

*Stress field equations in granular solids:
A shift of paradigm*

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Synopsis

- A key concept to the understanding of stress transmission in granular materials is the **Marginally Rigid State** and an experiment is described which establishes the relevance of this state.
- The **MRS** can be regarded as a critical point wherein a particular lengthscale diverges.
- Granular matter at the **MRS** is statically determinate (isostatic), **obviating** elasticity theory.
- A new theory – isostaticity theory - is formulated for stress transmission at the **MRS**. Isostaticity explains the force chains, frequently observed in experiments, and makes it possible to predict their trajectories.
- A new set of equations is presented for the yield flow of granular matter.

Overview

- The problem
- Marginal rigidity and isostatic states in granular matter - experimental evidence
 - Mean coordination number and density
 - Yield layer and critical behaviour
- The isostatic state and elasticity theory
- Constitutive stress-structure equations - Isostaticity theory
- Solutions in 2D and emergence of force chains
- Structure-property relations
- Yield flow equations for marginally rigid granular matter

The state of granular matter and the coordination number

- Granular matter behaves sometimes as fluid, sometimes as solid and often as both simultaneously
 - Why? What determines the state? Are there other states? What are the behaviours in the various states?
- Essential to understand stress transmission
- A key parameter on the grain scale is the mean coordination number (mean contact number), Z
- In principle, the intergranular contact forces are statically determinate when $Z = Z_c$:

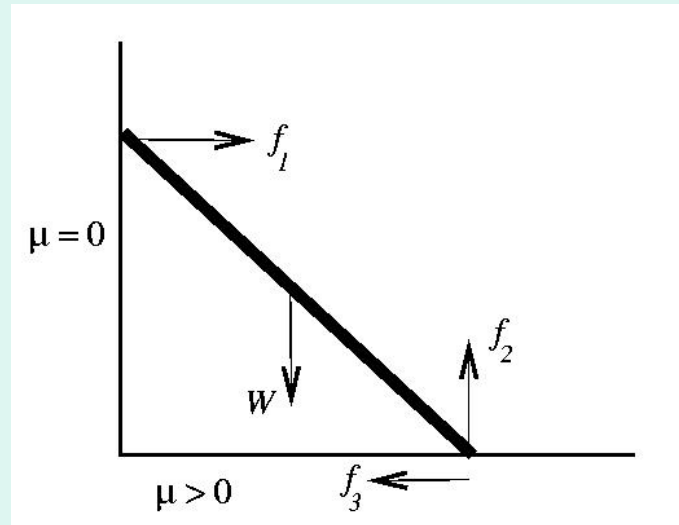
$Z_c = 3$ in $2D$ (4 in $3D$) - rough arbitrary grains

$Z_c = 6$ in $2D$ (12 in $3D$) - smooth arbitrary grains

$Z_c = 4$ in $2D$ (6 in $3D$) - smooth spherical grains

A familiar example of a statically determinate system.

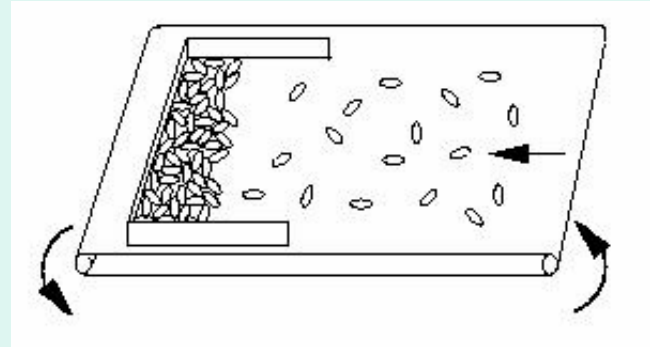
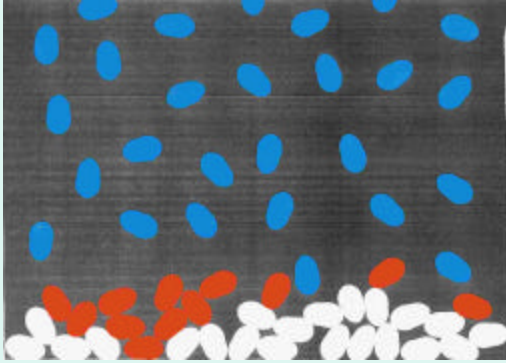
The forces f_1, f_2, f_3 are determined from balance conditions alone.



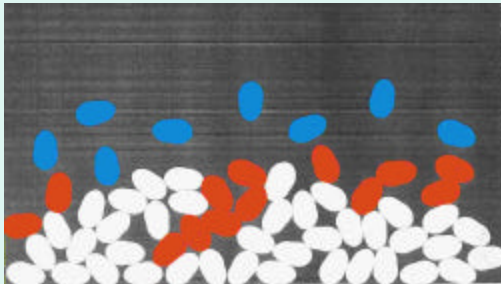
-
- $Z < Z_c$ - the forces are overdetermined, the structure is mechanically unstable → **Fluid**
 - $Z > Z_c$ - the forces are underdetermined, additional conditions are required → **Solid**
 - $Z = Z_c$ - the forces are exactly determined → **Marginal rigidity**
 - Is the isostatic state physically realisable? Is it relevant for practical purposes?

