{bk} \ll \beta_{mk}$, so the combined average strain $\beta_{cc}$ is dominated by $\beta_{bk}$:

$$\beta_{cc} \approx \frac{1}{1/\beta_{bk} + 1/\beta_{mk}} \approx \beta_{bk}, \quad (2.61)$$

i.e., the mean contact change strain is given by the mean breaking strain. The probability of making a contact in this regime is much smaller than breaking one:

$$\Pr(mk)^{LR} \sim \frac{1}{1 + \beta_{mk}/\beta_{bk}} \approx \frac{1}{1 + 1/N^2p} \approx N^2P \ll 1. \quad (2.62)$$

In Fig. 2.18(a), we show $\Pr(mk)^{LR}$ as a function of $N^2P$ for each ensemble, and find the derived scaling: $\Pr(mk) \sim N^2P$ for small $N^2P$ and $\Pr(mk) \sim 1/2$ for high $N^2P$. We then fit our data with a simple scaling function to ease comparison with the numerical data.
To compare the results to numerical simulations, we determine the frequentist probability
\[ \Pr(\text{mk})^{\text{DNS}} = \frac{N_{\text{mk}}}{N_{\text{total}}} \cdot \] (2.63)

We then plot this probability against \( N^2P \) in Fig. 2.18(b). To get an error estimate, we model the system as Poissonian [92, A1], and use
\[ s = \sqrt{N(1 - Pr)/N} , \] (2.64)
as standard deviation, where we take \( Pr = \Pr(\text{mk})^{\text{DNS}} \). If \( \Pr(\text{mk})^{\text{DNS}} = 0 \), we take \( Pr = 1/N_{\text{total}} \).

We find the scaling describes our data reasonably well for medium to high \( N^2P \), but at lower \( N^2P \), we find a large number of outliers on a plateau around \( \Pr(\text{mk})^{\text{DNS}} \approx 5 \cdot 10^{-3} \). We propose this deviation is caused by difference in the distributions of \( \gamma_{\text{mk}} \) and \( \gamma_{\text{bk}} \). In Fig. 2.19, we plot the distributions of \( \gamma_{\text{mk}} \) and \( \gamma_{\text{bk}} \). As we have seen in § 2.3.2, the distribution of \( \gamma_{cc} \) deviates from exponential for \( N^2P \ll 1 \), but here we
2.5 Multiple contact changes

In this section, we will discuss the behavior of our systems when strained beyond the first contact change. We will discuss the implications of contact changes for continuum elasticity, and will take a look at the effects of switching from free boundaries at zero strain to fixed boundaries in systems at finite strain.
2.5.1 Shear modulus

As we have seen, the first contact change happens at lower and lower strains as systems get larger. Schreck et al. [76] suggested that this implies that linear response is no longer valid for disordered systems at large $N$. It is clear that changing a single contact can have a large effect on small systems, but one would expect the effect to vanish in larger systems: in the thermodynamic limit, systems are expected to behave increasingly like an elastic solid, and this apparent paradox lead to a lively debate [77, 78, 93].

Here we show how the effect of a single contact change on the shear modulus becomes smaller and smaller when the system size is increased. We note that, as long as the shear modulus does not change significantly, we can consider the system to have an effective linear response, even though it is no longer strictly linear. To quantify the effect of a single contact change, we calculated the shear modulus before ($G_0$) and after ($G_1$) the first contact change.
change using Eq. (2.47). For each value of $N$ and $P$, we have calculated the probability distributions $\rho(G_1/G_0)$. From these, we determine in particular $\Pr(G_1 < 0)$ (Fig. 2.20(a)) and the width of these distributions (Fig. 2.20(c)). We find that the shape of these distributions varies strongly and that we can organize our data using the finite size parameter $N^2 P \log_{10}(N)^{-0.7}$, and as function of this parameter we distinguish three regimes.

(i) $N^2 P \log_{10}(N)^{-0.7} \ll 1$. In the small system size limit, we find that $\rho(G_1/G_0)$ is a strongly asymmetric distribution, with most weight around zero. We find that the mean $\langle G_1/G_0 \rangle \approx 0.2$, and that $0 < G_1 < G_0$. To understand this, we note that in this regime, the first contact change is a breaking event, which weakens the system. We find that $G_1$ is significantly smaller than $G_0$ because, in this regime, there is typically only a single excess contact (Fig. 2.10). Surprisingly, the system does not unjam immediately, for reasons we will discuss in § 2.5.2.

(ii) $N^2 P \log_{10}(N)^{-0.7} \approx 1$. In the intermediate regime, the number of excess contacts remains small, contact changes are predominantly contact breaking events, and we observe that $G_1 < G_0$. However, the probability that $G_1 < 0$ becomes finite, in contrast to the behavior in regime (i). This follows from the variation of forces on the contacts between particles, the prestress: without prestress, $G$ has to be non-negative [28, 94], but as $P$ increases in regime (ii) there is sufficient prestress to allow for negative values of $G_1$, and this happens in up to 35% of cases (Fig. 2.20(b)).

(iii) $N^2 P \log_{10}(N)^{-0.7} \gg 1$. For large systems, we enter the continuum regime, where the distribution $\rho(G_1/G_0)$ peaks around one and becomes increasingly symmetric and narrow. Hence $G_1 \approx G_0$, and this is the essence of the solution of the apparent paradox. The symmetry of the distribution is consistent with our observation that contact creation and contact breaking becomes equally likely in this regime.

Types of events. We observe a strong correlation between the type of events and the behavior of $G_1/G_0$, where, in the vast majority of cases, $G_1 < G_0$ is linked to broken contacts, and $G_1 > G_0$ to created contacts (Fig. 2.20(a)). In a minority of breaking events ($\approx 0.5\%$), we find $G_1 < G_0$, but a close inspection of anomalous events systematically reveals that for these events,
Contact changes of sheared systems

rearrangements happen at very nearby strains, or \( G_1 \approx G_0 \), which suggest that their small probability is a measure of numerical noise, and does not contain significant physics.

**Effective linear response.** A simple scaling argument for the width of the distribution of \( G_1/G_0 \) can be obtained from combining the scaling of \( G \) with \( P, G \sim \Delta z \sim \sqrt{P} \) with the observation that making and breaking of contacts is equally likely. As a single contact change modifies \( \Delta z \) by \( \pm 1/N \), we thus expect \( G_1^\pm \sim \Delta z_0 \pm 1/N \). The width of this distribution scales as

\[
s \sim \frac{G_1^+ - G_1^-}{G_0} \sim \frac{1}{N} \frac{\Delta z_0}{\sqrt{P}} = \frac{1}{\sqrt{N^2 P}}.
\]  

(2.65)

However, when we measure the width of the distribution using the standard deviation \( s \), we observe it vanishes as \((N^2 P \log_{10} N)^{-0.7}\) with \( \beta = 0.35 \pm 0.01 \) (Fig. 2.20(c)). We suggest that the contacts changed under a shear deformation have a relatively large impact on the shear modulus - a relatively small number of contacts contribute disproportionately to the elastic moduli [95].

