Kinetic theory and granular hydrodynamics

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Part I: Kinetic theory of granular gases

- Inelastic Hard Sphere model
- Homogeneous cooling
- Boltzmann equation
- Conservation equations and constitutive laws
- Applications
- Driven systems

Part II: Granular hydrodynamics of dense granular liquids

- Usual geometries
- Dimensional analysis
- The inertial number rheology
- Application of the local rheology to avalanches
- Extensions: tensorial form, hysteresis, non-locality
- Boundary conditions

Part I: Kinetic theory of granular gases

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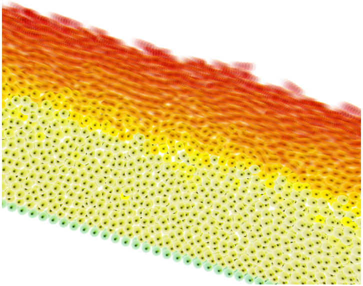
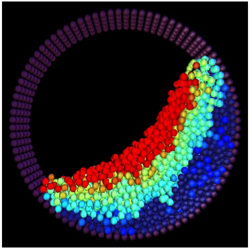
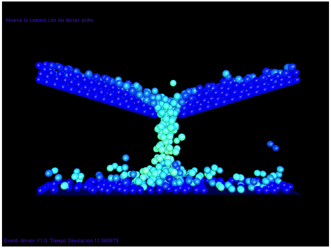
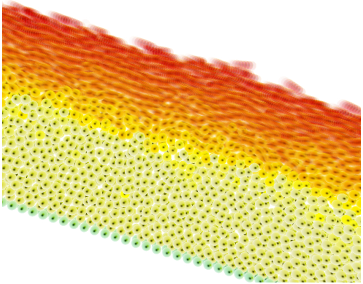
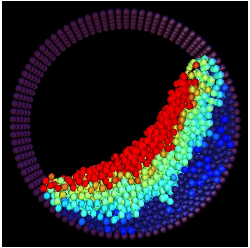
Some simple flows











Relevant fields:

- Density ρ or volume fraction ϕ
- Mean velocity $\mathbf{v}$

Navier-Stokes equations for molecular flows

$$\nabla \cdot \mathbf{v} = 0$$
$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} \right) = -\nabla p + \eta \nabla^2 \mathbf{v}$$

Is there an analogous for granular flows?

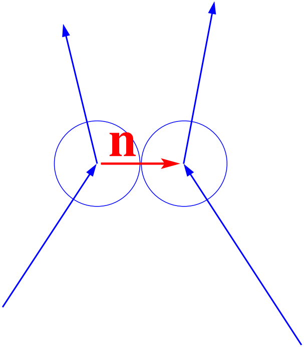
- Granular flows are compressible

$$\nabla \cdot \mathbf{v} = 0 \quad \rightarrow \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$
$$\eta \nabla^2 \mathbf{v} \quad \rightarrow \quad \eta \nabla^2 \mathbf{v} + \zeta \nabla(\nabla \cdot \mathbf{v})$$

- Mass and momentum are conserved but energy is not.
- The transport coefficients (viscosity, for example) depend on temperature. What is the analog here?

Properties

- Restitution coefficient $0 \leq \alpha \leq 1$
- Momentum is conserved
- Energy is not conserved:
  $\Delta E = -\frac{m}{4}[(\mathbf{v}_1 - \mathbf{v}_2) \cdot \hat{\mathbf{n}}]^2(1 - \alpha^2)$
- Particles align after collision
- The model can be extended to include rotation and friction



A collection of grains, with initial energy and no forcing

Energy per particle: $e = E/N$

Energy dissipated in each collision $\Delta E \sim -(1-\alpha^2)e$

Number of collisions per unit time $dN_{\mathrm{col}}/dt \sim Nn\sqrt{e}$

Then: $\dfrac{de}{dt} = -c(1-\alpha^2)ne^{3/2}$

Solution: $e = \dfrac{e_0}{[1+at]^2}$ Haff's law

There is a need for energy injection.

To make a more formal analysis, we use kinetic theory.

The basic concept is the velocity distribution function $f(\mathbf{r}, \mathbf{v}, t)$: average number of grains with given position and velocities.