A Simple experiment

(RB, Ball, Edwards, *Nature*, kicking about)



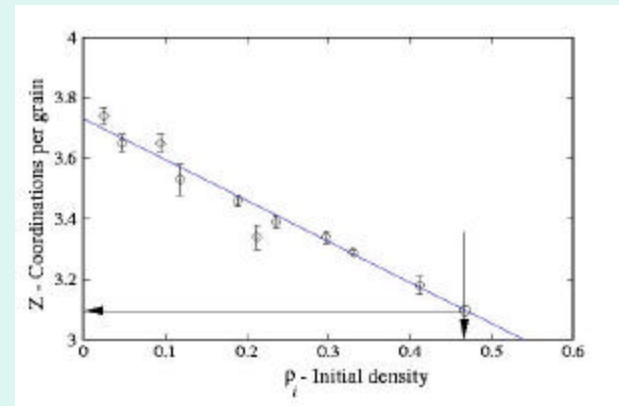
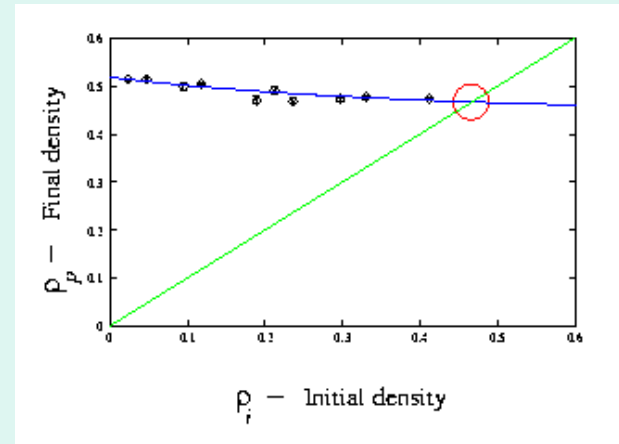
(*up*) Sketch of the experimental setup: grains are conveyed by a moving surface towards a stationary collector of similar material. The grains are effectively rigid, with high mutual friction, and the slow advance rate minimises inertial effects.



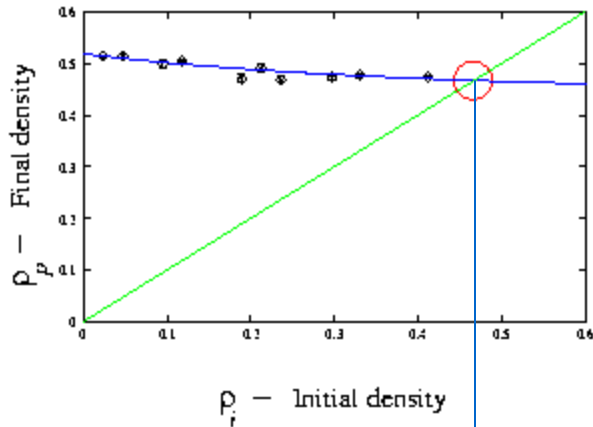
(*left*) The growth of a pile, with time running from top image to bottom. The grains coloured blue are ‘free-falling’ towards the growing pile. The white grains have come to permanent rest. Friction relative to the moving base supplies an analogue of gravitational force. The red grains have not fully consolidated.

Results I: pile density and coordination number

1. The pile density, ρ_p , decreases with increasing the initial density of falling particles – this a fingerprint of jamming!
2. The coordination number, Z , also decreases with increasing initial density
3. $Z(\rho_i \rightarrow 0) \rightarrow 3.7$ in good agreement with the sequential deposition value $4-e$

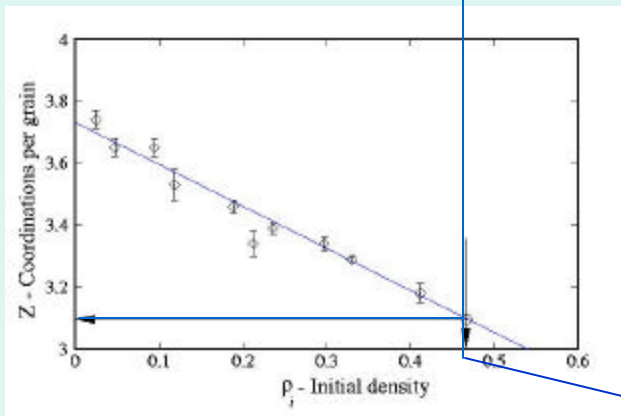


Final pile density, ρ_p , vs ρ_i



The line interpolates the experimental points.
The circled point is where the initial and final densities extrapolate to equal [$\rho_c = 0.465(5)$].
 ρ_c is the natural limiting density of the experiments.