Nevertheless, the observed diminishing of the width of the distribution \( \rho(G_1/G_0) \) is sufficiently strong to be consistent with an effective linear response picture. We call a material **effectively linear** if, for a small fixed deformation \( \gamma_t \), the standard deviation of \( G(\gamma_t) \) vanishes for \( N \to \infty \). In terms of contact changes, we need to establish how the number of contact changes experienced up to \( \gamma_t \) grows with \( N \), and how the effect of a single contact change decreases with \( N \). We estimate the number of contact changes between \( \gamma = 0 \) and the test strain \( \gamma_t \) as

\[
n = \frac{\gamma_t}{\gamma_{cc}} = \frac{\gamma_t}{(\sqrt{P}/N)}.
\]  

(2.66)

We then assume that all contact changes are independent of each other, and assume each contact change causes a change in \( G \) drawn from the distribution \( \rho(G_1/G_0) \) with standard deviation \( s \sim (N^2 P)^{-\beta} \). The central limit theorem then states that the standard deviation after \( n \) contact changes is given by

\[
s_n \sim \sqrt{n(N^2 P)^{-\beta}}.
\]  

(2.67)
2.5. Multiple contact changes

Figure 2.21: The number of contacts for systems with \( N = 16 \) particles at \( P = 10^{-6} \). The circle area represents the fraction of systems with a given number of contacts; the thickness of the lines represent transition probabilities. Initially, the systems start off with the minimum number of contacts \( 2N + 1 = 33 \) (31 or 29 when there are one or two rattlers, respectively). In the first and second contact change, the system loses one contact (three when a rattler is created). In the following events, the system alternately gains and loses a contact.

Combining these, we find that the standard deviation after a strain \( \gamma_t \) is given by

\[
s_{\gamma_t} \sim \sqrt{\gamma_t / (\sqrt{P} / N)} \left( N^2 P \right)^{-\beta} \sim \sqrt{\gamma_t} \cdot N^{\frac{1}{2} - 2\beta} P^{-\frac{1}{4} - \beta},
\]

which vanishes for large \( N \) as long as \( \frac{1}{2} - 2\beta < 0 \), or

\[
\beta > 1/4.
\]

Clearly, 0.35 > 1/4, so, for \( N \to \infty \), our systems approach the continuum limit. This is consistent with the picture where, for large \( N \), the effective value of \( G \) depends on the applied shear \( \gamma \) rather than the number of contact changes \( n \) [96, 97].

2.5.2 Alternating contact changes

Here, we investigate correlations between consecutive contact changes. In Fig. 2.21, we show the number of contacts in the system as a function...
CONTACT CHANGES OF SHEARED SYSTEMS

of the number of contact changes for systems with \( N = 16 \) particles, at \( P = 10^{-6} \). Initially, systems have \( 2N + 1 \) contacts, i.e., 33 if all particles are part of the contact network, 31 if there is one rattler and 29 if there are two rattlers. Surprisingly, we observe the first two contact changes are breaking events, bringing the contact number to \( 2N - 1 \). The system then alternately gains and loses a contact, switching between \( 2N - 1 \) and \( 2N \) contacts. This behavior stays apparent at least until the 10th contact change. This evidences correlations between subsequent events. In addition, we note that the same contact is often involved in multiple contact changes, although typically not in subsequent contact changes.

The subtle role of boundary conditions. One question this poses is why the system is allowed to lose contacts in the first place: after all, we are on the brink of losing rigidity, and a single broken contact should unjam the system. However, that does not take into account the change in boundary conditions between the initial relaxation and the strained state. In the initial relaxation, we require

\[
F_x = F_y = 0 \tag{2.70}
\]

for all particles, and

\[
\sigma_{yx} = \sigma_{xy} = 0 , \quad \tau = \frac{1}{2}(\sigma_{xx} - \sigma_{yy}) = 0 , \quad P_{\text{int}} = \frac{1}{2}(\sigma_{xx} + \sigma_{yy}) = P_{\text{ext}} , \tag{2.71}
\]

for the boundaries. This gives us \( 2N + 3 \) degrees of freedom. Two of these degrees are constrained by requiring zero global translation, and the other \( 2N + 1 \) need to be constrained by at least \( N_c = 2N + 1 \) contacts between particles to be jammed [28, 33]. When we strain the system, this changes. Instead of requiring a fixed stress on the boundaries, we require a fixed deformation

\[
L_{yx}(\gamma) = L_{yx}(0) + \gamma \cdot L(0) , \tag{2.72}
\]
\[
L_{xx}(\gamma) = L_{xx}(0) , \quad \text{and} \tag{2.73}
\]
\[
L_{yy}(\gamma) = L_{yy}(0) . \tag{2.74}
\]

Of the initial \( 2N + 3 \) degrees of freedom, we now only have \( 2N \) left, which means we need just \( 2N - 2 \) contacts for stability: our system is suddenly
overconstrained, and we expect we need to break *four* contacts to unjam. Surprisingly, we find that the system only loses *two* contacts before gaining a new contact, and that diving below $2N - 1$ contacts already unjams the system.
CONTACT CHANGES OF SHEARED SYSTEMS

\[ N^1.8 \gamma \sim P^1.6 \ldots 2.0 \text{ (vertical)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (blue border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (green border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (red border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (black border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (white border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (yellow border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (orange border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (pink border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (brown border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (light gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (medium gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (dark gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (black border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (white border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (yellow border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (orange border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (pink border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (brown border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (light gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (medium gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (dark gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (black border)} \]

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\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (pink border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (brown border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (light gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (medium gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (dark gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (black border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (white border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (yellow border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (orange border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (pink border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (brown border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (light gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (medium gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (dark gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (black border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (white border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (yellow border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (orange border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (pink border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (brown border)} \]

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\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (light gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (medium gray border)} \]

\[ N^1.8 \gamma \sim (d_{N \gamma})^{1.6} \text{ (dark gray border)} \]
2.6 Alternative scaling models

In this section, we will discuss our findings in the light of alternative scaling approaches that have surfaced in the literature recently. First, we will investigate how accurately we can determine the power laws via scaling collapse of our data, and will compare the log corrections we applied in § 2.3.3 to power law corrections. Then, we will compare our results to work on contact changes in closely related model systems. Schreck et al. [76] have investigated nonlinearities in jammed packings at finite temperature, and found a different scaling law for the onset of contact changes that we attribute to their averaging over modes. Combe and Roux [79] and Lerner et al. [80] have approached the problem from a hard particle perspective, and found a scaling law very close to the behavior we find close to jamming. Finally, we will approach the problem from a statistical perspective. Starting from the distribution of $\gamma^*_c$ of all contacts in all packings, we apply extreme value analysis to find the expected mean first contact change. We find that this does not yield a good prediction for the measured value, and determine that this cannot be explained by a few weak contacts, but rather points to correlations involving the whole system — i.e., the statistics of the first $n$ contact changes in a system are different from the statistics of the first contact change in $n$ systems.

