Stress in particulate media - theory
Synopsis

This short course aims to introduce postgraduate students to the physics, current modelling, and open questions of stress transmission in an important family of soft systems – particulate, granular and dense colloidal systems.

First, I will define the systems included within this remit and their distinction from conventional particle systems. Then, I will explain why this class of systems is important to study and introduce their strange stress transmission, which differs significantly from conventional matter.

I will then focus on an ideal class of dry particulate and dense colloidal systems - isostatic structures - and show why conventional elasticity theory is invalid for them. A first principles stress field theory – isostaticity theory - will be then introduced for these materials and we will discuss the stress fields, to which it gives rise. Misconceptions about this theory and its stress solutions will be discussed and a recent improvement in the theory for cylindrical geometries will be shown to be much more relevant to granular systems than the initial formulations.

Finally, I will outline directions in which the field needs to advance, the difficulties involved, and my own ideas how to extend the theory to realistic non-isostatic particulate systems.
# Stress in particulate media - theory

## 1. Synopsis

## 2. Table of contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Synopsis</td>
<td>2</td>
</tr>
<tr>
<td>2. Table of contents</td>
<td>3</td>
</tr>
<tr>
<td>3. Introduction</td>
<td></td>
</tr>
<tr>
<td>What do we mean by particulates and granular matter</td>
<td>5</td>
</tr>
<tr>
<td>Ubiquity and types of particulate materials</td>
<td>6</td>
</tr>
<tr>
<td>Unique features and properties of granular materials</td>
<td>12</td>
</tr>
<tr>
<td>The significance of particulates and granular materials</td>
<td>17</td>
</tr>
<tr>
<td>The strange physics of particulates and granular materials</td>
<td>19</td>
</tr>
</tbody>
</table>
4. Stress theory of particulate matter ........................................
   The Janssen model ..............................................................
   Isostatic systems ..............................................................
   Failure of theories based on stress-strain relations ............
   The stress field equations ...................................................
   Isostaticity theory ............................................................
   Aside: quantitative description of disordered particulate structures ..
   Voronoi tessellations .........................................................
   The Quadron tessellations ..................................................
   Closure of the isostaticity stress equations: 2D ..................
   General solution to the isostaticity stress equations
   .
   .
   .

5. Extension of isostaticity theory to real granular matter – stato-elasticity

Acknowledgments
What do we mean by particulate and granular matter?

- These are a family of soft matter, which is a subfield of condensed matter. Other soft systems include liquids, colloids, polymers, foams, gels, and most biological systems.

- In this course we focus on particulate, granular systems and, under some conditions, dense colloidal systems.

- A very broad range of relevant lengthscales, often much larger than atomic – often mesoscopic and sometimes macroscopic.

- The predominant techniques used in soft matter come from classical and statistical physics; quantum mechanics will not therefore be useful here.
Particulate matter (PM) is all around us

- The name particulate systems refers to a broad class of materials: sand, rocks, aerosols, dense colloidal suspensions, nano-particles, food stuff, powders, viruses, microbes.
The name *particulates* refers to a broad class of materials: sand, rocks, aerosols, dense colloidal suspensions, nano-particles, food stuff, powders, viruses, microbes.
The name *particulates* refers to a broad class of materials: sand, rocks, aerosols, dense colloidal suspensions, nano-particles, food stuff, powders, viruses, microbes.
• Most particulate and granular materials are immersed in a fluid, which could be gas or liquid.

• The particles distribution in space depends on the relative mass densities, which leads to buoyancy or sedimentation, and particle number density, which determines inter-particle interactions.
Types of PM

- We distinguish between dry PM, e.g. sand in the desert, and wet, e.g. beach sand near the waterline.
- The main difference between the two is in the inter-particle interactions:
  - in dry PM the interaction is hard-core if the particles are rigid or a combination of hard-core and elastic if they are not
  - in wet materials it can be hard-core at the smallest range, hydrodynamically-mediated if the particles move in a liquid, or capillary attraction if there are liquid ‘necks’ between particles otherwise immersed in air
  - The relative mass and number densities also affect interactions with external fields, such as gravitational, electrostatic and magnetic

Most of the theoretical analysis in this course will be on dry systems.

However, it must be remembered that most PM, which we call dry, is actually a suspension!
Unique features and behaviour of PM

- Most dry PM of interest on Earth is not affected by thermal fluctuations – it is non-Brownian.
- Thermal fluctuations are important only if they can move particles distances that are comparable, or larger, than their own size.

