Elasticity in particle packings near jamming

- Finite shear modulus and yield stress above a critical volume fraction, $\phi_J$.
- Linear response of static packings anomalous near $\phi_J$ beyond a lengthscale that diverges at $\phi_J$.
- Different characteristic lengths control longitudinal and transverse components of the point response.
- Rigid shear: Modulus dependent on scale
- Free shear: Surprisingly invariant with respect to jamming.

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[NSF logo]

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Outline

• Background and overview
  • Soft particle suspensions
  • Jamming and random close packing
  • Elasticity: Development of shear modulus
  • Plasticity: Development of yield stress
  • Simple models

• Elasticity
  • Scaling laws, (criticality?) and emergent lengthscales
  • Point response
  • Constrained homogeneous deformation
  • Unconstrained homogeneous deformation

• Plasticity:
  • Shear transformations, slip avalanches, and diffusion
  • Short-time intermittency
  • Long time diffusion
  • Plastic strain correlations
Soft glasses

• Particles suspended in liquids can behave like glasses or other conventional amorphous solids.

• Particles can be:
  • solid like in a paste
  • liquid like in an emulsion
  • air like in a foam or mousse

• Technological applications:
  • Device fabrication/assembly
  • Oil / Gas drilling/production
  • Food / personal care
  • Bio-related

• This work:
  • Athermal
  • Deformable
  • Jammed
Jamming: random close packing

A brief history of jamming:
• Key quantities: volume fraction, $\varphi$; contact #, $z$.
• Jamming: “Random close packing version 2.0”
• JD Bernal (1960): spheres “pack randomly” at $\varphi \sim 0.64$, $z \sim 6$.
• Donev et. al. (2004): M&M’s do better. $\varphi \sim 0.71$, $z \sim 10$.
• Maxwell constraint counting (frictionless spheres):
  • $dN$ translational DOFs
  • there are $zN/2$ contacts in the system
  • $z/2 > d$ is a necessary condition for rigidity
Jamming: development of a static shear modulus

- Monodisperse oil-in-water emulsion
- Viscosity vs. concentration
- Shear modulus jumps by 4 orders of magnitude at $\phi_{rcp}$
- Analagous to rigidity percolation?
Jamming: development of yield stress

- μ-gel suspension
- $\phi > \phi_{rcp}$: yield stress
- $\phi < \phi_{rcp}$: viscous fluid
Jamming: critical scaling at $\Phi_c$

- $\Phi, \sigma$ rheology scaling near “point J”
- Olsson and Teitel (bubbles), Hatano (grains)...
- Depinning-like transition (dynamical criticality) at yield surface: (CEM and Robbins -- Vandembroucq et. al.)
Bubble model (Durian)

- Repulsion, $F_{\text{rep}}$, linear in overlap, $s$:
  - $F_{\text{rep}} = ks$
  - (could be arbitrary power of $s$)
- Drag, $F_{\text{drag}}$, w/r/t imposed flow:
  - $F_{\text{drag}} = b (v_{\text{bubble}} - v_{\text{flow}})$
- For (massless) bubbles, $F_{\text{rep}} = F_{\text{drag}}$
  - $v_{\text{bubble}} = F_{\text{rep}} / b + v_{\text{flow}}$
- Single timescale: $\tau_D = b R^4 / k$
- Dimensionless shearing rate:
  - $\text{De} = (d\gamma / dt) \tau_D$
  - (Deborah number)
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Elasticity near jamming: $z, P, K, G$

- $F=s^\alpha$; Harmonic: $\alpha=1$; Hertz: $\alpha=3/2$
- Previous results from simple models:
  - Excess contacts: $\Delta z = z - z_{\text{Maxwell}} \sim \Delta \phi^{1/2}$
    - Independent of force law, dimension, and polydispersity!
    - Related to Bernal’s “almost-contacts”
  - Pressure, $P \sim \Delta \phi^\alpha \sim <s>^\alpha$ e.g. Harm: $P \sim \Delta \phi \sim \Delta z^2$
    - Naive expectation
    - Implies compression modulus: $K$
    - $K = \delta P/\delta \ln V \sim \delta P/\delta \phi \sim \Delta \phi^{\alpha-1} \sim <s>^{\alpha-1}$
  - Shear modulus, $G \sim \Delta \phi^{\alpha-3/2} \sim <s>^{\alpha-3/2}$
    - So $G/K \sim \Delta z \sim \Delta \phi^{1/2}$
    - Particle packings are incompressible at jamming!