Best collapse. Before describing the scaling functions found in other work, we will first investigate the range of scaling functions that gives an acceptable match to our data.

In § 2.3.3, we provided two arguments that predict the following scaling for the first contact change strain $\gamma_{cc}$:

$$N^2\gamma_{cc} \sim F\left(N^2P\right)$$  \hspace{1cm} (2.75)

where $F(x) \sim x$ for small $N^2P$ and $F(x) \sim x^{0.5}$ for large $N^2P$. In the same section, we have seen the results from the simulation collapse when plotted on these axes. Furthermore, we have seen that the collapse improves significantly by using the log correction

$$N^2\gamma_{cc} \sim F\left(N^2P \log_{10}(N)^{-0.7}\right),$$  \hspace{1cm} (2.76)

with the same $F(x)$. 

First, we investigate for which exponents in $N$ the collapse, without the log correction, is satisfactory, i.e., for what values of $q$ and $r$ does

$$N^q \gamma_{\text{cc}} \sim F(N^r P)$$

(2.77)

give an acceptable collapse? To make this quantitative, we measure the running maximum $M$ (starting at low $N^r P$) and the running minimum $m$ (starting at high $N^r P$), and calculate the effective area between the curves

$$\aleph = \int \left[ \log_{10}(M(N^r P)) - \log_{10}(m(N^r P)) \right] d \log_{10}(N^r P),$$

(2.78)

where

$$M(x) = \max(N^q \gamma_{\text{cc}}|N^r P \leq x),$$

(2.79)

$$m(x) = \min(N^q \gamma_{\text{cc}}|N^r P > x).$$

(2.80)

In Fig. 2.22, we show collapse plots for $q = 1.8 \ldots 2.2$ and $r = 1.6 \ldots 2.0$. We observe that all plots with

$$r \leq q \leq r + 0.4$$

(2.81)

are reasonable ($\aleph \lesssim 1$), and that $N^2 \gamma \sim F(N^{1.8} P)$ has the best overall scaling collapse ($\aleph = 0.32$). Our log-corrected collapse is very close to this, with $\aleph = 0.37$.

Second, we can wonder about the correct asymptotic behavior of $F(x)$. To find this behavior, we fit $F(x) = C \cdot x^\beta$ separately for both the upper ($N^{1.8} P > 10$) and lower ($N^{1.8} P < 0.1$) branches (Fig. 2.23(a)), and find

$$F(x) = \begin{cases} 
(1.7 \pm 0.1) \cdot x^{0.50 \pm 0.01} & (x \ll 1) \\
(2.7 \pm 0.3) \cdot x^{1.00 \pm 0.01} & (x \gg 1) 
\end{cases},$$

(2.82)

which means that the best overall scaling of $\gamma$ becomes

$$\gamma = \begin{cases} 
(1.7 \pm 0.1) \cdot P^{0.5} N^{-1.1} & (N^2 P \ll 1) \\
(2.7 \pm 0.3) \cdot P^1 N^{-0.2} & (N^2 P \gg 1) 
\end{cases}.$$

(2.83)

The error bars are given by the variation of the parameters when the fit range is increased or decreased by a decade. When $p$ and $q$ are varied within the collapse region, the exponents vary by $\sim \pm 0.05$. 

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2.6. ALTERNATIVE SCALING MODELS

\[ N^{2.0 \gamma} / (N^{1.8} P)^{\beta} = N^{2.0 \gamma} / (N^{1.8} P)^{0.5} \]

\( \beta = 1 \)
\( \beta = 0.5 \)

**Figure 2.23:** (a) Asymptotic behavior of \( F(x) \). Black lines show the result from the power law fit: \( F(x) \sim x^{1.0} \) for small \( x \) and \( F(x) \sim x^{0.5} \) for large \( x \). The crossover between the two regimes is at \( x = 0.4 \). (b) Residual plot \( F(x)/x^{1.0} \) (blue) and \( F(x)/x^{0.5} \) (red) show the fitted power laws match the behavior very well in their respective regimes, as they scatter around a constant value. (c) Log-correction \( c(N) = \log_{10}(N)^{-0.7} \) and power law correction \( c(N) = N^{2}/N^{1.8} = N^{-0.2} \) as function of system size \( N \). Both vary roughly by a factor of two in the range of \( N \) we probe. (d) The ratio of the two varies by less than 35%.

When we compare the power laws to our expected scaling (Eq. (2.31)), we find the scaling of \( \gamma \) with \( P \) is as expected, but note two differences from the expected scaling of \( \gamma \) with \( N \). First, we observe \( \gamma \) decreases as \( N^{-0.2} \) for small systems, instead of the independence of \( N \) our scaling model predicted. Second, for large systems, we observe \( \gamma_{cc} \) scales as \( N^{-1.1} \) instead of \( N^{-1} \).

**Comparison between power law and log corrections.** We can interpret the 1.8 exponent in \( N \) as a correction to the predicted \( N^2 P \) scaling: \( N^{1.8} P = N^{-0.2} (N^2 P) \). In Fig. 2.23(c), we compare this correction to the log correction described in § 2.3.3. We observe the corrections produce largely the same effect in the range of \( N \) that our simulations cover. When we plot the ratio of the two (Fig. 2.23(d)), we observe that the deviations between
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FIGURE 2.24: “The total energy per particle required to break a single contact averaged over $k$ (scaled by $A(\Delta \phi)(\Delta \phi)^2$, where $A(\Delta \phi)$ is only weakly dependent on $\Delta \phi$) versus $N$ for $\Delta \phi = 10^{-2}$ (crosses), $10^{-3}$ (pluses), $10^{-4}$ (triangles), $10^{-5}$ (diamonds), $10^{-6}$ (squares), and $10^{-7}$ (circles). The solid line has slope $-1.7$.” From Schreck et al. [76, Fig. 3(b)]; copyright 2011 by The American Physical Society.

both corrections are less than 35%, over a range where $N^2$ changes by three orders of magnitude.

It is thus very difficult to distinguish log corrections from power law corrections to scaling in 2D. To achieve a measurable difference of a factor three, systems of at least 60,000 particles are required. Alternatively, simulations can be performed in three dimensions, in which case log corrections will disappear [28].

To conclude, we find our deviations from the expected scaling can be described by both a log correction and a power law correction. Much larger systems or three-dimensional simulations are required to fully distinguish the two corrections.