Example:
The size of a grain of sand is

\[ l \approx 0.5 \text{mm} \approx 5 \times 10^{-4} \text{m} \]

Its mass (assuming it is mostly quartz) is

\[ m \approx 0.5 \text{µg} \approx 5 \times 10^{-7} \text{Kg} \]

The energy required to raise it to a height equal to its own size is

\[ E = mgl \approx 25 \times 10^{-10} \text{N} \times m \approx 2.5 \text{nJ} \approx k_B \times (1.8 \times 10^{14} \text{K})! \]
Thermal energy, gravitational potential energy, and size

\[ \frac{E_P}{E_T} = \frac{\rho gl^4}{k_B T} > 1 \]

\[ \frac{\rho gl^4}{k_B T} \ll 1 \]
• Thermal fluctuations at room temperature (Brownian motion) can only affect particles smaller than

\[ E = mgl = \rho gl^4 \approx k_B T \Rightarrow l \approx \left( \frac{k_B T}{\rho g} \right)^{1/4} \approx 0.7 \mu m \]

• Dry particles interact via repulsive potentials

- **Hard-core** potential

\[ V(r) = \begin{cases} \infty & r < a \\ 0 & r \geq a \end{cases} \]

- **Elastic** potential

\[ V(r) = \begin{cases} \frac{1}{2} k (r - a)^2 & r < a \\ 0 & r > a \end{cases} \]

- **Hertz** potential

\[ V_{3D}(r) = \begin{cases} C (r - a)^{5/2} & r < a \\ 0 & r > a \end{cases} \]
• Unlike molecular particles, the range of the interactions in dry PM is much smaller than the particle size

• Unlike molecular particles, the interactions in dry PM can be central (frictionless particles) or non-central (frictional particles)

• Examples of frictionless particles
  – Emulsions, e.g. oil droplets in water

• Examples of frictional particles
  – Sand, rocks, cereals, most foods,…

*From the work of Brujic*
• Unlike molecular particles, in PM the particles have **internal degrees of freedom** (variables). This has several implications:

I. the interaction may dissipate energy through **rubbing** (and rolling) friction during slow dense flow

II. **collisions** dissipate energy – often occur during fast flows; energy dissipation is parameterised by a **restitution coefficient**

III. the particles may have a **surface topography**, i.e. shape, roughness

• For hard-core interaction we need to define the concepts of contact and touching
  
  – nothing in nature really touches; granular particles are considered to be in contact when the distance between their surfaces at some region of space is below their surface roughness and comparable to the range of Van der Waals forces
  
  – the region where this touching occurs is the ‘**contact**’ and it is shared by both particles
Significance of PM

- PM are abundant in nature and in human society
  - Powders in nature (snow) and in the industry
  - processing of food, mineral, metal, laundry products, …
  - grounds, coffee beans, sand, gravel, cereals, agricultural grains and seeds, pharmaceutical products, boulders, rings of Saturn, …

- PM are significant economically
  - in the chemical industry: about ½ the products and over ¾ of the raw materials are in particulate form
  - in the chemical industry: particulate technology in the USA alone engages over $60 billion
  - 1.3% of all USA electrical power goes toward grind particles and ores
  - 10% of the world’s energy supply goes toward handling particulates
  - in Mexico, 5 million tonnes of corn are handled every year; 30% of these grains are lost because of inefficient handling and transportation methods
  - over 50% of the world’s energy resources are extracted from GM, such as soils and rocks
- **PM are important to health and hazard prevention**
  - Land- and mud-slides cause annually damages of up to $2 billion and over 25 fatalities in the USA
  - California lost $140 million in 1997-8 to land slide damages
  - over 1000 silos, bins and hoppers collapse or fail in the USA every year

- **PM exhibit very rich behaviour**
  - behave sometimes as **fluid**, sometimes as **solid**, and often as both states simultaneously
Physics of PM

- PM dynamics lead to rich and exquisite pattern formation
• PM seems to be a *state of matter* in its own right
  ➢ The state of matter is commonly determined by the way the medium responds to stress
    ✓ gas has to be contained otherwise it disperses
    ✓ under gravity liquid assumes the shape of the container
    ✓ solids first deform and then support the stress
  ➢ So, to determine the state of matter we need to understand how GM transmit stress; this will be the focus of this course.

• Pose unique fundamental problems - difficult to model theoretically
  ➢ the physics is well understood on the scale of single particles – but the coarse-graining to the continuum is more difficult than for traditional phases of matter
  ➢ we need continuous theories is in three main directions:
    ✓ stress transmission;
    ✓ statistical mechanics
    ✓ flow dynamics
Physics of granular systems

Sir Sam F. Edwards (1928 - 2015)
Cavendish Professor 1984-1995
winner of many medals and prizes in physics

His two papers with Oakeshott jump-started the field of granular science in the physics community


(Notice the low impact factor of these journals, in contrast to the high impact these papers had in Physics)
Rich statics and peculiar stress transmission

From the works of the groups of: Behringer, Nagel, Revuzhenko
Quasi-statics: stick-slip structural organisation

From the works of Behringer’s group
A silo collapse.
This happens because we don’t understand well enough how PM support and transmit forces (stress).
Arching and force chains

From the work of Behringer’s group
Rich behaviour: peculiar dynamics and patterns
Stress theory

Experimental observations of non-uniform stresses

Difficult to explain with conventional theories

In particular, elasticity theory fails

*From the work of Behringer’s group*
A silo collapse.
This happens because we don’t understand well enough how PM support and transmit stress.

