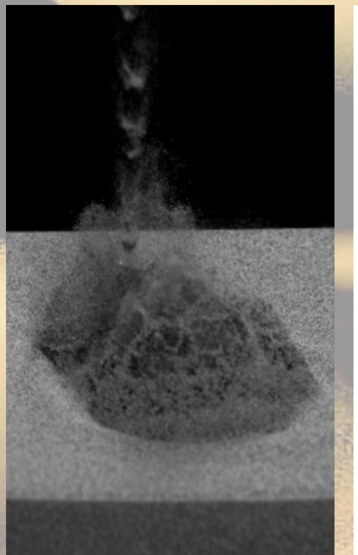
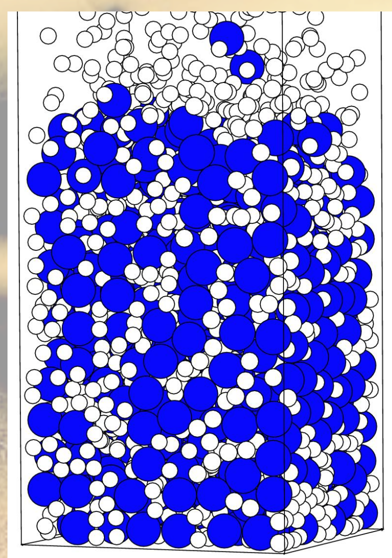
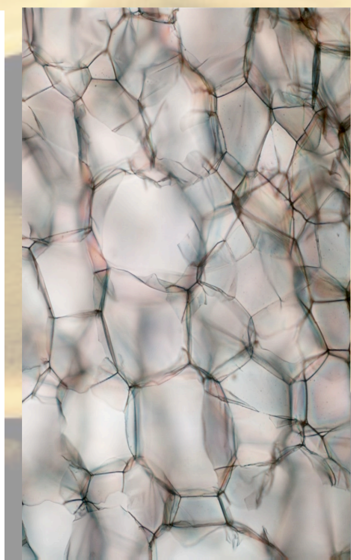
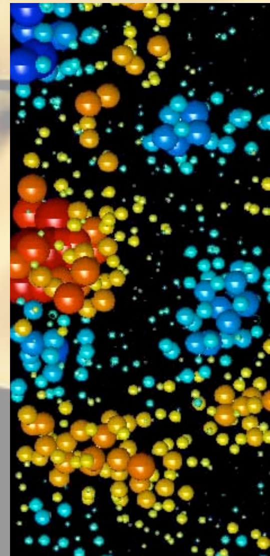
JMBC Workshop
“Statics and dynamics of soft and granular materials”
Drienerburght, University of Twente, March 21 - March 24, 2016

Speakers: Günter Auernhammer - Dirk van der Ende - Nico Gray - Daniela Kraft - Detlef Lohse - Stefan Luding - Martin van der Hoef - Vanessa Magnanimo - Devaraj van der Meer - Peter Schall

Many materials, often grouped together using the term ‘soft matter’, share common characteristics and behavior: For example, the materials consist of macroscopic particles, larger than the molecules that build up the world around us. They jam when flow is about to stop, and unjam just before flow starts. The static (‘solid’) situation is often characterized by a high degree of disorder, inhomogeneity and anisotropy, while the dynamic (‘fluid’) situation is frequently dominated by dissipative interaction forces leading to a dissipation time scale that interacts with other time scales in the system. Finally, there is the role of the interstitial fluid that resides between the particles and may mediate thermal (Brownian) motion, in the case of colloids, or hydrodynamic interactions (drag) in the case of macroscopic grains. This course, aimed at graduate students, will provide an introduction to this type of materials and discuss many of the phenomena mentioned above both as an overview and in the context of actual research.

PROGRAM JMBC Workshop "Statics and dynamics of soft and granular materials"
(Drienerburght, University of Twente, March 21 - March 24, 2016)

	MONDAY March 21, 2016	TUESDAY March 22, 2016	WEDNESDAY March 23, 2016	THURSDAY March 24, 2016	FRIDAY March 25, 2016
09:00 - 10:45		**Granular materials: from physics to engineering applications Vanessa Magnanimo)**	**Simulation of granular two-phase flows (Martin v/d Hoef)**	**Impact on granular solids (Detlef Lohse)**	
10:45 - 11:15	**Welcome**	coffee & tea	coffee & tea	coffee & tea	
11:15 - 12:15	**Introduction (Devaraj v/d Meer)**	**Granular matter and interstitial fluids (Devaraj v/d Meer)**	**Colloidal self-assembly (Daniela Kraft)** [11:15 - 12:45]	**Student talks**	
12:15 - 13:30	lunch	lunch	lunch [12:45 - 13:30]	lunch	
13:30 - 15:15	**Granular Avalanches (Nico Gray)**	**Nonequilibrium transitions in flowing colloidal glasses and grains (Peter Schall)**	**Introduction to Rheology: Does soft matter have a memory? (Dirk v/d Ende)**	**Experiments in two and three dimensions (Günter Auernhammer)**	
15:15 - 15:45	coffee & tea	coffee & tea	coffee & tea		
15:45 - 17:30	**Particle size segregation in granular free surface flows (Nico Gray)**	**Modeling jamming and unjamming in soft and granular matter (Stefan Luding)**	**Dispersion Rheology: How flow determines the structure of a suspension and how structure determines flow (Dirk v/d Ende)**		
18:30 - 21:00			**Workshop dinner**		

Registration: http://www.jmburgerscentrum.nl/formulier/6/JMBC-PhD-Course.htm
Tuition fee: University PhDs/postdocs/staff Netherlands: €250; idem other countries: €400; others: €1,000
More information: d.vandermeer@utwente.nl


What is Soft Matter ?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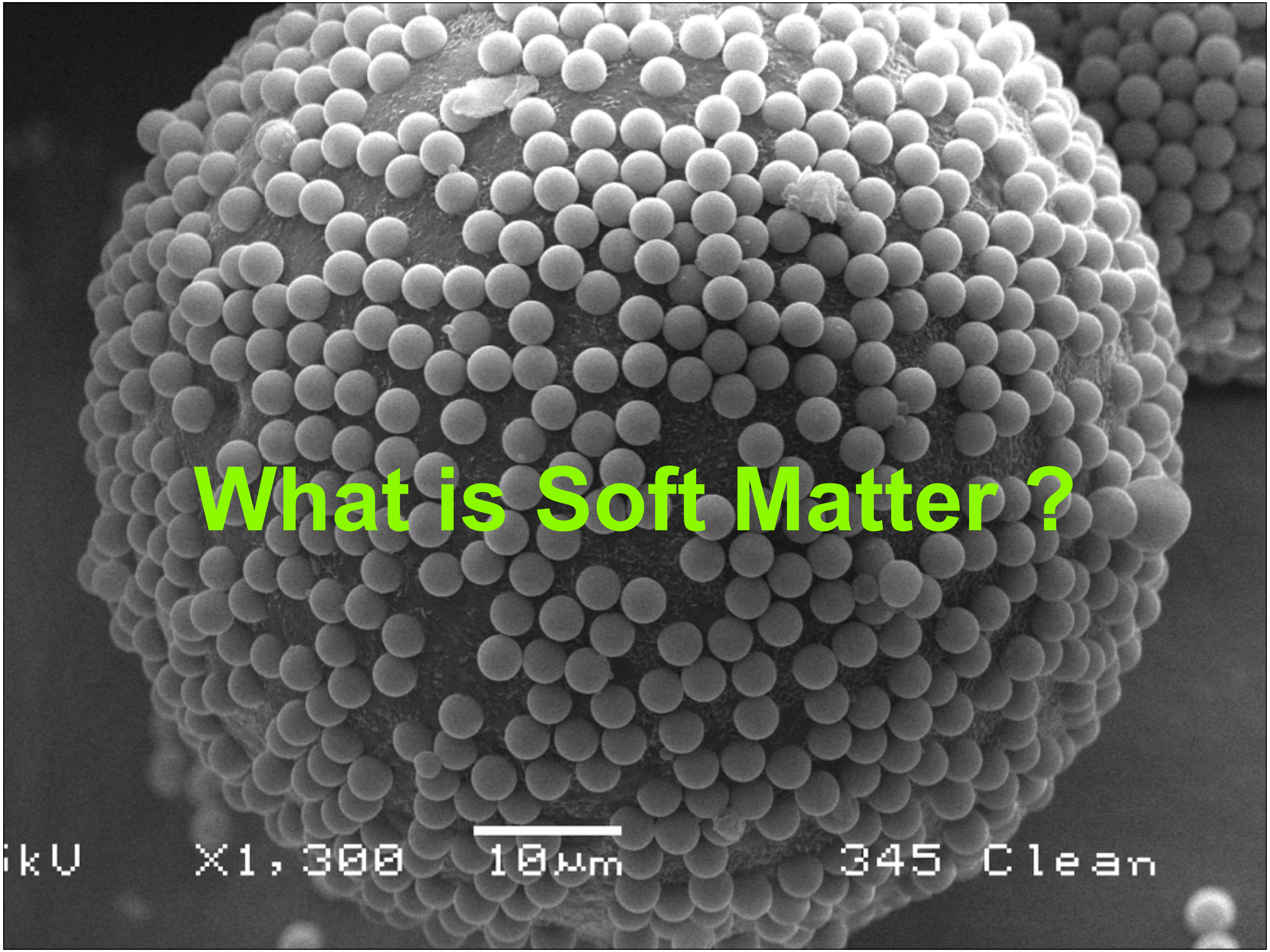


What is Soft Matter ?

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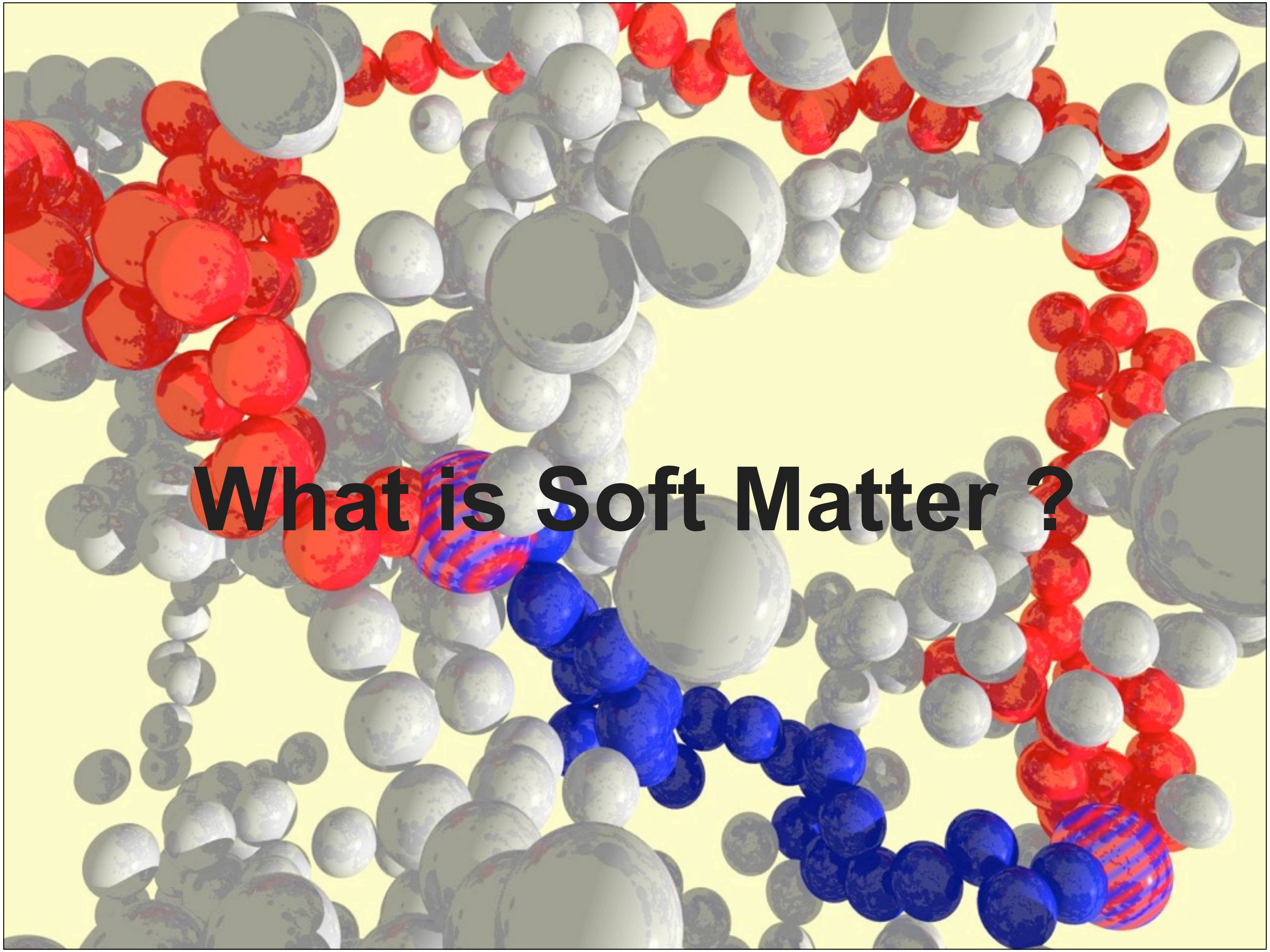
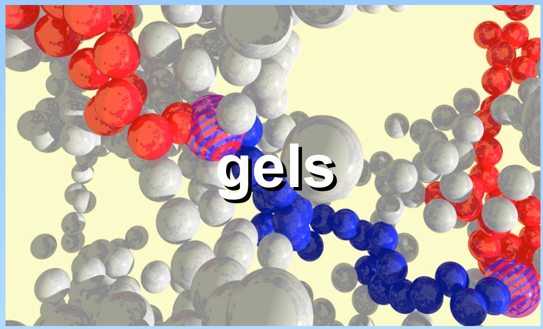
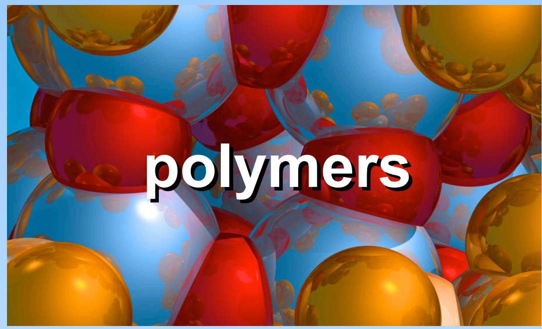


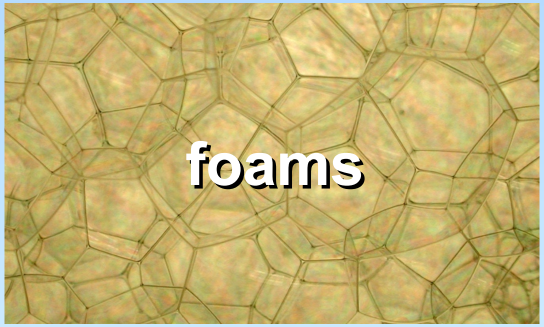
Soft Matter physics is:

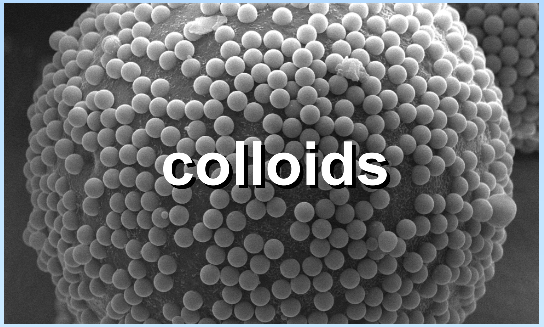
the physics (statics/dynamics) of a system consisting of many particles at a scale on which quantum effects are not important.

Soft Matter includes:

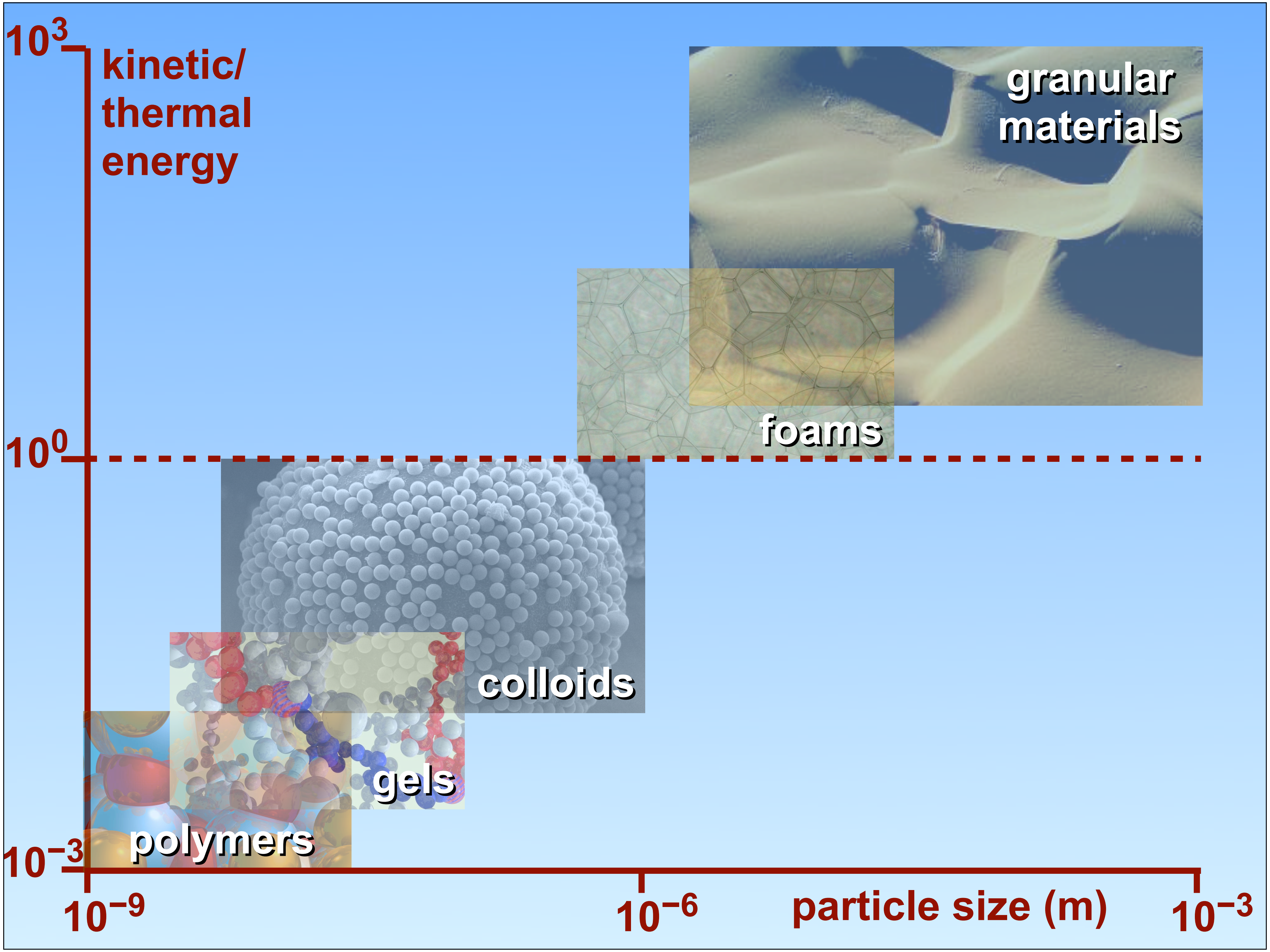








and many biological materials.