**Naive expectation**

**Non-trivial**
Diverging lengthscales and criticality at $\Phi_J$

- $\Phi_J$ critical point? Analogy to rigidity percolation? Diverging lengthscale?

- Goodrich et. al. (Soft Matter 2014): rigidity length $l^* \sim 1/\Delta z \sim \delta \Phi^{-1/2}$.
  - $O(L^d \Delta z)$ excess geometrical constraints
  - Free surface: release $O(L^{d-1})$ of them
  - For some $l^* \sim \Delta z^{-1}$, $L < l^*$ underconstrained

- Silbert et. al. (PRL 2005): dynamical structure factor at $\omega^*$. $\xi_T \sim \delta \Phi^{-1/4}$

- Ellenbroek et. al. (PRE 2009): longitudinal force fluctuations in response to local dilation. $l^* \sim \delta \Phi^{-1/2}$

- Lerner et. al. (Soft Matter 2014): single bond extension $\xi_T \sim \delta \Phi^{-1/4}$

- **Our goal**: measure both lengths in a single, simple, **experimentally realizable** procedure
Measurement 1: Point response

$(\lambda + G) \nabla (\nabla \cdot \mathbf{u}) + G \nabla^2 \mathbf{u} = 0$

- Standard model and prep. protocol
- harmonic, 50:50, $R_{\text{big}}=1.4R_{\text{small}}$
- Infinitesimal point load on single particle
- (Slight difference with both Ellenbroek et. al. and Lerner et. al.)

Motivation: Leonforte et. al. PRB 2004 (Lennard-Jones)
Measurement 1: Point response

\[(\lambda + G)\nabla(\nabla \cdot u) + G \nabla^2 u = 0\]

- Elasticity: Lame’-Navier equation.
- Singular solution: Kelvin
- Lame’ coefficients, G (shear modulus) and \(\lambda\) determined by homogeneous loading of large system with PBCs.
- “Continuum” solution computed at particles using Debye-like cutoff and linear dispersion (\(\omega^2 \sim k^2\))
- Slight dependence on Poisson ratio.
- Point response becomes less and less Kelvin-like near \(\phi_J\)

\(\phi = 0.85\)

\(\phi = 0.90\)
Measurement 1: Point response

\[(\lambda + G)\nabla (\nabla \cdot \mathbf{u}) + G\nabla^2 \mathbf{u} = 0\]

- Averaged power spectrum at \(\phi=0.85\)
- Look at Longitudinal and Transverse contribution separately.
- Kelvin:
  \[
u_L(q) = \frac{\sin(\theta)}{(K + G)q^2}
\]
  \[
u_T(q) = \frac{\cos(\theta)}{Gq^2}
\]
  
- Note: \(u_L\) should be zero along \(\theta=0\) and \(u_T\) should be zero along \(\theta=\pi/2\).
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Measurement 1: Point response

- Take isotropic average of Log(S) for better statistics.
- S=1 means Kelvin.
- Note: long wavelength behavior determined by "macroscopically" measured G and K.
- No free parms. in fit to low-q.

$(\lambda + G)\nabla (\nabla \cdot u) + G\nabla^2 u = 0$
Point response: scaling with pressure

As We Approach Jamming, Departure Occurs At Smaller $q$.

Transverse Is Less Dependent On Jamming
Point response: scaling with pressure

- Scaling function with pressure:
  \[ \xi_T \sim p^{-0.25} \]

- Long. scaling function more severe than transverse.