Basic definitions

$$n(\mathbf{r}, t) = \int dv\, f(\mathbf{r}, \mathbf{v}, t) \qquad \text{number density}$$

$$\rho(\mathbf{r}, t) = mn \qquad \text{mass density}$$

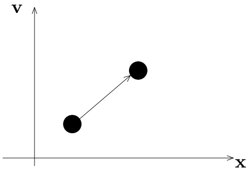
$$\mathbf{u}(\mathbf{r}, t) = n^{-1} \int dv\, \mathbf{v}\, f(\mathbf{r}, \mathbf{v}, t) \qquad \text{mean velocity}$$

$$\frac{3}{2} T(\mathbf{r}, t) = n^{-1} \int dv\, \frac{m}{2} (\mathbf{v} - \mathbf{u})^2 f(\mathbf{r}, \mathbf{v}, t) \qquad \text{granular temperature}$$

If we know f we have the full evolution

The distribution function $f(\mathbf{r}, \mathbf{v}, t)$ changes by two mechanisms:

Particles change position by the free motion or their velocities change by the action of external forces



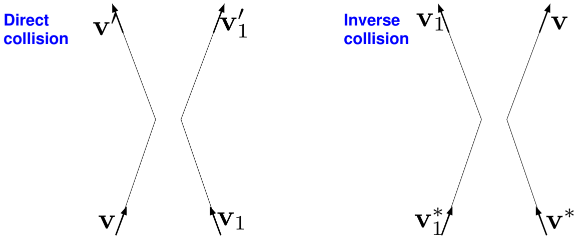
This contribution is considered exactly, tracking the particles

$$f(\mathbf{r}, \mathbf{v}, t + \Delta t) = f(\mathbf{r} - \Delta t\, \mathbf{v}, \mathbf{v} - \Delta t\, \mathbf{F}/m, t)$$

Taylor expanding leads to

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0$$

Collisions between particles change their velocities



Direct collisions destroy particles. Inverse collisions create particles. The collision rate is proportional to

$$\sigma^2 |(\mathbf{v} - \mathbf{v}_1) \cdot \hat{\mathbf{n}}| f(\mathbf{v}) f(\mathbf{v}_1)\, d^2\hat{\mathbf{n}}\, d^3\mathbf{v}\, d^3\mathbf{v}_1$$

For the inverse collisions we have to change variables from $\mathbf{v}^*$ to $\mathbf{v}$. Two considerations

$$|(\mathbf{v}^* - \mathbf{v}_1^*) \cdot \hat{\mathbf{n}}| = \alpha^{-1} |(\mathbf{v} - \mathbf{v}_1) \cdot \hat{\mathbf{n}}|, \quad d^3\mathbf{v}^*\, d^3\mathbf{v}_1^* = \alpha^{-1} d^3\mathbf{v}\, d^3\mathbf{v}_1$$

Combining the contributions of the change of f by the particle motion and the collisions, we obtain the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = J[f]$$

with the collision term

$$J[f] = \sigma^2 \int \left[\frac{f(\mathbf{v}^*) f(\mathbf{v}_1^*)}{\alpha^2} - f(\mathbf{v}) f(\mathbf{v}_1) \right] |(\mathbf{v} - \mathbf{v}_1) \cdot \hat{\mathbf{n}}| \, d^2\hat{\mathbf{n}} \, d^3\mathbf{v}_1$$

The Boltzmann equation has the property that

$$\int dv\,\psi(\mathbf{v})J[f] = 0 \text{ if } \psi \text{ is a conserved quantity: } 1, \mathbf{v}$$

Multiplying the Boltzmann equation by $1, m\mathbf{v}$, and $mv^2/2$ we get

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0$$

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) = -\nabla \cdot \mathbb{P} + \mathbf{f}_{\mathrm{ext}}$$

$$\frac{3}{2}\rho \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = -\nabla \cdot \mathbf{Q} - \mathbb{P} : \nabla \mathbf{u} - \Gamma$$

Hydrodynamic equations with $\mathbb{P}$ stress/pressure tensor, $\mathbf{Q}$ energy flux, and Γ energy dissipation rate.

Conservation equations and constitutive laws

To obtain $\mathbb{P}$, $\mathbf{Q}$, and Γ we need to solve the Boltzmann equation. It is a non-linear equation, complex to solve in general.

The Chapman Enskod method solves the Boltzmann equation in a perturbation scheme for small inhomogeneities

$$
\begin{aligned}
f_0 &= f_0[n, \mathbf{u}, T] \quad \text{depends on the forcing mechanism} \\
f_1 &= g_1 \nabla n + h_1 \nabla \mathbf{u} + j_1 \nabla T \\
&\dots
\end{aligned}
$$

Keeping up to first order

$$
\begin{aligned}
\mathbb{P} &= nT\mathbb{I} - \eta_0 \sqrt{T} \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \\
\mathbf{Q} &= -\mu_0 \sqrt{T} \nabla n / n - \kappa_0 \sqrt{T} \nabla T \\
\Gamma &= \gamma_0 (1 - \alpha^2) n^2 T^{3/2}
\end{aligned}
$$

Transport coefficients: η_0, κ_0, μ_0, and γ_0, depend on f_0 and α.

