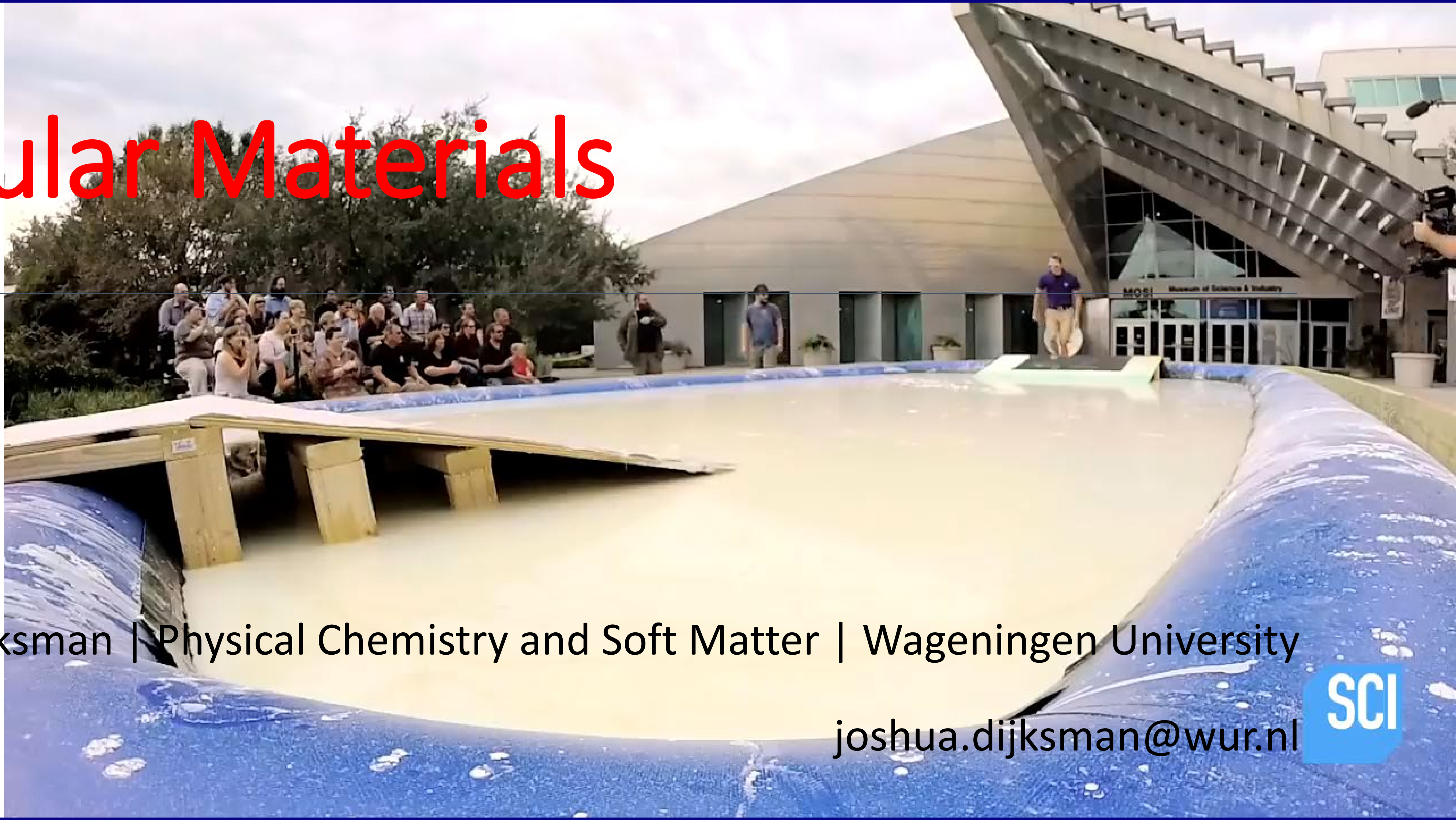
Granular Materials



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Granular materials are everywhere

Sugar

Klamath National Forest

67P Churyumov-Gerasimenko

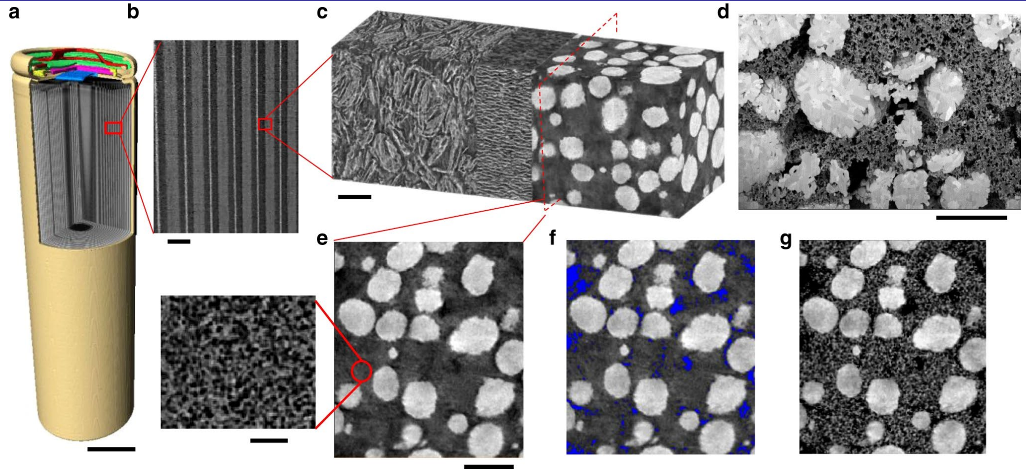
https://commons.wikimedia.org/wiki/File:AcucarCubosDSC6111.jpg

https://inciweb.nwcg.gov/incident/photograph/7699/0/

Granular materials are everywhere

Granular gas

The Guardian



Li-ion battery

Shear thickening suspensions

330 feet per second
100 meters per second

0.20 gram
Plastic BB

https://www.youtube.com/watch?v=Esz6ne9x9yM

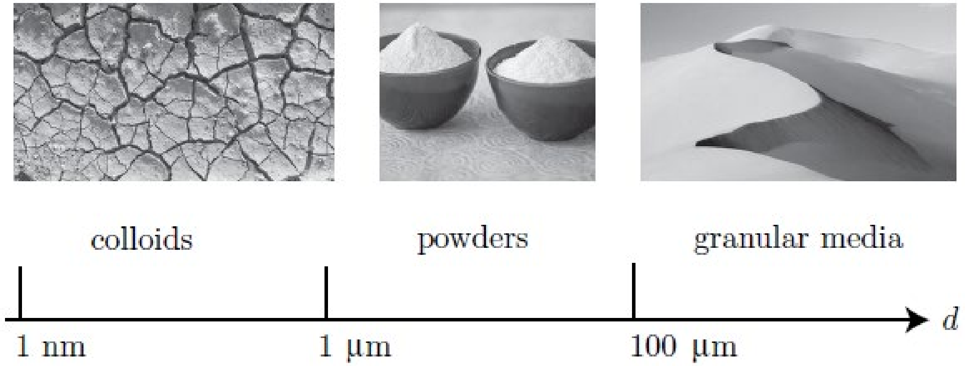
https://www.nature.com/articles/s41467-020-15811-

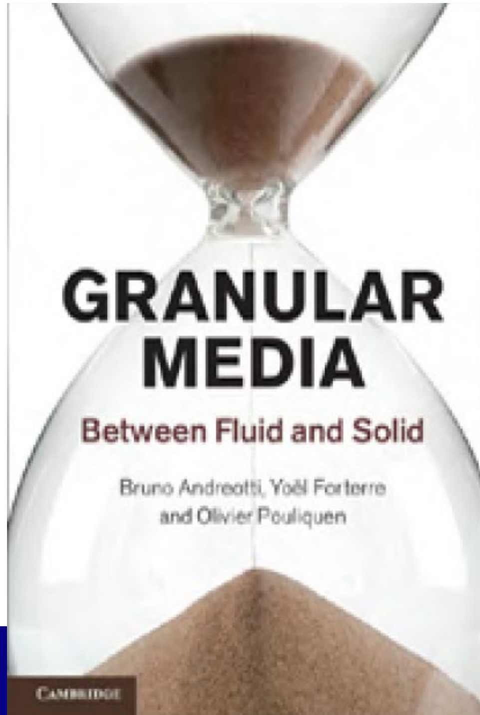
and an interesting model system for materials

of mobility. I took a box which, when closed, just held 100 marbles, with five specially coloured ones placed near the centre, and then noted how many had to be removed from the box to allow the five coloured ones to scatter on agitation; a slight motion of the five as a body was not accepted as a sign of mobility. It was necessary to remove 16 to get slow and partial scattering of the central 5, and 20 or 25 to get quick and decided scattering. Thus for mobility among a set of marbles the free volume must be between 25 and 33 per cent. of the volume of the marbles. Of course the circumstances are in most ways vastly different from those of perfectly rebounding swiftly moving molecules, but the comparison was worth making in passing. In the case of mole-

Sutherland (1891)

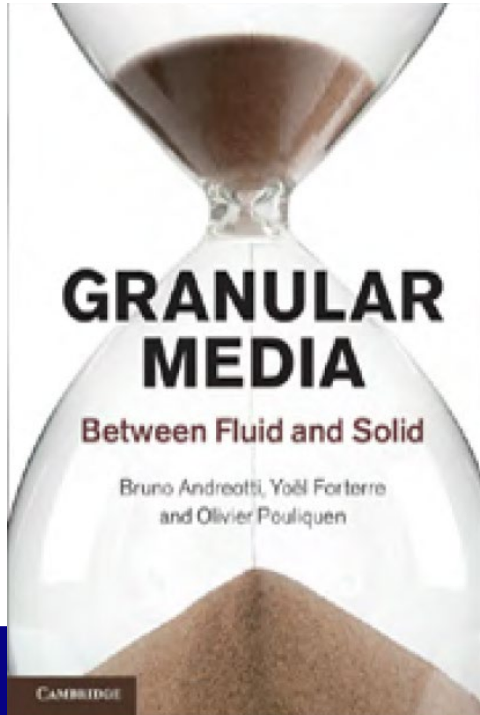
Figure 1.1 Examples of granular media.