2.6.1 Excited eigenmodes

We now turn to comparing our results to other work on contact changes in amorphous systems. We first focus on work by Schreck et al. [76], who investigated contact breaking in jammed sphere packings using excited eigenmodes. They displace particles along an eigenmode:

$$\vec{r} = \vec{r}_0 + \sqrt{N} \delta \hat{e}_k ,$$

(2.84)
where \( r_0^* \) is the original state, \( r^* \) the excited state, \( N \) the system size, \( \delta_k \) the eigenvector for eigenmode \( k \), and \( \delta \) the excitation amplitude. The system is then allowed to evolve at fixed energy. For small excitations \( \delta \), the system oscillates around a base state, and most energy is contained in the initial eigenmode. However, for excitations larger than a critical excitation amplitude \( \delta_c(k) \) there is a sharp increase in how much energy spreads into the other eigenmodes of the system. Schreck et al. find that \( \delta_c \) is directly related to the first contact change in the system. Surprisingly, they find that contacts only break, even for large systems \((N = 1920)\) at high densities \((\Delta \phi = 10^{-2})\).

For each system, \( \delta_c(k) \) is calculated for every eigenmode \( k \). The authors then measure the average energy required to break a contact

\[
E = \langle (\omega_k \delta_c(k))^2 \rangle_k ,
\]

where \( \omega_k \) is the eigenfrequency of eigenmode \( k \) and the mean is taken over all eigenmodes.

Fig. 2.24 shows the scaling of the energy per particle \( E/N \) as a function of density \( \Delta \phi \) and system size \( N \). Schreck et al. find a relationship

\[
\frac{E/N}{A(\Delta \phi) \cdot (\Delta \phi)^2} \sim N^{-\beta} ,
\]

“where \( A(\Delta \phi) \) is only weakly dependent on \( \Delta \phi \) and \( \beta \approx 1.7 \)” [76]. Close to jamming \((N \Delta z = 0 \ldots 2)\), they find \( A(\Delta \phi) \) is constant and \( \beta = 1 \ldots 2 \) [98]. When we rewrite Eq. (2.86) in terms of \( E \), take \( A(\Delta \phi) \) as constant and use \( \Delta \phi \sim P \), we find

\[
E \sim N^{1-\beta}(\Delta \phi)^2 \sim N^{1-\beta}P^2 .
\]

To compare this with our results, we note that

\[
E \sim \sigma \gamma L^2 \sim \sigma \gamma N \sim GN\gamma^2 ,
\]

so

\[
\gamma \sim \sqrt{E/GN} \sim N^{-\beta/2}PG^{-1/2} .
\]

Using the known finite-size scaling of \( G \) [34], we then find

\[
\gamma \sim \left\{ \begin{array}{ll}
PN^{(1-\beta)/2} & (N^2P \ll 1) \\
N^{0.75}P^{-\beta/2} & (N^2P \gg 1)
\end{array} \right.
\]
To test whether this matches the data, we plot $N^{(\beta+3)/2}r$ as a function of $N^2P$ in Fig. 2.25(a), using the published value $\beta = 1.7$. We find, firstly, that the collapse is not very good. Secondly, we find the 0.75 power law for the upper branch overestimates the actual strains. To a lesser extent, the lower branch also deviates from Eq. (2.90). This is also reflected in the residuals in Fig. 2.25(b) — neither branch collapses onto a constant value.

We expect these differences arise because Eq. (2.85) calculates the energy as an average over $2N$ modes within the same system. In § 2.6.3, we will see that averaging over all contacts loses many of the features we find for the first contact change.

### 2.6.2 Hard particle systems

The question of contact breaking and plasticity has also been studied in systems of hard particles. These systems are isostatic [100], which means a contact change is always a breaking event, and each breaking event will

---

**Figure 2.25:** (a) Our data rescaled as in Schreck et al. [76] (Eq. (2.90)). Black lines indicate power laws with exponent 1 and 0.75. (b) The residuals $F(x)/x^{1.0}$ (blue) and $F(x)/x^{0.75}$ (red) do not have a plateau, indicating these power laws do not well describe the data. (c,d) Same, but with data rescaled as in Wyart [99] (Eq. (2.94)), where we have chosen $r = 1.8$, as in our best collapse. The corresponding $q = 1.8 + 0.15 = 1.95$ is indistinguishable from our best choice $q = 2.0$. 
cause the system to unjam. Contact changes are therefore directly connected to plastic events. Isostaticity also implies that the force distribution is unique, and can be derived directly from the contact network [101]. Because the systems are isostatic, the results can only describe the $N^2 P \ll 1$ limit of soft particle systems.

Combe and Roux [79] investigated the prevalence of and distance between strain jumps in a system under uniaxial stress-controlled compression. The system is deformed by increasing $\sigma_{yy}$ while keeping $\sigma_{xx}$ constant. Combe and Roux find that the spacing between events is described by an exponential distribution in $\delta q (N/1024)^{1.16}$, where $\delta q$ is the relative uniaxial stress increment $\Delta \sigma_{yy} / P$. This is consistent with modeling events as a Poisson process.

Because the mean of the distribution

$$\langle \delta q (N/1024)^{1.16} \rangle = \langle \Delta \sigma \rangle (1/P) (N/1024)^{1.16} \sim \text{constant}$$

is independent of $N$ and $P$, the mean stress required to break the first contact scales as

$$\langle \Delta \sigma \rangle \sim P \langle \Delta q \rangle \sim P/N^{1.16}.$$  \hspace{1cm} (2.92)

We can then calculate the $\gamma_{bk}$ using the uniaxial compression modulus $E$. Using that $K \sim 1$ and $G \sim 1/N \ll K$ near jamming, $E$ is given by [102]

$$E = \frac{4}{1/K + 1/G} \sim G \sim \frac{1}{N}$$

and the expected mean strain to break the first contact is thus given by

$$\gamma_{bk} \sim \langle \Delta \sigma \rangle / E \sim P/N^{0.16},$$

which is very close to the $P/N^{0.20}$ scaling we found by fitting our data to a pure power law (Eq. (2.83)).

A theoretical argument for this power law, based on the concept of "weak" contacts that connect to local motion, and "strong" contacts that are connected to global motion, was introduced by Lerner et al. [80]. Wyart [99] uses this to predict that the strain for the first contact change should scale as

$$\gamma \sim P/N^{0.15},$$

which is close to the value found by Combe and Roux [79].
In Fig. 2.25(c), we show this scaling also provides a good match to our data — the 0.15 exponent can be seen as a power law correction to our initial $\gamma \sim P$ scaling near jamming, and is essentially indistinguishable from either log or 0.2 power law corrections.