This collapse is because most of the weight is supported by the silo walls, rather than by the silo base.
A phenomenological model: Janssen model

\[ \sigma_{zz} = \sigma_0 - \sigma_1 e^{-h/h_0} \]

Engineering-based; we will not go over it in this short course because we aim at a more fundamental approach.
Stress theory

Experimental observations of non-uniform stresses

Difficult to explain with conventional theories

In particular, elasticity theory fails

To understand why that is let us consider ideal systems – *isostatic* packings

*From the work of Behringer’s group*
Isostatic systems

In an isostatic state a packing of grains is statically determinate (SD)!
This means that the inter-granular forces can be determined from balance conditions alone.

Question:
What are the conditions for a packing to be statically determinate?
Coordination number and isostatic states: 2D

\[ N = \text{number of grains} >> 1 \]

\[ z_g = \text{number of contacts of grain } g \]

\[ \bar{z} = \frac{1}{2} \sum_g z_g = Nz_c = \text{total number of contacts} \]

Number of unknowns = vector components

Force balance

\[ \left( \frac{1}{2} N\bar{z} \right) 2 = N[2+1] \rightarrow \bar{z} = 3 \]

\[ \frac{1}{2} N\bar{z} = N[2+1] \rightarrow \bar{z} = 6 \]

\[ \frac{1}{2} N\bar{z} = 2N \rightarrow \bar{z} = 4 \]

- rough arbitrary grains
- smooth arbitrary grains
- smooth spheres
Coordination number and isostatic states: $d$ dimensions

$N = $ number of grains $\gg 1$

$z_g = $ number of contacts of grain $g$

$\frac{1}{2} \sum_g z_g = N z_c = $ total number of contacts

$d = $ dimension

Number of unknowns = vector components

Force balance

Torque balance

- rough arbitrary grains

- smooth arbitrary grains

- smooth spheres
Important conclusion: For a packing to be statically determinate it is sufficient that the mean number of force-carrying contacts per grain (or the mean coordination number), $\bar{z}$, attains a particular value – $z_c$.

$$z_c = \begin{cases} 
  d(d+1) & \text{rough grains} \\
  d + 1 & \text{smooth non-spherical grains} \\
  2d & \text{smooth spherical grains} 
\end{cases}$$

Assumptions in the above calculations:
1. particles are convex, i.e. grains can only contact at one ‘point’;
2. there is no redundancy of torque balance equations
Important conclusion: For a packing to be statically determinate it is sufficient that the mean number of force-carrying contacts per grain (or the mean coordination number), $\bar{z}$, attains a particular value – $z_c$.

$z_c$ is (in principle) the lowest possible value for which the packing can be mechanically stable. Such states are marginally rigid – they are on the verge of failure.
Important conclusion: For a packing to be statically determinate it is sufficient that the mean number of force-carrying contacts per grain (or the mean coordination number), $\bar{z}$, attains a particular value – $z_c$.

$z_c$ is (in principle) the lowest possible value for which the packing can be mechanically stable. Such states are *marginally rigid* – they are on the verge of failure.

$\bar{z}$ is a key parameter:
- $\bar{z} < z_c$ – forces are overdetermined, the structure is unstable $\rightarrow$ *Fluid*
- $\bar{z} > z_c$ – forces are underdetermined, the structure is unstable $\rightarrow$ *Solid*
- $\bar{z} = z_c$ – forces are exactly determined, $\rightarrow$ *Marginally rigid, SD=isostatic*
Important conclusion: For a packing to be statically determinate it is sufficient that the mean number of force-carrying contacts per grain (or the mean coordination number), $\bar{z}$, attains a particular value $- z_c$.

$z_c$ is (in principle) the lowest possible value for which the packing can be mechanically stable. Such states are marginally rigid – they are on the verge of failure.

$\bar{z}$ is a key parameter:

$\bar{z} < z_c$ – forces are overdetermined, the structure is unstable $\rightarrow$ Fluid

$\bar{z} > z_c$ – forces are underdetermined, the structure is unstable $\rightarrow$ Solid

$\bar{z} = z_c$ – forces are exactly determined, $\rightarrow$ Marginally rigid, SD=isostatic

It is possible to come very close to a SD state experimentally

$\Rightarrow (i)$ large $SD$ regions are physically realizable

$\Rightarrow (ii)$ real granular materials contain $SD$ regions

$\Rightarrow (iii)$ $SD$ regions get larger, the closer the material is to marginal rigidity

= (criticality)
The significance of static determinacy

A familiar example of a SD system:

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

\[ f_1 = f_3 \]
\[ f_2 = W \]
\[ f_1 h = WL / 2 \]
A familiar example of a SD system:

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

Statics suffice $\Rightarrow$ isostatic materials

Key point:

To solve for the forces, there is no need to know the elastic properties of the ladder – the balance conditions suffice.
Failure of theories based on stress-strain relations