Lecture overview

- Granular Materials: why are they interesting?
- Curiously, intermediate flow speed is easiest!
- And how did we find out?
- What happens if you go slower?
- Or spill some water over the grains?



Learning objectives

- Identify the main microscopic features of granular materials and their link to other subfields of soft matter or materials science.
- Derive the relevant dimensionless numbers to quantify the effect of a particular mechanical variable.
- Select optimal measurement methods to extract the consequence of changing a particular mechanical variable.

Lecture overview

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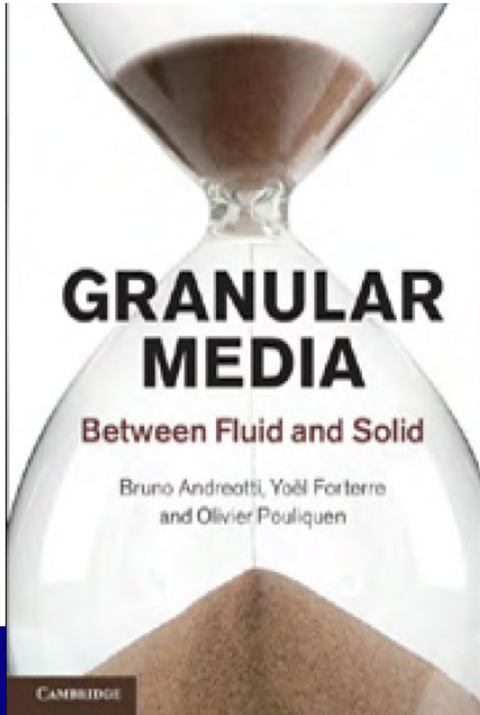


Granular materials satisfy Newton's Laws!

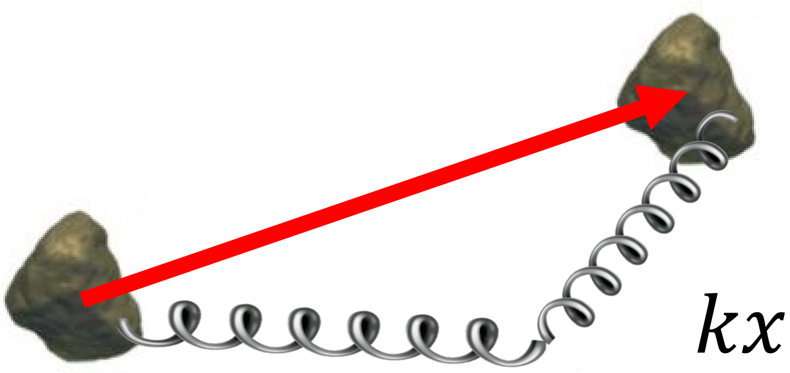
$$F = ma = m\frac{d^2x}{dt^2}$$

Newton wrote it differently

$$F = ma = m\frac{d^2x}{dt^2} = \frac{d}{dt}(mv)$$

Works like a charm for a single grain

$$F = ma = m\frac{d^2x}{dt^2} = \frac{d}{dt}(mv)$$



$$kx = F$$

Now... SHOCKER

Usually there is more than one grain

What if we have more than one grain?

$$F = ma = m\frac{d^2x}{dt^2} = \frac{d}{dt}(mv)$$

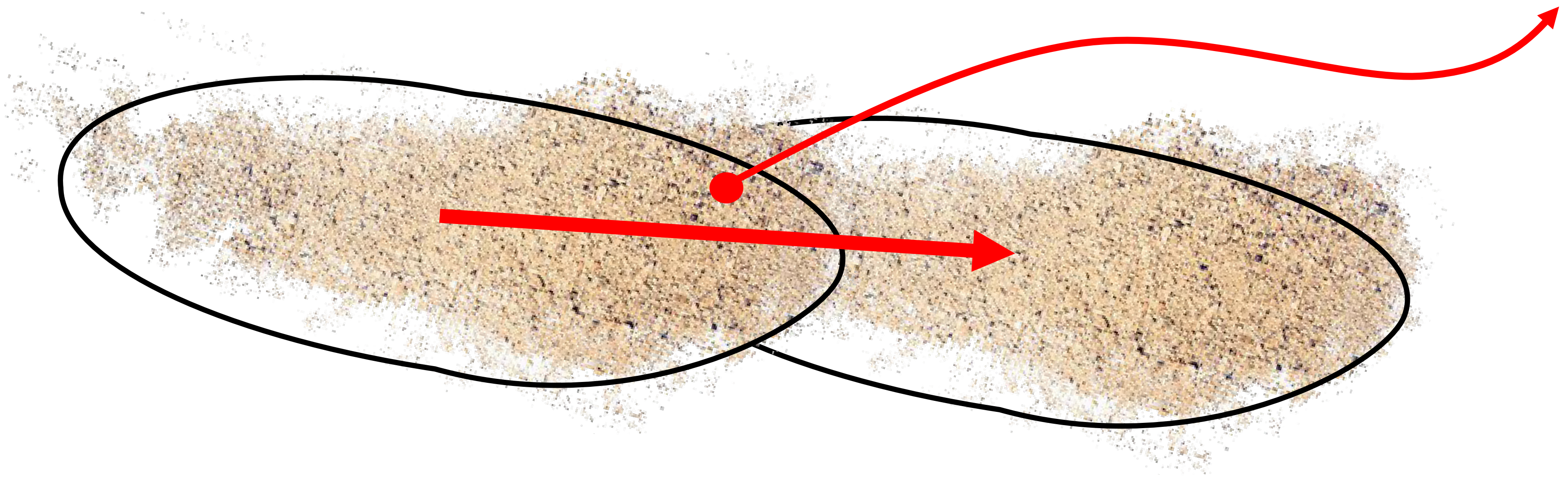
2 grains!

F from interactions

What if we have many grains?

$$F = ma = m\frac{d^2x}{dt^2} = \frac{d}{dt}(mv)$$

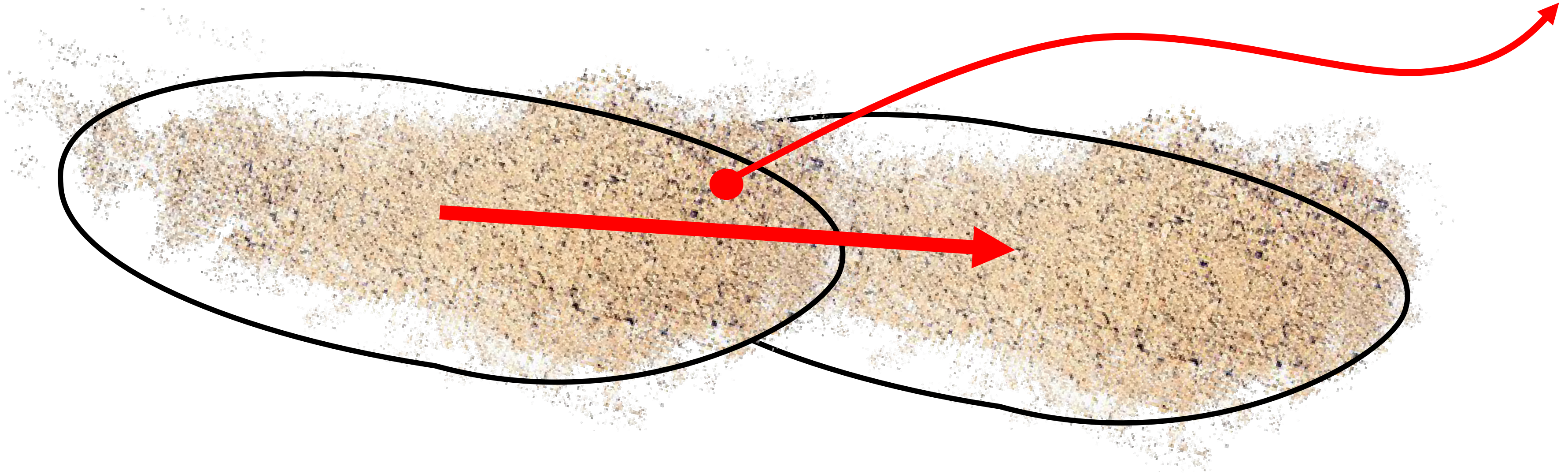
- Which m?
- Which v?
- Which x?



...the curse of the continuum

$$F = ma = m\frac{d^2x}{dt^2} = \frac{d}{dt}(mv)$$

- Which m?
- Which v?
- Which x?