- \( S_L \sim q^2 \), \( S_T \sim q^1 \)

- Note: longitudinal scaling more severe than transverse.
Measurement 2: Constrained shear modulus

Detour: non-affine elastic formalism
Aside: non-affine elastic formalism

- Single particle toy problem:
  - Start at F=0

- CEM+Lemaître (PRL 2004)
Aside: non-affine elastic formalism

- Single particle toy problem:
  - Start at $F=0$
  - Apply affine shear
  - Forces remain zero
  - No correction necessary
Aside: non-affine elastic formalism

- Single particle toy problem:
  - Start at $F=0$
Aside: non-affine elastic formalism

- Single particle toy problem:
  - Start at $F=0$
  - Apply strain

Disordered Case
Aside: non-affine elastic formalism

- Single particle toy problem:
  - Start at $F=0$
  - Apply strain

Use Hessian to compute "Affine force"

\[ \vec{\Xi}_i = \gamma \sum_j H_{ij} \hat{x} \delta y_j \]
Aside: non-affine elastic formalism

- **Single particle toy problem:**
  - Start at $F=0$
  - Apply strain

Use Hessian to find position correction

\[
\vec{\Xi}_i = \mathbf{H}_{ii} \vec{d}r_i \\
\vec{d}r_i = \mathbf{H}_{ii}^{-1} \vec{\Xi}_i
\]
Aside: non-affine elastic formalism

• Back to full assembly:

\[ \vec{\Xi}_i = \gamma \sum_j H_{ij} \hat{x} \delta y_{ij} \]

• Measure of local disorder.

• Only short range correlations in our samples.
Force balance: Affine forces, $\Xi$, must be balanced by correction forces, $H^{-1}_{ij}dx_j$.

Aside: non-affine elastic formalism

Back to full assembly:

$$\vec{dr}_i = \gamma \sum_j H^{-1}_{ij} \vec{\Xi}_j$$
Aside: non-affine elastic formalism

- **Tangent modulus**

\[
\sigma = \frac{dU}{d\gamma} = \frac{\partial U}{\partial \dot{r}_{i\alpha}} \frac{d\dot{r}_{i\alpha}}{d\gamma} + \frac{\partial U}{\partial \gamma} = \frac{\partial U}{\partial \gamma} \\
\mu = \frac{d\sigma}{d\gamma} = \frac{\partial^2 U}{\partial \gamma^2} - \Xi_{i\alpha}H_{i\alpha j\beta}^1 \Xi_{j\beta} = \mu_a - \mu_{na}
\]

Crucial for this talk:
Non-affine motion gives negative definite correction to any physical modulus.

\( \mu_{\text{net}} < \mu_{\text{affine}} \text{ and } K_{\text{net}} < K_{\text{affine}} \) (but not necessarily \( \lambda \))

Parenthetical:
Tangent modulus goes to negative infinity at bifurcation points
Measurement 2: Constrained shear modulus

Detour finished... back to results
Measurement 2: Constrained shear modulus

- As usual: modulus, $\mu = \Delta \text{stress/strain}$
- Apply homogeneous shear at boundaries, but material responds inhomogeneously in interior
- Inhomogeneous motion always lowers $\mu$ relative to “naive” value
- Q) How big a chunk of material do I need before I converge to a well defined elastic modulus?
Measurement 2: Constrained shear modulus

- Small R, inhomogeneous corrections are suppressed (Cauchy-rule enforced).
- $\mu$ decays to $\mu_\infty$ as $R \to \infty$
- known: near $\phi_{rcp}$ $\mu(R=0) \to$ constant and $\mu(R=\infty)$ goes to zero.
- so what?: at $\phi=0.88$ $R=100$ gives $\mu$ to 10%, at $\phi=0.85$, need $R=500$!