10^3
kinetic/
thermal
energy
10^0
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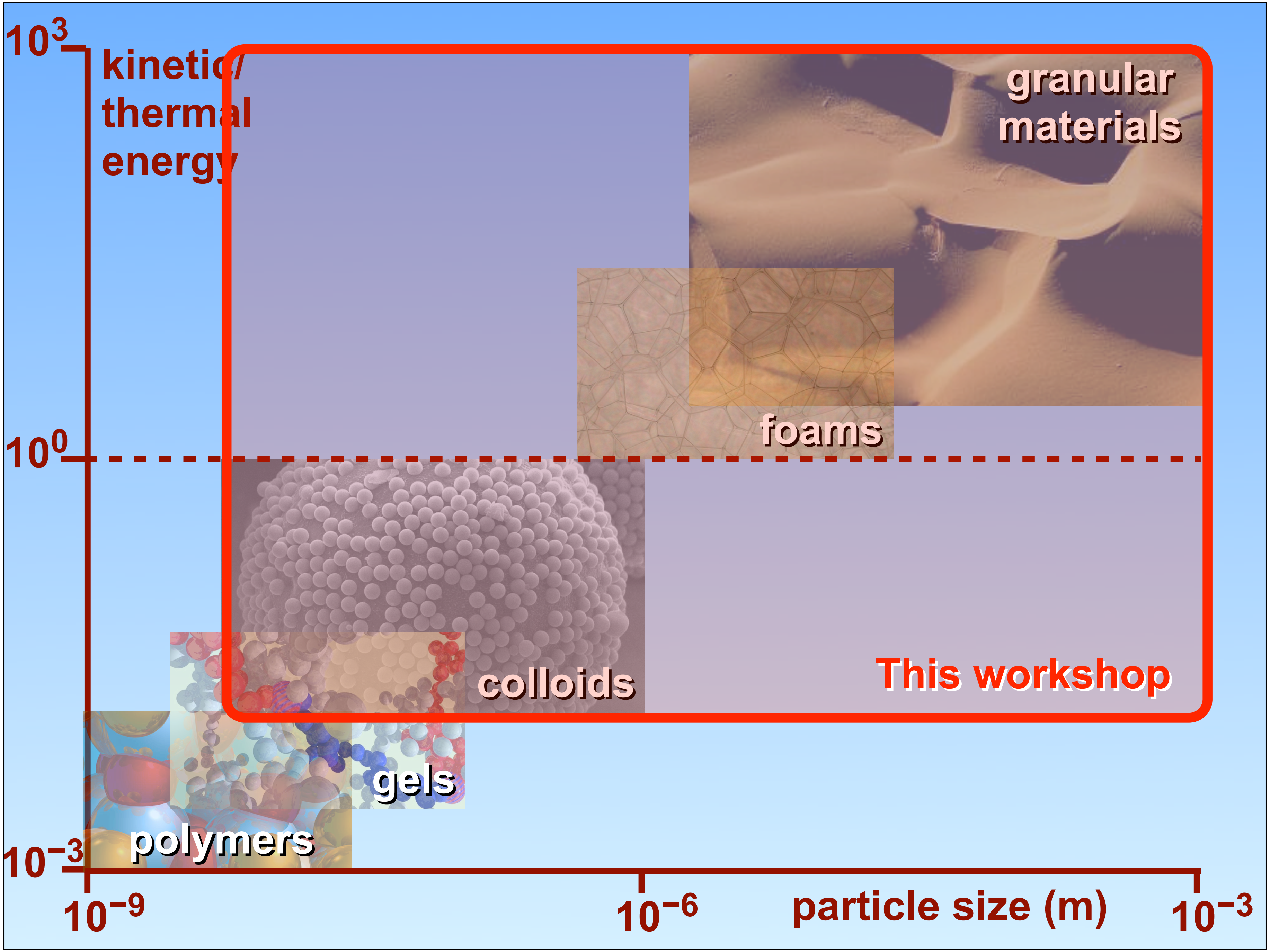
granular
materials
foams
colloids
gels
polymers
10^{-9}
10^{-6}
particle size (m)
10^{-3}



10^3
kinetic/
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foams
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This workshop
gels
polymers
10^{-3}
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particle size (m)
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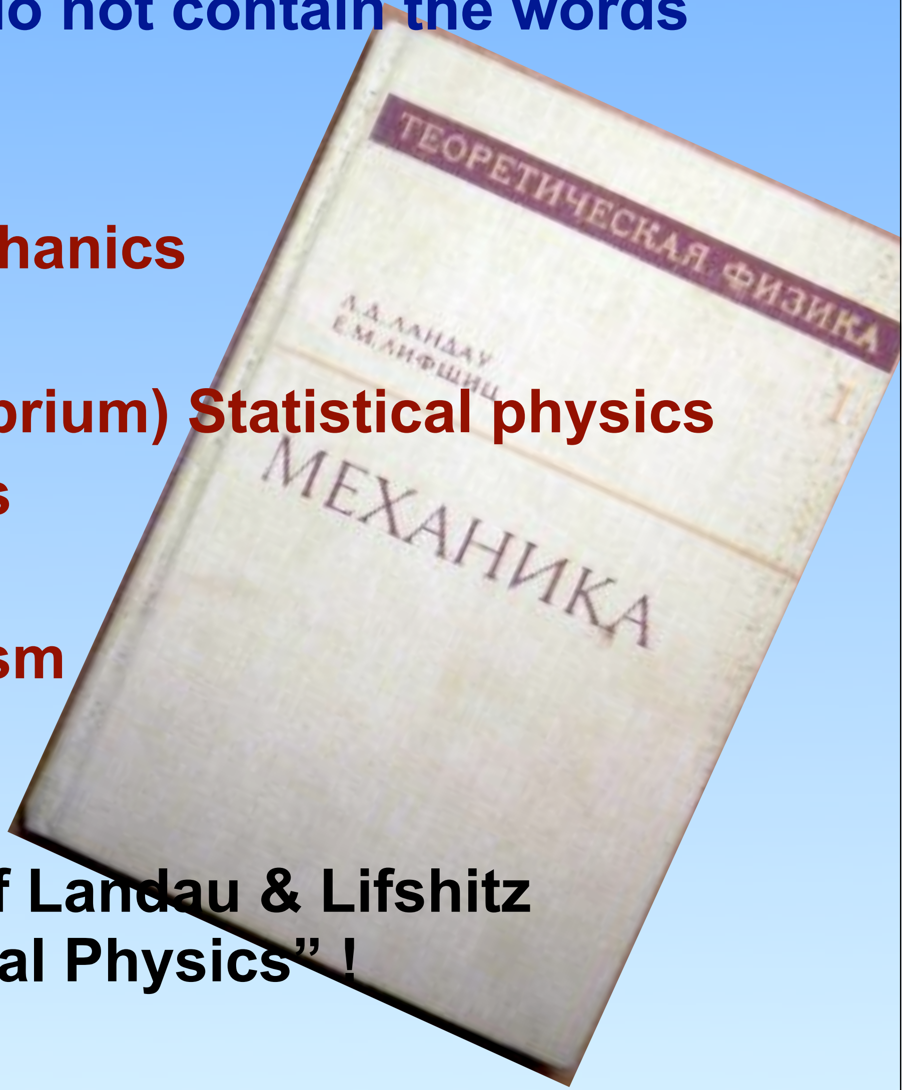
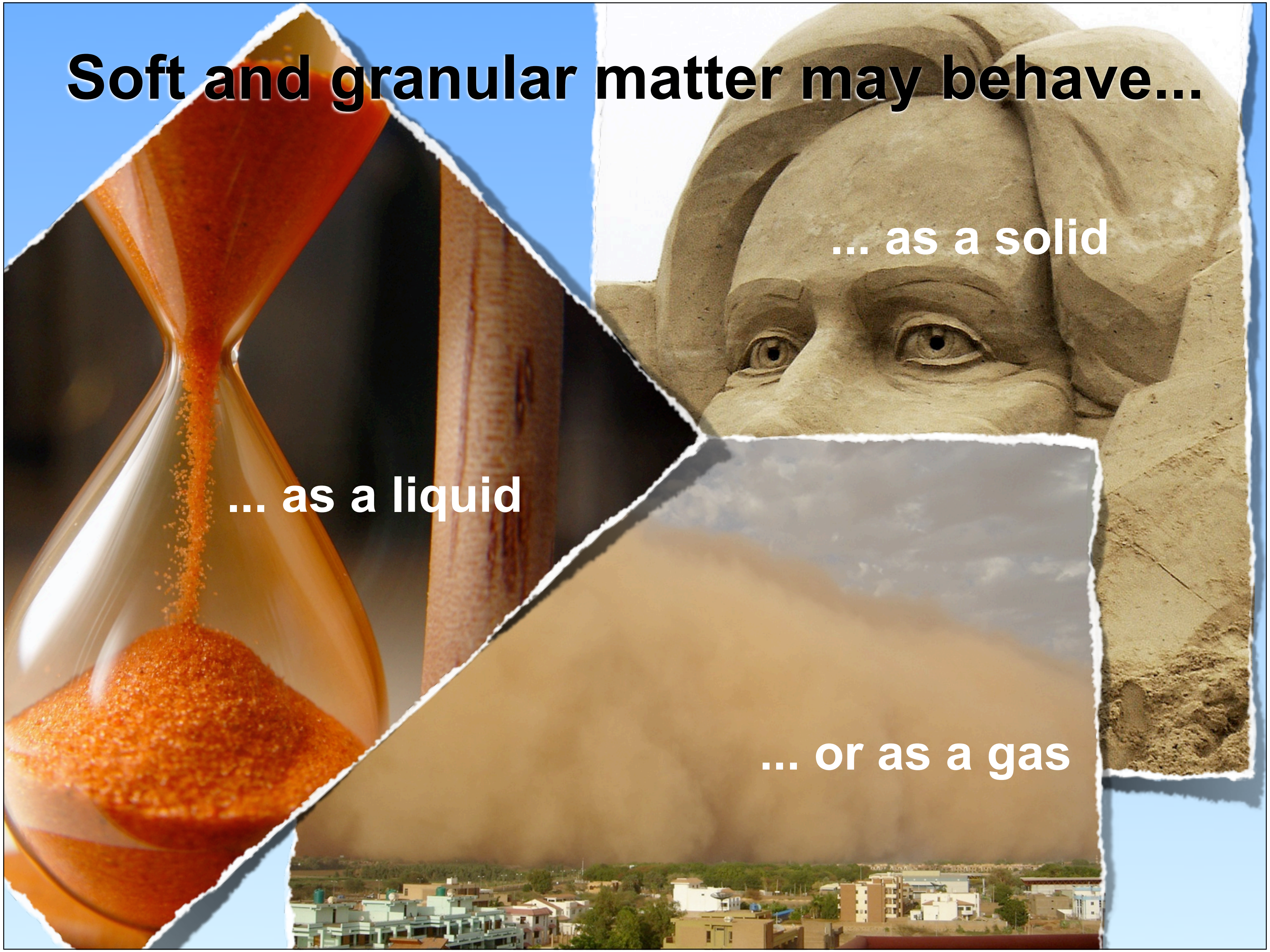
The tools of Soft Matter physics

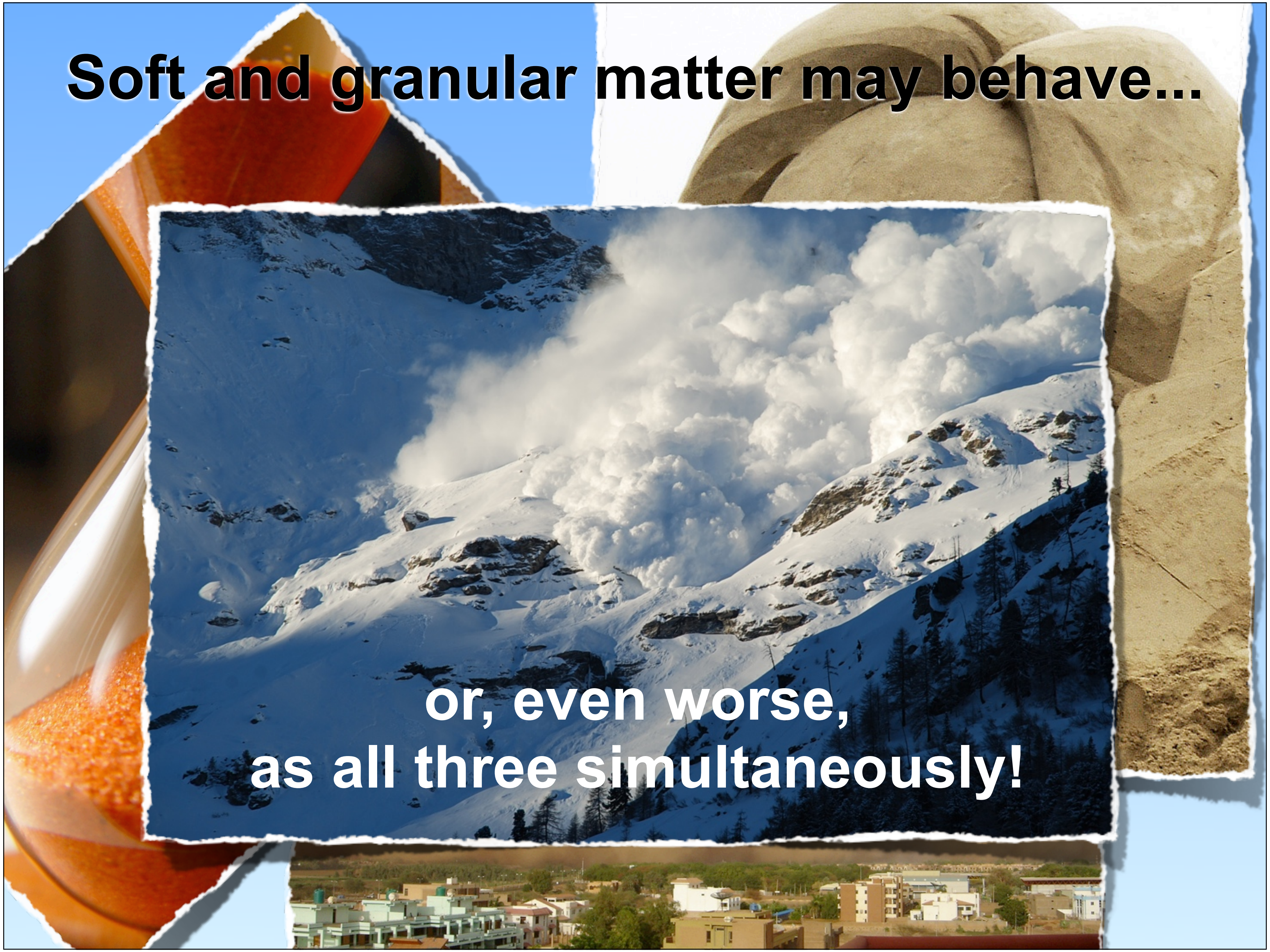
All the tools of physics that do not contain the words "quantum" or "high energy":

V1	(Nonlinear) Mechanics
V2	Classical fields
V5 & V9	(Far from equilibrium) Statistical physics
V6	Fluid Mechanics
V7	Elasticity
V8	Electromagnetism
V10	Kinetic Theory



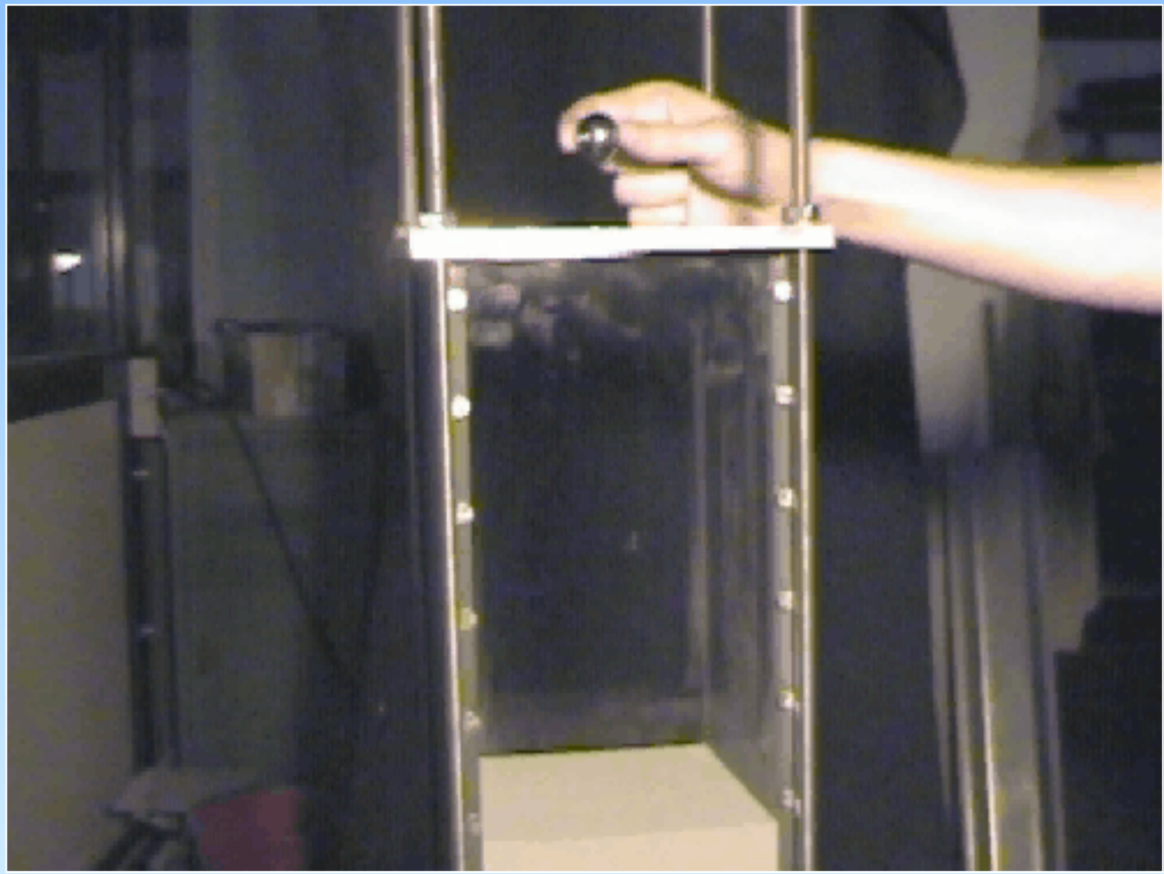
This is 8 out of 10 volumes of Landau & Lifshitz famous "Course of Theoretical Physics" !


Soft and granular matter may behave...
... as a solid
... as a liquid
... or as a gas


Soft and granular matter may behave...
or, even worse,
as all three simultaneously!

Impact on a granular solid

Ball dropped onto loose, very fine sand



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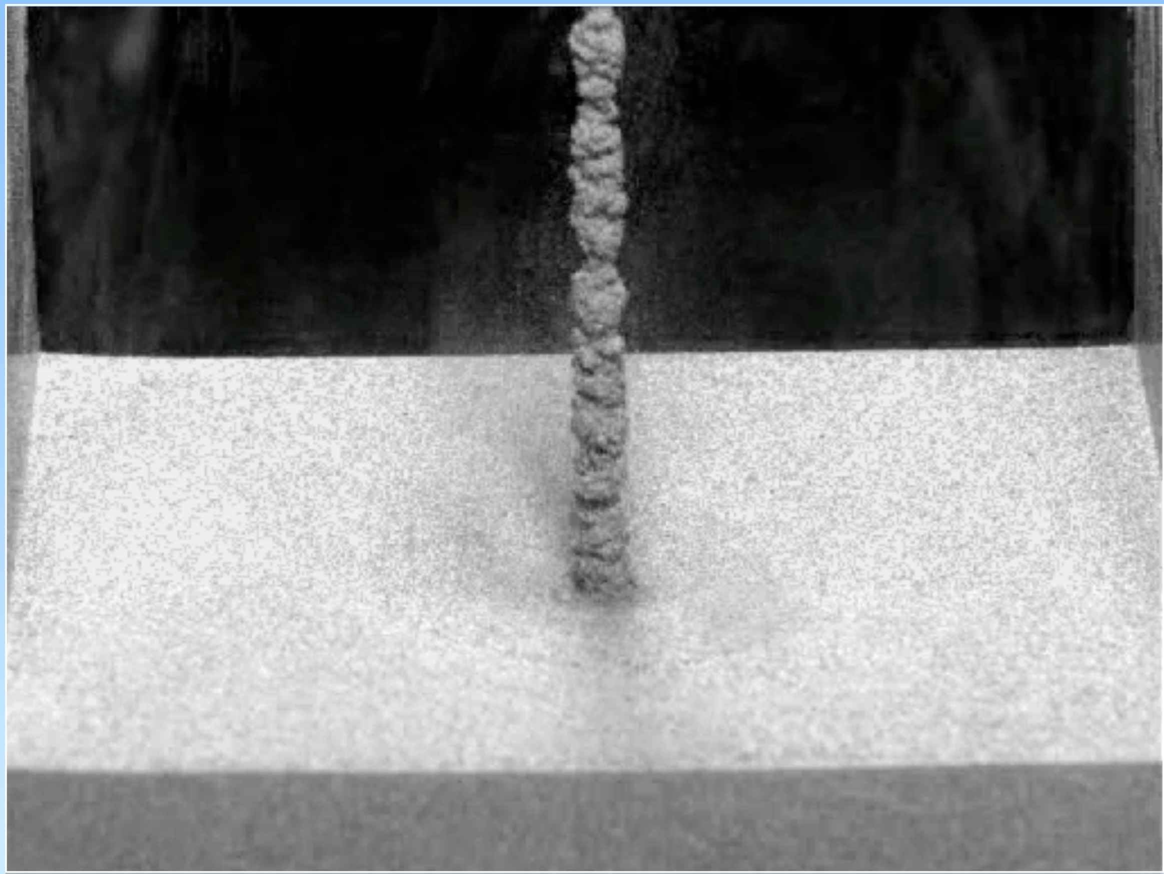