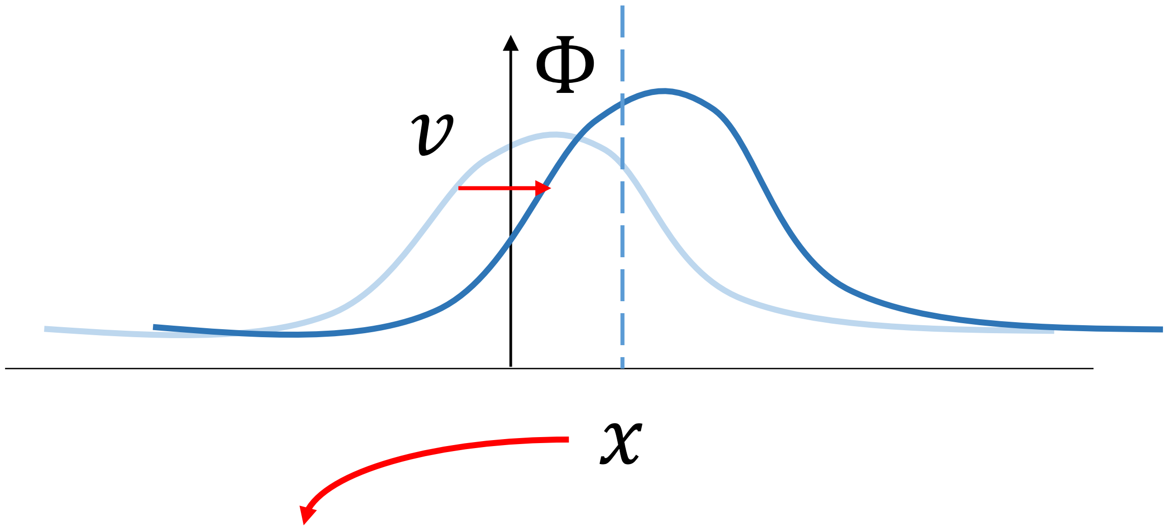


...the curse of the continuum

- Which x?
- Which v?
- Which m?

Total derivative – one dimension

For any field Φ



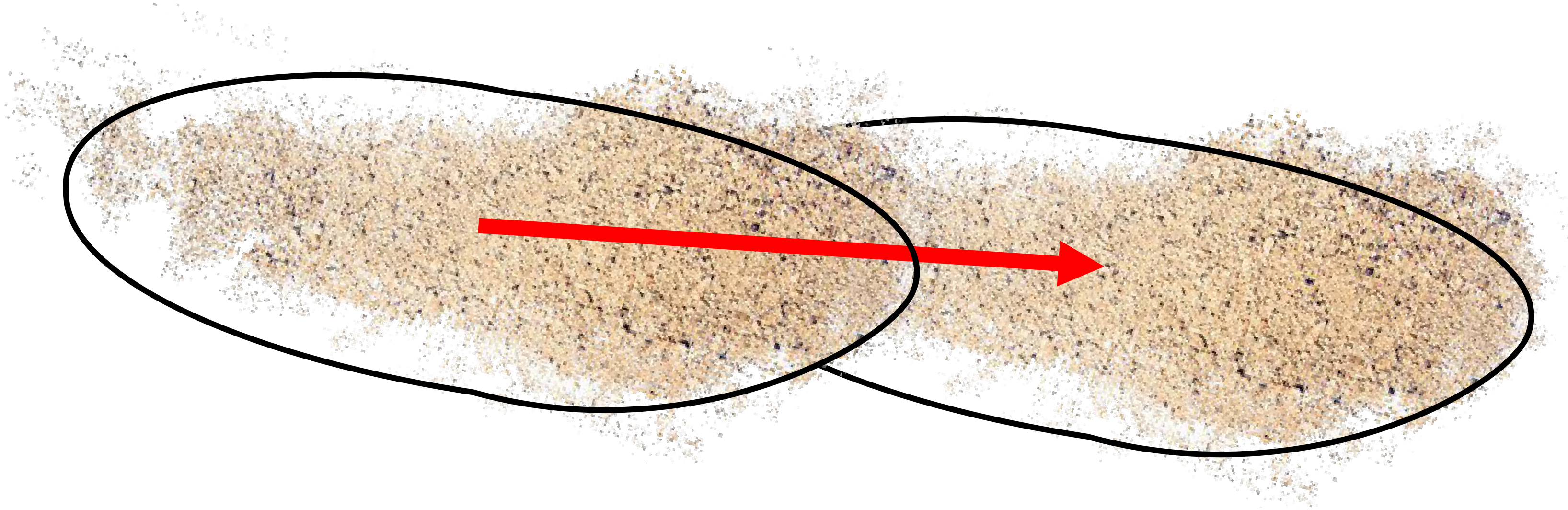
$$\frac{D\Phi}{Dt} = \frac{\partial \Phi}{\partial t} + v\,\frac{\partial \Phi}{\partial x}$$

Also known as

- “Lagrangian derivative”
- “convective derivative”
- “substantial derivative”
- “particle derivative”

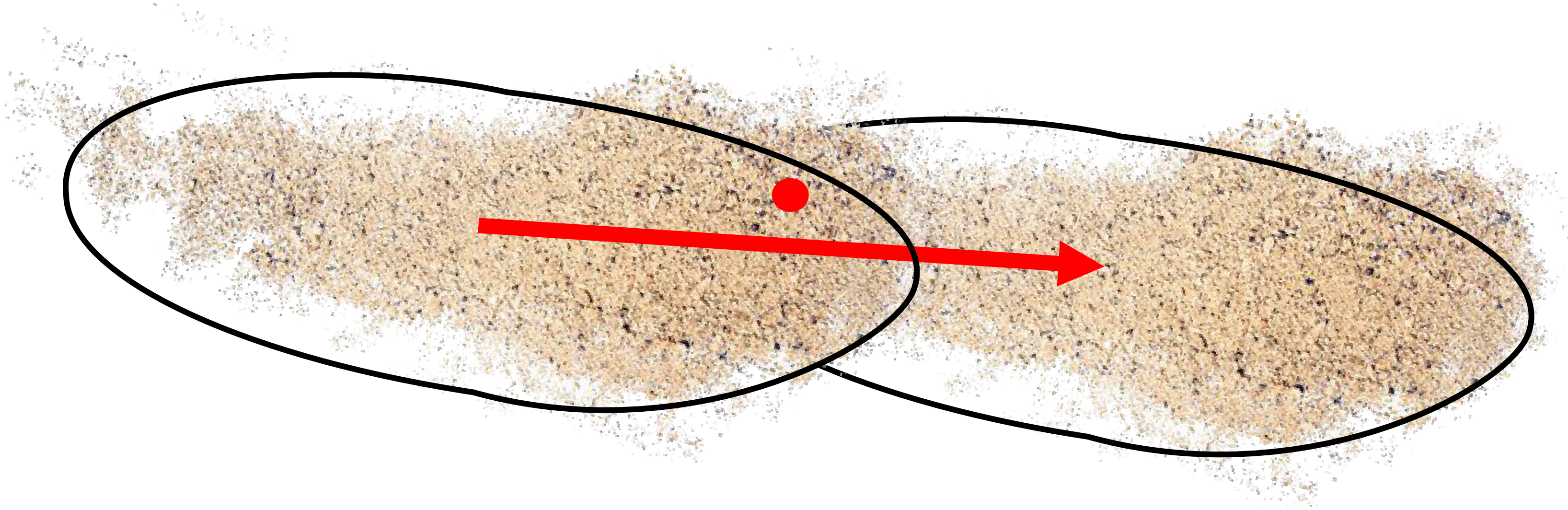
Include the finite volume

$$\frac{F}{V} = \frac{d}{dt}\left(\frac{m}{V}v\right) = \frac{d}{dt}(\rho v)$$



Include the finite volume and total derivative

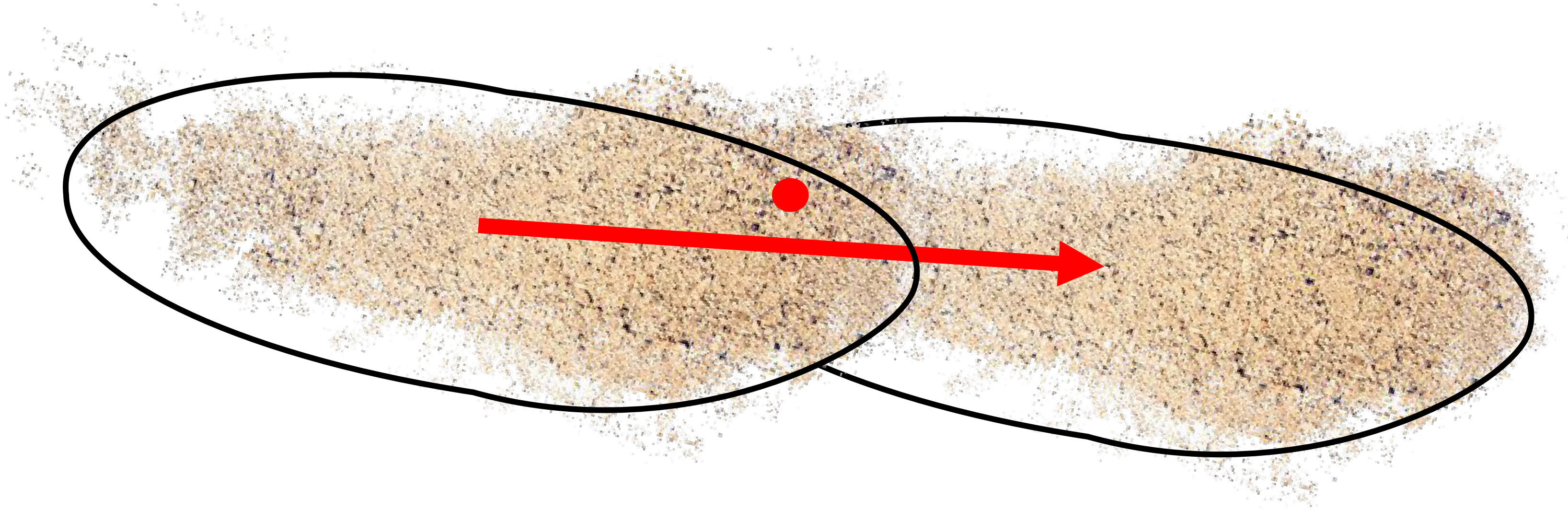
$$\frac{F}{V} = \frac{D}{Dt}(\rho v) = \frac{\partial(\rho v)}{\partial t} + v\,\frac{\partial(\rho v)}{\partial x}$$



But an additional ambiguity arises

- Which F?