- Suggestions that granular materials are a **state of matter** in its own right

- Observations of force chains that cannot be explained easily by elasticity theory (**Seelig et al. 1946; Wakabayashi 1957; Dantu 1957**)

- Force chains suggest that the equations are probably hyperbolic

- In SD granular packs elasticity is a **redundant** theory!
Force balance

\[
\begin{align*}
\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} &= g_x \\
\frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} &= g_y
\end{align*}
\] \rightarrow \text{d eqs.}

Torque balance

\[\sigma_{ij} = \sigma_{ji} \rightarrow \text{d(d - 1)/2 eqs.}\]

\(\sigma\) is a \(d \times d\) stress tensor \(\Rightarrow\) to solve for the stress we need \(d^2\) eqs.

\[d^2 - [d + d(d - 1)/2] = d(d - 1)/2\]

\(\Rightarrow\) \(d(d - 1)/2\) further (constitutive) eqs. required = one in 2D, three in 3D
The stress field equations

\[ \text{div} \cdot \sigma = g \]  
\[ \sigma_{ij} = \sigma_{ji} \]

Force balance  
Torque balance

Closure relations
In elasticity theory we use the Saint Venant’s closure: compatibility conditions

\[
\begin{align*}
\partial_{xx} e_{yy} - 2\partial_{xy} e_{xy} + \partial_{yy} e_{xx} &= 0 \\
\end{align*}
\]

but these conditions are on the strain rather than the stress

introduce then stress-strain relations
Closure procedure in elasticity theory

(i) impose compatibility conditions on the strain
(ii) relate strain to stress, $\sigma = \sigma(e)$
$\Rightarrow$ i.e. closure is based on compliance and hence on displacement

But this leads to a conundrum

in discrete SD systems = all contact forces determinable only from balance eqs.
$\Rightarrow$ no information required about compliance (e.g. elastic constants) or displacements

The macroscopic stress field is a continuous coarse-grained description of the discrete field of contact forces
$\Rightarrow$ no compliance data should be required for the continuous description
$\Rightarrow$ stress-strain relations are irrelevant; the wrong constitutive information

Since elasticity theory is based on such relation then
$\Rightarrow$ elasticity theory is not useful for isostatic media.
$\Rightarrow$ In fact, any theory based on displacements is ineffective!
Isostaticity theory as a baseline model for stress transmission in granular solids
Isostaticity theory – timeline:

1989 - suggestion to consider *arching effects* (*Edwards et al.*)

90’s - empirical suggestion of *hyperbolic* isostaticity equations, initial solutions in Cartesian geometries (*Bouchaud, Cates et al.*)

2002 - *first-principles particle-scale derivation* of the stress equations (*Ball & RB*)

2004 - (i) *Coarse-graining* of the equations to the continuum (RB); (ii) suggestion that realistic granular matter is a *two-phase composites* (RB)

2008 - isostatic solutions for *non-uniform* structures (beyond force chains) in rectangular geometries (*Gerritsen et al.*)

2017 - isostatic solutions in *cylindrical geometries* (*RB & Ma*)

Present - Development of *two-phase stress theory* initiated (*King & RB*)
Empirical suggestion in the early 90’s:

\[ \text{div} \cdot \sigma = g \quad \text{Force balance} \]
\[ \sigma_{ij} = \sigma_{ji} \quad \text{Torque balance} \]

Closure of the stress equations with a linear relation between the stress components

\[ A_{xx} \sigma_{xx} + A_{xy} \sigma_{xy} + A_{yy} \sigma_{yy} = 0 \]

where

\[ \det\{A\} < 0 \]

The significance of this condition is that it makes the stress equations \textit{hyperbolic}!
Example of a well-known hyperbolic equation: the wave equation

\[ (\nabla^2 - \partial^2) f(\vec{r}, t) = F(\vec{r}) \]

In 1 + 1 dimensions

\[ f(x, t) = f_1(x - ct) + f_2(x + ct) \]

The solution of the Green function is non-zero only on the characteristics
In elasticity theory we use the Saint Venant’s closure: compatibility conditions

\[ \sigma_{ij} = \sigma_{ji} \]

but these conditions are on the strain rather than the stress

\[ \partial_{xx} e_{yy} - 2 \partial_{xy} e_{xy} + \partial_{yy} e_{xx} = 0 \]

introduce then stress-strain relations
The balance conditions:

\[ \text{force balance} \]

\[ \text{torque balance} \]

\[
\begin{align*}
\text{Elasticity theory} \\
\sigma_{ij} = \sigma_{ji}
\end{align*}
\]

\[
\begin{align*}
\text{Isostaticity theory} \\
P_{xx} \sigma_{yy} - 2P_{xy} \sigma_{xy} + P_{yy} \sigma_{xx} = 0
\end{align*}
\]
Like any modelling in physics, we need to start with more idealisation:
- particles are rigid (infinite elastic moduli)
- the interaction is pure hard-core repulsion
- friction between particles

We need to quantify the structure with a constitutive fabric tensor $P$
Quantitative description of the disordered particulate structures

What is the difference between the following structures?