### 2.6.3 Extremal value scaling

In this section we probe whether we can predict the scaling of $\gamma_{cc}$ and distribution of $\gamma_*$ based on the distribution of all contact change strains $\rho(\gamma_{ij})$ for a given ensemble $(N, P)$. Note that before (§§ 2.3 and 2.4), we have determined the scaling of $\gamma_{cc}$ by determining $\gamma_*$ for each packing, and averaging over those values. We found that the distribution of $\gamma_*$ is close to a exponential distribution. Assuming that large enough packings are statistically similar, it should be possible to predict $\gamma_{cc}$ from the distribution of $\rho(\gamma_{ij})$ using extremal statistics. In particular, one might expect that $\rho(\gamma_{ij})$ takes on a simple form for sufficiently large $N$, possibly even amenable to a theoretical description. Deviations from this picture may point to lack of self-averaging or other subtleties, and as such provide important information for developing a deeper theoretical understanding for the characteristic strains of the first contact change. Before starting, we note that for contact creation, it is difficult to establish which potential contacts should be considered, and we therefore focus on the breaking of contacts only, using $\gamma_{*,bk}^{LR}$ from linear response. We will also limit our discussion to contacts that break under shear in the positive direction, i.e., $\gamma > 0$. As a first probe of the usefulness of extremal value statistics for contact breaking, we compare the results of two distinct methods of calculating the mean contact breaking strain. First, we define $\gamma_{bk}^{LR} = \langle \gamma_{*,bk}^{LR} \rangle$, the mean of the contact breaking strains determined for an ensemble of packings, as we have done in § 2.4. Second, we determine $\gamma_{bk}^{dist}$ from the distribution of positive contact change strains $\rho(\gamma_{ij}^\dagger)$ by solving

$$\frac{1}{\langle N_{bk} \rangle} = \int_{0}^{\gamma_{bk}^{dist}} \rho(\gamma_{ij}^\dagger) d\gamma_{ij}^\dagger.$$  

To implement this, we first compute the numerical CDF $\Pr(\gamma_{ij}^\dagger < \gamma)$ based on the breaking strain $\gamma_{ij}$ for every contact in every packing in the ensemble and then solve

$$\Pr(\gamma_{ij}^\dagger < \gamma_{bk}^{dist}) = 1/\langle N_{bk} \rangle,$$  

(2.97)
2.6. ALTERNATIVE SCALING MODELS

\[ \Pr(\gamma_{ij}^+ < \gamma) = 1/N_c \]

\[ \langle N_{bk} \rangle = 1147 \]

Figure 2.26: (a) CDF of \( \gamma_{ij}^+ \) for every contact for every packing in the \( N = 1024, P = 10^{-2} \) ensemble. The strain at which \( \Pr(\gamma_{ij}^+ < \gamma_{bk}^{\text{dist}}) = 1/\langle N_c \rangle \) is the expected contact breaking strain for this ensemble: \( \gamma_{bk}^{\text{dist}} = 1.4 \times 10^{-4} \). The mean breaking strain from linear response is \( \gamma_{bk}^{\text{LR}} = 1.5 \times 10^{-4} \), and is indicated with the dashed line. (b) Colored symbols: resulting scaling of \( \gamma_{bk}^{\text{dist}} \). Gray background: scaling of \( \gamma_{bk}^{\text{LR}} \), as in Fig. 2.17(b). (c) The ratio \( \gamma_{bk}^{\text{dist}} / \gamma_{bk}^{\text{LR}} \) varies slowly with \( N^2 P \log_{10}(N)^{-0.7} \), from \( \gamma_{bk}^{\text{dist}} / \gamma_{bk}^{\text{LR}} \approx 0.5 \) to \( \gamma_{bk}^{\text{dist}} / \gamma_{bk}^{\text{LR}} \approx 1.0 \).

where \( \langle N_{bk} \rangle \approx 0.5 \langle N_c \rangle \) is the mean number of contacts that break under positive strain, for which we take the numerical ensemble average. This procedure is illustrated in Fig. 2.26(a) for the \( N = 1024, P = 10^{-2} \) ensemble, where \( \langle N_{bk} \rangle = 1147 \). For this particular example we find that \( \gamma_{bk}^{\text{LR}} = 1.5 \times 10^{-4} \) whereas \( \gamma_{bk}^{\text{dist}} = 1.4 \times 10^{-4} \). These values are close but distinct \( (\gamma_{bk}^{\text{dist}} / \gamma_{bk}^{\text{LR}} = 0.93) \) — as we will show below, there are systematic deviations between these numbers which provide insight into the statistics of contact breaking.

As comparison, we repeat this procedure for a synthetic ensemble of systems where all contacts are uncorrelated. To build this ensemble, we draw \( N_{bk} = 1147 \) contacts for each of \( N_s = 1000 \) systems from the measured frequentist distribution of contact breaking strains \( \rho(\gamma_{ij}^+) \) of the \( N = 1024, P = 10^{-2} \) ensemble (bootstrapping). For each system, we calculate the minimum strain \( \gamma^* \). We then compare the mean breaking strain \( \gamma_{bk} = \langle \gamma^* \rangle = (1.34 \pm 0.04) \times 10^{-4} \) to \( \gamma_{bk}^{\text{dist}} = 1.4 \times 10^{-4} \), and find
\( \gamma_{\text{bk}} / \gamma_{\text{bk}} = 1.05 \pm 0.04 > 1 \). Values below 1 thus indicate significant deviations from uncorrelated systems.

**Distribution of strains.** We now probe the distribution of strains of first contact breaks. Consider an ensemble of \( M \) packings of \( N \) particles, each with \( N_{\text{bk}}(m) \) contacts for which we calculate the breaking strains \( \gamma_{ij}^{\dagger} \). This yields a total of \( \Sigma_{m=1}^{M} N_{\text{bk}}(m) = M \langle N_{\text{bk}} \rangle \) samples (values of \( \gamma_{ij}^{\dagger} \), as illustrated in Fig. 2.27 for a synthetic data set, as well as for two data sets at fixed \( P \) and \( N \). First, we can collect all breaking strains in a distribution \( \rho(\gamma_{ij}^{\dagger}) \) (black curves in panels b,e,h). As illustrated in Fig. 2.27 there are now two operations we can perform. Equivalent to what we do to determine \( \gamma_{\text{LR}}^{\text{bk}} \) in linear response, we can determine the minimum breaking strain for each of the \( M \) packings, obtaining \( M \) breaking strains (red crosses in panels a,d,g) and the corresponding distribution \( \rho(\gamma_{LR}^{\text{bk}}) \) (shown as red curves in panels b,e,h, as a fraction of \( \rho(\gamma_{ij}^{\dagger}) \)). Alternatively, we may also consider the \( M \) smallest values out of \( M \langle N_{\text{bk}} \rangle \) samples taken out of the distribution \( \rho(\gamma_{ij}^{\dagger}) \) (blue circles), which yields the distribution \( \rho(\gamma_{<}) := \rho(\gamma|\gamma \leq \gamma_{\text{dist}}^{\text{bk}}) \) (blue curve). The mean values considered above are related to these distributions as follows: \( \gamma_{\text{bk}}^{\text{LR}} \) is the mean of the \( \rho(\gamma_{*,\text{bk}}^{\text{LR}}) \), whereas \( \gamma_{\text{bk}}^{\text{dist}} \) is the maximum value of \( \gamma_{<} \) in \( \rho(\gamma_{<}) \). Clearly, the distributions \( \rho(\gamma_{*,\text{bk}}^{\text{LR}}) \) and \( \rho(\gamma_{<}) \) in general will be different, but if the different packings are statistically indistinguishable and large enough to allow for self-averaging, so that \( \gamma_{\text{bk}}^{\text{LR}} \approx \gamma_{\text{bk}}^{\text{dist}} \), these distributions are directly related (see below), which yields a statistical test on the nature of the contact breaking strains.