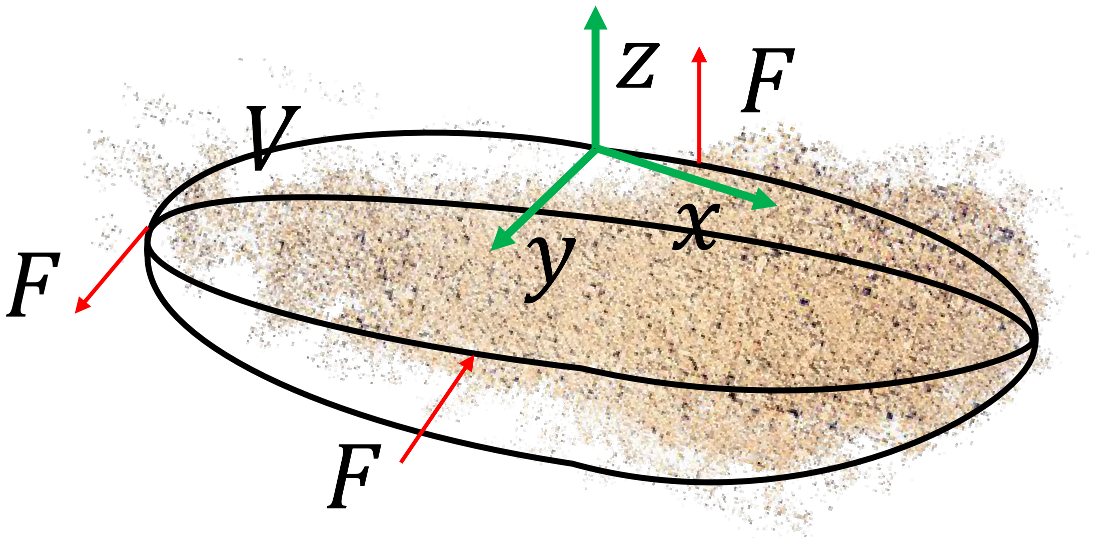
$$\frac{F}{V} = \frac{D}{Dt}(\rho v) = \frac{\partial(\rho v)}{\partial t} + v\,\frac{\partial(\rho v)}{\partial x}$$



There are multiple ways to consider F

- Which F?

$$\frac{F}{V} = \frac{D}{Dt}(\rho v) = \frac{\partial(\rho v)}{\partial t} + v\,\frac{\partial(\rho v)}{\partial x}$$



$\rightarrow F_{ij}$

Split up tensor in three components

F_{ij} has nine terms but three main "parts"

- "offset" = body forces $\frac{F}{V} \equiv f$ (gravity, magnetic, etc)
- "diagonal elements" = compression / dilation
- "off-diagonal element" = shear

Where do the components act?

F_{ij} has nine terms but three main “parts”

- “offset” = body forces $\frac{F}{V} \equiv f \rightarrow$ acts on all elements
- “diagonal elements” $\rightarrow$ acts on surface
- “off-diagonal element” $\rightarrow$ acts on surface

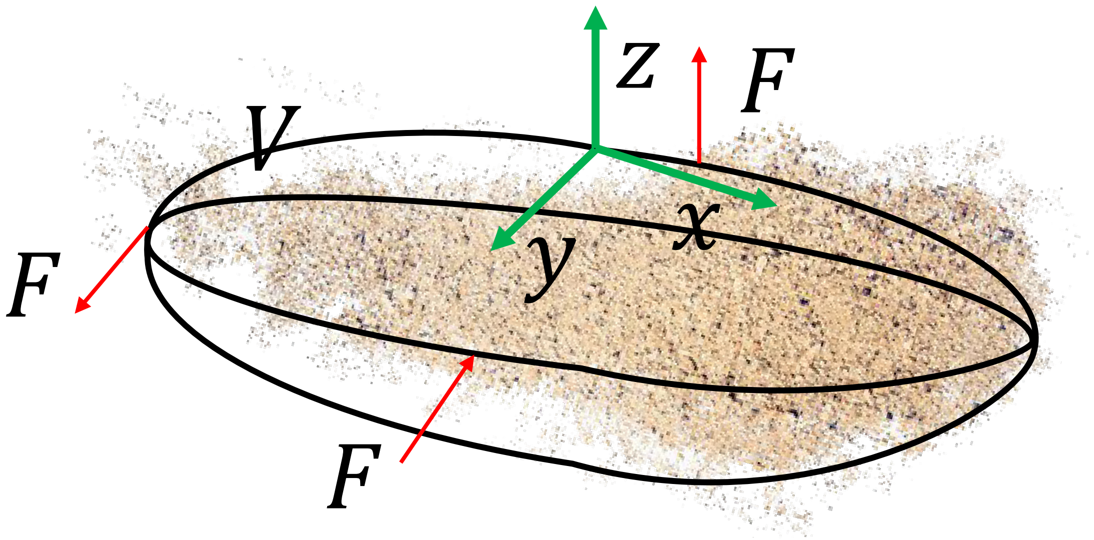
Surface forces are "stresses"

F_{ij} per unit surface area A: $\frac{F}{A} = \sigma$

- "diagonal elements" → $\sigma_{xx}; \sigma_{yy}; \sigma_{zz}$ "Normal stress"
- "off-diagonal element" → $\sigma_{xy};\ \sigma_{yz}, \ldots$ "Shear stress"

Kinetics come from stress gradients in volume

$$f + \frac{\partial \bar{\sigma}}{\partial x} = \frac{D}{Dt}(\rho \vec{v})$$



https://pngimg.com/image/37220

Total derivative in three dimensions

Also known as

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- “convective derivative”
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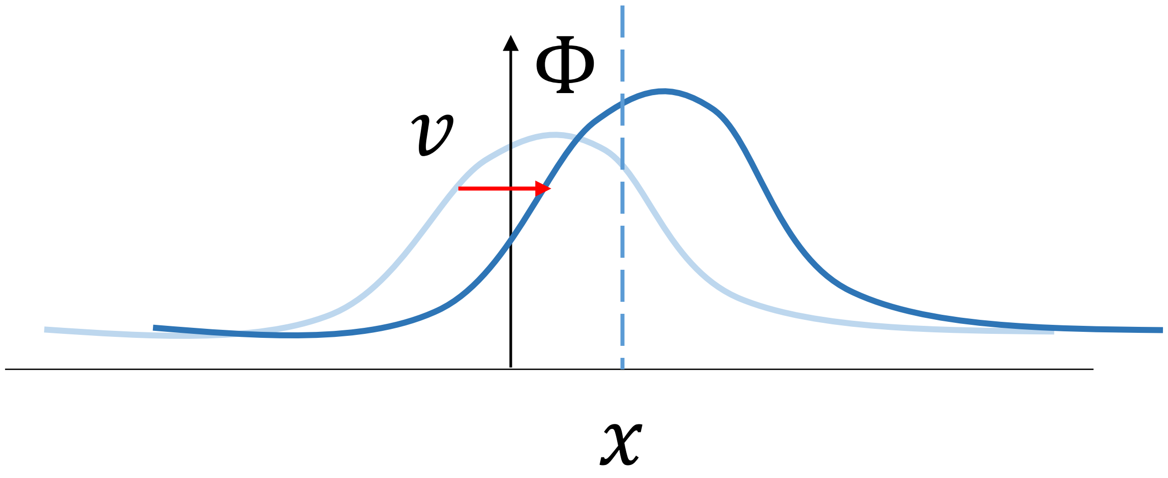
For any field Φ



$$\frac{D\Phi}{Dt} = \frac{\partial \Phi}{\partial t} + (\vec{v} \cdot \nabla)\Phi$$

Equation of motion for continuum

$$\vec{f} + \nabla\bar{\sigma} = \frac{\partial(\rho\vec{v})}{\partial t} + (\vec{v}\cdot\nabla)(\rho\vec{v})$$

Additional information needed to solve!

→ all terms expressed in $\vec{x}, \frac{\partial\vec{x}}{\partial t}, \frac{\partial^2\vec{x}}{\partial t^2}$ (cf. Hooke)

Equation of motion for continuum

$$\vec{f} + \nabla\bar{\sigma} = \frac{\partial(\rho\vec{v})}{\partial t} + (\vec{v} \cdot \nabla)(\rho\vec{v})$$

- Continuity: $\nabla \cdot (\rho\vec{v}) = -\frac{\partial \rho}{\partial t}$
- “Constitutive equation”: $\bar{\sigma}(\vec{v}, \nabla \cdot \vec{v})$

Who knows an example of this?

"Constitutive equation": $\bar{\sigma}(\vec{v}, \nabla \cdot \vec{v})$

Equation of motion for continuum

$$\vec{f} + \nabla\bar{\sigma} = \frac{\partial(\rho\vec{v})}{\partial t} + (\vec{v}\cdot\nabla)(\rho\vec{v})$$

... And what else?