Final pile mean coordination number, z , vs ρ_i

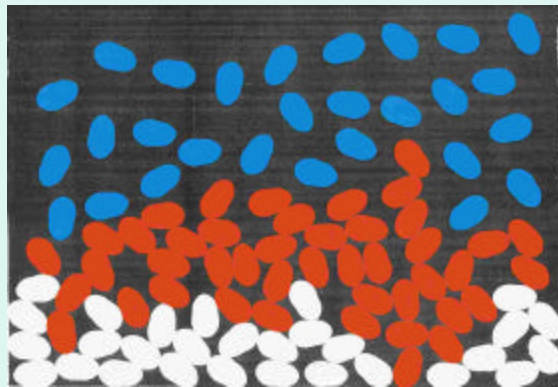
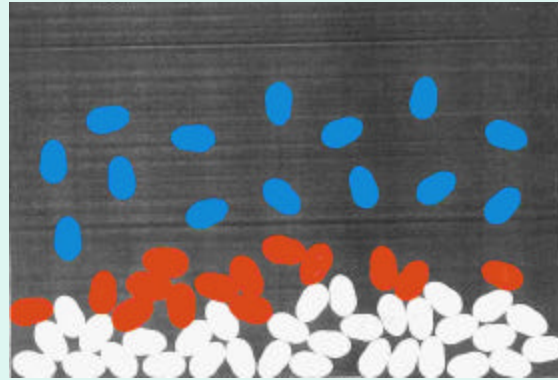
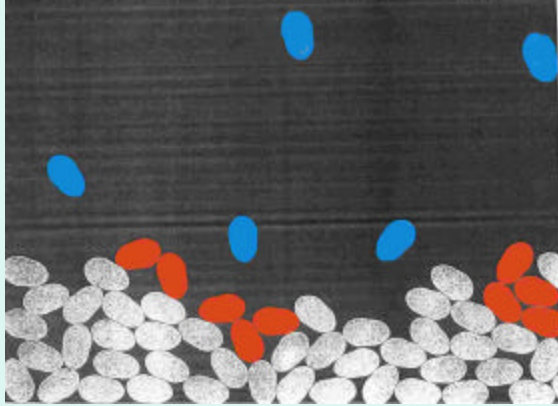


$Z(\rho \rightarrow \rho_c) \rightarrow 3.1$ in good agreement with **MRS** value.
 $Z(\rho \rightarrow 0) \rightarrow 3.7$ in good agreement with theoretical sequential deposition value.

Interpretation: at ρ_c the pile is marginally rigid -

MRS

Results II: The yield front

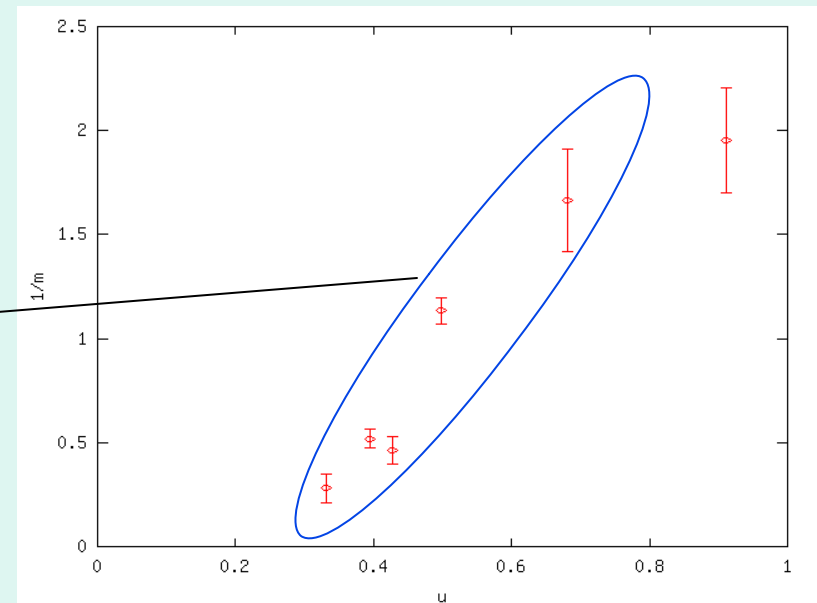


The front (coloured **red**) of grains that have encountered the pile but not yet reached their final consolidated positions. Three different experiments are shown at initial densities: 0.024 (top), 0.142 (middle), and 0.236 (bottom). At the low density the front is less than one grain deep; at the high density it is more than half the pile and the consolidation is highly cooperative.

1. The size of the yield front becomes as large as the pile when $\mathbf{r} \rightarrow \mathbf{r}_c$, implying divergence
 $\Rightarrow \mathbf{r}_c$ is a **critical point**

2. Effective medium analysis:
 - (a) The front propagates at a speed $v = v_0 \mathbf{r}_i / (\mathbf{r}_p - \mathbf{r}_i)$
 - (b) The front size $m \propto (\mathbf{r}_p - \mathbf{r}_i)^{-1}$

Consistent with our effective medium analysis which predicts a straight line (but not too close to the origin)



A plot of $1/m$ vs $u = (\rho_p - \rho_i) / (\rho_p + \rho_i)$.