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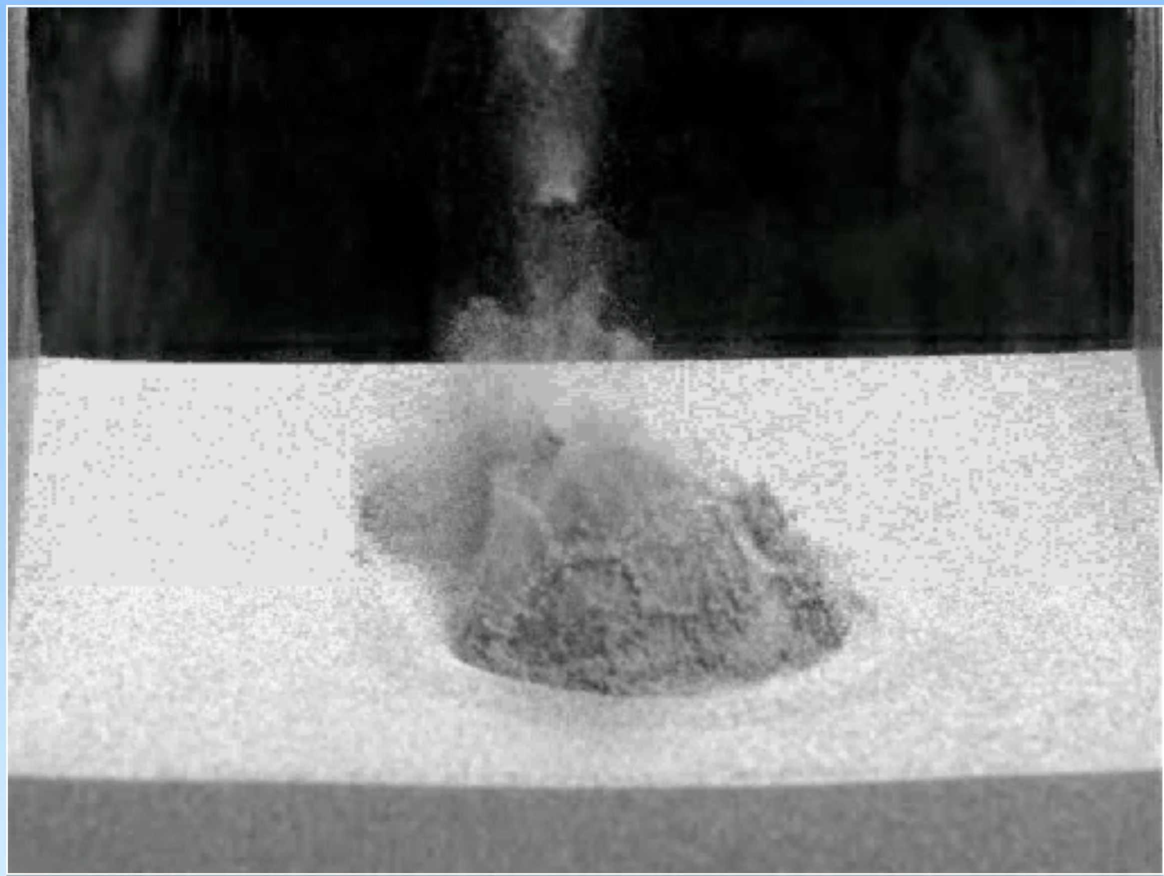


What sets these materials apart from their molecular counterparts ?

To some or large extent, they:

1. are *athermal*

2. interact through *contact forces*

3. have *dissipative* interactions

4. are *inhomogeneous*

1. Granular matter is *athermal*

Definition:

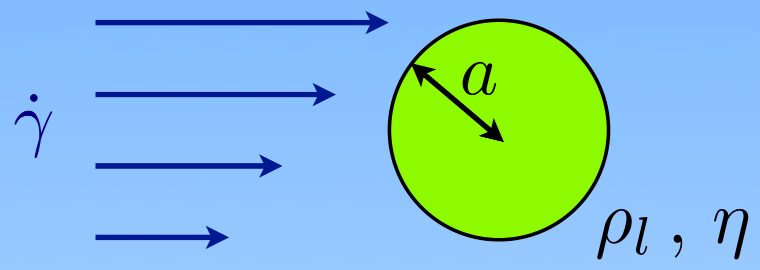
Granular matter =
many body system in which the typical particle size > 10 μm

$$\frac{1}{2} m v_{\text{thermal}}^2 = \frac{3}{2} k_B T \quad \Rightarrow$$ (at room temperature)

$$v_{\text{thermal}} = \sqrt{\frac{3 k_B T}{\frac{4}{3}\pi r^3 \rho}} \approx \sqrt{\frac{10^{-20}}{10^{-11}}} \approx 3 \cdot 10^{-5}\ \mathrm{m/s}$$

Thermal energy is negligible for such particles !

When does thermal motion matter?



Droplet (radius *a*) in liquid with viscosity *η* and density *ρ*ₗ. Flow with shear rate $\dot{\gamma}$.

Péclet number:

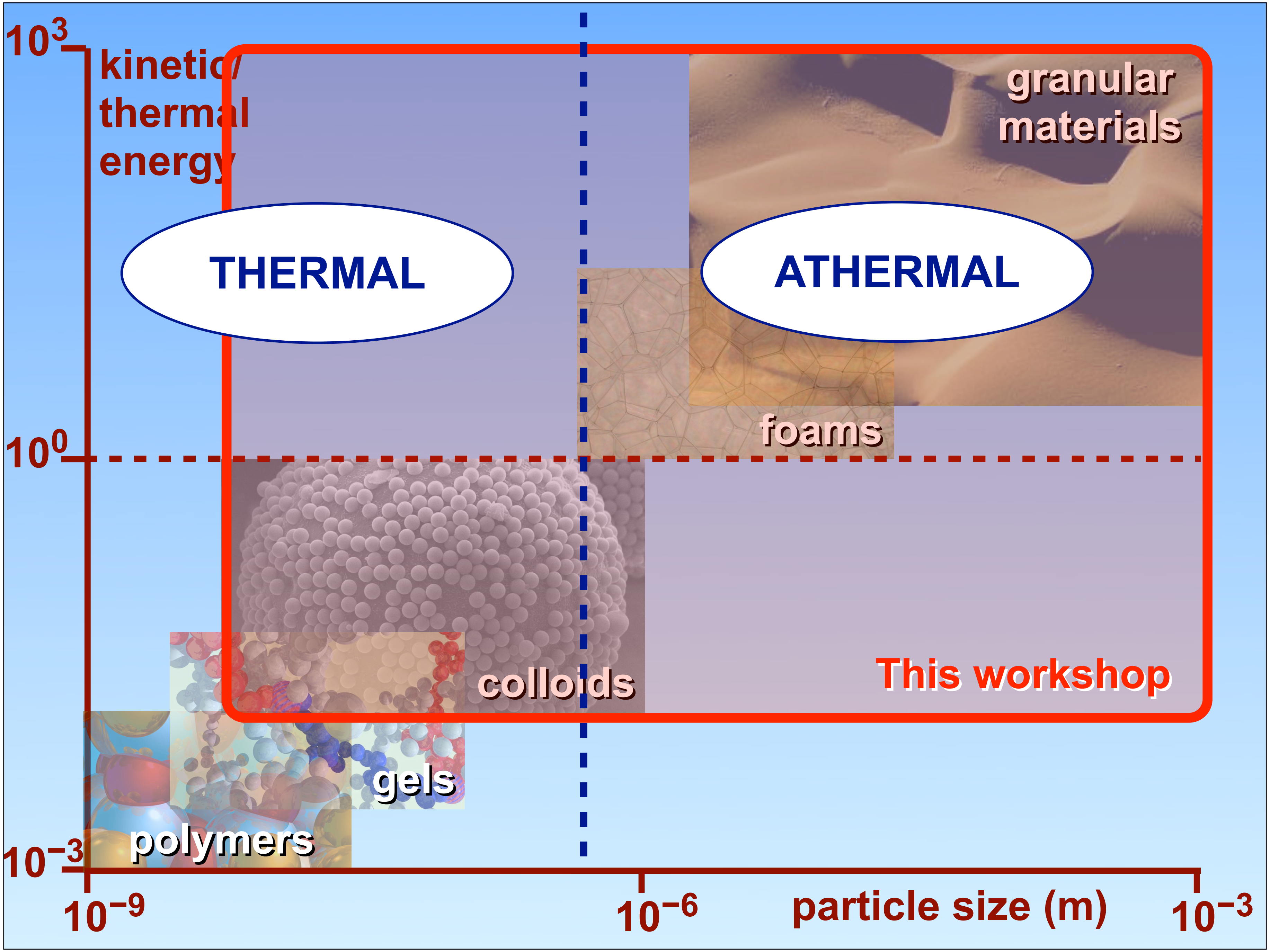
$$\mathrm{Pe} = \frac{\tau_{\mathrm{thermal}}}{\tau_{\mathrm{shear}}} = \dot{\gamma}\,\frac{a^2}{D_0} = 6\pi\,\frac{\eta\dot{\gamma}a^3}{k_B T} = 6\pi\,\frac{\tau a^3}{k_B T}$$

$$D_0 = \frac{k_B T}{6\pi\eta a}$$ **(Stokes-Einstein FDR)**

Péclet number (sedimentation):

$$\mathrm{Pe_s} = \tfrac{4}{3}\pi\,\frac{\Delta\rho\, g\, a^4}{k_B\, T}$$

$$\boxed{\mathrm{Pe_s} \approx 1 \quad \Rightarrow \quad a \approx 500\,\mathrm{nm}}$$



10^3
kinetic/
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THERMAL
ATHERMAL
granular
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This workshop
10^{-9}
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particle size (m)
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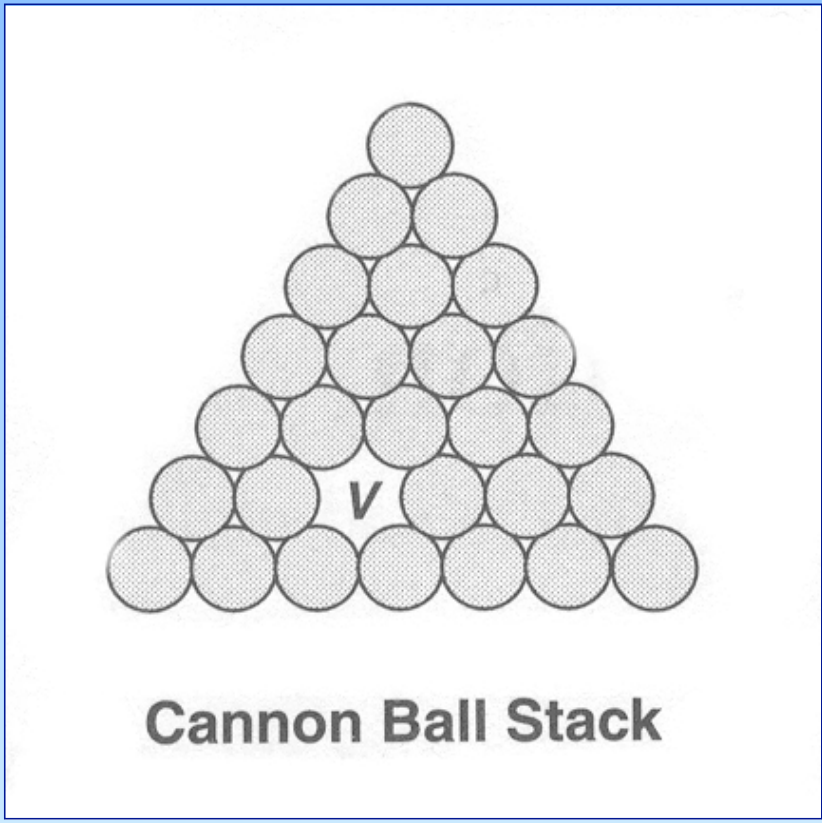
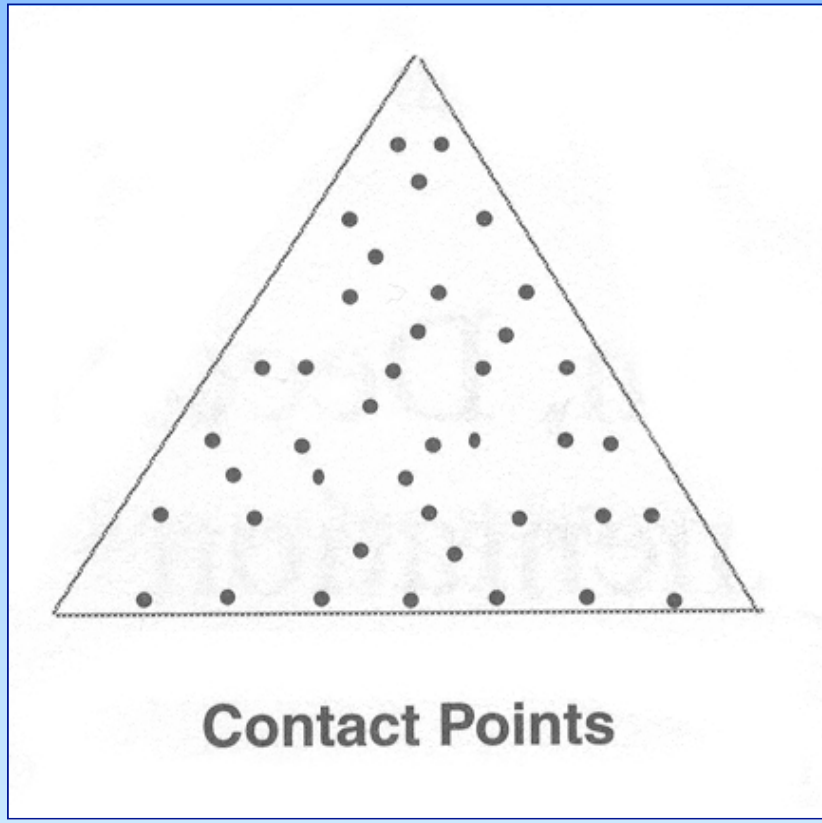
2. Contact forces

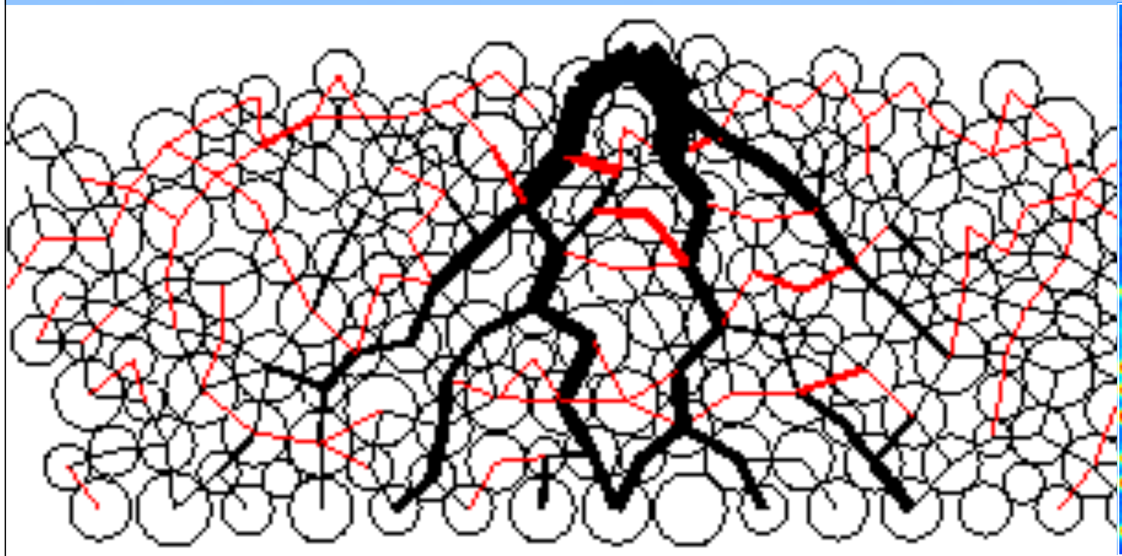
Dominant for granular materials at rest

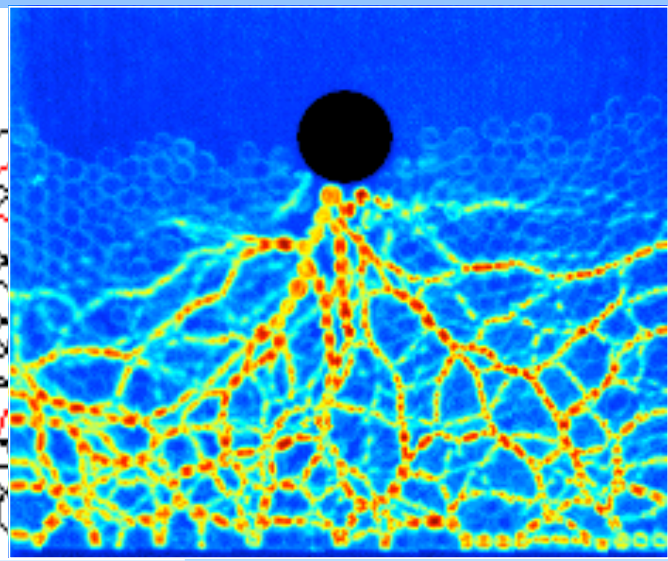




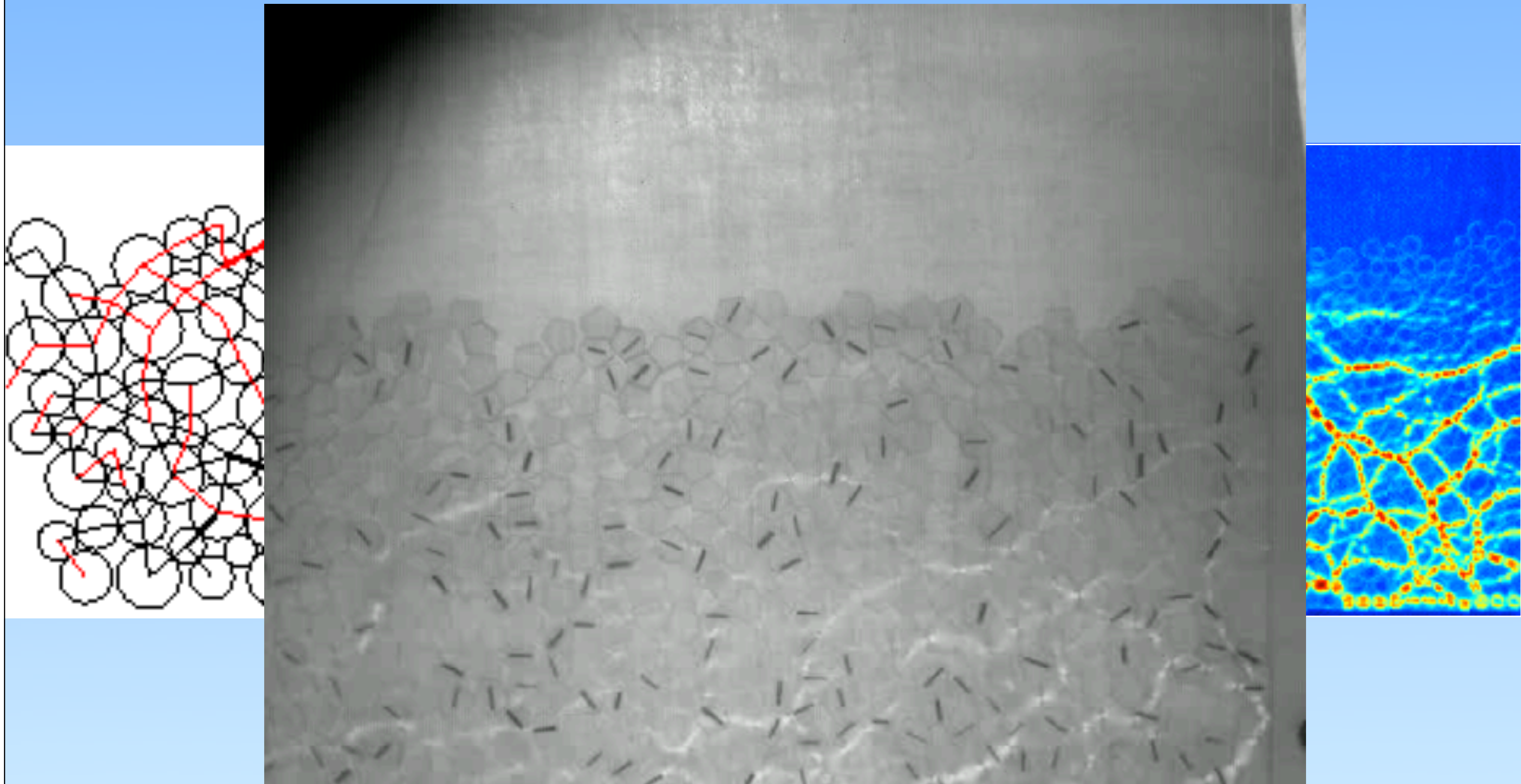
"Chaotic" network of contact points and forces !