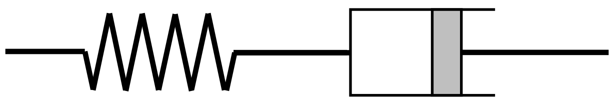
Constitutive equation for continuum media: 1D examples

$$\sigma = \sigma_0 + k\dot{\gamma}^n$$

Herschel-Bulkley

$$\lambda \frac{\partial \sigma}{\partial t} + \sigma = \eta \dot{\gamma}$$

Maxwell

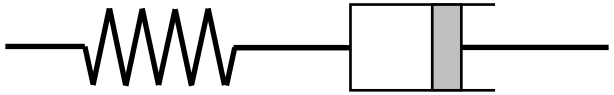


$$\eta_{\text{eff}} = \eta_\infty + \frac{\eta_0 - \eta_\infty}{1 + (k\dot{\gamma})^n}$$

Cross fluid

Constitutive equation for continuum media: 3D example

$$\bar{\sigma} + \lambda \frac{\partial \bar{\sigma}}{\partial t} = 2\eta\dot{\bar{\gamma}}$$

Maxwell 

$$\mathbf{T} + \lambda \overset{\nabla}{\mathbf{T}} = 2\eta_0 \mathbf{D}$$

“Upper Convected Maxwell”

https://en.wikipedia.org/wiki/Upper-convected_Maxwell_model

For n = 1

$$\sigma = \sigma_0 + k\dot{\gamma}^n$$

Constitutive equation for continuum media?

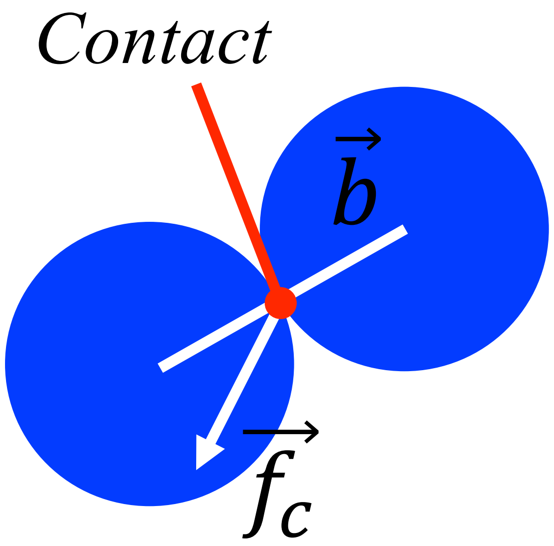
Dynamics: $\bar{\sigma}(\vec{v}, \nabla \cdot \vec{v})$

But also statics: $\bar{\sigma}(\vec{x})$

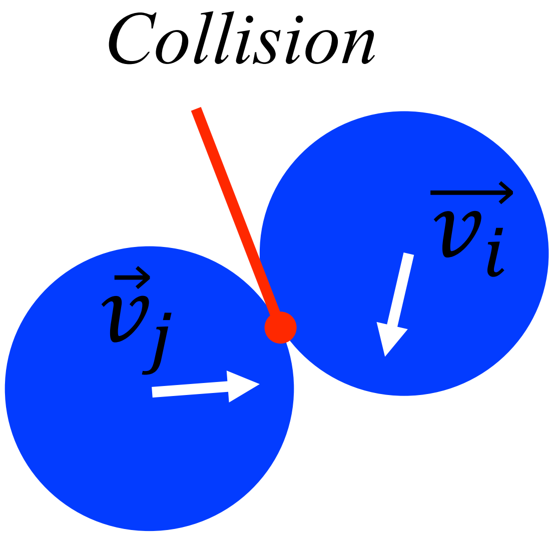
Can we understand $\bar{\sigma}(x)$ from microscopics?

Yes: Irving-Kirkwood-Noll procedure

$$\bar{\sigma} \cong \frac{1}{V_c} \sum_{\text{Contacts}} \vec{b} \otimes \vec{f_c} + \frac{1}{V_c} \sum_{\text{Collisions}} \vec{v_i} \otimes \vec{v_j}$$



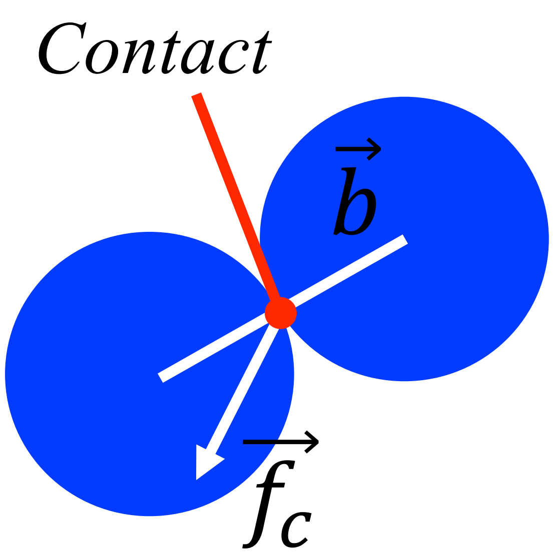
Generally true
for all materials!



goes back to Cauchy, Piola, Kirchhoff, Love, Weber,...

Recall Alexey: Virial Theorem

$$P = \mathrm{Tr}(\bar{\sigma}) \cong \frac{1}{V_c} \sum_{\mathrm{Contacts}} \vec{b} \cdot \vec{f_c}$$



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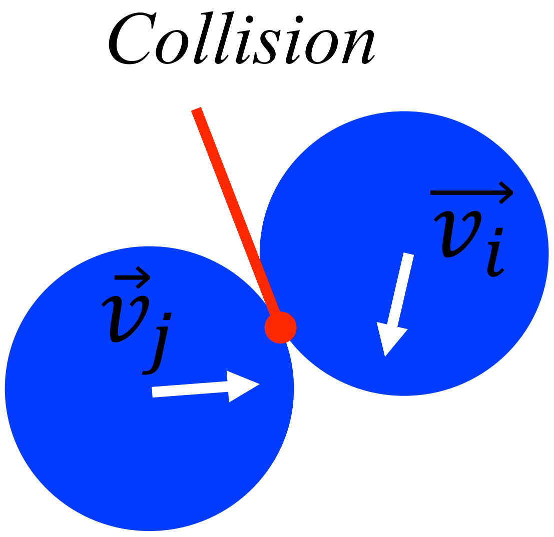

goes back to Cauchy, Piola, Kirchhoff, Love, Weber,...

Applying this to granular materials

$$\bar{\sigma} \cong \frac{1}{V_c} \sum_{\text{Contacts}} \vec{b} \otimes \vec{f_c} + \frac{1}{V_c} \sum_{\text{Collisions}} \vec{v_i} \otimes \vec{v_j}$$

Let's calculate a stress tensor!

Applying this to granular materials

$$\bar{\sigma} \cong \frac{1}{V_c} \sum_{\text{Contacts}} \vec{b} \otimes \vec{f_c} + \frac{1}{V_c} \sum_{\text{Collisions}} \vec{v_i} \otimes \vec{v_j}$$

What are the key assumptions for this material choice?

Applying this to granular materials

$$\bar{\sigma} \cong \frac{1}{V_c} \sum_{\text{Contacts}} \vec{b} \otimes \vec{f_c} + \frac{1}{V_c} \sum_{\text{Collisions}} \vec{v_i} \otimes \vec{v_j}$$

Let’s make an inventory for the simplest case:
a collection of glass beads

Applying this to granular materials

$$\bar{\sigma} \cong \frac{1}{V_c} \sum_{\text{Contacts}} \vec{b} \otimes \vec{f_c} + \frac{1}{V_c} \sum_{\text{Collisions}} \vec{v_i} \otimes \vec{v_j}$$

- Discrete particles
- Spherical, convex particles
- Frictional contacts
- Hard: no deformation of particles
- Large particles: no thermal motion
- Particles are “loose”
- “Passive” particles

- Weakly elastic collisions
- Mono/bidisperse
- Embedded in air; no viscous drag
- Only repulsive forces, no attraction
- Steady state situation
- Disordered arrangement
- Mechanical interactions, no electrons

Applying this to granular materials

$$\bar{\sigma} \cong \frac{1}{V_c} \sum_{\text{Contacts}} \vec{b} \otimes \vec{f_c} + \frac{1}{V_c} \sum_{\text{Collisions}} \vec{v_i} \otimes \vec{v_j}$$

Increasing velocity of particles →

"Inertial number" $I(\vec{v})$

Static packing

Slow flow

Fast flow

Granular gas

2D scenario:

$$\frac{\sigma_{xy}}{\sigma_{yy}} = \mu(I(\vec{v}))$$

Lecture overview

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- What happens if you go slower?
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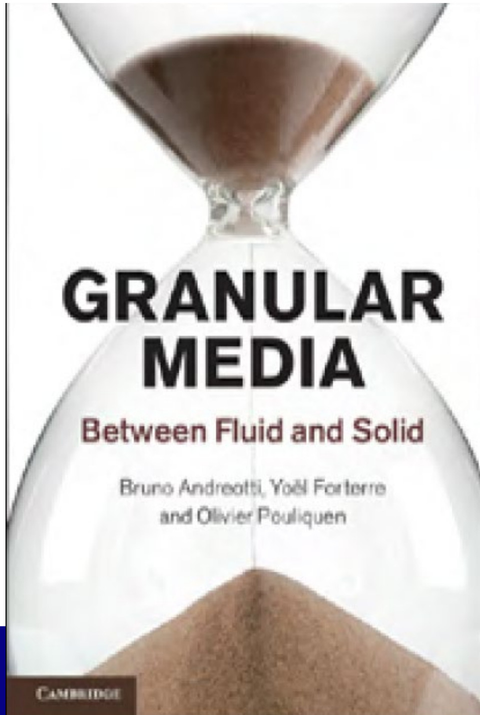
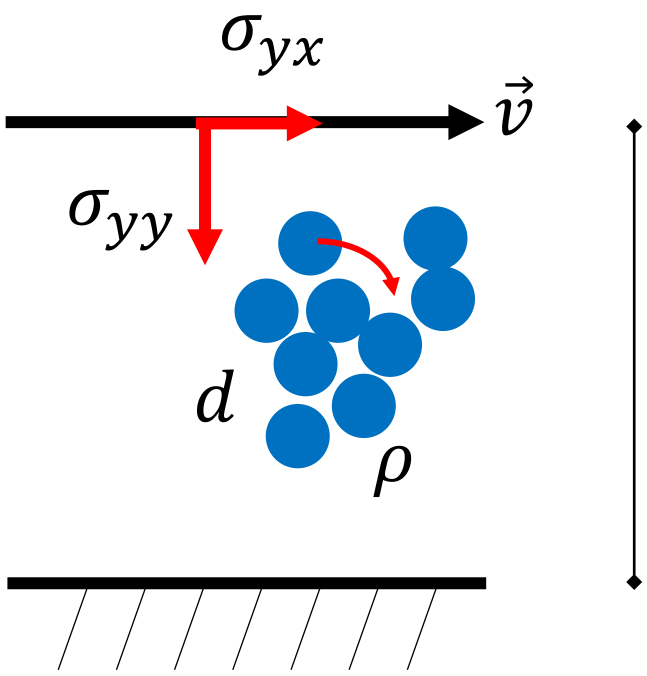


Part II: Sometimes, medium is best

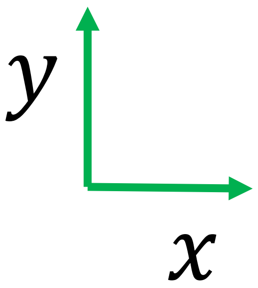
Try to come up with the definition

What is the most reasonable dimensionless number possible?