How do we quantify structures in general? How do we put local numbers inside a structure? What is the structure here?
We use the word *structure* often and we even believe we know what we are talking about. But it is an abstract concept – there is no systematic way to quantify disordered structures with *local* numbers.

Yet, most of the structures in nature are *disordered*.

Traditionally, much of structural characterisation is done with spectroscopy. Spectroscopic methods involve radiating energetic particles or quasi-particles or photons on the material and deducing features of the structure from the frequency spectrum of the radiation that results from the radiation-matter interaction. This can be through scattering, absorption, refraction, etc.

The radiation can be electromagnetic (light, x-ray, seismic, etc.), acoustic (ultrasound and pressure waves), or of high energy particles (electrons, neutrons, ions, etc.).
These methods are very well established but they are *not local*. What one obtains is a *sum* over many material points. For example, most scattering techniques are practically measuring the Fourier transform:

\[ \text{Re} \int \rho(\vec{r}) e^{i\vec{k} \cdot \vec{r}} \, d\vec{r} \]

These methods are very common and we are used to characterise the structure with *integrated* global quantities.

The mean density is an example of one such quantity. It is an average (i.e. an integrated quantity) over the volume of material particles, divided by the total volume that they occupy including the voids between them.

This is insufficient for the stress field equations: we want a constitutive quantity that quantifies the *local structure* - we cannot use an integrated quantity.
In particulate systems the way to quantify structures is by associating a local volume with every particle and quantifying it.

The method of associating a volume with a specific particle inside a large system of many particles is called *tessellation* or *partition*. We will use the word tessellation because statistical mechanics of granular matter involves a quantity called a *partition function*, which describes a different concept.
Voronoi tessellations

This is the name given to a family of methods that associate a volume with a specific point in space within a collection of other points.

Given a collection of $N$ points in space, $\{P_1, P_2, ..., P_N\}$, the volume associated with a specific point is the locus of all the space points that are closer to $P_n$ than to any other $P_{k \neq n}$.
The dual of the Voronoi tessellation is the Delaunay (pronounced *de-lonie*) map, so, sometimes this method is called Voronoi-Delaunay tessellation.

There are several variants of this method: the Medial Axis, the Navigation Map, ...
These methods are visually pleasing, and have the advantage that there are out there many free routines on the net to compute them.

However, they have some disadvantages when one tries to quantify particulate spaces.

In particulate systems most of the relevant physics is based on the force transmission through the inter-particle contacts. The main disadvantage of the Voronoi tessellations is that they are based on proximity and are blind to the real contacts.

The second disadvantage is that the Voronoi tessellations produce polytopes with arbitrary numbers of ‘sides’: in two dimensions, these are polygons with a range of number of edges and the result is polyhedra with a range of number of faces.
This makes it difficult to assign unambiguous numbers to these polytopes; the quantification of the local structure depends on local choice, and this makes quantifying the structure arbitrary.

The second problem can be resolved by using Delaunay triangulation – all the volume elements in two dimensions are triangles and in three dimensions they are all tetrahedra.

But what to do about the first problem?

To solve both problems, a new method was proposed: the *Quadron* tessellation
**The Quadron tessellations**

Tessellation means coverage of the space occupied by a structure with a set of volume elements. The tessellation has to:

i) be *complete*;
ii) correspond *uniquely* to the structure;
iii) be *general and flexible*;
iv) be *useful* and capture relevant information.

Significantly, for PM the connectivity of the structure affects much of the physical properties of the system. Therefore the tessellation must preserve it (which is why we cannot use straightforward Voronoi tessellations).
Two dimensions

We want to tessellate the space occupied by a packing of $N$ particles in contact with their neighbours. This is done in several steps.
1. Identify contacts points (if the contacts are small surfaces – their centroids)
2. Connect contacts around particles, rotating clockwise = contact network
Example of result (by G. Frenkel)
3. Identify centroids of contacts around every particle
4. Identify centroids of cells = the centroids of contacts around them.
5. Construct the conjugate of the contact network – vectors from grains to cells
6. Construct quadrons
Definitions:

vector of the contact network, \( \vec{r}_{cg} \equiv \vec{r}_q \)

centroid of loop \( \mathbf{c} \)

centroid of particle \( \mathbf{g} \)

vector of the conjugate network, \( \vec{R}_{cg} \equiv \vec{R}_q \)
7. Consider only the contact network and its conjugate – delete particles
8. Construct all quadrons
9. Consider only the quadron tessellation – delete the networks
10. Assign each quadron a *shape tensor* (sometimes called *structure tensor*)

quadron volume $V_q$

vector of the contact network, $r_q$

vector of the conjugate network, $R_q$

quadron shape tensor:

$$C'_q = R_q \otimes r_q \quad \text{or} \quad (C'_q)_{ij} = (r_q)_i (R_q)_j$$
The quadron volume