Static granular matter: Force Chains



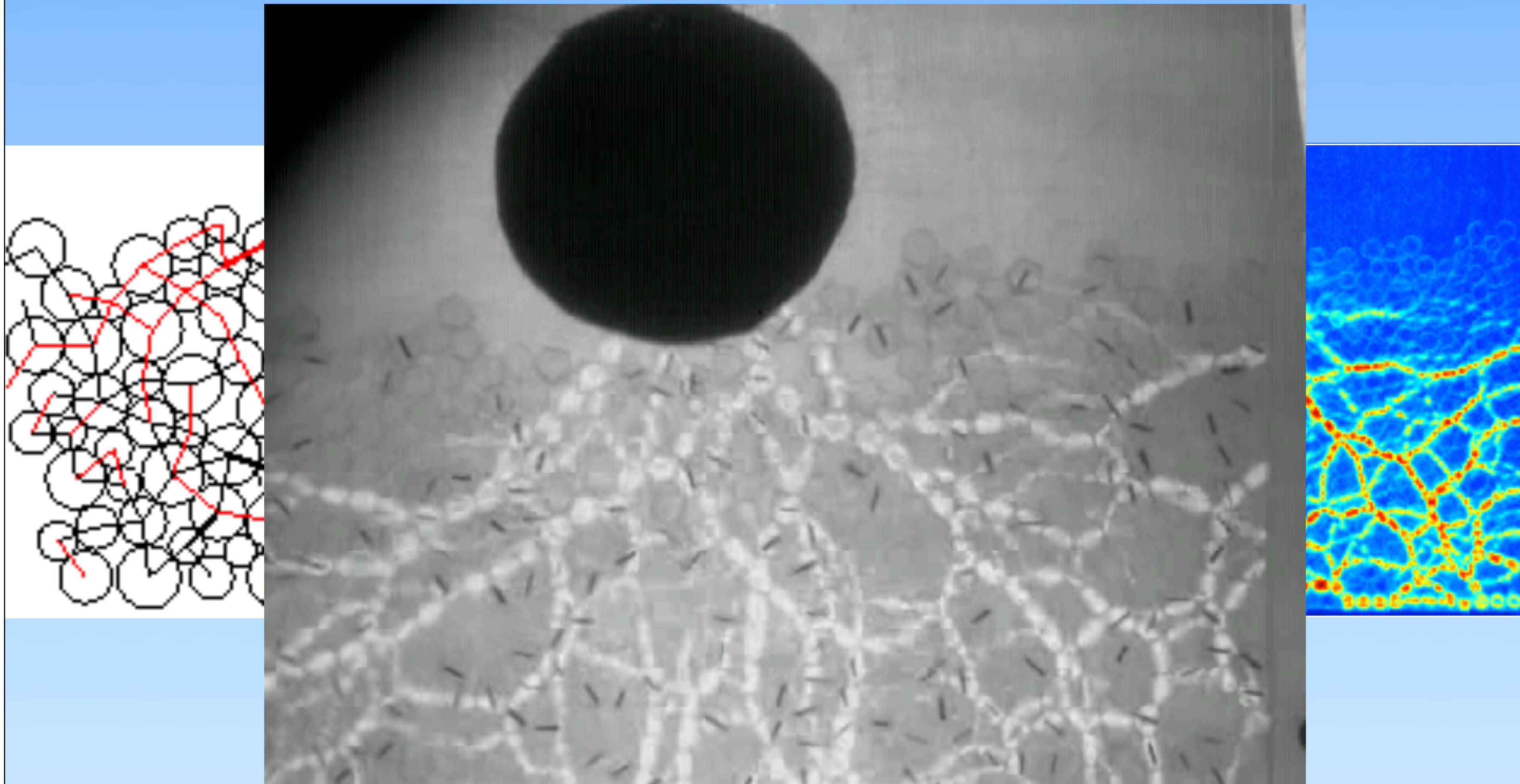


Static granular matter: Force Chains



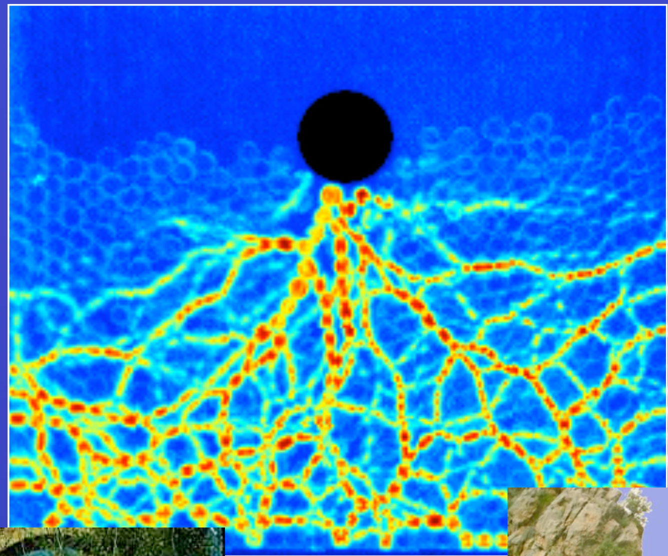
(Bob Behringer, Duke)

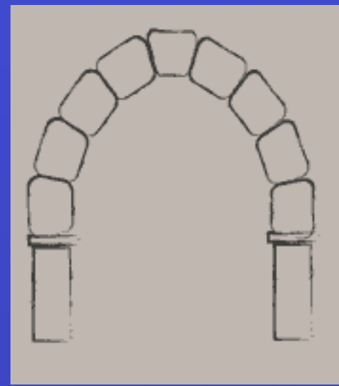
Static granular matter: Force Chains

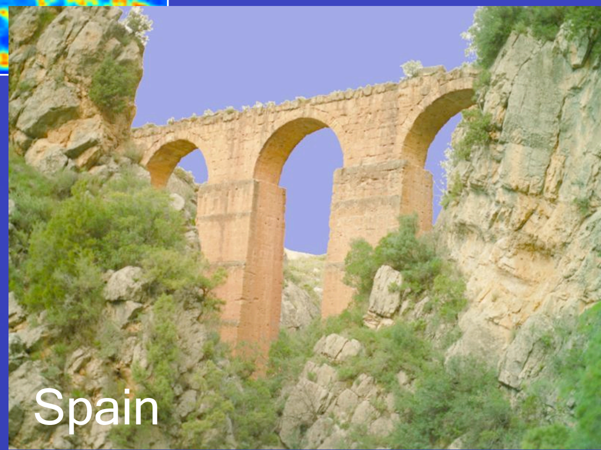


(Bob Behringer, Duke)

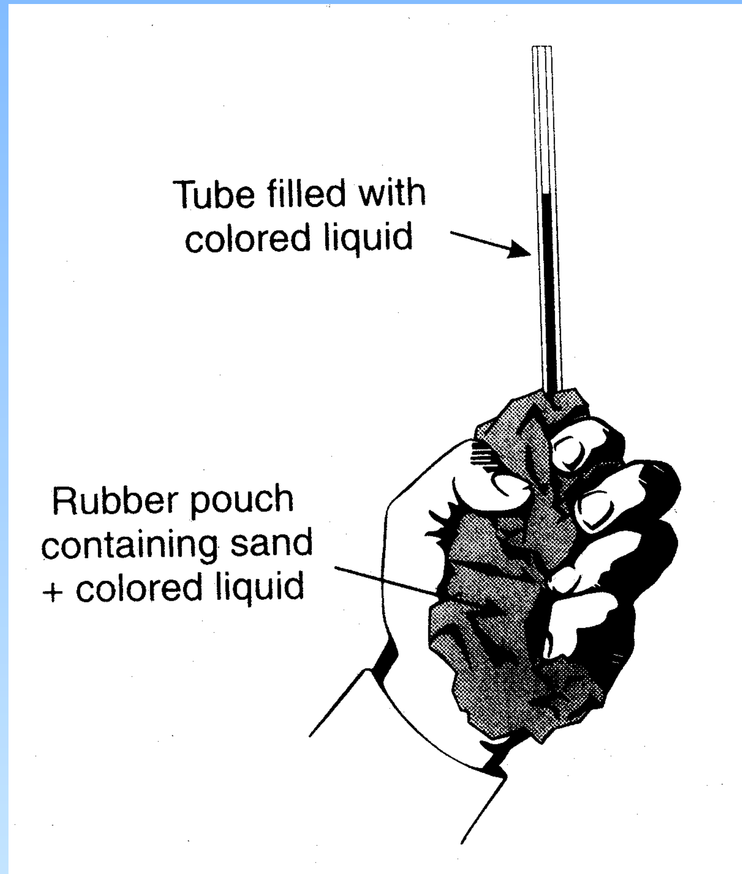
In stalling flow, force chains manifest themselves as arches







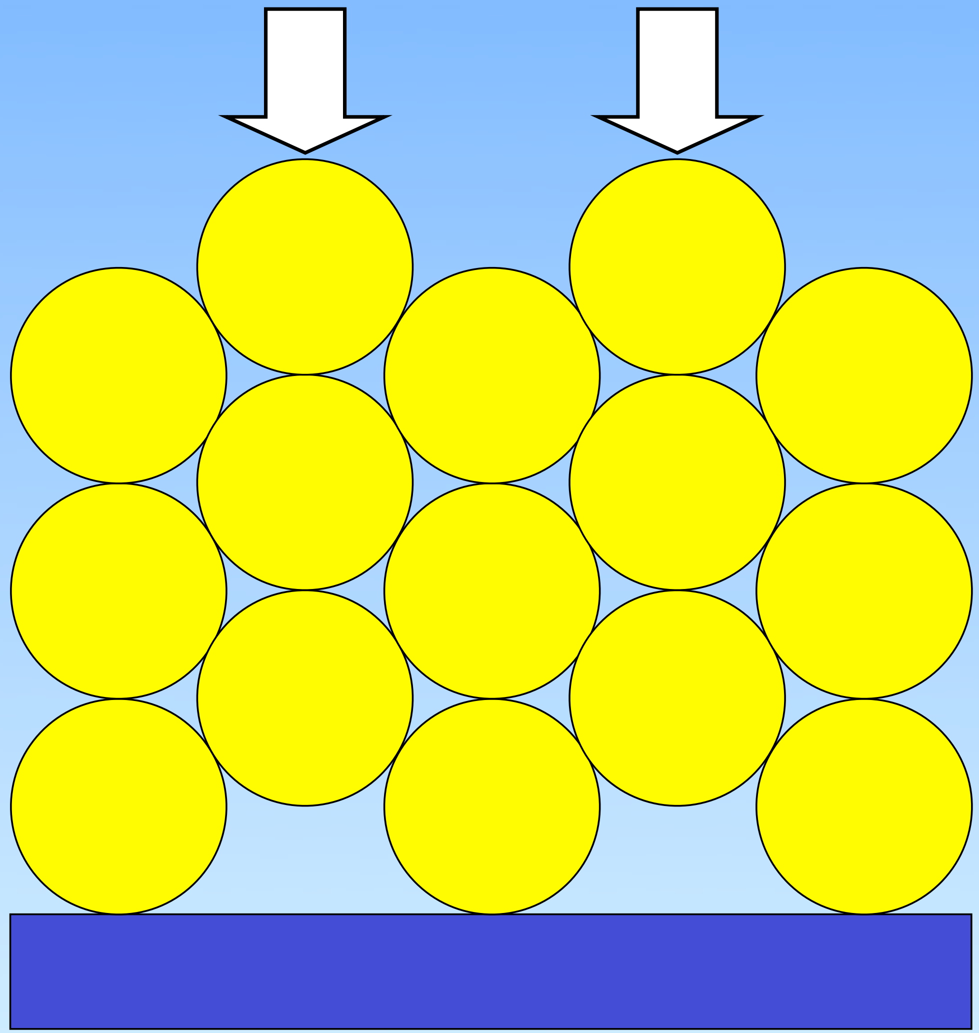
Reynolds dilatancy



Osborne Reynolds (1885):

"A strongly compacted granular medium dilates under pressure".

What causes the dilatancy ?

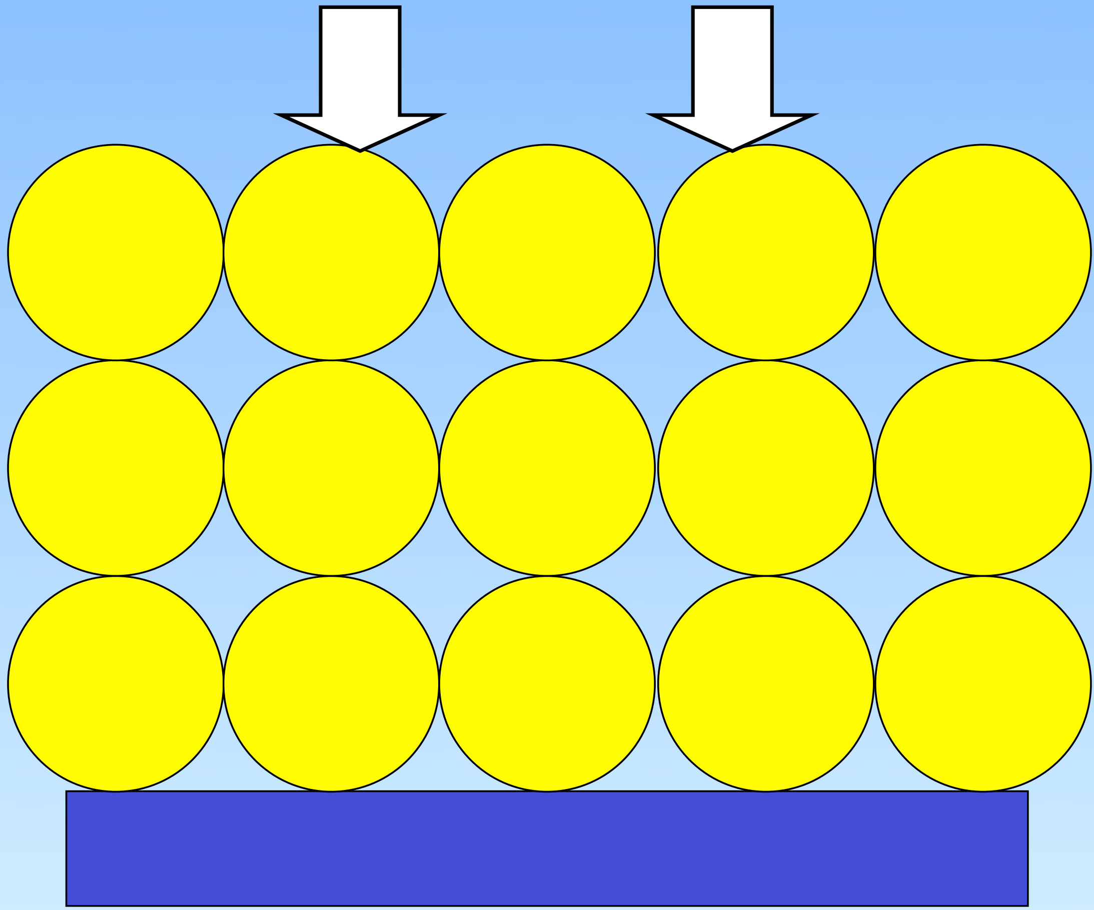


$\varphi = 0.907$

φ = packing fraction

$= V_{solids}/V_{total}$

What causes the dilatancy ?