Microscopic interpretation



$$L \rightarrow \dot{\gamma} = \frac{|\vec{v}|}{L}$$



$$I = \frac{\dot{\gamma} d}{\sqrt{\sigma_{yy}/\rho}}$$

Applying this to granular materials

Increasing velocity of particles

“Inertial number” $I(\vec{v})$

Static packing

Granular gas

Applying this to granular materials

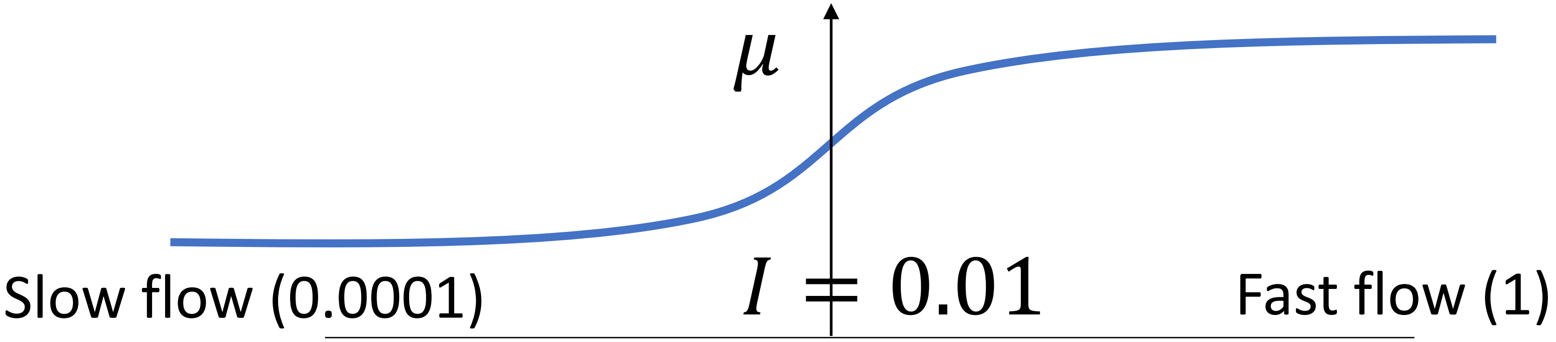
$$\frac{\sigma_{xy}}{\sigma_{yy}} = \mu\left(I(\vec{v})\right) = \mu_s + \frac{\mu_0 - \mu_s}{I/I_0 + 1}$$