\[ V_q = \frac{1}{2} \left( r_{q,x} R_{q,y} - r_{q,y} R_{q,x} \right) = \frac{1}{2} Tr \left( C_q \right) \]

where

\[ C_q \equiv \varepsilon \cdot C'_q \ ; \ \varepsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \]

particle volume = sum over its quadron volumes

\[ \Rightarrow V_g = \sum_{q \in g} V_q = \frac{1}{2} Tr \left( \varepsilon \cdot C_g \right) \]

and we have

\[ V_{\text{system}} = \sum_{g=1}^{N} V_g = \sum_{\text{all } q} V_q \]
The *skewness* of the quadron is

\[ S_q = \left( r_{q,x} R_{q,x} + r_{q,y} R_{q,y} \right) = \text{Tr}\left( C'_q \right) \]

or

\[ \text{Antisymm}\left( C_q \right) = S_q \varepsilon \]

* The skewness determines the *chirality* of the structure around the particle, which plays an important role in the theory of stress in granular matter [Ball and Blumenfeld, Phys. Rev. Lett. (2002)]
The same concept: First, tessellate the space occupied by the system into volume elements of the same polyhedra types, the quadrons, then quantify the shape of each quadron.

* In fact, the quadrons need not all have exactly the same polytope. In 2d, for grains with only two contact points, the quadrons degenerate from quadrilaterals to triangles and still can be described by the structure tensor $C$. In 3d, for grains with only three contact points, the quadrons degenerate from octahedra to hexahedra and still can be described by the structure tensor $C$. 

Three dimensions
Step 1.
Connect the contacts the contact points (the green dots) around a grain. The contacts may be surfaces, rather than points, when the grains are not perfectly rigid. Then connect the centroids of the contact surfaces.

These connections make polyhedra that represent grains (in the figure this is a tetrahedron). As much as possible, every face of the polyhedron should be a triangle. The polyhedra are connected at their corners, which are the original contacts.
Example: packing of spheres

Transformation to the polyhedral structure
This is an example of a polyhedral structure for a special system, where every grain has exactly four contacts.

This is the exact equivalent of a cellular structure.
Step 2.

Tessellate the volume with volume elements – the 3D quadrons

Again, one of the requirements is that the tessellation preserves the connectivity of the structure – it has to be based on the contacts.

The next several slides outline the tessellation procedure in detail.
Consider the inside of a cell (also known as a `void’ or a `pore’).

The transparent sphere in the figure is there only to visualise the cell.

The cell surface is made of the blue triangles and the polygons that they enclose.

The triangles are the faces of the grain polyhedra.

The polygons are the ‘throats’ to neighbouring cells.
The cell seen from inside

**Face of grain polyhedron**

**Polygon p**

**Vertex v** = **Centroid of grain g**

**Cell c**
1. Define: the edge between two contacts is a \textit{vector}, \( \vec{r}_{cvp} \) \( = \vec{r}_{cgp} \)

\( c \) = cell;
\( v \) = vertex (same as grain);
\( p \) = polygon (same as throat)

\textit{Face of grain polyhedron}

\textit{Vertex} \( v \) = \textit{Centroid of grain} \( g \)
2. Connect the two ends of $\vec{r}^{cvp}$ with:

(i) the centroid of face $\vec{S}^{cv}$

(ii) the centroid of polygon $p$

This makes a (non-planar) quadrilateral with $\vec{r}^{cvp}$ one of its diagonals.
3. Connect the corners of the quadrilateral with the centroid of the grain \( v \) (the blue dashed lines)

This generates a *pyramid-like* polyhedron with apex at \( v \) but non-planar basis.
Pyramid-like 1
4. Connect the corners of the quadrilateral with the centroid of the cell.
the joined pyramids = quadron
The quadrons cover the volume perfectly – no gaps and no overlaps
5. Define the structure tensor

The structure of the quadron is described by the structure tensor

\[
(C_q)_{ij} = (\vec{\xi}_q \times \vec{r}_q)_i (R_q)_j \quad \text{or} \quad C_q = (\vec{\xi}_q \times \vec{r}_q) \otimes \vec{R}_q
\]

The quadron volume is

\[
V_q = \frac{1}{3!} Tr \{ C_q \}
\]

The grain structure tensor and volume are

\[
C_g = \sum_{q \in g} C_q \quad \text{and} \quad V_g = \sum_{q \in g} V_q
\]
Similarly, the structure and volume of the entire system are:

\[
C_{\text{system}} = \sum_{g \in \text{system}} C_g = \sum_{g \in \text{system}} \sum_{q \in g} C_q \\
V_{\text{system}} = \sum_{g \in \text{system}} V_g = \sum_{g \in \text{system}} \sum_{q \in g} V_q
\]

These tensors are additive and they quantify the structure at every point in the system.
The same method can be used to quantify disordered *cellular structures*, such as soap froths, foams, biological tissues, compressed suspensions of soft colloids, and arbitrary Voronoi graphs.
Extension of the method to cellular structures

A cellular structure is made of some material enclosing cells

(i) *Skeletonise* the material phase
(ii) construct a *polyhedral representation*
The resulting structure is the same as in the particulate systems: a network of connected polyhedra, but simpler – all tetrahedra. Equivalent to granular systems, where each grain has exactly four contacts.