**Results.** We have determined \( \gamma_{\text{bk}} \) and \( \gamma_{\text{bk}}^{\text{dist}} \) for all \( (N, P) \) ensembles. In Fig. 2.26(b) we plot \( N^{2} \gamma_{\text{bk}}^{\text{dist}} \) vs \( N^{2} P \log_{10}(N)^{-0.7} \), and in Fig. 2.26(c) we plot the ratio \( \gamma_{\text{bk}}^{\text{dist}} / \gamma_{\text{bk}}^{\text{LR}} \) vs \( N^{2} P \log_{10}(N)^{-0.7} \). At low \( N^{2} P \log_{10}(N)^{-0.7} \), we find that \( \gamma_{\text{bk}}^{\text{dist}} \) and \( \gamma_{\text{bk}}^{\text{LR}} \) exhibit similar scaling with \( N^{2} P \log_{10}(N)^{-0.7} \), but that their ratio \( \gamma_{\text{bk}}^{\text{dist}} / \gamma_{\text{bk}}^{\text{LR}} \approx 0.6 < 1.05 \pm 0.05 \) points to deviations from self-averaging. At very high \( N^{2} P \log_{10}(N)^{-0.7} \), \( \gamma_{\text{bk}}^{\text{dist}} \) increases faster than \( \gamma_{\text{bk}}^{\text{LR}} \) and appears to reach equality for the highest values of \( N^{2} P \) — we suggest that here the packings are large enough to be self-averaging.

To further characterize the origins of this breakdown of self averaging in small systems, we take a closer look at the distributions \( \rho(\gamma_{*,\text{bk}}) \) and

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**CONTACT CHANGES OF SHEARED SYSTEMS**

\[ \gamma_{\text{bk}} / \gamma_{\text{bk}} = 1.05 \pm 0.04 > 1. \] Values below 1 thus indicate significant deviations from uncorrelated systems.

**Distribution of strains.** We now probe the distribution of strains of first contact breaks. Consider an ensemble of \( M \) packings of \( N \) particles, each with \( N_{\text{bk}}(m) \) contacts for which we calculate the breaking strains \( \gamma_{ij}^{\dagger} \). This yields a total of \( \Sigma_{m=1}^{M} N_{\text{bk}}(m) = M \langle N_{\text{bk}} \rangle \) samples (values of \( \gamma_{ij}^{\dagger} \), as illustrated in Fig. 2.27 for a synthetic data set, as well as for two data sets at fixed \( P \) and \( N \). First, we can collect all breaking strains in a distribution \( \rho(\gamma_{ij}^{\dagger}) \) (black curves in panels b,e,h). As illustrated in Fig. 2.27 there are now two operations we can perform. Equivalent to what we do to determine \( \gamma_{\text{bk}}^{\text{LR}} \) in linear response, we can determine the minimum breaking strain for each of the \( M \) packings, obtaining \( M \) breaking strains (red crosses in panels a,d,g) and the corresponding distribution \( \rho(\gamma_{LR}^{\text{bk}}) \) (shown as red curves in panels b,e,h, as a fraction of \( \rho(\gamma_{ij}^{\dagger}) \)). Alternatively, we may also consider the \( M \) smallest values out of \( M \langle N_{\text{bk}} \rangle \) samples taken out of the distribution \( \rho(\gamma_{ij}^{\dagger}) \) (blue circles), which yields the distribution \( \rho(\gamma_{<}) := \rho(\gamma|\gamma \leq \gamma_{\text{dist}}^{\text{bk}}) \) (blue curve). The mean values considered above are related to these distributions as follows: \( \gamma_{\text{bk}}^{\text{LR}} \) is the mean of the \( \rho(\gamma_{*,\text{bk}}^{\text{LR}}) \), whereas \( \gamma_{\text{bk}}^{\text{dist}} \) is the maximum value of \( \gamma_{<} \) in \( \rho(\gamma_{<}) \). Clearly, the distributions \( \rho(\gamma_{*,\text{bk}}^{\text{LR}}) \) and \( \rho(\gamma_{<}) \) in general will be different, but if the different packings are statistically indistinguishable and large enough to allow for self-averaging, so that \( \gamma_{\text{bk}}^{\text{LR}} \approx \gamma_{\text{bk}}^{\text{dist}} \), these distributions are directly related (see below), which yields a statistical test on the nature of the contact breaking strains.

**Results.** We have determined \( \gamma_{\text{bk}} \) and \( \gamma_{\text{bk}}^{\text{dist}} \) for all \( (N, P) \) ensembles. In Fig. 2.26(b) we plot \( N^{2} \gamma_{\text{bk}}^{\text{dist}} \) vs \( N^{2} P \log_{10}(N)^{-0.7} \), and in Fig. 2.26(c) we plot the ratio \( \gamma_{\text{bk}}^{\text{dist}} / \gamma_{\text{bk}}^{\text{LR}} \) vs \( N^{2} P \log_{10}(N)^{-0.7} \). At low \( N^{2} P \log_{10}(N)^{-0.7} \), we find that \( \gamma_{\text{bk}}^{\text{dist}} \) and \( \gamma_{\text{bk}}^{\text{LR}} \) exhibit similar scaling with \( N^{2} P \log_{10}(N)^{-0.7} \), but that their ratio \( \gamma_{\text{bk}}^{\text{dist}} / \gamma_{\text{bk}}^{\text{LR}} \approx 0.6 < 1.05 \pm 0.05 \) points to deviations from self-averaging. At very high \( N^{2} P \log_{10}(N)^{-0.7} \), \( \gamma_{\text{bk}}^{\text{dist}} \) increases faster than \( \gamma_{\text{bk}}^{\text{LR}} \) and appears to reach equality for the highest values of \( N^{2} P \) — we suggest that here the packings are large enough to be self-averaging.

To further characterize the origins of this breakdown of self averaging in small systems, we take a closer look at the distributions \( \rho(\gamma_{*,\text{bk}}) \) and
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FIGURE 2.27: (a) Scatter plot of each positive contact breaking strain $\gamma_{ij}^\dagger$ for 100 synthetic systems drawn (bootstrapped) from the distribution $\rho(\gamma_{ij}^\dagger)$ for $N = 1024$, $P = 10^{-2}$ (black dots). For each system, $\gamma_* \equiv \min \gamma_{ij}^\dagger$ is indicated with a red +. All values below the $1/N_c$ percentile are indicated with a blue ◦. (b) The PDF $\rho(x_{ij})$ (black). The distribution of per system minima ($\rho(\gamma_*)/M$, red dashed) and values below the $1/N_c$ percentile ($\rho(\gamma_<)/M$, blue dash-dotted) as part of the whole are indicated. (c) Same as (b), but with a linear PDF axis. (d,e,f) Same as (a,b,c), with numerical data from the $N = 1024$, $P = 10^{-2}$ ensemble. (g,h,i) Same, with numerical data from the $N = 16$, $P = 10^{-6}$ ensemble.
\(\rho(\gamma_<)\) in Fig. 2.27 and 2.28. In Fig. 2.27(a–c), we plot each value of \(\gamma_{ij}^+\) for the first 100 systems in the synthetic ensemble described above. When we compare the PDFs of the per system \(\rho(\gamma_{*,bk})\) (red curves in panel b) and distribution minima \(\rho(\gamma_<)\) (blue curves in panel b), we note they are similar for small values of \(\gamma_{ij}^+\), but different for larger values of \(\gamma_{ij}^+\).