$\varphi = 0.907$

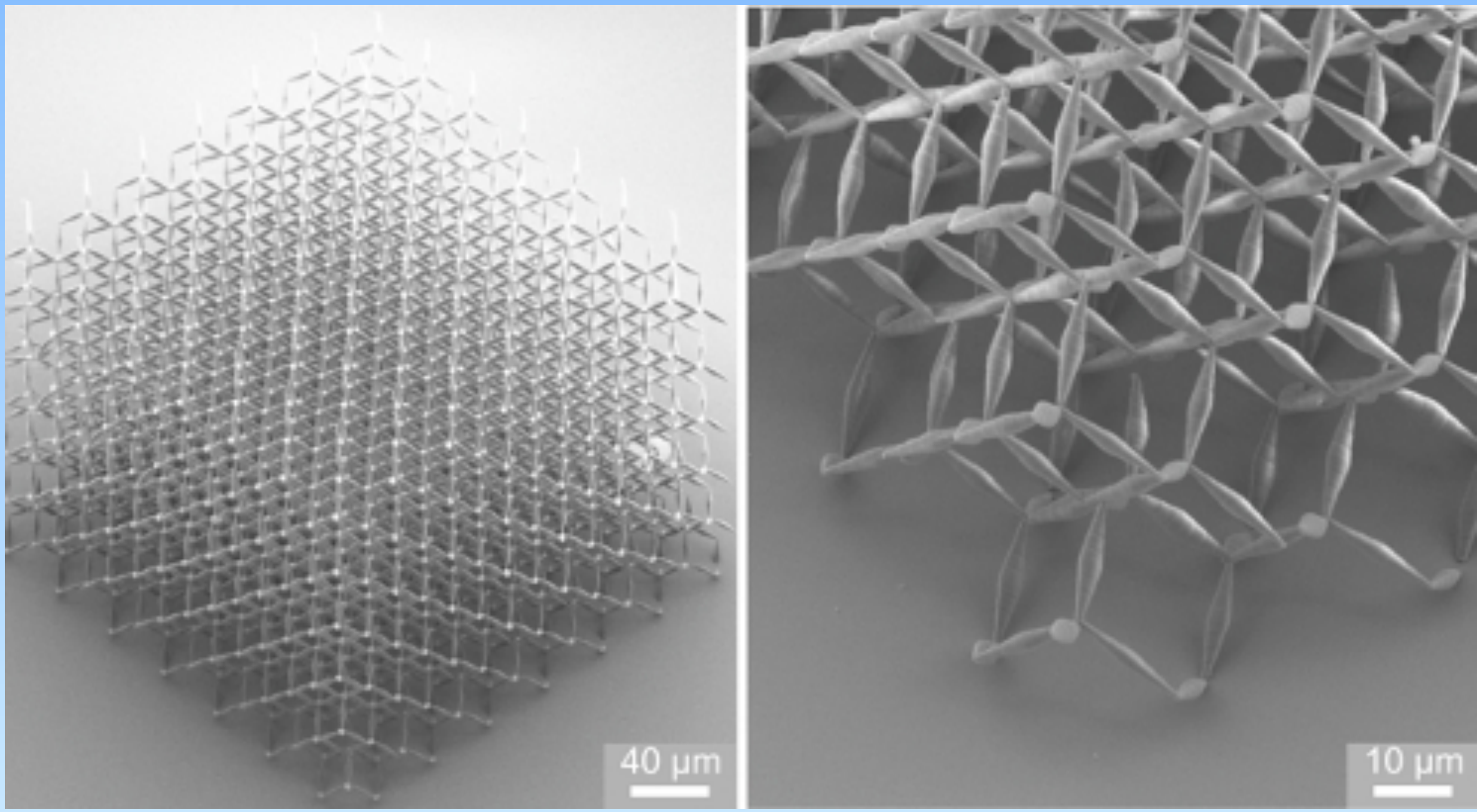
$\downarrow$

$\varphi = 0.785$

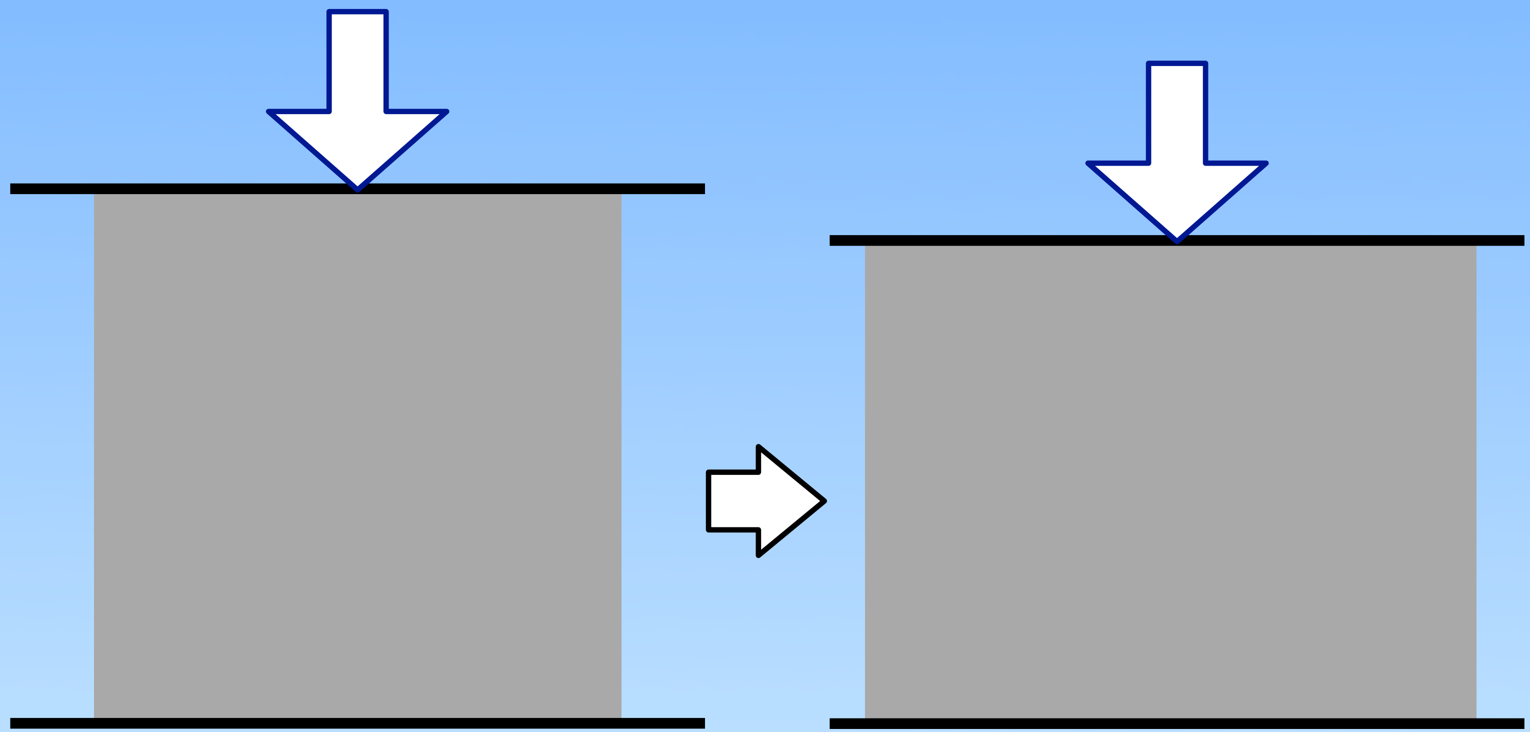
φ = packing fraction

$= V_{solids}/V_{total}$

Metamaterials



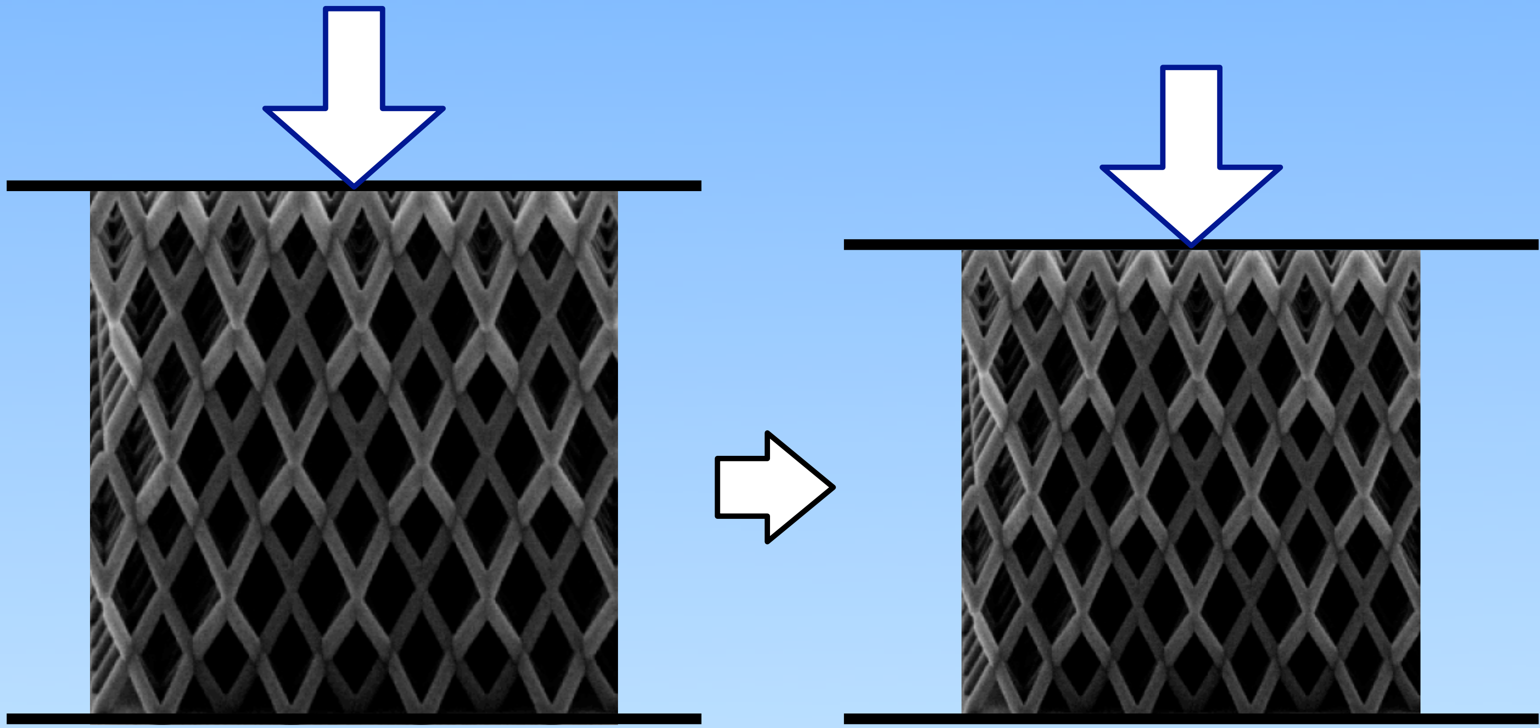
Positive Poisson ratio ν



When compressed vertically, ordinary materials expand horizontally.

$\nu > 0$

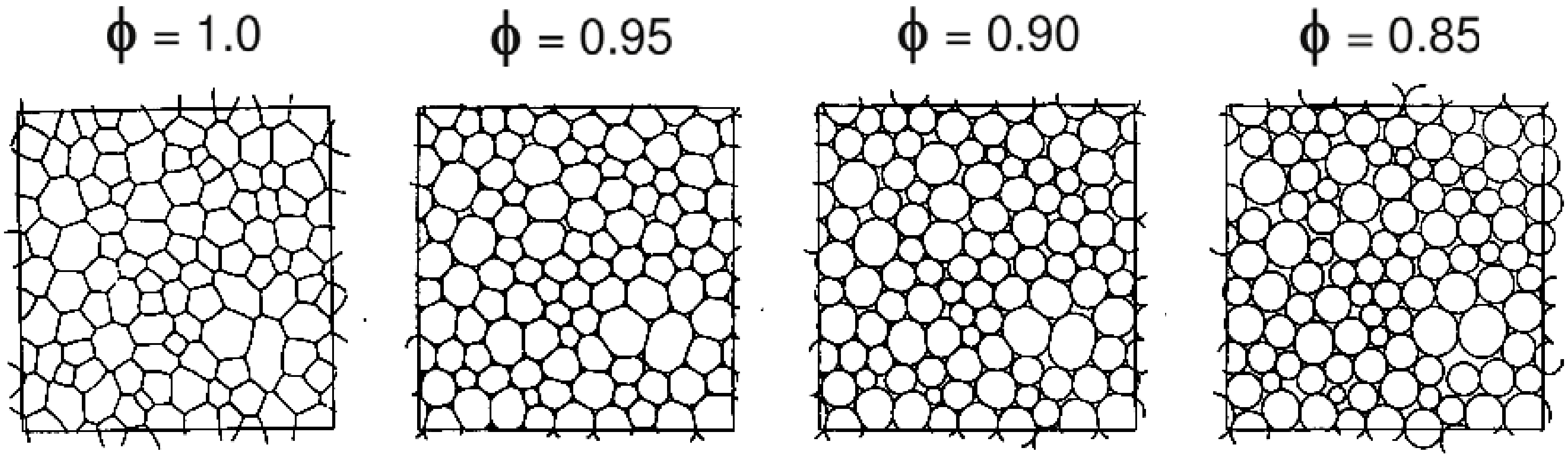
Negative Poisson ratio *ν*



When compressed vertically, tailored metamaterials compress horizontally.

$\nu < 0$

Stability of foams

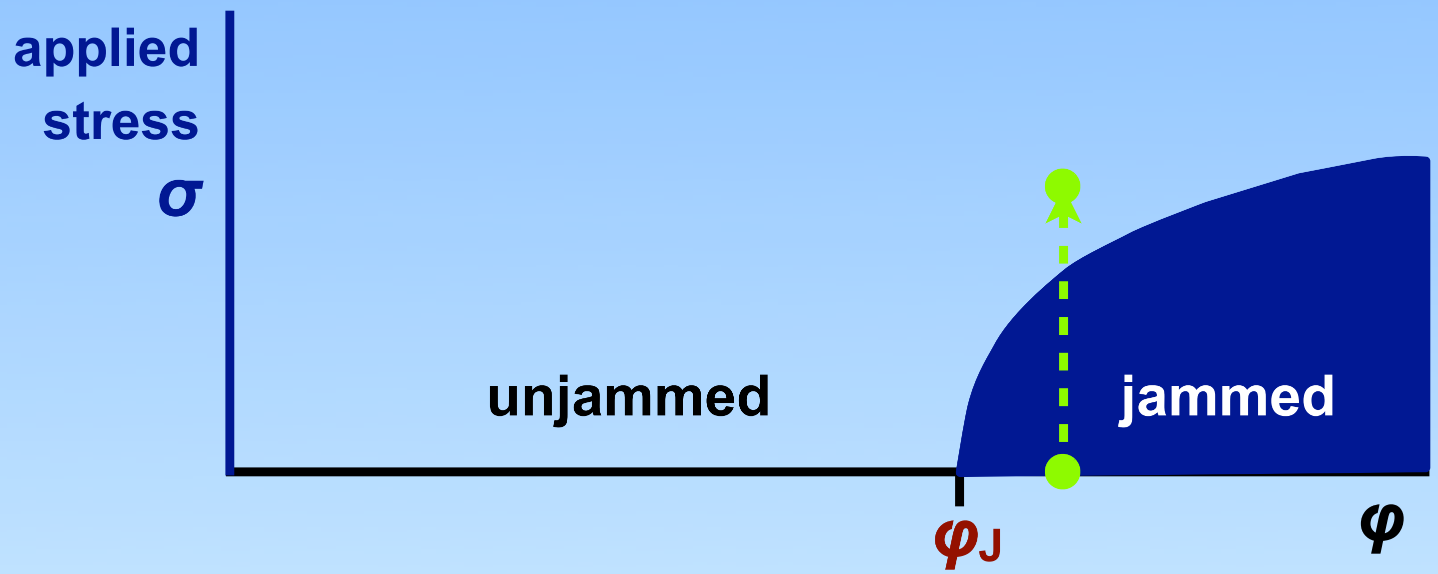


Bolton, Weaire, PRL (1990)

The foam looses stability at $\varphi \approx 0.84$

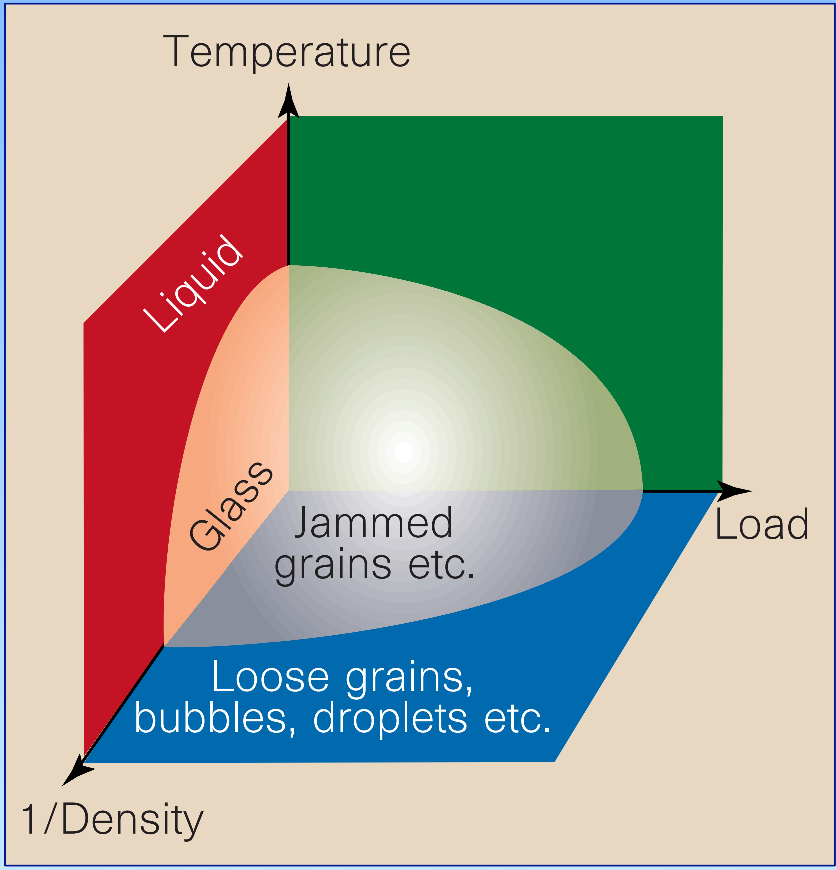
Jamming

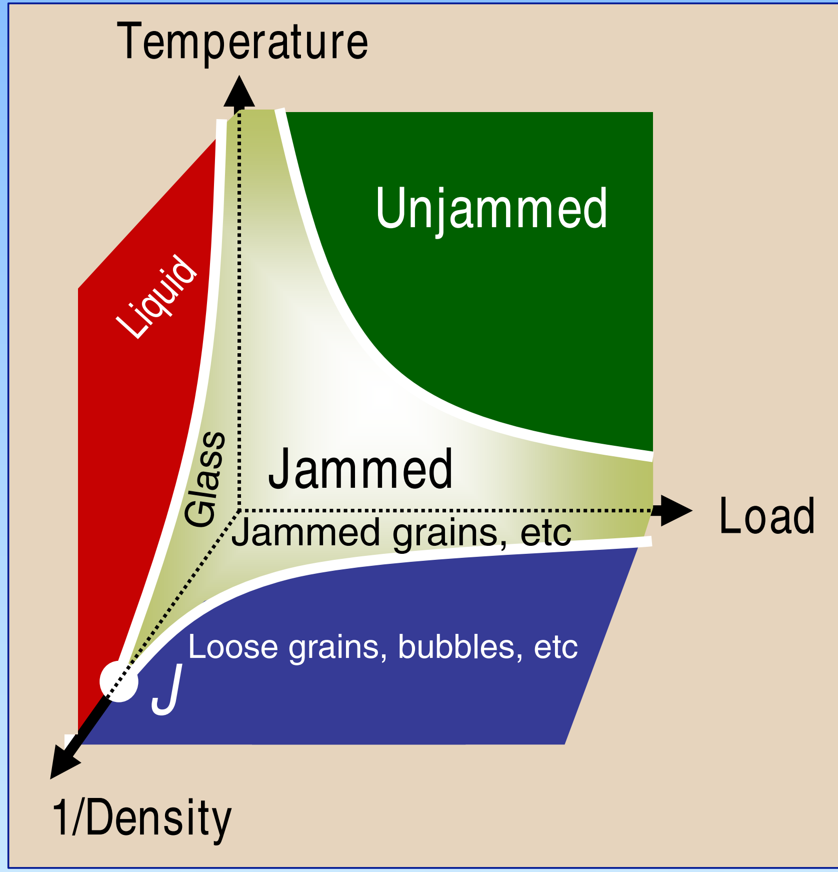
A granular material with a packing fraction above a critical value φ_J is stable.



At φ_J the packing is marginally stable: any stress will destroy the packing

Jamming diagrams



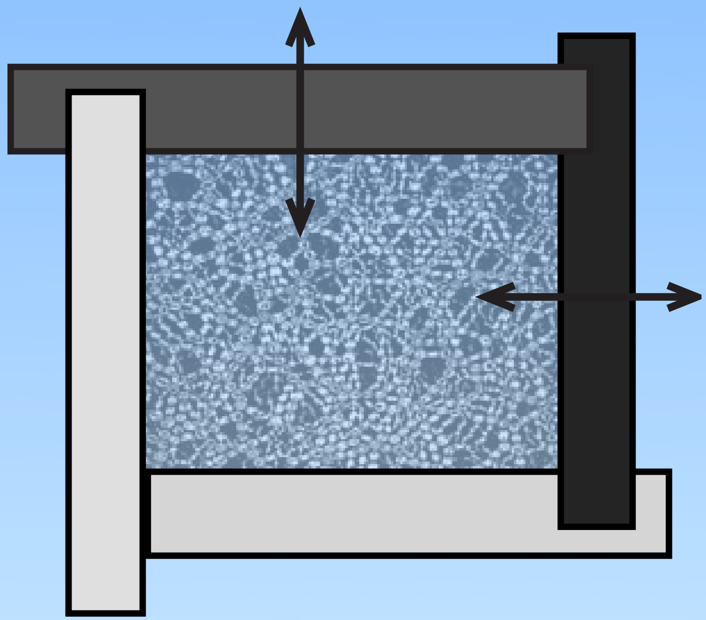


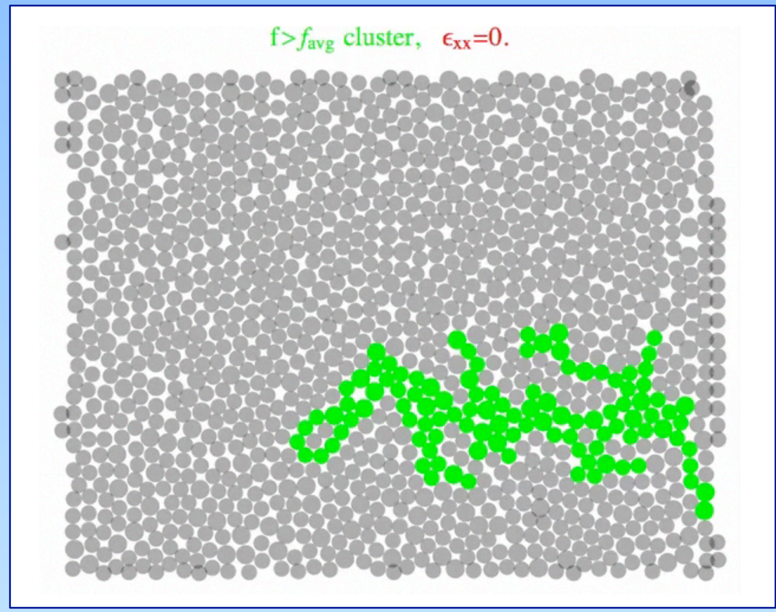
Andrea Liu, Sid Nagel
Nature (1998)

Martin van Hecke,
J. Phys.: Cond. Matt. (2010)

The controversy continues...