From here the description is identical.
(iii) construct the same *quadron representation*

Comment: because all the polyhedra are generically tetrahedra, the quadron construction is easier for cellular structures.
$P$ is a ‘fabric tensor’ characterizing the structure
On the granular level $P$ is defined as:

\[ P_{ij}^{cv} = \frac{1}{2} \sum_{\text{All cells } c \text{ around } v} \left( r_i^{cv} R_j^{cv} + r_j^{cv} R_i^{cv} \right) \]

[Ball & RB, Phys.Rev.Lett. 88, 115505 (2002)]

$P$ can be coarse-grained to the continuum

[RB, Physica A 336, 361 (2004)]
A first-principles 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 \( p_{ij} = \frac{1}{2} \sum_{l \in g} (r_{il}^{lg} R_{lj}^{lg} + r_{jg}^{lg} R_{ig}^{lg}) \)

is a new *fabric tensor*
1. Construct the vectors $r_{cg}$ and $R_{cg}$

2. Assign each loop a force $f_c$

3. Parameterise the granular forces, $f_{gg'}$, in terms of the loop forces $f_c$:

$$f_{gg'} = f_{c'} - f_c$$

(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 force moment around grain \( g \) is
\[
S_{g}^{ij} = \Sigma_{c} r_{cg}^{i} f_{c}^{j} ; \quad \sigma_{g}^{ij} = S_{g}^{ij} / A_{g}
\]

6. In terms of the continuous field
\[
S_{g} = \Sigma_{c} r_{cg} (f_{g} + R_{cg} * \nabla f_{g}) = C_{g} * \nabla f_{g}
\]
where
\[
C_{g} = \Sigma_{c} r_{cg} R_{cg} = P_{g} + V_{g} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}
\]
is the structure tensor
7. Over any connected part of the system, $\Gamma$
\[
\sigma_{\Gamma} = \langle S_g \rangle_{\Gamma} = \langle C_g \cdot \nabla f_g \rangle_{\Gamma} \cong \langle C_g \rangle_{\Gamma} \langle \nabla f \rangle_{\partial \Gamma}
\]

8. Now impose torque balance condition
\[
\{ C_g \varepsilon^{-1} \langle \sigma \rangle \} = \{ C_g \varepsilon^{-1} \langle \sigma \rangle \}^T
\]

9. This gives two conditions:
(i) $\langle \sigma \rangle = \langle \sigma \rangle^T$ (as expected)
(ii) $\{ P \varepsilon^{-1} \langle \sigma \rangle \} = \{ P \varepsilon^{-1} \langle \sigma \rangle \}^T$

\[
\Rightarrow \quad p_{xx} \sigma_{yy} + p_{yy} \sigma_{xx} - 2p_{xy} \sigma_{xy} = 0 \quad \text{or} \quad \text{Tr}[(\varepsilon P \varepsilon^{-1}) \cdot \sigma] = 0
\]

Conclusions:
1. the fabric tensor $P$ can be calculated directly from images of the granular assembly;
2. the fabric tensor can be then coarse-grained to the continuum consistently.
General solutions to the Isostaticity stress field equations
Conclusions

• Isostaticity theory makes it possible to solve for stress fields in marginally rigid granular systems from first-principles.

• The solutions are not just the force chains, as commonly believed, there appear secondary (and higher-order) chains even when $P$ is uniform.

• In non-uniform granular packs, the stress field becomes ever more uniform as the distance from the stress sources increases.

• Force chain meander, forces attenuate along chains, forces ‘leak’ from chains into the material, and force chains branch where the fabric tensor changes sharply.

• Stress fields in isostatic systems are much richer than previously thought.
Extension of isostaticity theory to real granular matter – stato-elasticity theory

Changsha, Sept 2014
Motivation

- Most real granular materials are not isostatic – $z > z_c$

- Does that mean that we need to discard isostaticity theory altogether?

- This question was at the heart of a big controversy between the those who rely on strain-based theories and those who use isostaticity theory.

- The answer to the question is No!
  - increasing $z > z_c$ gradually adds over-connected regions in the medium;
  - in these regions isostaticity theory does not hold;
  - this introduces increasingly larger corrections to the theory;
  - only when $z - z_c \geq 1$ fully strain-based theories (elasticity, plasticity, etc.) apply.

- Evidence for this comes from an experiment, which we have no time to go over
  
**A piling experiment** [Blumenfeld, Edwards & Ball, J. phys. C (2005)]

*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. The slow advance rate minimizes inertial effects.