The stress field - back to basics

In d -dimensions force balance translates into

$$\operatorname{div} \boldsymbol{\sigma} = \boldsymbol{g}_{ext} \rightarrow d \text{ equations}$$

Torque balance translates into

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T \rightarrow d(d-1)/2 \text{ equations}$$

To solve for the stress we need $(d \times d)$ equations

$$\begin{aligned} \Rightarrow & d(d-1)/2 \text{ further equations required} \\ & = \text{one in 2D, three in 3D} \end{aligned}$$

Why not use elasticity theory?

Conventional elasticity theory teaches:

Impose compatibility (Saint Venant) conditions on the strain,

e.g. in 2D

$$\mathbb{I}_{xx}e_{yy} + \mathbb{I}_{yy}e_{xx} - 2\mathbb{I}_{xy}e_{xy} = 0$$

Next relate the strain to the stress, $\boldsymbol{\sigma} = \boldsymbol{\sigma}(e)$

e.g.
$$\sigma_{ij} = C_{ijkl}e_{kl}$$

This conveniently gives a constitutive closure of the equations

Or does it?

The conundrum

- In isostatic systems the contact forces can be uniquely determined from balance equations alone (static determinacy)
⇒ no additional (in particular compliance) information required
- The macroscopic stress field is a continuous coarse-grained description of the discrete field of contact forces
⇒ no additional information required to determine the stress
- It follows that **stress-strain relations are redundant!**

- Question: How do we close the stress field equations for isostatic systems without stress-strain relation?
- The global balance equations relate the stress only to external fields (force, torque) \Rightarrow the closure must involve constitutive data.
- The only constitutive information available is the structure.
- **Conclusion:** the closure, or ‘missing equations’, must comprise relations between **stress** and **structure**.

The constitutive equation in planar systems

Ball and RB, *Phys.Rev.Lett.* **88**, 11505 (2002); RB, *J. Phys. A* **36**, 2399 (2003);
RB, *Physica A* **336**, 361 (2004)

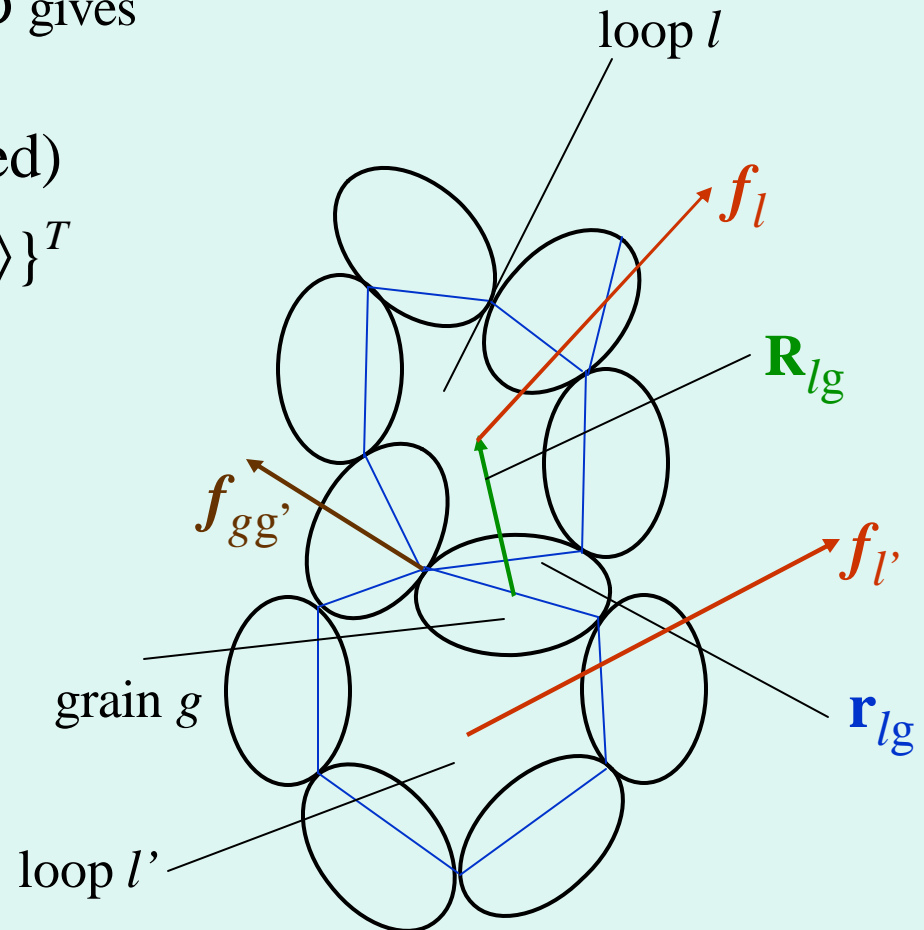
A new theory for isostatic systems in 2D gives **two conditions** from torque balance:

- (i) $\langle \sigma \rangle = \langle \sigma \rangle^T$ (as expected)
- (ii) $\{P \varepsilon^{-1} \langle \sigma \rangle\} = \{P \varepsilon^{-1} \langle \sigma \rangle\}^T$

Where $\varepsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

and $p_{ij} = \frac{1}{2} \sum_{l \in g} (r_i^{lg} R_j^{lg} + r_j^{lg} R_i^{lg})$

is a new geometric tensor



Explicitly, the new constitutive equation reads:

$$p_{xx}\sigma_{yy} + p_{yy}\sigma_{xx} - 2p_{xy}\sigma_{xy} = 0 \quad \text{or} \quad \mathbf{Q} : \mathbf{S} = 0$$

$$Q_{ij} \equiv (\varepsilon^{-1})_{ik} p_{kn} \varepsilon_{nj}$$

Interpretation

- * p_{ij} is the symmetric part of $C_{ij} = \sum_l \mathbf{r}_i^{lg} \mathbf{R}_j^{lg} = P_{ij} + A \varepsilon_{ij}$
- * It characterises geometric **fluctuations** around grains on a **mesoscopic** (\sim few grains / loops) scale
- * The constitutive equation couples the stress to local structural information; **stress-structure** relation

Stress propagation and force chains

(*RB, Phys.Rev.Lett.*, 93, 108301 (2004))

Question:

How to understand and predict force chains from a continuous theory of stresses?

The field equations

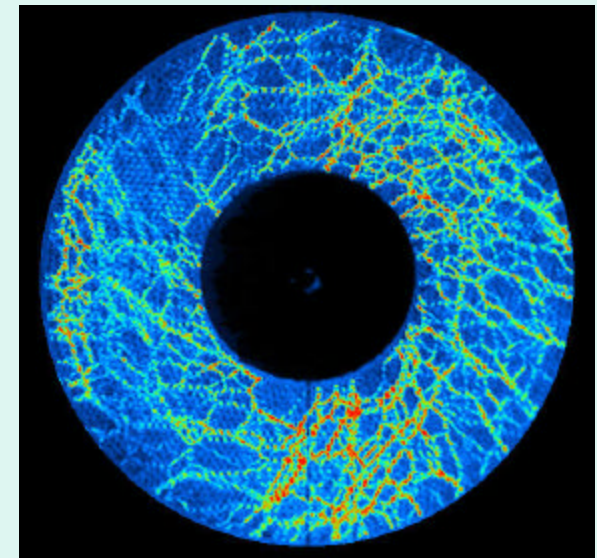
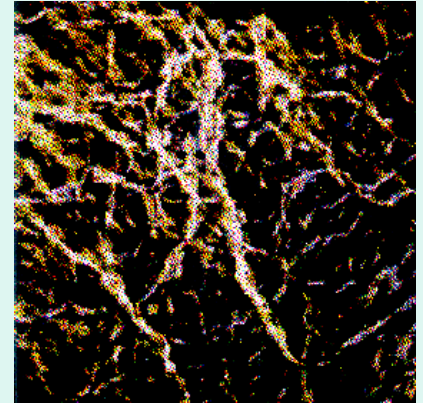
$$\mathbb{I}_x \sigma_{xx} + \mathbb{I}_y \sigma_{xy} = g_1$$

$$\mathbb{I}_x \sigma_{xy} + \mathbb{I}_y \sigma_{yy} = g_2$$

$$p_{xx} \sigma_{yy} + p_{yy} \sigma_{xx} - 2p_{xy} \sigma_{xy} = 0$$

The latter is the (non-trivially) **coarse-grained** form of the mesoscopic constitutive equation

(*R.B., Physica A 336*, 361 (2004))



Under a suitable change of variables

$$\begin{pmatrix} u \\ v \end{pmatrix} = M(p_{ij}) \bullet \begin{pmatrix} x \\ y \end{pmatrix}$$

The equations for the σ_{ij} become

$$\left(\frac{\partial^2}{\partial u^2} - \frac{\partial^2}{\partial v^2} \right) \sigma_{ij} = f_{ij} \left(P_{ij}, \frac{\partial g_a}{\partial x_b} \right)$$

This equation is **hyperbolic*** (resolving a long-standing dispute)

Its solutions propagate as **meandering** (not diffusive-like!) **force chains** along characteristic trajectories $u \pm v$

Structure-property relationship

- The conventional approach:
 - Find a general relation between the microstructure and a stress-strain relation (e.g. elastic constants in linear elasticity)
 - Upscale the relation by integration over small-scale degrees of freedom, to obtain a macroscopic relation $(C_{eff})_{ijkl}$
- Isostaticity theory redefines the structure-property problem in granular materials:
 - The ‘property’ is the local value of the geometric tensor P .
 - No need to go to derive elastic constants from the structure and coarse-grain those; all we need is to coarse-grain P directly.
 - The coarse-graining is not trivial (RB, *Physica A* **336**, 361 (2004)).