Jamming by shear

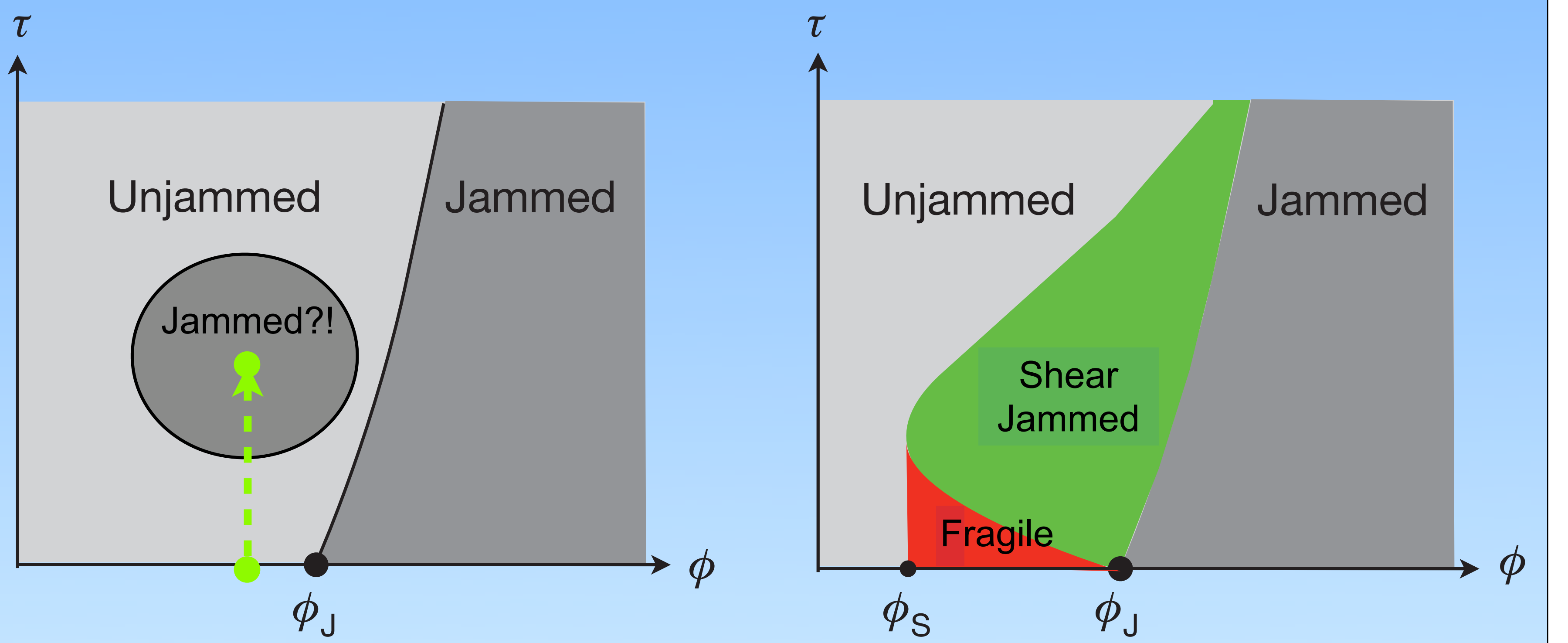




Dapeng Bi, Jie Zhang, Bulbul Chakraborty, Bob Behringer, Nature (2011)

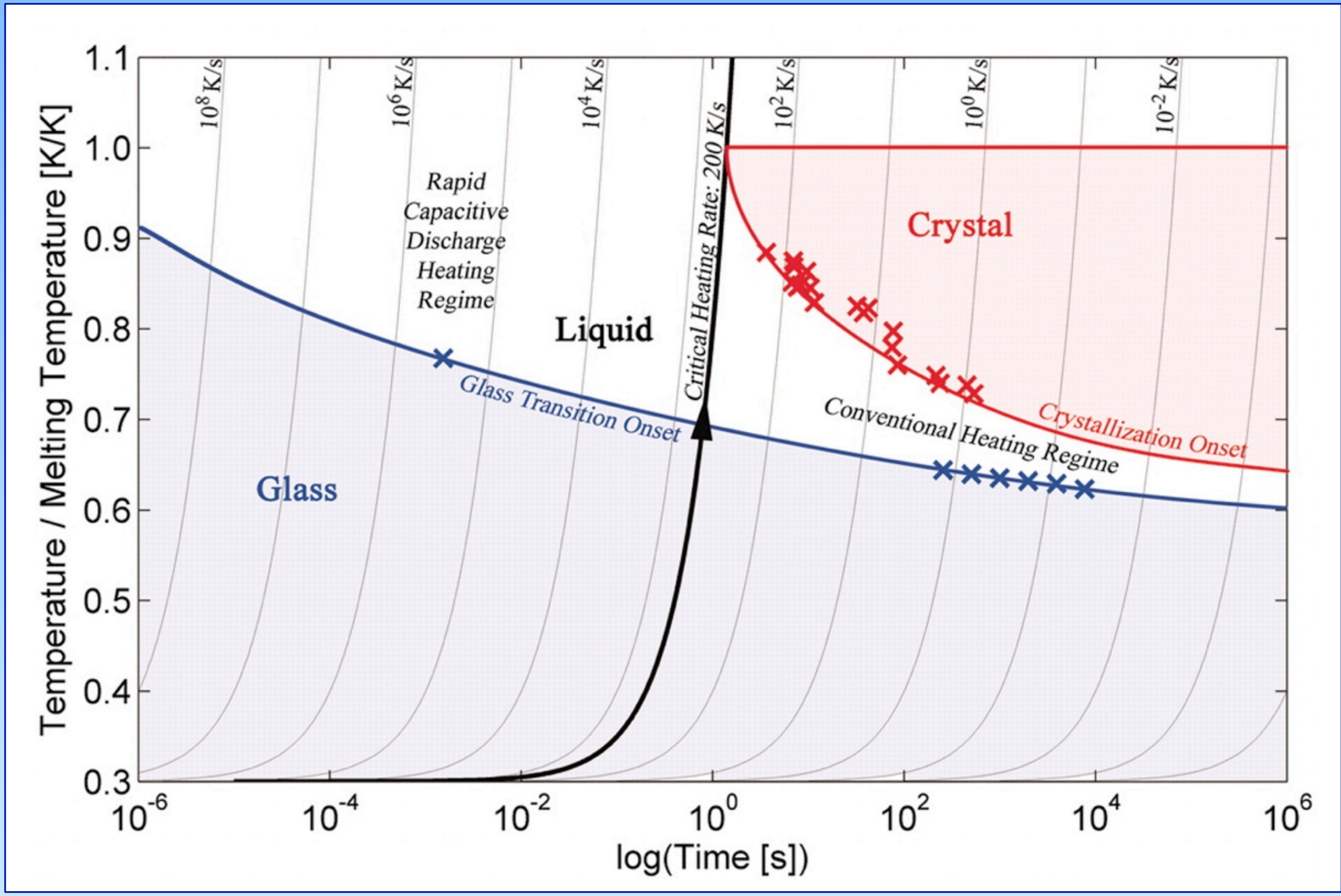
The controversy continues...

Jamming by shear



Dapeng Bi, Jie Zhang, Bulbul Chakraborty, Bob Behringer,
Nature (2011)

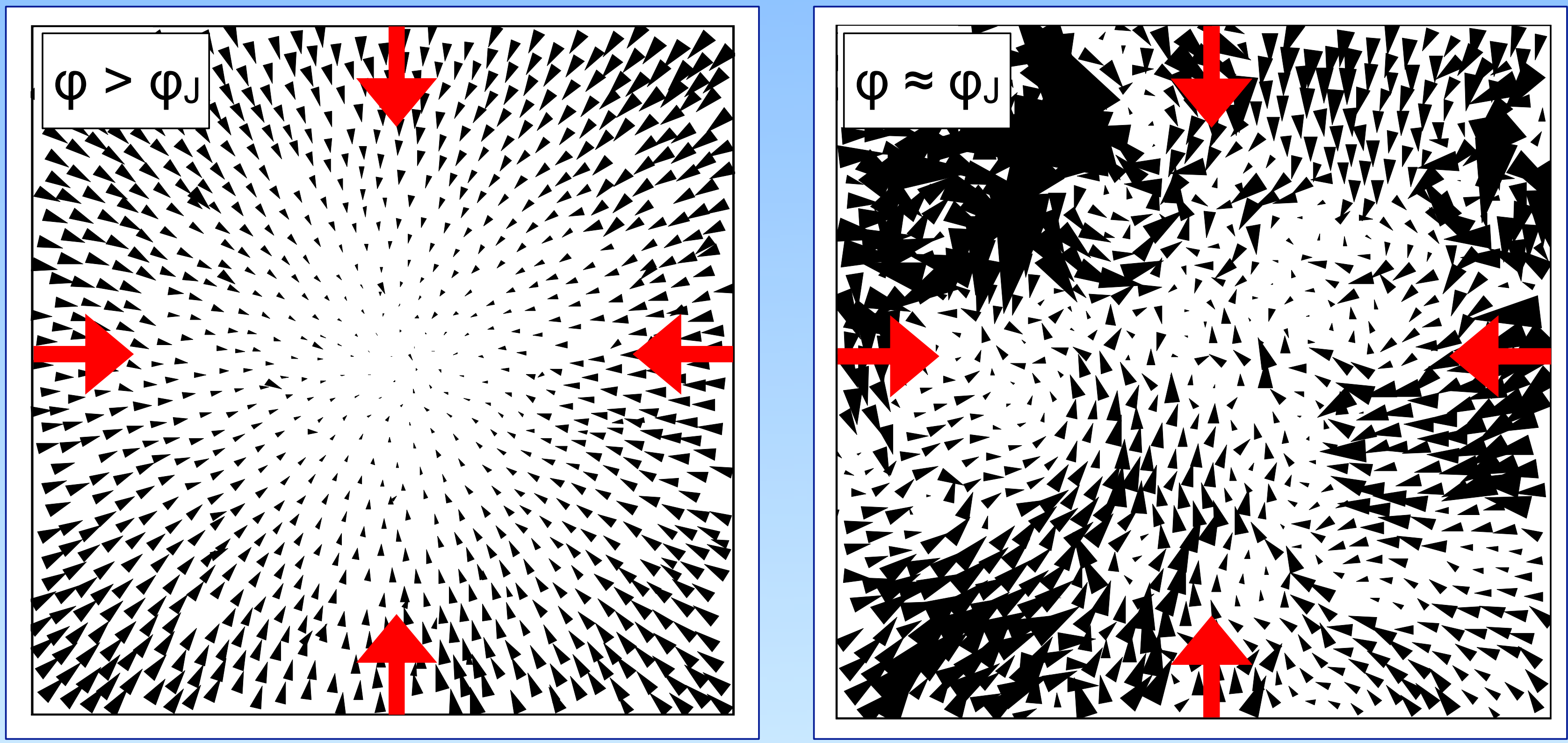
Finite temperature: glassy behavior



System quenched in a jammed or glass state

Close to point J:
Very loose contact networks

response to uniform compression



close to φ_J: displacement field has non-affine response

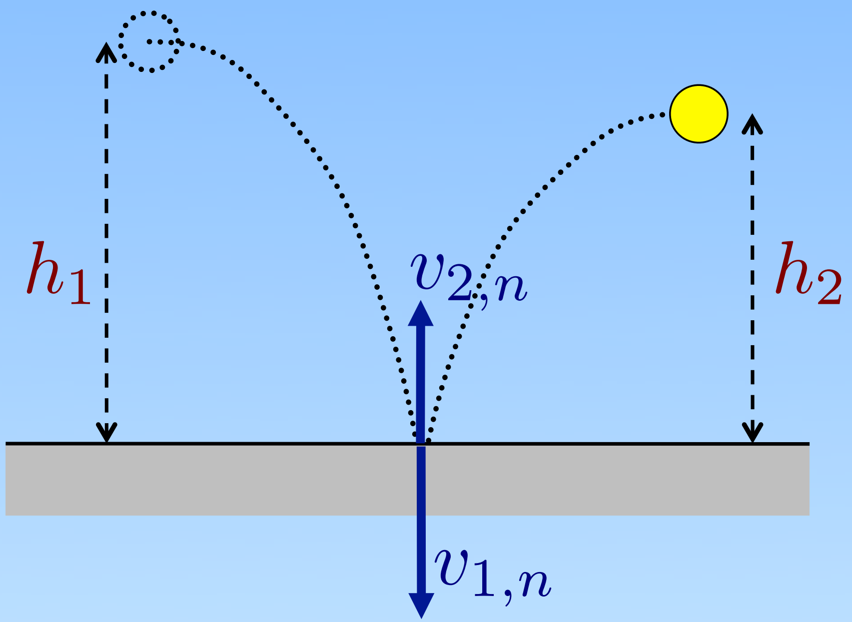
3. Dissipative interactions

Dissipative interactions may arise:

- **as a result of motion through another medium (see 4)**
  - **Brownian motion (fluctuation-dissipation)**
  - **dissipation in medium (viscosity, turbulence)**
- **as a result of contact forces:**
  - **friction**
  - **inelastic collisions**

transfer of kinetic energy into other degrees of freedom.

Dissipative collisions



coefficient of normal restitution:

$$e = \frac{v_{2,n}}{v_{1,n}} \left(= \sqrt{\frac{h_2}{h_1}} \right)$$

Grains have many internal degrees of freedom through which kinetic energy is dissipated.

(sound, heat, deformation)

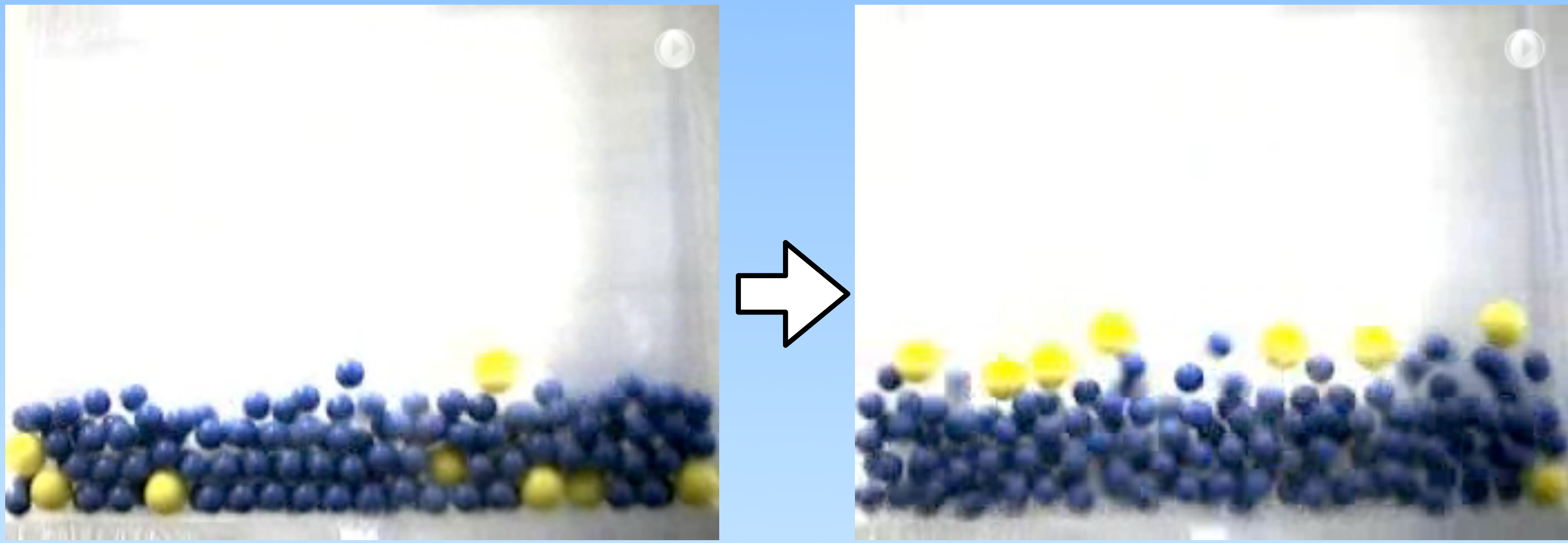
4. Inhomogeneous

Soft Matter is usually inhomogeneous. There are two main causes:

1. **The inhomogeneity is caused by the (unavoidable) presence of an interstitial fluid (*intrinsic*).**
   - **colloids are particles subject to Brownian motion and hydrodynamic interactions with the embedding fluid.**
   - **polymers are modeled as Brownian particle-springs**

2. **The inhomogeneity is due to inhomogeneity of the material (*external).***
   - **granular materials can be bidisperse or polydisperse**
   - **clay is a material made up of clay (nanoscale) and silica particles**

Vibrated bidisperse mixture



Segregation !

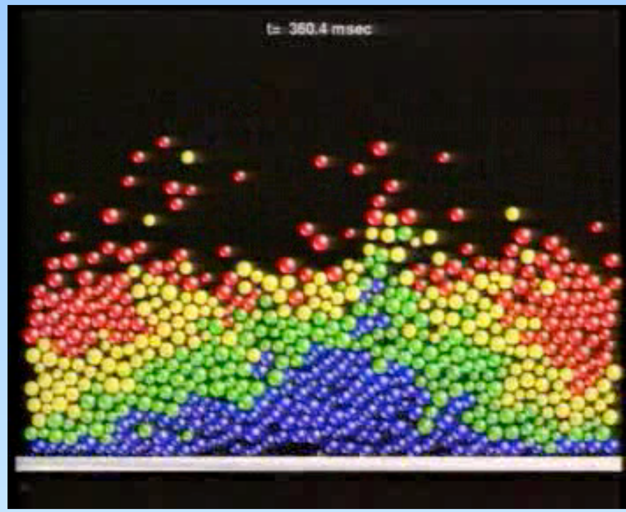
"Brazil Nut Effect"

Three explanations BNE

1. percolation: small grains percolate the empty spots between the large ones.

2. exclusion: while vibrating small grains fill space below the large ones, not vice versa.

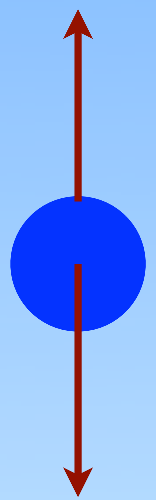
3. convection: interaction with walls trigger convection rolls.



large grains can follow the upward, but not the downward flow.

Role of intersitial air: single particle

$$F_{drag} = 3\pi\eta dV$$



$$F_g = \frac{1}{6}\pi d^3 \rho_p g$$

d = particle diameter
V = typical particle velocity
η = air viscosity ($2\cdot10^{-5}$ Pa·s)
ρ_p = part. density ($2.5\cdot10^{3}$ kg/m^3)
g = grav. acceleration (10 m/s^2)

$$\boxed{B \equiv \frac{F_{drag}}{F_g} = \frac{18\eta V}{\rho_p g d^2}}$$

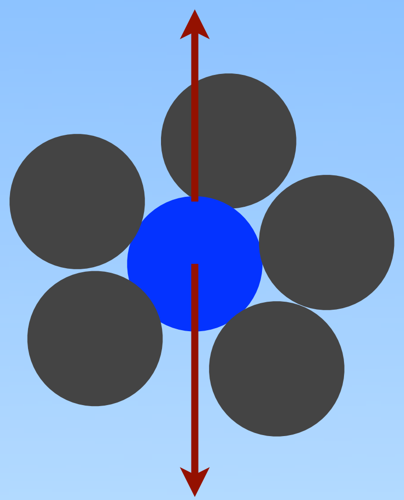
$$B \approx 1 \to d \approx \sqrt{\frac{18\eta V}{\rho_p g}}$$

$$V \approx 1 \text{ m/s} \to d \approx 120\ \mu\text{m}$$

$$V \approx \sqrt{2gd} \to d \approx 16\ \mu\text{m}$$

Role of interstitial air: packed particle

$$F_{f\to s} = 2k\frac{1-\varepsilon}{\varepsilon^3}F_{drag}$$



$$F_g = \tfrac{1}{6}\pi d^3 \rho_p g$$

$\varepsilon = 1 - \varphi =$ porosity (≈ 0.5)
$k =$ Kozeny constant (≈ 5)

$$\boxed{B_p \equiv \frac{F_{f\to s}}{F_g} \approx 40\frac{18\eta V}{\rho_p g d^2}}$$

$$B_p \approx 1 \to d \approx \sqrt{40}\sqrt{\frac{18\eta V}{\rho_p g}}$$

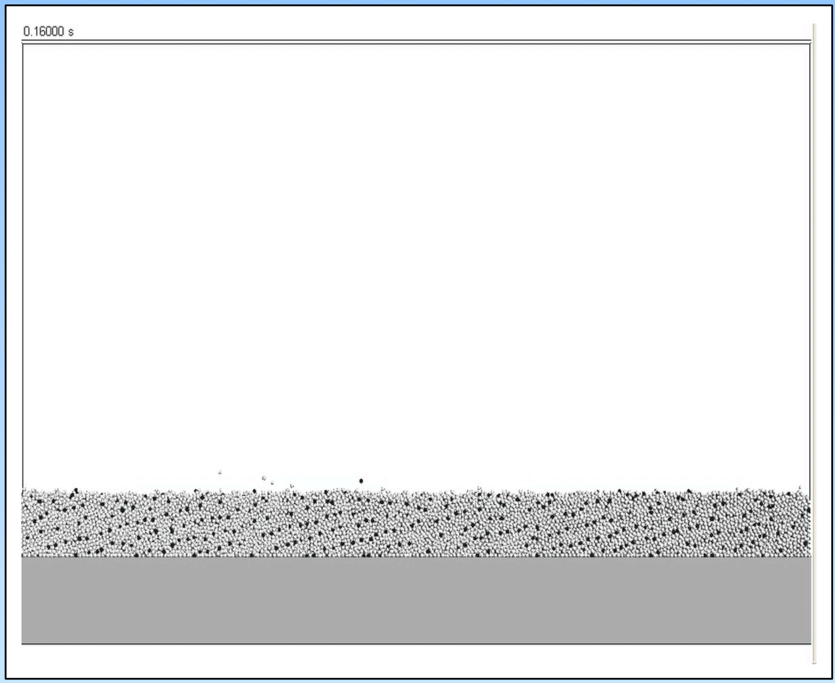
$$V \approx 1 \text{ m/s} \to d \approx 760\ \mu\text{m}$$

$$V \approx \sqrt{2gd} \to d \approx 190\ \mu\text{m}$$

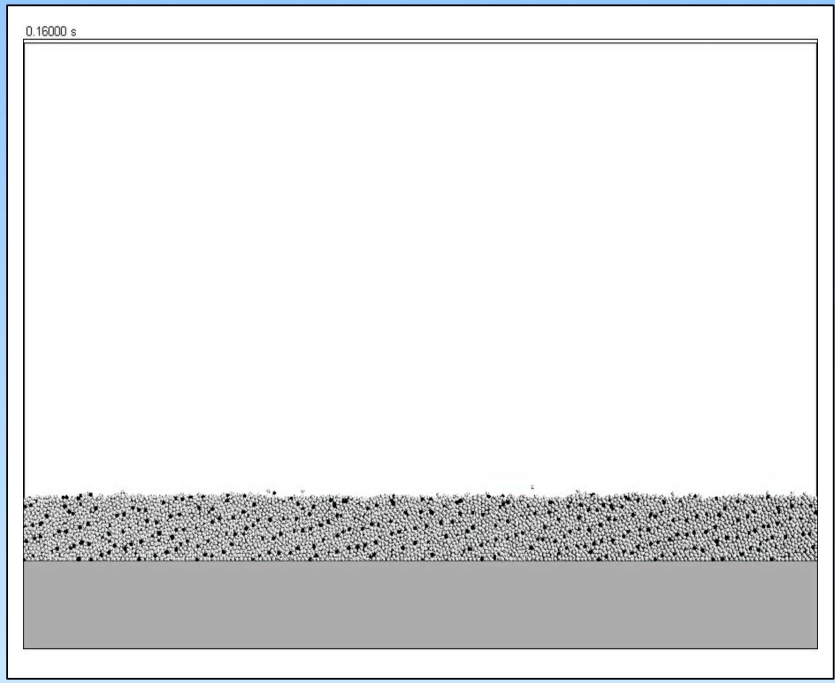
Faraday heaping

Vertically vibrated granular layer:

Numerical simulation of heaping with a hybrid GD-CFD code



without air



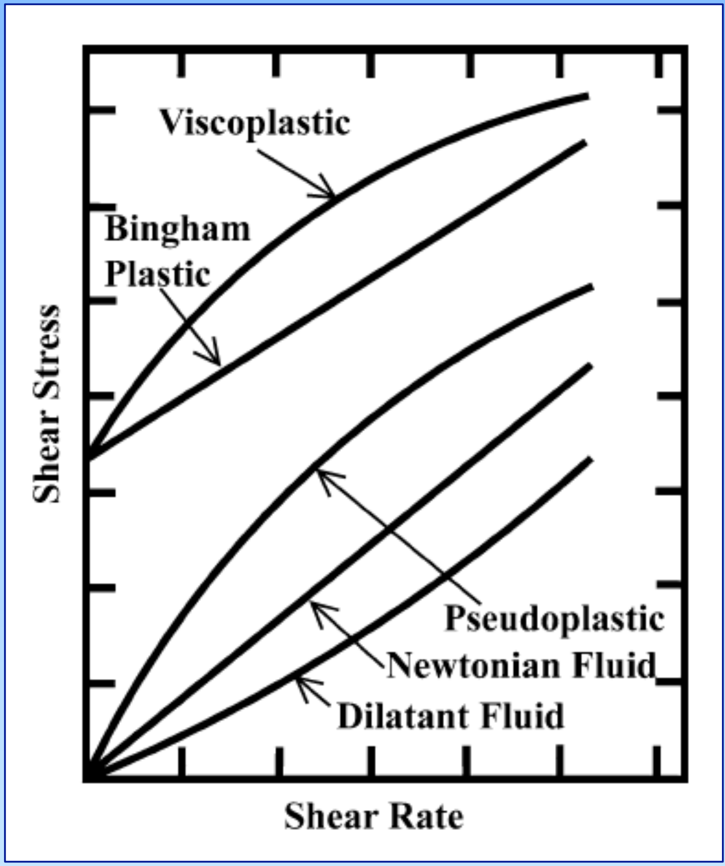
with air

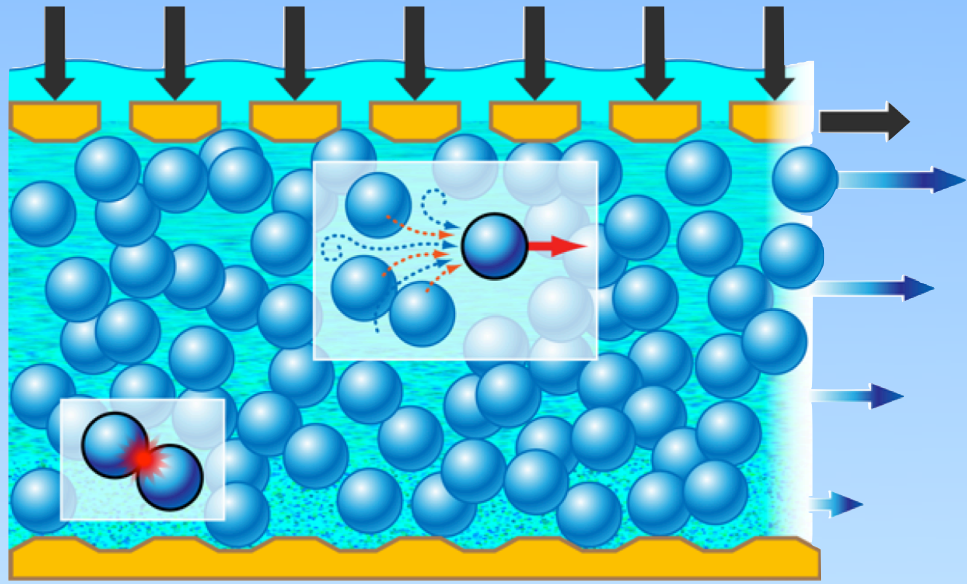
Interstitial liquids: suspensions

a granular suspension: cornstarch on a shaker

Walking on cornstarch

Macroscopic vs microscopic





Why is Soft Matter a booming subject in physics ?

There are many reasons,
but one has been absolutely crucial:

NUMERICS

Some numerical techniques

- Brownian dynamics
- Monte Carlo
- molecular dynamics
- lattice Boltzmann
- Event driven hard sphere dynamics
- Hard sphere dynamics
- Soft sphere dynamics
- Two or multiple fluid models
- Multi-particle collision dynamics
- Hybrid MD lattice Boltzmann
- Stochastic rotation dynamics
- Hybrid granular dynamics computational fluid dynamics

Some examples

Granular packing (for spheres)

fluid

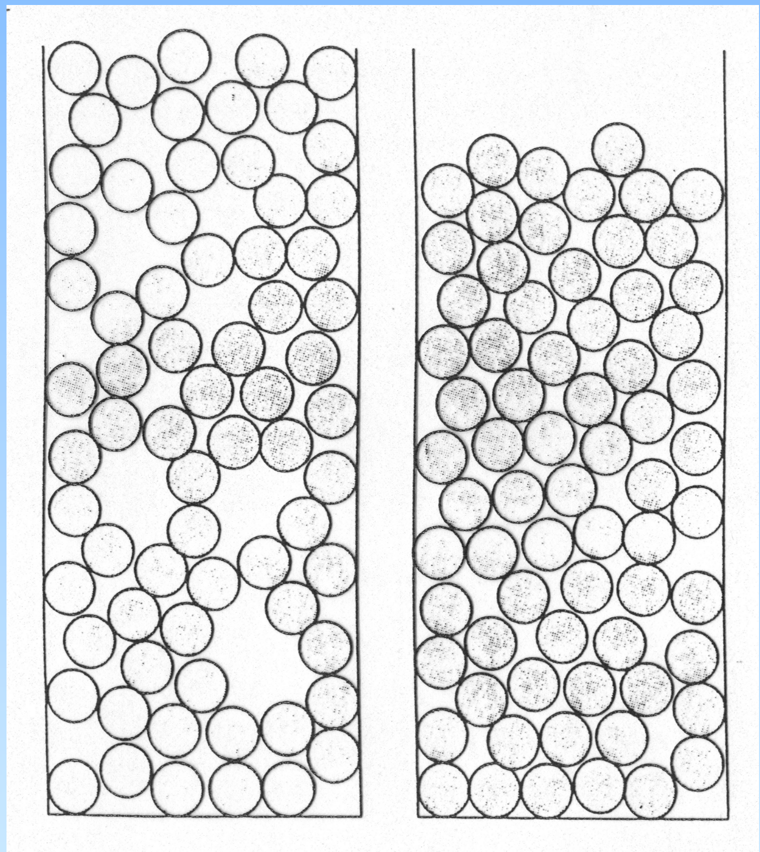
0.57, RLP =
random loose packing

solid

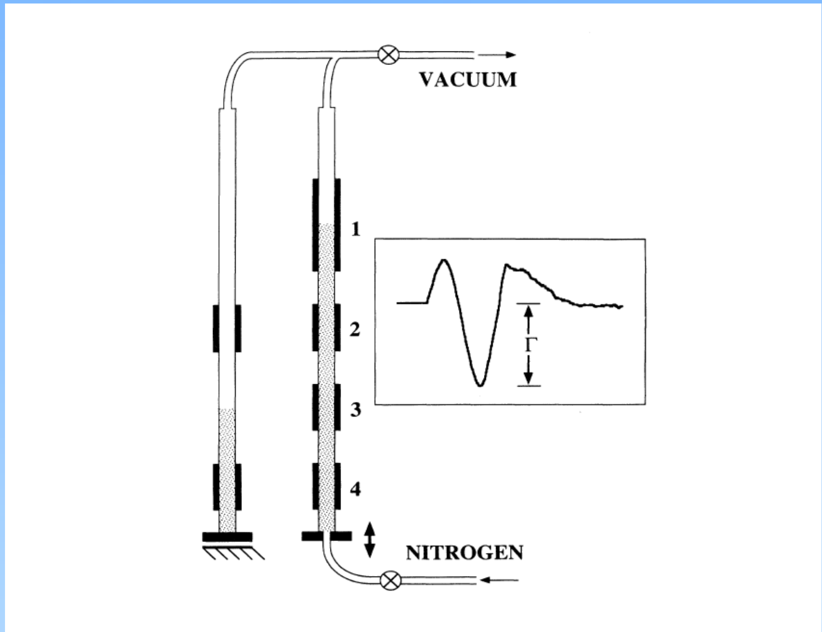
0.64, RCP =
random close packing

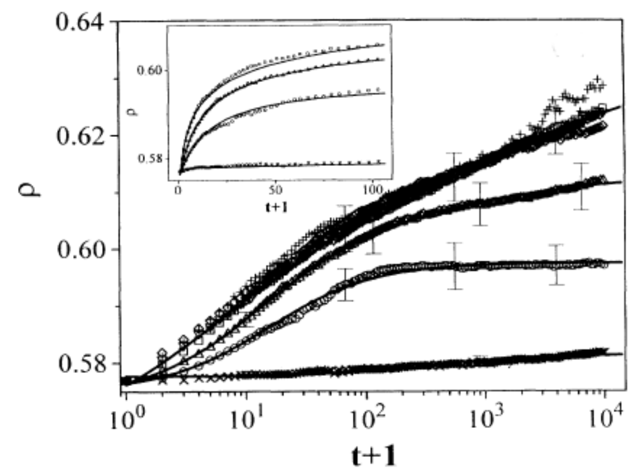
0.74, crystal =
perfectly hexagonal

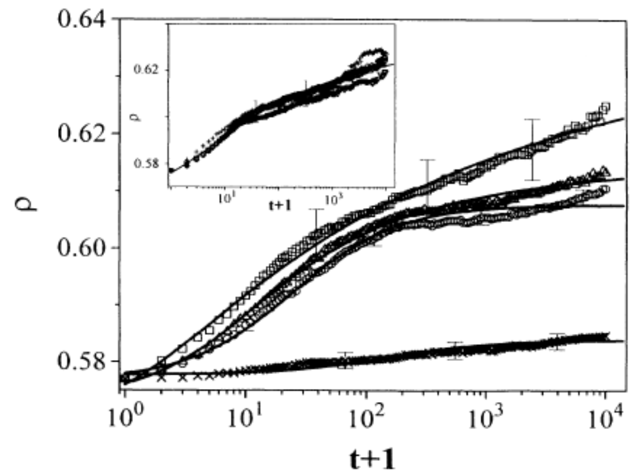
solid
fraction



Compactification experiment







$$\rho(t) = \rho_f - \frac{\rho_f - \rho_0}{1 + B \log(1 + t/\tau)}$$

$$\rho(t=0) = \rho_0 \ ; \ \rho(t \to \infty) = \rho_f$$

regime 1: local reorganization

regime 2: global reorganization

Analogy: car-parking in street

Model (Ben-Naim):

- Initial state: randomly parked cars (no extra fit in)
- Start to move cars randomly. Whenever there is a large enough gap, a new car jumps in.

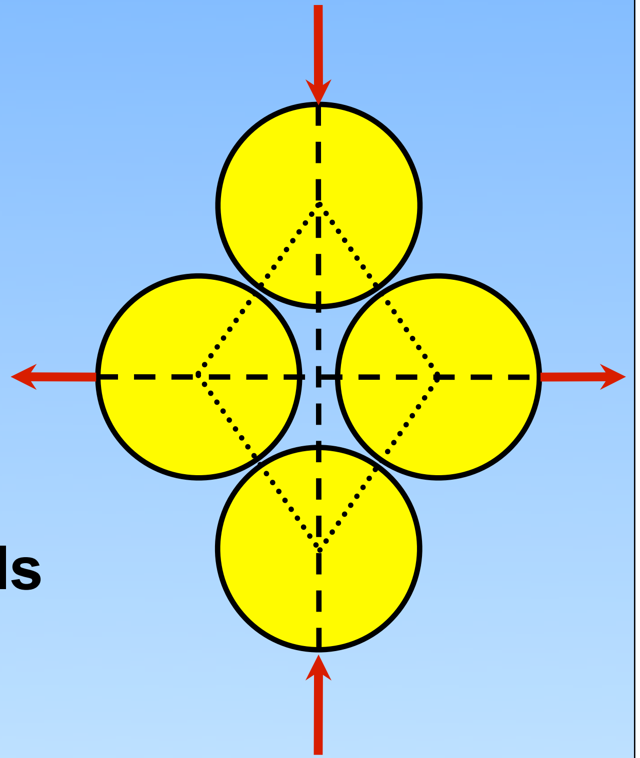
<u>regime 1</u>: movement of a single car creates gap

<u>regime 2</u>: more than one car has to move:

required time for gap to open grows exponentially:

$$\frac{\rho(t)-\rho_f}{\rho_0-\rho_f} \propto \frac{1}{\log(t/\tau)}$$

Importance of sidewalls: Rayleigh-Janssen model



Force parallelogram as unit cell of a 2D granular medium

vertical forces ⇒ horizontal forces

balanced by sidewalls

Lord Rayleigh:

$$\boxed{p_h = K\, p_v}$$

K **= coefficient of redirection;**
p_h, p_v = horizontal, vertical pressure

Importance of sidewalls: Rayleigh-Janssen model (2)

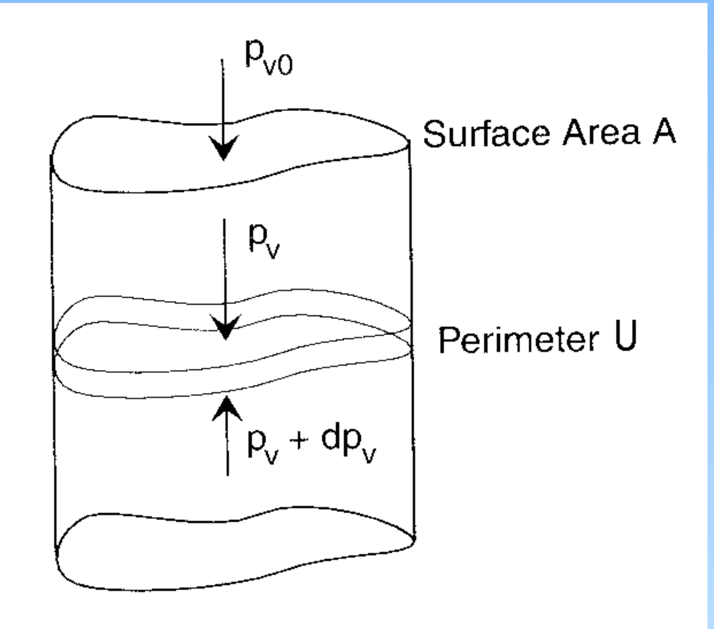
Slice experiences friction force with sidewalls:

$$dF_{\text{friction}} = \mu_s p_h U \, dh$$
$$= \mu_s (K p_v) U \, dh$$

Vertical force balance on slice:

$$[p_v(h+dh) - p_v(h)] \, A \; + \; \mu_s K p_v U \, dh = \rho g A \, dh$$

$$\boxed{\frac{dp_v}{dh} + \mu_s K \frac{U}{A} p_v = \rho g}$$

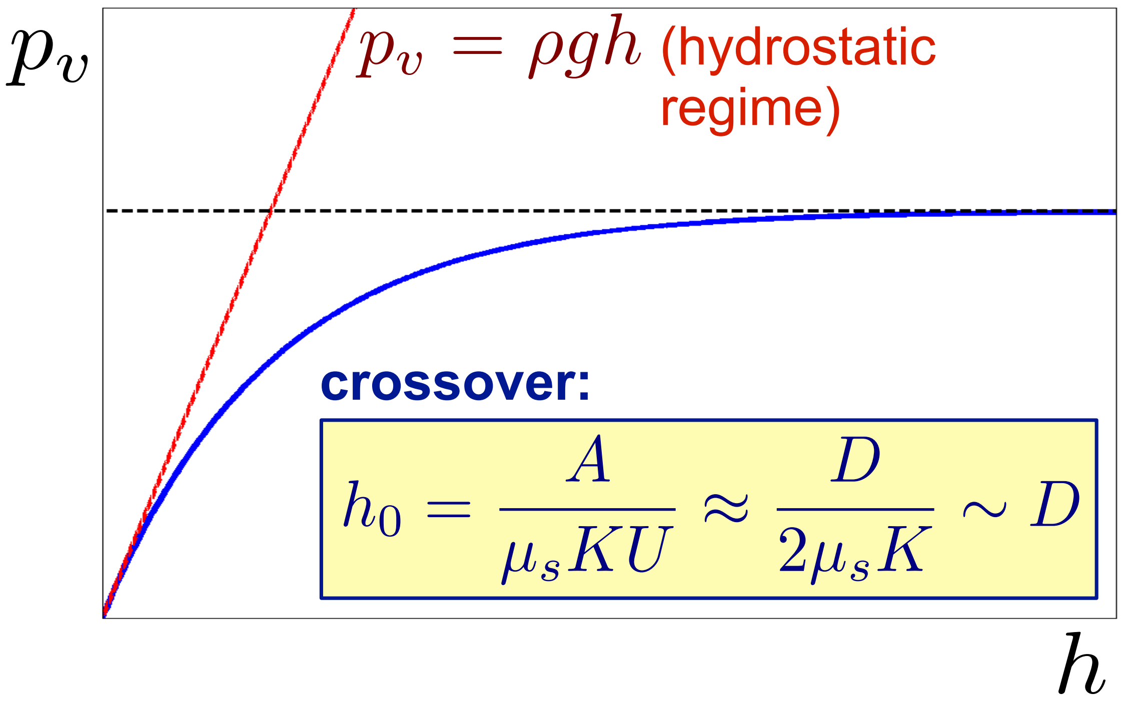


Integration gives:

$$\boxed{p_v(h) = \frac{\rho g A}{\mu_s K U} \left[1 - \exp\left(-\mu_s K \frac{U}{A} h \right) \right]}$$

Janssen's equation

Importance of sidewalls: Rayleigh-Janssen model (2)



$$p_v = \frac{\rho g A}{\mu_s K U}$$

(saturated regime)

$$p_v(h) = \frac{\rho g A}{\mu_s K U}\left[1 - \exp\left(-\mu_s K \frac{U}{A} h\right)\right]$$

Janssen's equation

Effective weight of granulate in silo

$$\boxed{\chi \equiv \frac{\mu_s K U}{A} h}$$ **(decompaction parameter)**

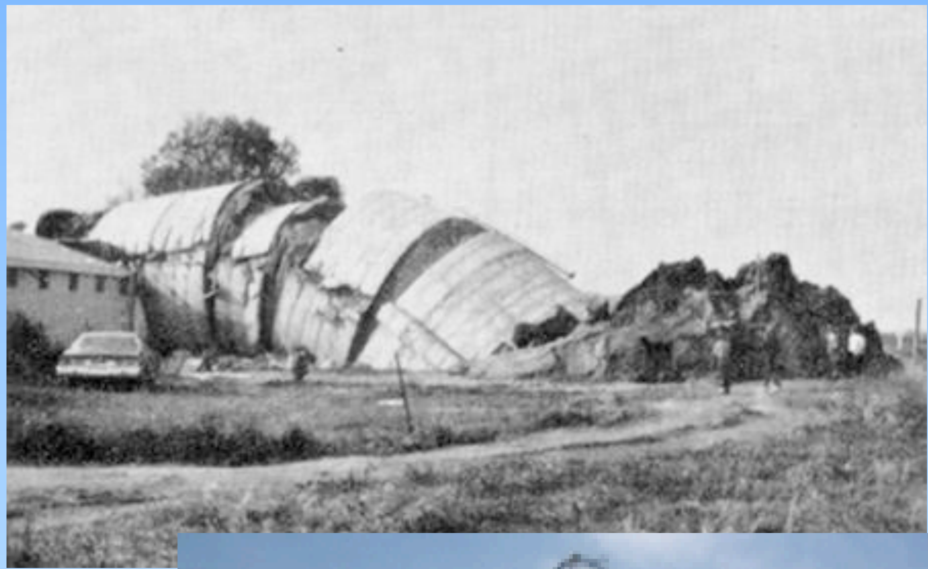
Effective weight on bottom = $F_v(h) = p_v(h)\,A$

$$\boxed{F_v(h) = mg\frac{1-\exp(-\chi)}{\chi} \approx \frac{mg}{\chi}}$$

($\rightarrow$ 0 for large χ, i.e., large h)

What happens to the remaining weight?