In Fig. 2.28(a) we compare the CDF of the per system minima to the CDF of the whole distribution. In the synthetic data, we can deduce that the inverse CDF of minima \(\Pr(\gamma_* \geq \gamma)\) relates to the CDF of the distribution \(\Pr(\gamma_{ij} < \gamma)\) as

\[
\Pr(\gamma_* \geq \gamma) = (1 - \Pr(\gamma_{ij} < \gamma))^{\langle N_{bk} \rangle} = \left[1 - \frac{\#_{\gamma_{ij} < \gamma}}{N_s \langle N_{bk} \rangle}\right]^{\langle N_{bk} \rangle} \\
\approx \exp\left(-\frac{\#_{\gamma_{ij} < \gamma}}{N_s}\right) \\
= \exp\left(-\langle N_{bk} \rangle \Pr(\gamma_{ij} < \gamma)\right),
\]

(2.98)

for large enough \(\langle N_{bk} \rangle\) for a given \(\langle N_{bk} \rangle \Pr(\gamma_{ij} < \gamma)\). In Fig. 2.28(a), we plot \(\Pr(\gamma_* \geq \gamma)\) as a function of \(\langle N_{bk} \rangle \Pr(\gamma_{ij} < \gamma)\) for both the synthetic distribution described above, as well as for a synthetic distribution with small \(\langle N_{bk} \rangle\). We observe the exponential scaling predicted in Eq. (2.98) for both. Hence, one expects 63% of the \(N_s\) per-system minima \(\gamma_*\) to be present in the set of \(N_s\) global minima \(\gamma_<\).

In Fig. 2.27(d–f), we plot each value of \(\gamma_{ij}^+\) for the first 100 systems, taken from the \(N = 1024, P = 10^{-2}\) ensemble. The relation between the PDFs of the per system \(\rho(\gamma_{bk}^{LR})\) (red curves in panel e) and distribution minima \(\rho(\gamma_<)\) (blue curves in panel e) are similar to those of the synthetic data, and \(\gamma_{bk}^{\text{dist}} = 1.4 \times 10^{-4}\) and \(\gamma_{bk}^{LR} = 1.5 \times 10^{-4}\) are quite similar. Consistent with this, a plot of \(\Pr(\gamma_* \geq \gamma)\) as a function of \(\langle N_{bk} \rangle \Pr(\gamma_{ij} < \gamma)\) is approximately exponential, although slight deviations can be seen in the tails of these distributions (Fig. 2.28(b)).

In Fig. 2.27(g–i), we plot each value of \(\gamma_{ij}\) for the first 100 systems, taken from the \(N = 16, P = 10^{-6}\) ensemble. The differences between the PDFs of the per system \(\rho(\gamma_{bk})\) (red curves in panel h) and distribution minima \(\rho_<(\gamma_{bk}^{\text{dist}})\) (blue curves in panel h) are more significant, and \(\gamma_{bk} = 1.6 \times 10^{-6}\)
2.6. ALTERNATIVE SCALING MODELS

![Diagram](image_url)

**Figure 2.28:** \( \Pr(\gamma_* \geq \gamma) \) as a function of \( \langle N_{bk} \rangle \Pr(\gamma_{ij} < \gamma) \) (see text). (a) Solid black curve: Synthetic data, drawn from \( \rho(\gamma^*_{ij}) \) in the \( N = 1024, P = 10^{-2} \) ensemble (\( \langle N_{bk} \rangle = 1147 \)). For the same ensemble, data with a single value from a distribution with lower mean (dot-dashed blue curve) and for systems with an overall per-system scale (dashed purple curve) are also shown. Dotted red curve: Synthetic data, from \( \rho(\gamma^*_{ij}) \) in the \( N = 16, P = 10^{-6} \) ensemble (\( \langle N_{bk} \rangle = 16 \)). The gray line indicates \( \Pr(\gamma_* \geq \gamma) = \exp(-\langle N_{bk} \rangle \Pr(\gamma_{ij} < \gamma)) \). (b) Data from our simulations. We observe the curves decay slower than exponential, indicating correlations between contacts. (c) Data from (b), but with all strains rescaled to the mean of strains within one system. This reduces the effect of a per-system scale (dashed purple curve), but does not completely negate it. The behavior for the packing-derived data is unchanged as compared to (b).

and \( \gamma^*_{bk} = 1.1 \times 10^{-6} \) are quite distinct. Consistent with this, a plot of \( \Pr(\gamma_* \geq \gamma) \) as a function of \( \langle N_{bk} \rangle \Pr(\gamma_{ij} < \gamma) \) deviates significantly from an exponential (Fig. 2.28(b)). This deviation points to a lack of self-averaging in small systems.

*Interpretation.* We now discuss two possible scenarios to explain the deviations for small \( N^2P \log_{10}(N)^{-0.7} \). First, each finite packing could have a different distribution of \( \gamma_{ij} \), but between packings these distributions are related by an overall scale factor. The data shown in Fig. 2.27(g) suggests that this is possible. To understand the effect of such ‘overall scale factor’ for the statistics, we draw an overall system scale from a uniform distribution
\[ U(0, 1) \] for each of the synthetic systems, and multiply the strains for each system with this scale factor. The resulting behavior is shown in Fig. 2.28(a), where we see the decay is much slower than for uncorrelated systems. The reason for this is that packings with a low minimum will typically come from a system which contains other low strains. This saturates the low strain region of the overall distribution with strains that are not system minima. The data extracted from our direct simulations (Fig. 2.28(b)) show a similar decay, slower than exponential, with slower decays for lower pressures. To directly check whether a per-system scale can explain the behavior, we divide all strains by the mean strain for each system, and show the results in Fig. 2.28(c). In the case of a simple scale incorporated in synthetic data, this brings the behavior closer to the simple exponential (dashed purple line). The behavior is still not purely exponential because this normalization step overcorrects deviations. Nevertheless, we note that the rescaling has very little effect on the contact change strains shown in Fig. 2.28(b). We therefore conclude the correlations cannot be simply explained by an overall system scale.