The growth of a pile, with time running from top image to bottom. The blue grains 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.
Pile density $\rho_f$ vs initial density $\rho_i$
Pile density $\rho_f$ vs initial density $\rho_i$

- $\rho_f$ decreases with $\rho_i$ - fingerprint of jamming
- The line extrapolates the experimental points
- $\rho_f = \rho_I = \rho_c$ - a natural limit density

Pile mean coordination number, $z$, vs $\rho_i$

- $z$ also decreases with $\rho_i$.
- $z(\rho \rightarrow 0) \rightarrow 3.7$ agrees with sequential deposition value ($z = 4 - \varepsilon$).

$z(\rho \rightarrow \rho_c) \rightarrow 3.1$
Pile density $\rho_f$ vs initial density $\rho_i$

- $\rho_f$ decreases with $\rho_i$ - fingerprint of jamming
- The line interpolates the experimental points
- $\rho_f = \rho_I = \rho_c$ - a natural limit density

Pile mean coordination number, $z$, vs $\rho_i$

- $z$ also decreases with $\rho_i$.
- $z(\rho \to 0) \to 3.7$ agrees with sequential deposition value ($z = 4 - \varepsilon$).

$z(\rho \to \rho_c) = 3.1$

is in excellent agreement with $z_c$

At $\rho_c$ the pile is minimally connected
$\Rightarrow$ marginally rigid $\Rightarrow$ isostatic
• $\rho_f$ decreases with $\rho_i$ - fingerprint of jamming
• The line interpolates the experimental points
• $\rho_f = \rho_I = \rho_c$ - a natural limit density

• $z$ also decreases with $\rho_i$.
• $z(\rho \to 0) \to 3.7$ agrees with sequential deposition value ($z = 4 - \varepsilon$).

Isostatic states are approachable and realisable!
Isostaticity is a critical state

- Example experiments at three densities
- The red grains constitute a yield front: grains that have ‘collided’ with the pile but have not yet consolidated
- At low density the front is less than one grain deep; at high density it is a finite fraction of the pile - the consolidation is highly cooperative

⇒ In the ‘thermodynamic’ limit, the yield front size diverges

Interpretation: the stress response length diverges

Experimental evidence

Blumenfeld et al 2005, Sibil & Mullin 2007
Conclusions

- As the value of $z$ increases
- the system moves further from the isostatic critical point
- over-connected regions form and grow
- the isostatic stress response length decreases
- ‘force chains’ get shorter

Enter stato-elasticity theory
Isostaticity (when \( p_{oc} = 0 \)) acts as a critical point – stress response length diverges

As \( p_{oc} \) increases: regions governed by non-isostatic equations form and grow
the stress response length decreases
the typical length of force chains gets shorter

Very reminiscent of percolation theory and superconductivity!

\( p_{oc} \) - area fraction of OC regions
The first step is to identify the isostatic regions in a given particulate media. These are results from analysis of a number of DEM simulations at different proximities to the jamming point (from above).
Indeed, we can see that the fraction of the area occupied by the isostatic regions increases as the connectivity is reduced to the isostatic limit $z \to z_c$. 

![Graph showing the relationship between ln(Fraction Isostatic) and ln(z - z_c)]
also to verify that the average size of the isostatic regions increases as the connectivity is reduced to the isostatic limit \( z \to z_c \)
Conclusion: there is a need to formulate a *stato-elasticity* theory

⇒ a theory for stress transmission in *two-phase composites*: SD and OC

To formulate such a theory, we need to solve for stresses in both regions and *match solutions* at the region boundaries

Not easy: elasticity eqs. are elliptic, isostaticity eqs. are hyperbolic

⇒ Naïve matching of solutions can lead to *Cauchy ill-posedness*!

Has been done: (i) in 1D-like system and (ii) for one OC inclusion in an SD medium (in preparation)

\( p_{oc} \) - area fraction of OC regions
**Acknowledgements**

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Robin Ball</td>
<td>(Physics, Warwick, UK)</td>
<td>- expm’n’t, statics, yield</td>
</tr>
<tr>
<td>Sam Edwards</td>
<td>(Cavendish, Cambridge, UK)</td>
<td>- expm’n’t, discussions</td>
</tr>
<tr>
<td>Bill Proud</td>
<td>(Cavendish, Cambridge, UK)</td>
<td>- discussions, new expm’n’ts</td>
</tr>
<tr>
<td>Margot Gerritsen</td>
<td>(ERE, Stanford, USA)</td>
<td>- variable $P$ solutions</td>
</tr>
<tr>
<td>Gunilla Kreiss</td>
<td>(IT, Uppsala, Sweden)</td>
<td>- variable $P$ solutions</td>
</tr>
<tr>
<td>Golnaz Alipour</td>
<td>(ERE, Stanford, USA)</td>
<td>- yield of force chains</td>
</tr>
<tr>
<td>Julian Ma</td>
<td>(Cavendish, Cambridge, UK)</td>
<td>- Isostaticity in cyl. coor.</td>
</tr>
<tr>
<td>David King</td>
<td>(Cavendish, Cambridge, UK)</td>
<td>- Stato-elasticity</td>
</tr>
</tbody>
</table>