Relations between isostaticity and elasticity

Start from an unstrained system and strain slightly

$$\nabla \cdot \boldsymbol{\sigma} + F_{\text{ext}} = 0$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$$

Elasticity theory

$$\mathcal{I}_{xx} e_{yy} + \mathcal{I}_{yy} e_{xx} - 2\mathcal{I}_{xy} e_{xy} = 0$$

$$e_{ij} = D_{ijkl} \sigma_{kl}$$

Isostaticity theory

$$p_{xx} \sigma_{yy} + p_{yy} \sigma_{xx} - 2p_{xy} \sigma_{xy} = 0$$

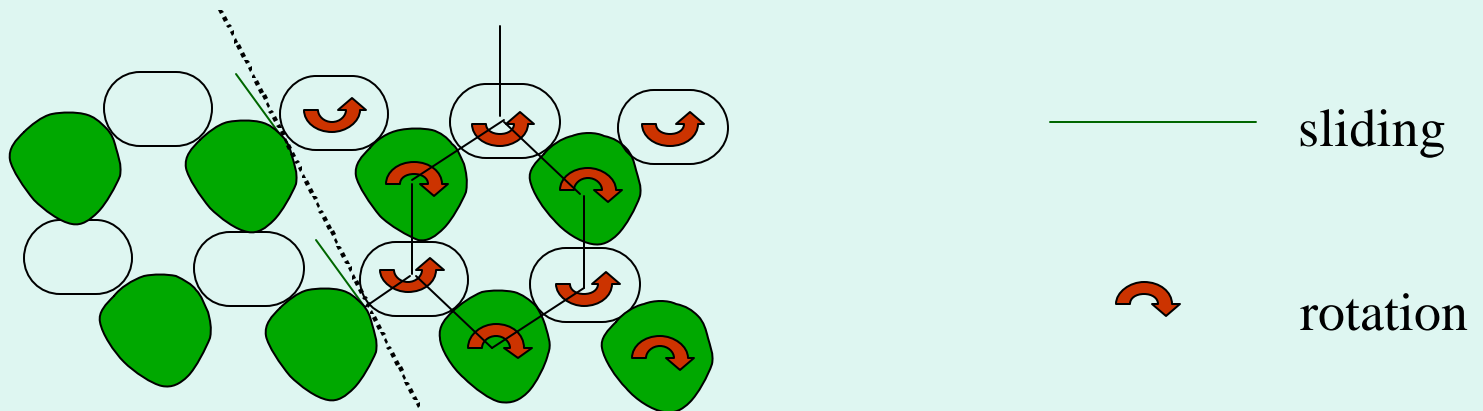
D is constrained by P

Can we find $D(P)$?

Understanding the yield front:

Yield flow equations

- Grains can either roll or slide on one another
- Both mechanisms contribute to the strain rate



- In lattices* the contributions can be separated

* *In fact, true in all systems possessing a staggered order*

- The following yield equations are exact for systems with staggered order and a conjecture for general (3D) systems

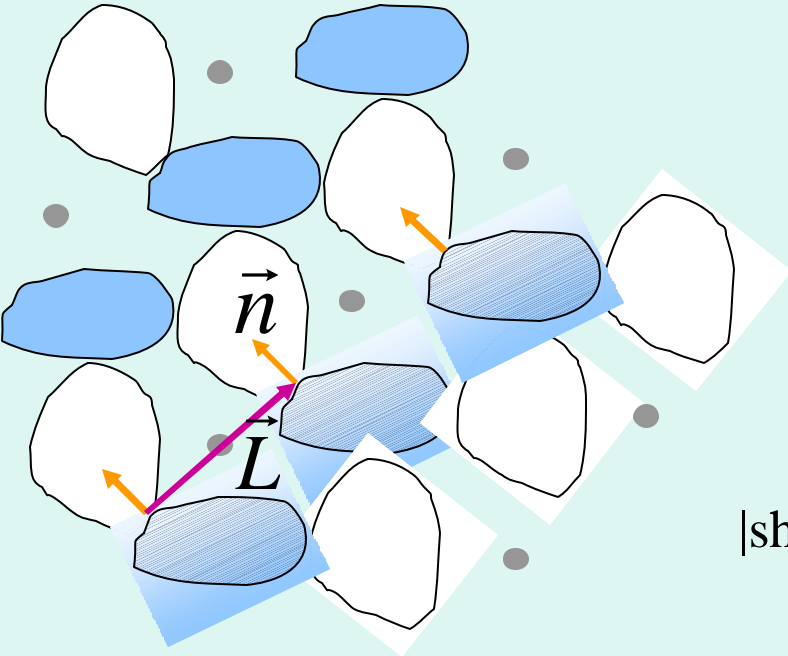
Traditional plasticity

Grain rolling

- 1. $\partial_i u_j + \partial_j u_i = A(\mathbf{r}, t) g_{ij}(\mathbf{s}) + \omega_{kl}(\mathbf{r}, t) q_{ijkl}(\mathbf{r})$