Second, inspired by Lerner et al. [103], we now investigate whether we can recover the behavior of \( \gamma_{LR} \) using extremal value statistics by assuming that most contacts are drawn from a distribution with mean \( k \), but a limited number of ‘weak’ contacts are drawn from a distribution with mean \( k' \ll k \). In the case of one extraordinarily weak contact in each packing, we expect most of the \( k \) system minima to show up in the lowest \( k \) values of the entire set of strains. We have simulated this by dividing one strain in each of the synthetic packings by \( 10^3 \). As we see in Fig. 2.28(a), \( \Pr(\gamma_s \geq \gamma) \) decreases much more rapidly than exponential, and drops to \( \Pr(\gamma_s \geq \gamma) = 0 \) around \( \langle N_{bk} \rangle \Pr(\gamma_{ij} < \gamma) \approx 3 \) — in other words, the \( k \) minima are all found in the lowest \( 3k \) values of the full set. The exact point of intersection depends on how weak the contact is, and on how many weak samples are in the packing. However, our data for actual packings shows a slower than exponential decay, thus discounting the ‘weak contact’ hypothesis as source for the correlations in our systems.

Hence, in conclusion: for sufficiently large systems, packings are self averaging, and extremal value statistics may be sufficient to determine the mean value and distribution for the first contact break strains. For small systems, correlations between contacts need to be taken into account for a correct prediction.
2.A. Finite size scaling of $\rho(u_{\parallel})$ and $\rho(u_{\perp})$

In this appendix, we will discuss the distributions of $u_{\parallel}$ and $u_{\perp}$, which provide a continuum description of the inter-particle motion. For each particle pair $i, j$, we split the inter-particle velocity $\vec{u}_{ij} = \partial \vec{x}_{ij} / \partial \gamma$ in components parallel and perpendicular to the contact:

$$u_{\parallel,ij} = \vec{u}_{ij} \cdot \hat{r}_{ij}, \quad (2.99)$$

$$u_{\perp,ij} = \sqrt{u_{ij}^2 - u_{\parallel,ij}^2}. \quad (2.100)$$

Using every contact in every packing in an ensemble, we then build the frequentist distributions $\rho(u_{\parallel})$ and $\rho(u_{\perp})$.

In the following, we will discuss the relationship between the shape and scale of these distributions and $N$ and $P$. Earlier work [31] has focused on Hertzian systems at intermediate to high pressure ($P^{2/3} \sim \langle \delta \rangle \geq 3 \cdot 10^{-4}$). They find the shape of the distribution does not depend on $P$, and find a simple single scaling of the overall scale with $P$. We extend this with harmonic systems much closer to jamming ($P \sim \langle \delta \rangle \geq 10^{-7}$). At high pressures, we recover the same behavior, but close to jamming, we find (i) the shape of the distributions depends on the pressure $P$, and (ii) the widths of the distributions scale with $N^2P$, with two distinct scaling regimes.

Shape of distributions. In Fig. 2.29, we plot the probability density functions of $u_{\parallel}$ and $u_{\perp}$, rescaled by their standard deviations $s_{\parallel}$ and $s_{\perp}$, for ensembles with different system sizes and pressures. We note that, even though the different distributions cannot be collapsed with a single scale parameter, the majority of the behavior is captured in the standard deviation $s$. For both distributions, we observe the distributions become increasingly peaked near 0, and, although neither PDF diverges, their peaks appear to develop a sharp kink for small pressures. We observe the shape changes with $P$, and, for large enough $N$, is largely independent of $N$. $N^2P$ is not the relevant scaling parameter here. Surprisingly, this means the overabundant low values are still present for large systems at $P \approx 10^{-3}$, which would normally not be considered ‘close to jamming’. 

Appendix
**Figure 2.29:** (top) Distributions of $u_\parallel$, rescaled by their standard deviation $s_\parallel$, for ensembles with $N = 16, 256, \text{ or } 1024$ particles at $P = 10^{-6} \ldots 10^{-1}$. $s_\parallel$ is indicated in each figure. The distributions develop a sharp kink around 0 for low pressures, and become smooth for $P \gtrsim 10^{-2}$. There is a weak dependence on $N$, with the distribution becoming more peaked for high $N$. (bottom) Same, for $u_\perp$. Here, the distributions depend less on $N$ and $P$, although also here the distribution gains weight near 0 for decreasing $P$. 
2.A. Finite size scaling of $\rho(u_\parallel)$ and $\rho(u_\perp)$

Figure 2.30: (a) Scaling of the standard deviation $s_\parallel$ as a function of $N$ and $P$. At low $N^2P$, $s_\parallel$ is independent of pressure and at high $N^2P$ we recover $s_\parallel \sim \delta^{0.25}$, consistent with [31]. (b) Same, for $s_\perp$. At low $N^2P$, $s_\parallel$ is independent of pressure. At high pressure we find a scaling $s_\parallel \sim \delta^{-0.25-0.15}$, somewhat slower than the $\delta^{-0.25}$ found in [31].

Scaling of standard deviations. Ellenbroek et al. [31] find the width of the distributions scale as

\[ s_\parallel \sim \langle \delta \rangle^{1/4} , \tag{2.101} \]
\[ s_\perp \sim \langle \delta \rangle^{-1/4} , \tag{2.102} \]

where $\langle \delta \rangle$ is the mean overlap between pairs of particles in contact in the ensemble. If we assume (i) the standard deviations will scale with $N^2P$ and (ii) the distributions are independent of $N$ for large $N$, Eq. (2.101) and Eq. (2.102) suggest plotting

\[ N^{0.5}s_\parallel \sim F(N^2P) , \tag{2.103} \]
\[ N^{-0.5}s_\perp \sim F(N^2P) , \tag{2.104} \]

should collapse our data. We note that, because the shape of the distribution varies, the choice of the measurement (e.g. a percentile rather than the standard deviation) can have a rather large effect on the collapse (which can reach $\pm 0.2$ in the scaling exponent), and we therefore do not expect a perfect match.
In Fig. 2.30(a), we find the best scaling collapse for $s_{\parallel}$ is close but not equal to the expected scaling: we find $s_{\parallel} \sim N^{-0.4}$ at low $N^2P$ rather than $s_{\parallel} \sim N^{-0.5}$. Nonetheless, we suggest that the scaling is close enough to be consistent with the proposed scaling. At low pressures, we find that $s_{\parallel}$ only depends on $N$, and no longer depends on $P$. For $N^2P \gg 1$, we find the expected $s_{\parallel} \sim P^{0.25}$ power law.

For $s_{\perp}$, we find Eq. (2.104) provides a rather good collapse (Fig. 2.30(b)). At low $N^2P$, we find $s_{\perp}$ becomes independent of $P$, and at high $N^2P$, we find behavior similar, but different from the expected $s_{\perp} \sim P^{-0.25}$ power law.

Surprisingly, we find both $s_{\perp}$ and $s_{\parallel}$ reach a pressure-independent plateau for low $N^2P$. This has important implications for the behavior close to jamming — in contrast to what is generally assumed, $s_{\perp}/s_{\parallel}$ does not diverge for low pressures, but reaches a plateau whose value diverges as $s_{\perp}/s_{\parallel} \sim N^{0.9}$ in the thermodynamic limit.