Collapsing silos



Walls take this weight!

Is a general hydrodynamic description of granular matter possible ?

VOLUME 74, NUMBER 8 PHYSICAL REVIEW LETTERS 20 FEBRUARY 1995

Breakdown of Hydrodynamics in a One-Dimensional System of Inelastic Particles

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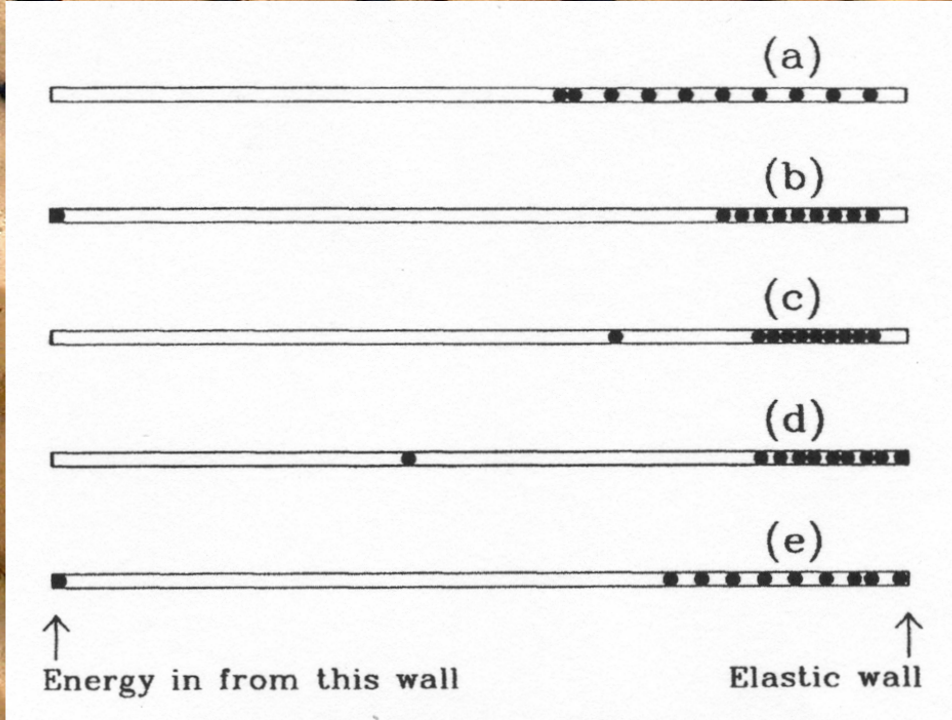


A) Hydrodynamic approach

Coarse graining over small intervals Δx, Δt to define macroscopic quantities:

density:

$$\rho(x,t) = \left\langle \sum_i \delta(x_i(t) - x) \right\rangle_{\Delta x, \Delta t}$$

velocity:

$$u(x,t) = \left\langle \sum_i v_i(t)\, \delta(x_i(t) - x) \right\rangle_{\Delta x, \Delta t}$$

temperature:

$$T(x,t) = \left\langle \sum_i \left(v_i(t) - u(x,t)\right)^2 \, \delta(x_i(t) - x) \right\rangle_{\Delta x, \Delta t}$$

Assuming local "thermal" equilibrium, one can derive mass, momentum, and energy conservation laws:

Conservation laws

In the dilute limit, using the ideal gas law:

$$\cancel{\partial_t \rho} + \cancel{\partial_x (\rho u)} = 0$$

$$\cancel{\rho\, \partial_t u} + \cancel{\rho u\, \partial_x u} = -c_1\, \partial_x (\rho T)$$

$$\cancel{\rho\, \partial_t T} + \cancel{\rho u\, \partial_x T} + c_1 \cancel{\rho T\, \partial_x u} - c_2\, \partial_x^2 (T^{3/2}) = -c_3 \varepsilon \rho^2 T^{3/2}$$

$\varepsilon = (1-e)/2$ expresses inelasticity

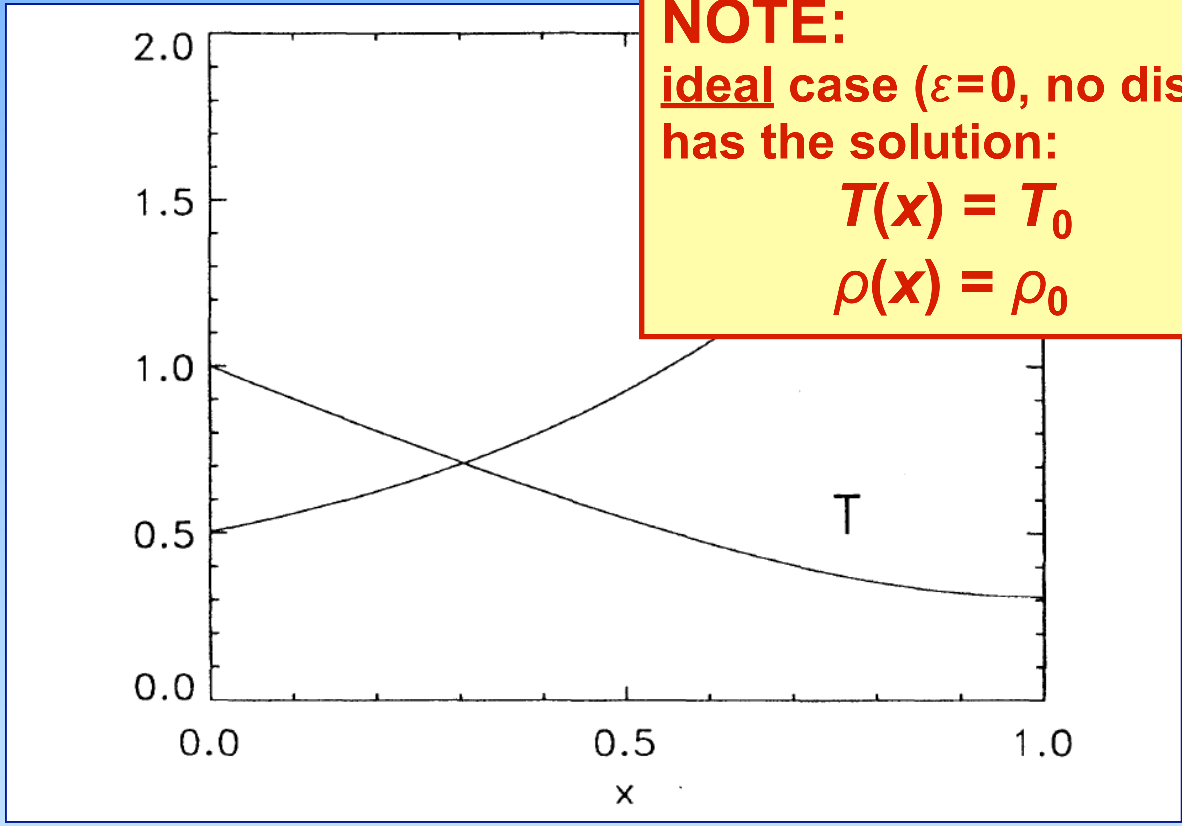
In the stationary limit (*u*=0, ∂_t=0) this becomes:

$$\rho T = \text{constant}$$

$$\partial_x^2 (T^{3/2}) = \frac{c_3 \varepsilon}{c_2} \rho^2 T^{3/2}$$

These equations can be solved analytically:

Hydrodynamic solution:



NOTE:
<u>ideal</u> case (ε=0, no dissipation) has the solution:

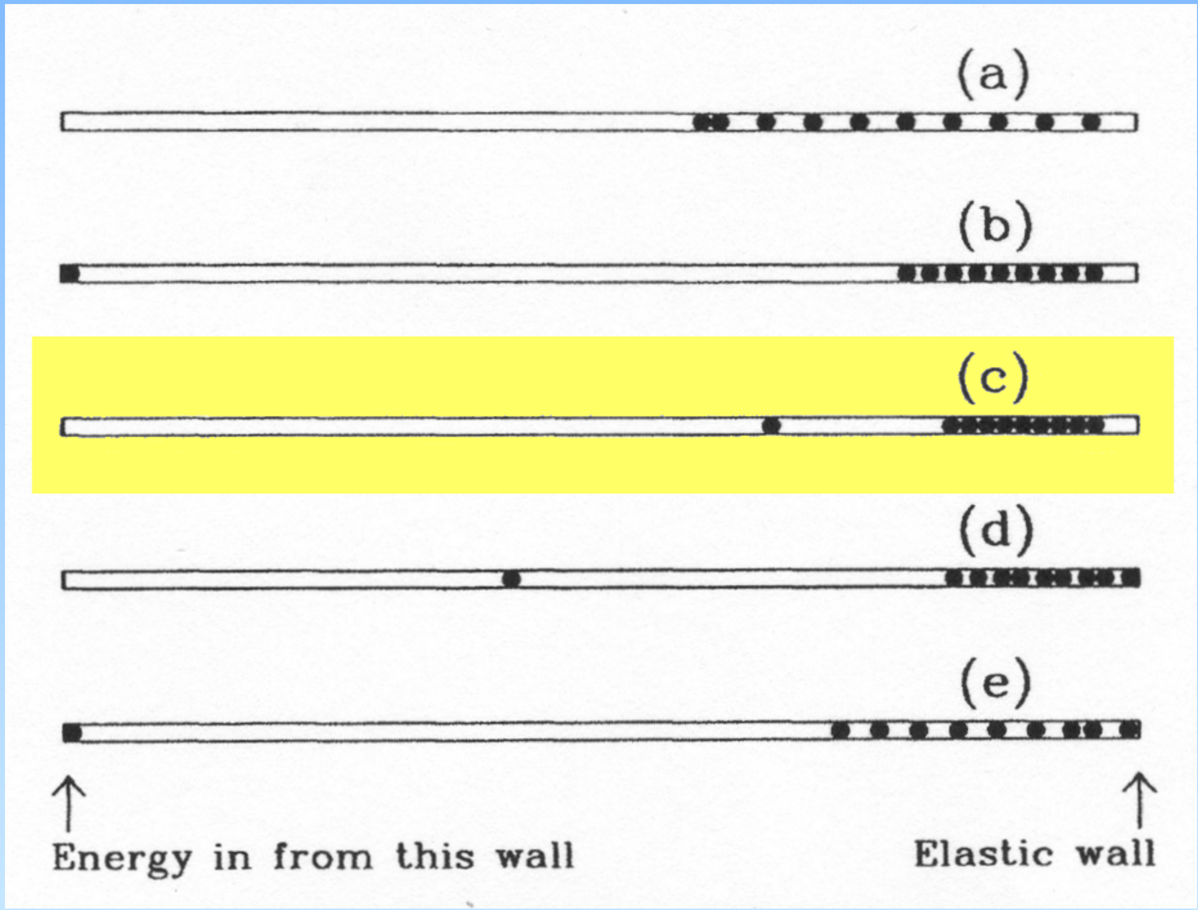
$$T(x) = T_0$$
$$\rho(x) = \rho_0$$

Using the boundary conditions:

$$T(0) = T_0$$ **[constant T at left border]**

$$\partial_x T(1) = 0$$ **[elastic wall (no heat flux) at right border]**

Particle dynamics solution:



(using MD simulations)

B) Discrete description

2-particle collision with

*** momentum conservation:**

$$v_1' + v_2' = v_1 + v_2$$

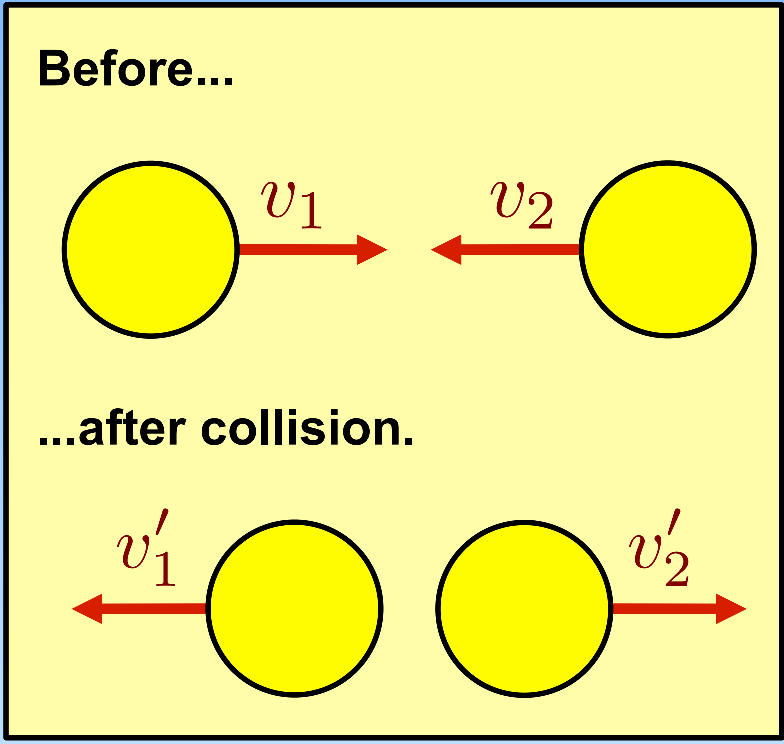
*** energy dissipation:**

$$v_1' - v_2' = e(v_1 - v_2)$$

This implies:

$$\boxed{\begin{aligned} v_1' &= \varepsilon\, v_1 + (1-\varepsilon)\, v_2 \\ v_2' &= (1-\varepsilon)\, v_1 + \varepsilon\, v_2 \end{aligned}}$$

with: $\varepsilon = (1-e)/2$



Ideal case $\varepsilon = 0$:

$v_1' = v_2$, $v_2' = v_1$, exchange of velocities.

Finally all velocities will be given by the PDF of velocities on the left.

Uniform distribution of particles, consistent with continuum description.

Non-ideal case $\varepsilon > 0$:

Numerical result very different from continuum result!

1 fast particle $v_N \sim \sqrt{T_0}$ and $(N-1)$ slow particles, clustering to the right and dissipating energy. Fast particle transports energy from left to right.

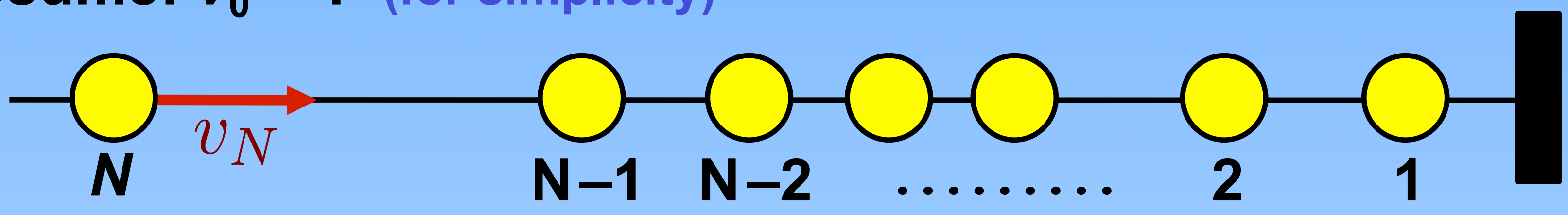
No longer local "thermal" equilibrium !

Breakdown of continuum approach !

Velocity center o

$$v_1' = \varepsilon\, v_1 + (1-\varepsilon)\, v_2$$
$$v_2' = (1-\varepsilon)\, v_1 + \varepsilon\, v_2$$

assume: v_0 = 1 (for simplicity)



before first collision:

$$v_N = v_0 = 1\,,\;\; v_i = 0 \;\text{ for } i < N$$

after first collision (between *N* and *N*–1):

$$v_N = \varepsilon\,,\;\; v_{N-1} = 1-\varepsilon\,,\;\; v_i = 0 \;\text{ for } i < N-1$$

after second collision (between *N*–1 and *N*–2):

$$v_N = \varepsilon\,,\;\; v_{N-1} = (1-\varepsilon)\varepsilon\,,\;\; v_{N-2} = (1-\varepsilon)^2\,,\;\; v_i = 0 \;\text{ for } i < N-2$$

...

after (N-1)th collision (between 2 and 1):

$$v_N = \varepsilon\,,\;\; v_{N-1} = (1-\varepsilon)\varepsilon\,,\;\; v_{N-2} = (1-\varepsilon)^2\varepsilon\,,\;\dots,$$
$$v_2 = (1-\varepsilon)^{N-2}\varepsilon\,,\;\; v_1 = (1-\varepsilon)^{N-1}$$

Velocity center of mass (2)

Mean velocity of cluster particles *N*,*N*−1,...,3,2:

$$v_{\mathrm{CM}} = \frac{1}{N-1}(v_N + v_{N-1} + v_{N-2} + \ldots + v_3 + v_2)$$
$$= \frac{1}{N-1}\left[\varepsilon + (1-\varepsilon)\varepsilon + (1-\varepsilon)^2\varepsilon + \ldots + (1-\varepsilon)^{N-2}\varepsilon\right]$$
$$= \frac{\varepsilon}{N-1}\left(\sum_{k=0}^{N-2}(1-\varepsilon)^k\right) = \frac{1}{N-1}\left(1-(1-\varepsilon)^{N-1}\right)$$
$$\approx \frac{1}{N-1}\left(1-\exp\left[-(N-1)\varepsilon\right]\right)$$

for large N

- **ε = 0, ideal case:**

  $$v_{\text{CM-cluster}} = 0$$

- **ε ≠ 0, real case:**

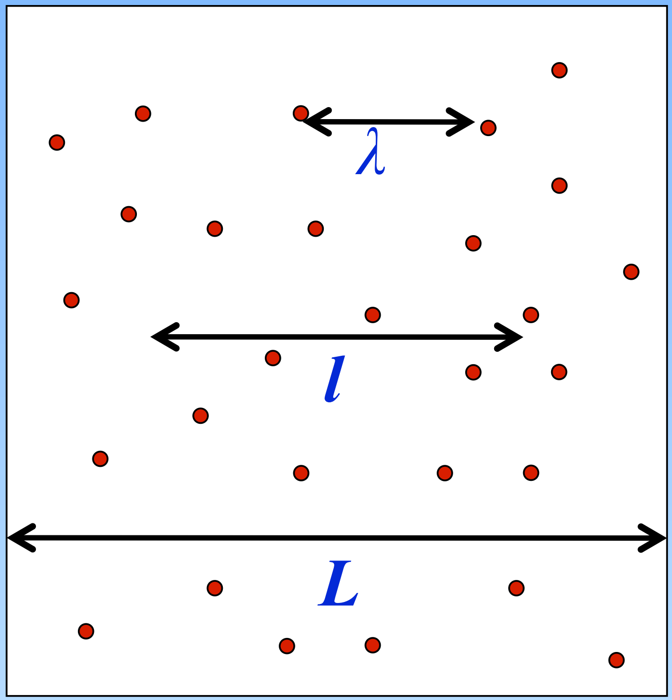
  $$v_{\text{CM-cluster}} > 0$$

drift of cluster towards wall !

In an isolated 1D case granular hydrodynamics does not work.

What about the general case?

Knudsen number



λ = mean free path

l = typical length at which macroscopic quantities vary

L = typical system size

$\mathrm{Kn} = \lambda/L$ (global Knudsen number)

$\mathrm{Kn}_{loc} = \lambda/l$ (local Knudsen number)

Hydrodynamics work if $\mathrm{Kn} << 1$!

Molecular system: local $\mathrm{Kn} <<1$ **(not a Knudsen gas!)**

Granular system: local Kn large !


Thank you!