Increasing velocity of particles

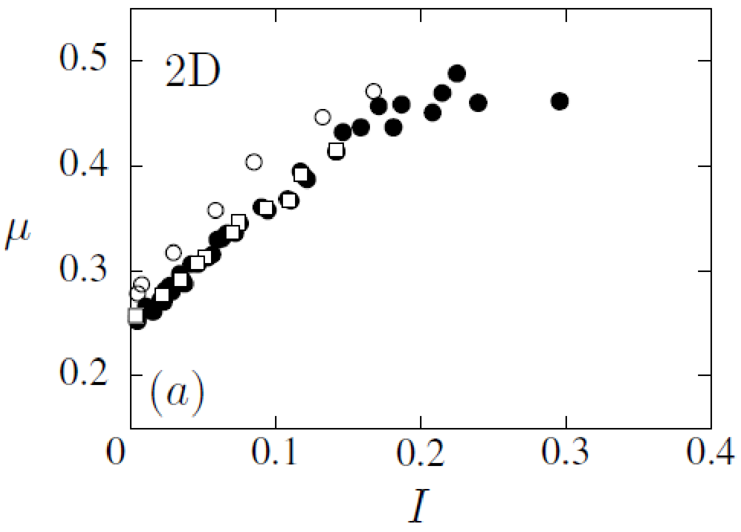
"Inertial number" $I(\vec{v})$

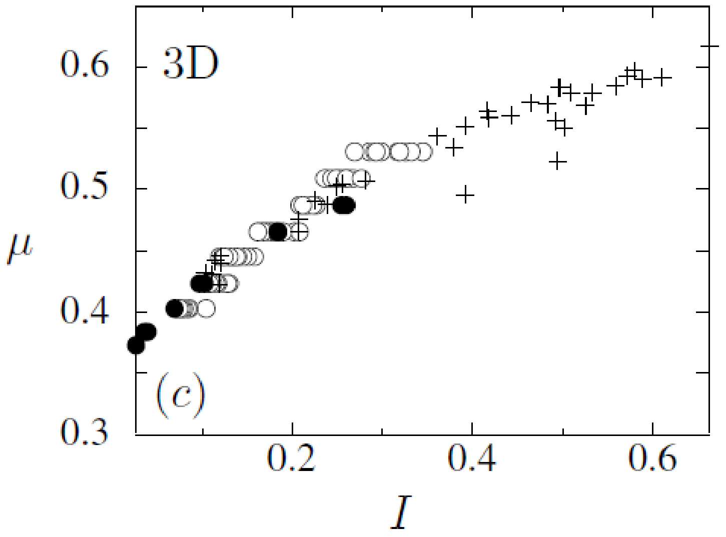
Static packing

Granular gas



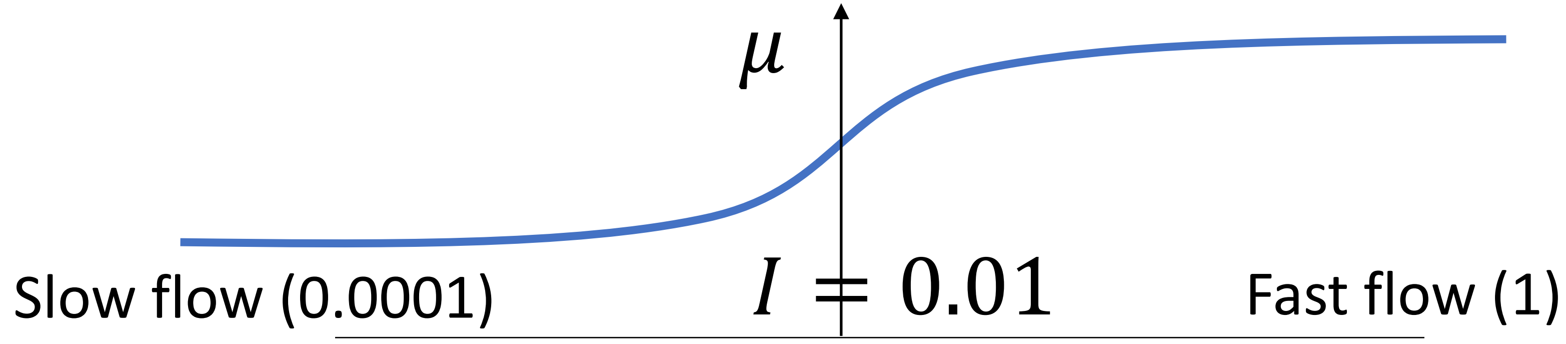
Works in flow fields





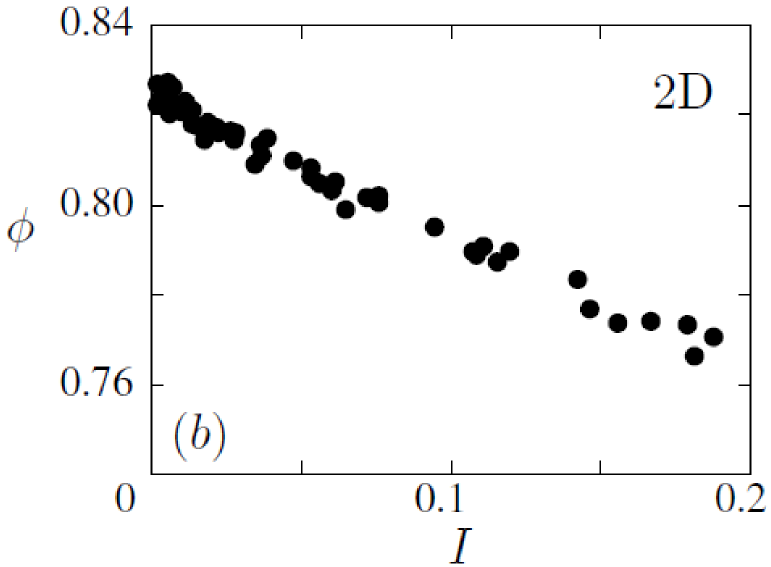
"Inertial number" $I(\vec{v})$

Static packing



Granular gas

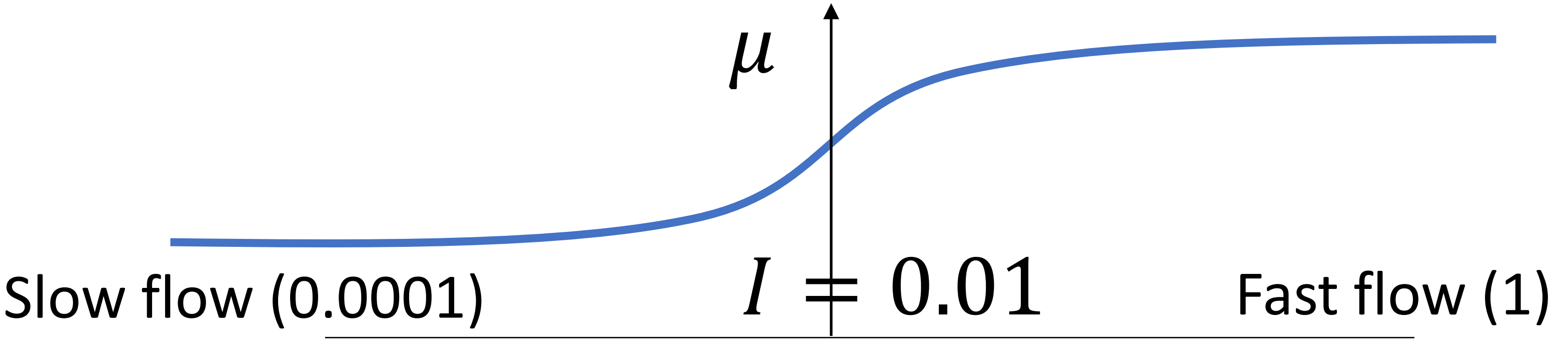
And for density or packing fraction



“Inertial number” $I(\vec{v})$

Static packing

Granular gas

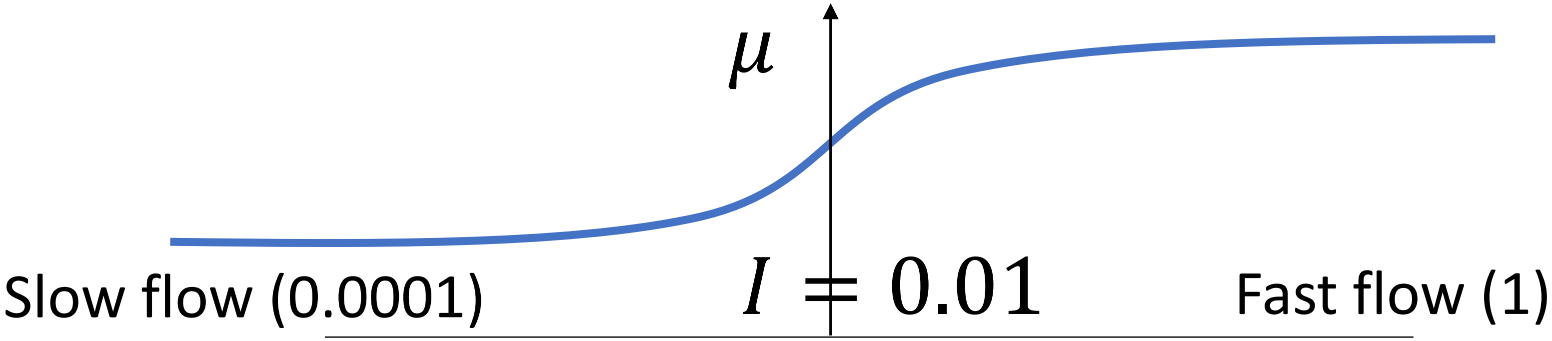


And for density or packing fraction

“Inertial number” $I(\vec{v})$

Static packing

Granular gas



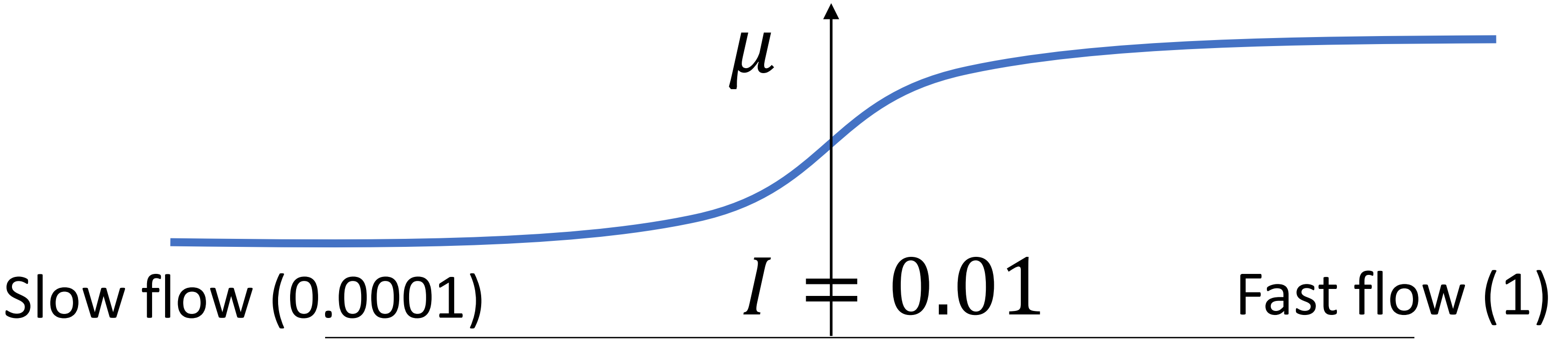
But why?

- Why this function?
- Where do constants come from?

“Inertial number” $I(\vec{v})$

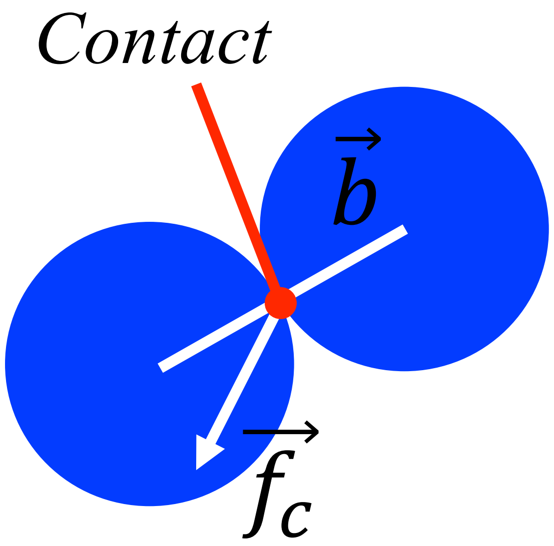
Static packing

Granular gas

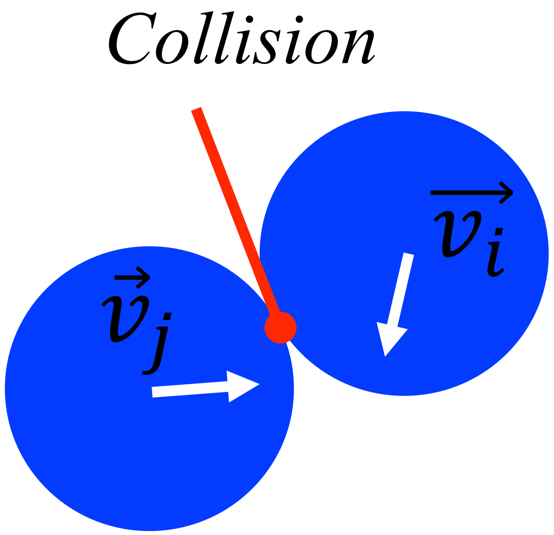


Material constants derive from microscopics

$$\bar{\sigma} \cong \frac{1}{V_c} \sum_{\text{Contacts}} \vec{b} \otimes \vec{f_c} + \frac{1}{V_c} \sum_{\text{Collisions}} \vec{v_i} \otimes \vec{v_j}$$



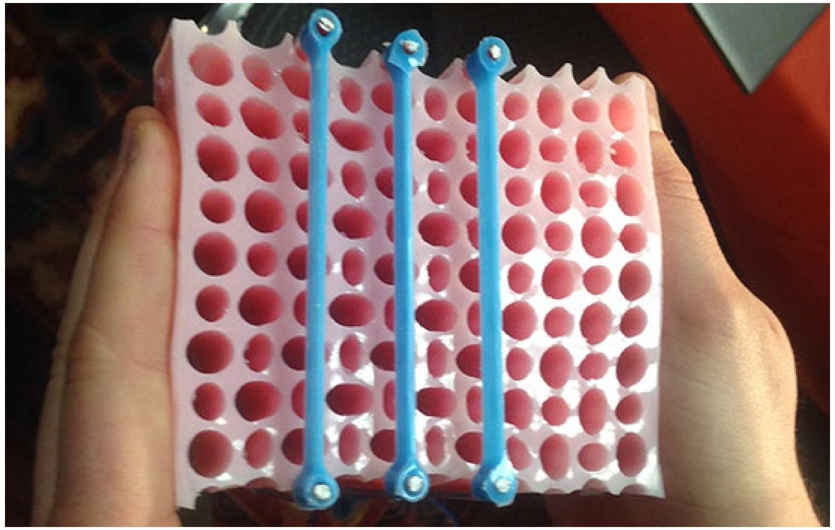
The science is e.g. in identifying emerging simplicity in $V_C < V_{sample}$