- The coefficients $q_{ijkl}(\mathbf{r})$ are **exactly** the components of the tensor $Q(\mathbf{r})$ of the constitutive equation
- Note: multiplying the equation by σ and expecting no energy dissipation due to pure rolling gives the static constitutive equation

$$q_{ijkl}(\mathbf{r}) \sigma_{ij} = 0 \quad \text{or} \quad Q : \mathbf{s} = 0 !$$



Condition for sliding at plane:

$$|\vec{n} \times \vec{S} \times \vec{L}| > \mathbf{m} (-\vec{n} \cdot \vec{S} \times \vec{L})$$

|shear force|

coeff friction

normal force

$$Y(\vec{S}) = \prod_{\text{sliding planes}} \left(|\vec{n} \times \vec{S} \times \vec{L}| + \mathbf{m} \vec{n} \cdot \vec{S} \times \vec{L} \right) > 0 \quad \text{yielding}$$

$$Y(\vec{S}) = 0 \quad \text{creeping yield} \Rightarrow \text{plastic flow,} \quad \text{direction} = g(\vec{S})$$

$$Y(\vec{S}) < 0 \quad \text{unyielding}$$

This equation is supplemented by:

The yield locus criterion

Force balance

The ‘constitutive’ relation

$$2. Y(\mathbf{s}) = 0$$

$$3. \mathbf{div} \boldsymbol{\sigma} + \mathbf{F}_{ext} = 0$$

$$4. q_{ijkl}(\mathbf{r}) S_{kl} = 0$$

Major advantage:

The number of unknowns is exactly equal to the number of equations. No need for undetermined internal variables.

<i>Variable</i>	<i>Unknowns</i>	<i>Equations</i>
\mathbf{s} (symmetric tensor)	$d(d+1)/2$	1. Strain rate kinetics
A (scalar)	1	2. Yield criterion
\mathbf{u} (vector)	d	3. Force balance
$\boldsymbol{\omega}$ (angular velocity)	$d(d-1)/2$	4. Constitutive equations
	$d^2 + d + 1$	

Summary

- The state of granular matter is directly related to the intergranular **coordination number**, Z .
- An experiment establishes existence and relevance of **marginal rigidity**:
 - The density and coordination number of consolidated piles decrease with increasing density of falling grains, reaching **MRS** at a critical density
 - The size of the yield layer between the falling grains and the consolidating pile **diverges** at the critical density
- A new **isostaticity theory** gives the stress equations in $2D$ isostatic systems
- The theory predicts **propagating force chains**

- Relations between elasticity and isostaticity theories
- Equations for the **yield** and failure of granular matter

Extensions / future work

- Extension to **non-isostatic** granular systems - *in progress*
- Stress-structure relations and isostaticity theory in **3D** – *in progress*
- Stress field solutions in 3D - any force chains there?
- The new theory simplifies the problem of **structure-property** relationship in isostatic solids, but it also makes it possible to derive new relationships between the elastic constants and the geometric tensor – *not much progress*
- Many applications: advanced materials, metal foams, biomaterials, porous media - *in progress*
- Coarse-graining and applications of the **yield equations**– *in slow progress*

Collaborators:

Prof. Sir Sam Edwards, Cavendish Laboratory

Prof. Robin Ball, Warwick University

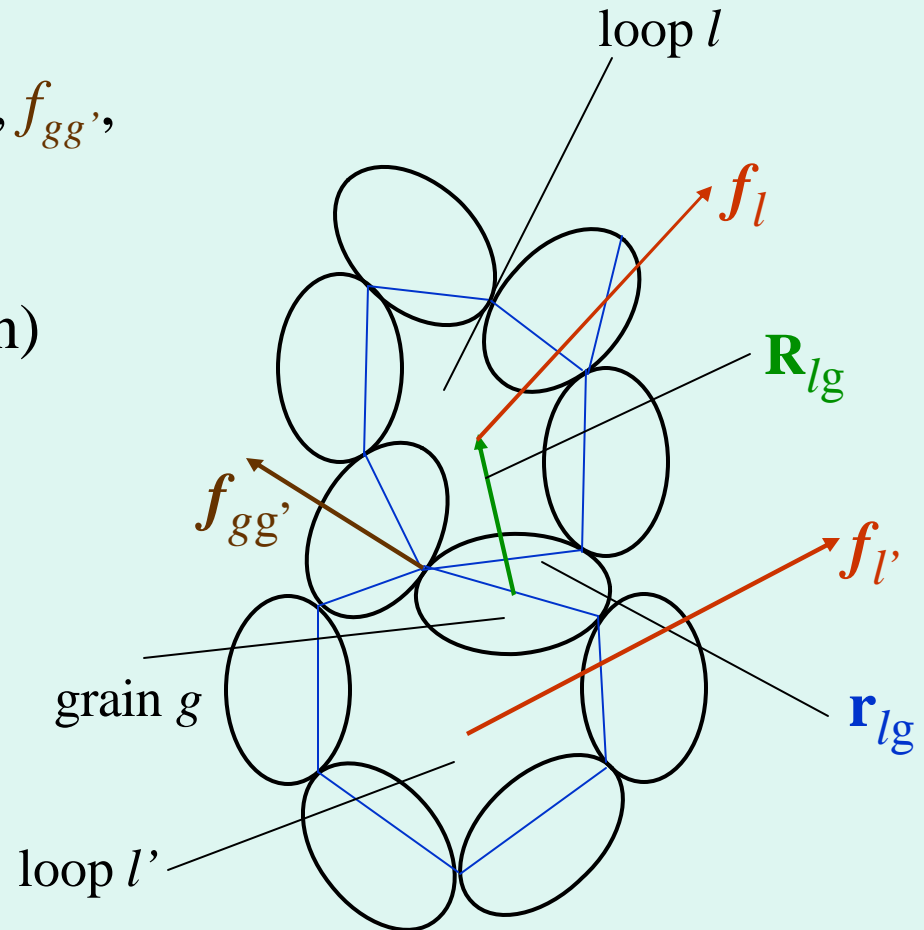
The constitutive equation in planar systems