- Simple scaling form: bulk vs. boundary says $\mu(R)/\mu-1 \sim 1/R$
- Collapse to $1/R$ form when R scaled by $p^{-0.5}$.
- Reminiscent of Goodrich rigidity percolation procedure and $l^* \sim 1/\Delta z \sim 1/p^{1/2}$
Measurement 3: Unconstrained (wave)

- Wave forcing: Impose external field
- Measure projected response to infer modulus: $\mu(\lambda)$

Inferred $\mu(\lambda)$ rapidly approaches bulk value.
Small $\lambda$ error can be understood as pseudo-Brillouin-boundary effects
Move it along... nothing to see here...
Recent update. Private conversation w/S Teitel... interesting scaling for $K(\lambda)$
Measurement 3: Unconstrained deformation

- Unconstrained homogeneous deformation with periodic boundary conditions.
- Moduli (both K and G) rapidly converge with system size to bulk values. (as in seminal work by O’Hern et. al. PRE 2003)
- Consistent with 2D Lennard-Jones (Tanguy et. al. PRB 2002)
Measurement 3: Unconstrained deformation ($\varphi=92\%$)

- Measure local dilatancy (longitudinal), $\Phi$, and local vorticity (transverse), $\omega$ in response to both compression ($\Phi_c, \omega_c$) and shear ($\Phi_s, \omega_s$).

- One or two dominant displacement quadrupoles (“STZ”s?) in a typical 320x320 box.

- Shear: disp. quadrupoles align (vertical compression, horizontal extension)

- Compression: quadrupoles random orient.

- $\Phi=92\%$ just like Lennard-Jones

- Effective-medium-like calculations (Didonna & Lubensky PRE 2005, Maloney PRL 2006) imply Gaussian random white noise for both $\Phi$ and $\omega$ fields. (Obvious: not strictly true)
Measurement 3: Unconstrained deformation ($\phi=85\%$)

- At $\phi=85\%$, dilatancy is less “coherent” in both compression and shear.

- Shear induced vorticity very similar to $\phi=92\%$. **VERY SURPRISING!** (Related to Ellenbroek, et. al. “sliding only” result?)

- Shear induced quadrupoles are no longer visible in long-range dilatancy field.

- Very small hint of compression induced quadrupoles in the vorticity (but not dilatancy)

- Idea: dilatancy must vanish outside STZ cores, but may be non-zero inside.
Measurement 3: Unconstrained deformation ($\varphi=92\%$)

- Power spectra for dilatancy (longitudinal) and vorticity (transverse)

- EMT says $q^2 S(q)$ should be flat and isotropic for both dilatancy and vorticity

- Clear deviations from both $S \sim q^{-2}$ and isotropy (compression response is isotropic by construction for $qL_{\text{cell}} \gg 1$)... that is: quadrupoles align with the shear.

- Anisotropy much more pronounced in dilatancy than vorticity (agreement with impression from real-space images).
Measurement 3: Unconstrained deformation

• Compression
• Shear

- Take isotropic average of \( \log(q^2S(q)) \)

- EMT says \( q^2S(q) \) should be flat and isotropic for both dilatancy and vorticity

- Clear deviations from both \( S \sim q^{-2} \) and isotropy (compression response is isotropic by construction for \( qL_{\text{cell}} >> 1 \))... that is: quadrupoles align with the shear.

- Anisotropy much more pronounced in dilatancy than vorticity (agreement with impression from real-space images).
Conclusions (Elasticity)

- **Method 1)** Point response:
  - $\xi_L \sim p^{-0.4}$, $\xi_T \sim p^{-0.25}$
  - hard to see $\xi_L$ since $G/K \to 0$ so $S_L/S_T \sim 0$
  - shape of scaling function $S(\xi q)$?

- **Method 2)** Constrained deformation:
  - $\mu(R)/\mu - 1 \sim 1/(Rp^{-0.5})$
  - analogous to rigidity-based approaches and $l^*$

- **Method 3)** Unconstrained deformation:
  - “Wave method” $G(\lambda)$
    - quick convergence $G_\infty$ beyond $\lambda \sim 5$
    - insensitive to $\phi_J$
    - (Should also check $K$)!
  - $S_T$
    - effective medium (uncorrelated strains) good approx
    - puzzle: insensitive to $\phi$!
  - $S_L$
    - effective medium only OK approx
    - details depend on $\phi$
    - “incoherent” beyond “shear zone size”.
    - peak position independent of $\phi$
    - shear transformation zones / soft spots???