Structure – material relation is a general perspective

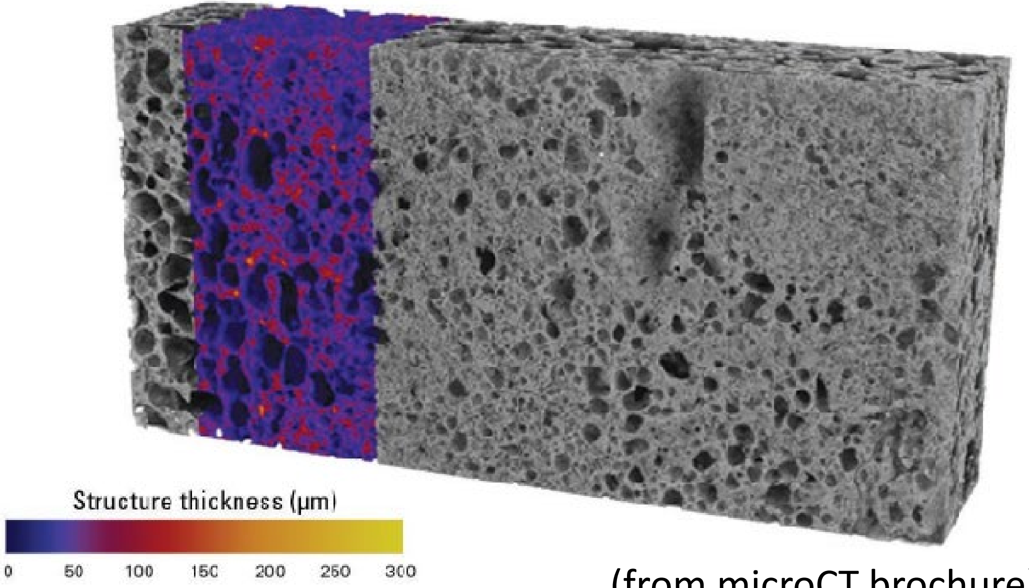
"Metamaterials are man-made materials with extraordinary properties that come from their geometrical structure rather than their chemical composition."

-- press release about successful funding application



General perspective

"Foams are man-made materials with extraordinary properties that come from their geometrical structure rather than their chemical composition."



(from microCT brochure)

General perspective

"Foams are man-made materials with extraordinary properties that come from their geometrical structure rather than their chemical composition."

...but now structure is disordered and at ~100 micron scale

General perspective

"Glasses are man-made materials with extraordinary properties that come from their geometrical structure rather than their chemical composition."

...but now structure is disordered and at ~10 nm scale

General perspective

"Mayonnaise is a man-made material with extraordinary properties that comes mostly from its geometrical structure rather than its chemical composition."

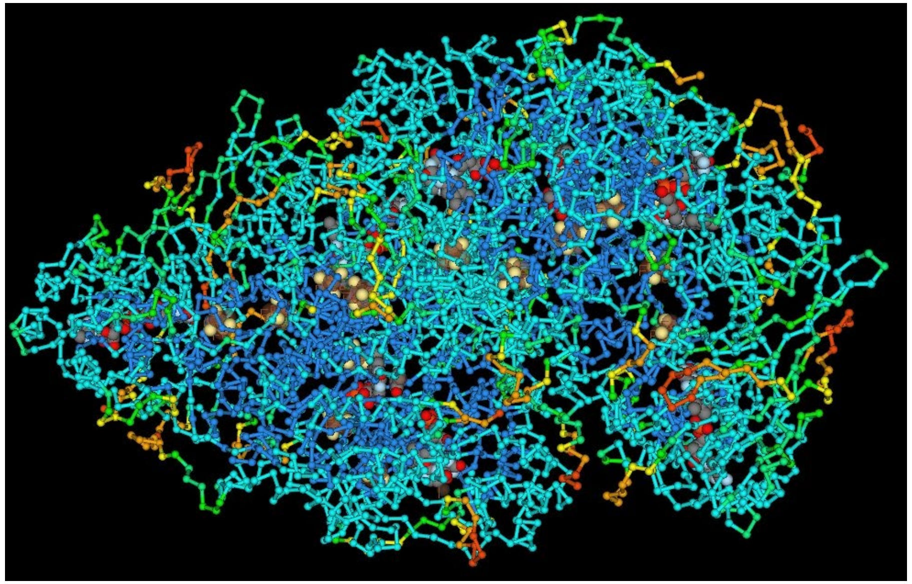
...but now structure is disordered and at ~10 micron scale

"Chemistry is more about electrons than elements"

-- P. Ball, Chemistry World (2010)

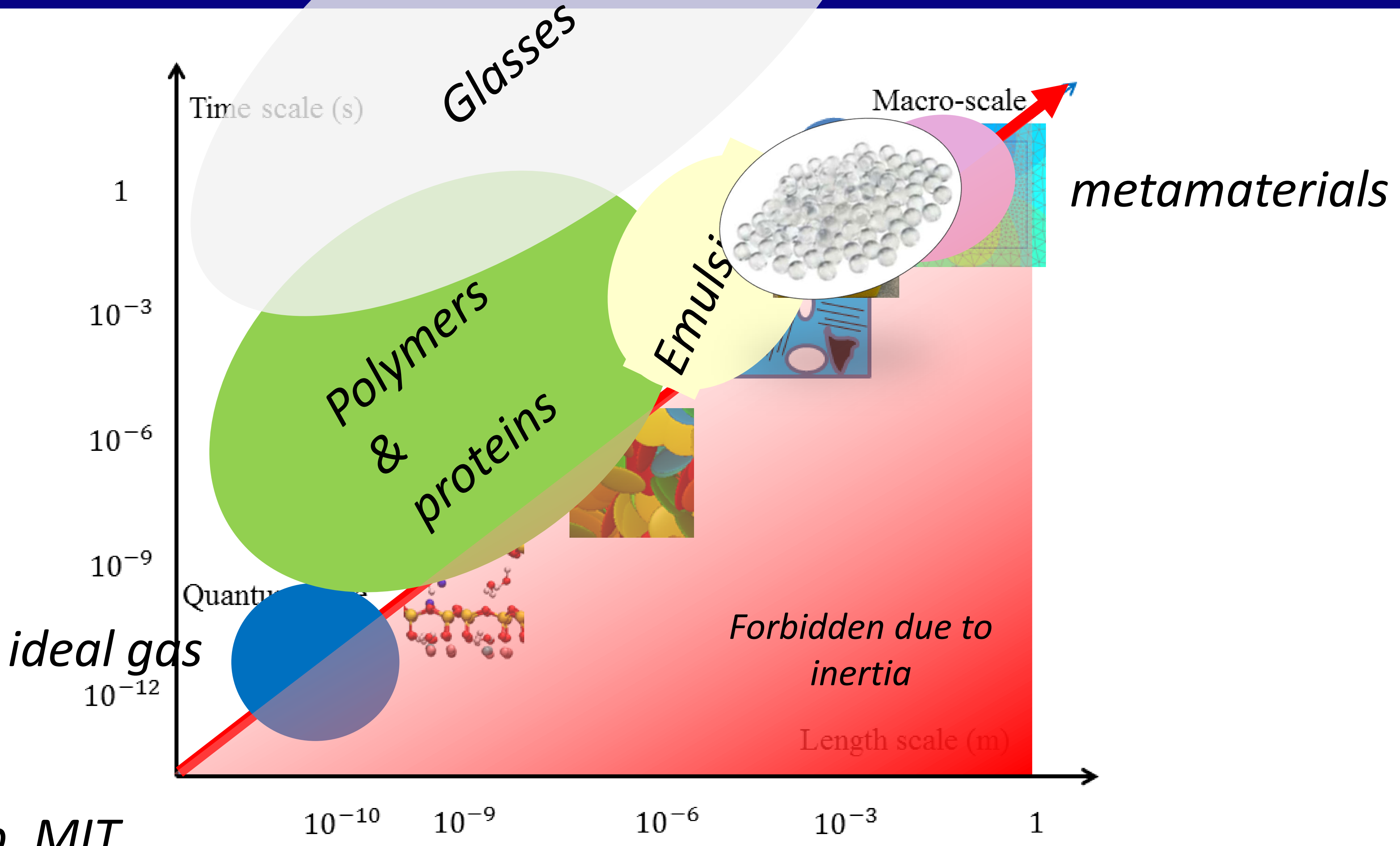
General perspective

"Proteins can be man-made materials with extraordinary properties that come partly from their geometrical structure, partly from their electronic structure."



...but now structure is ordered and at ~1 nm scale

Structure – interaction games in a universe of materials



Davoud Lab, MIT

Structure – material relation is a general perspective

"..the distinction between a material and a structure is never very clear."

-- J.E. Gordon, The New Science of Strong Materials

What other materials can we consider?

$$\bar{\sigma} \cong \frac{1}{V_c} \sum_{\text{Contacts}} \vec{b} \otimes \vec{f_c} + \frac{1}{V_c} \sum_{\text{Collisions}} \vec{v_i} \otimes \vec{v_j}$$

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What is the following material?

$$\bar{\sigma} \cong \frac{1}{V_c} \sum_{\text{Contacts}} \vec{b} \otimes \vec{f_c} + \frac{1}{V_c} \sum_{\text{Collisions}} \vec{v_i} \otimes \vec{v_j}$$

- Discrete particles
- Spherical, convex particles
- Frictional contacts
- Hard: no deformation of particles
- ~~Large particles: no thermal motion~~
- Particles are "loose"
- "Passive" particles

- Weakly elastic collisions
- Mono/bidisperse
- ~~Embedded in air; no viscous drag~~
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Hard sphere colloids

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Metamaterials

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Emulsions

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Polymeric gels

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How about your own research?

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Discuss for three minutes with your neighbor

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