1. Construct the vectors \mathbf{r}_{lg} and \mathbf{R}_{lg}
2. Assign each loop a force f_l
3. Parameterise the granular forces, $f_{gg'}$,
in terms of the loop forces f_l :

$$f_{gg'} = f_{l'} - f_l \text{ (note sign convention)}$$

Advantages:

- a. The loop forces automatically satisfy force balance
- b. They automatically satisfy Newton III
- c. Coarse-graining - fewer loop forces than granular forces



4. Interpolate the loop forces piecewise linearly around each grain into a continuous field $f_g = f(x_g)$

5. The stress around grain g is the (normalised) force moment

$$S_g^{ij} = \sum_l r_{lg}^i f_l^j$$

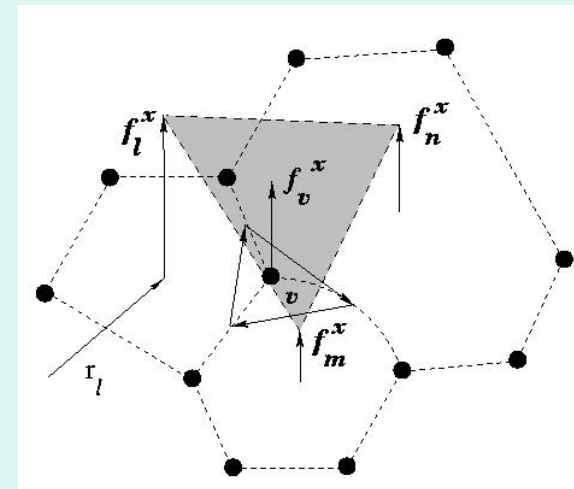
6. In terms of the continuous field

$$S_g = \sum_l r_{lg} (f_g + \mathbf{R}_{lg} \cdot \tilde{\mathbf{N}} f_g) = \mathbf{C}_g \cdot \tilde{\mathbf{N}} f_g$$

where

$$\mathbf{C}_g = \sum_l r_{lg} \mathbf{R}_{lg} = \mathbf{P}_g + \mathbf{A}_g \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

is a new geometric tensor.



The stress is the force moment normalised by the area

7. Over any connected part of the system, Γ

$$\boldsymbol{\sigma}_\Gamma = \langle \mathcal{S}_g \rangle_\Gamma = \langle \mathbf{C}_g \cdot \tilde{\mathbf{N}} f_g \rangle_\Gamma = \langle \mathbf{C}_g \rangle_\Gamma \cdot \langle \tilde{\mathbf{N}} f \rangle_{\partial\Gamma}$$

8. Impose now torque balance

$$\{ \mathbf{C}_g \boldsymbol{\varepsilon}^{-1} \langle \boldsymbol{\sigma} \rangle \} = \{ \mathbf{C}_g \boldsymbol{\varepsilon}^{-1} \langle \boldsymbol{\sigma} \rangle \}^T$$

This gives **two** conditions:

(i) $\langle \boldsymbol{\sigma} \rangle = \langle \boldsymbol{\sigma} \rangle^T$ (as expected)

(ii) $\{ P \boldsymbol{\varepsilon}^{-1} \langle \boldsymbol{\sigma} \rangle \} = \{ P \boldsymbol{\varepsilon}^{-1} \langle \boldsymbol{\sigma} \rangle \}^T$

\Rightarrow

$$p^{xx} \sigma_{yy} + p^{yy} \sigma_{xx} - 2p^{xy} \sigma_{xy} = 0 \quad \text{or} \quad \text{Tr}[(\mathbf{e} \mathbf{P} \mathbf{e}^{-1}) \times \mathbf{S}] = 0$$