The analysis has been improved by:

- Extending the kinetic equation to dense regimes using the Enskog equation: spatial correlations, finite particle sizes and excluded volume
  Now, for example
  $$\mathbb{P} = nTH(n)\mathbb{I} - \eta(n)\sqrt{T}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)$$
- Considering rotation: equation for the conservation of angular momentum
  Granular rotational temperature, but $T_{\rm rot} \neq T_{\rm trans}$
- Other collision models

Applications: Homogeneous cooling again

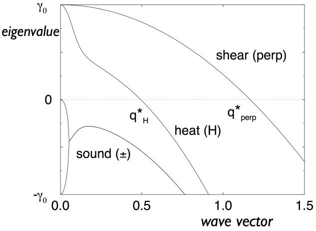
Assuming homogeneity, the hydrodynamic equations reduce to

$$
\begin{aligned}
\rho &= \rho_0 \\
\mathbf{u} &= 0 \\
\frac{dT}{dt} &= -\frac{2}{3}\gamma_0(1-\alpha)^2 n T^{3/2}
\end{aligned}
$$

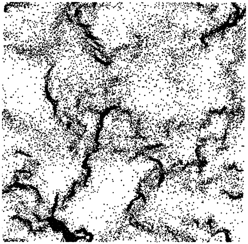
and we recover Haff's law.

What happens if there is no perfect homogeneity. Perturbation analysis. To eliminate the explicit time dependence, time is changed to $dt = ds/\sqrt{T}$. The fields are rescaled $T = T_0(t)\hat{T}$, $\mathbf{u} = \sqrt{T}\hat{\mathbf{u}}$

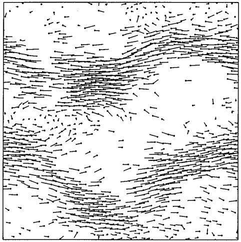
$$\rho = \rho_0 + \epsilon\rho_1 \qquad \hat{\mathbf{u}} = \epsilon\hat{\mathbf{u}}_1 \qquad \hat{T} = 1 + \epsilon\hat{T}_1$$



[Orza *et al.* 1997]



[Goldhisrsch and Zanetti 1993]



[McNamara and Young 1996]

Clustering instability mechanism:

A density increase ⇒ energy dissipation increases ⇒ temperature drops ⇒ pressure drops ⇒ mass influx ⇒ density increases

Applications: Bagnold scaling

Consider a granular gas in a uniform shear. If we want the density to be homogeneous, the temperature should be homogeneous

$$\frac{3}{2}\rho\cancelto{0}{\left(\frac{\partial T}{\partial t}+(\mathbf{u}\cdot\nabla)T\right)} = -\cancelto{0}{\nabla\cdot\mathbf{Q}} + \eta(\nabla\mathbf{u})^2 - \gamma(1-\alpha^2)\rho^2 T^{3/2}$$

The viscosity goes as $\eta = \eta_0\sqrt{T}$. Then

$$T \sim (\nabla\mathbf{u})^2/[\rho^2(1-\alpha^2)] \quad \text{Bagnold scaling}$$

The viscosity depends on the shear rate: $\eta = \eta_0\sqrt{T} \sim \eta_0|\nabla\mathbf{u}|$

For hydrodynamics to be valid, the change on velocities in a mean free path ℓ should be small (compared to the typical sound velocity $c \sim \sqrt{T/m}$).

That is, $\Delta u = \ell \nabla u \ll \sqrt{T/m}$

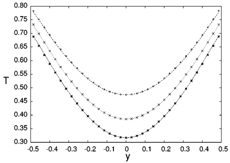
Using $\ell \sim 1/n$, and the Bagnold scaling $T \sim (\nabla \mathbf{u})^2/[\rho^2(1-\alpha^2)]$ we get the condition

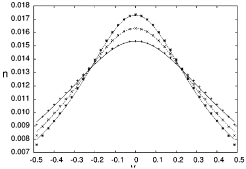
$$(1-\alpha^2) \ll 1$$

For large inelasticities, there is no temporal or spatial scale separation.

Applications: Boundary effects

Consider a granular gas that is driven by two vibrating walls, modeled as thermal to impose a granular temperature T_0.





[Cordero and Risso 2002]

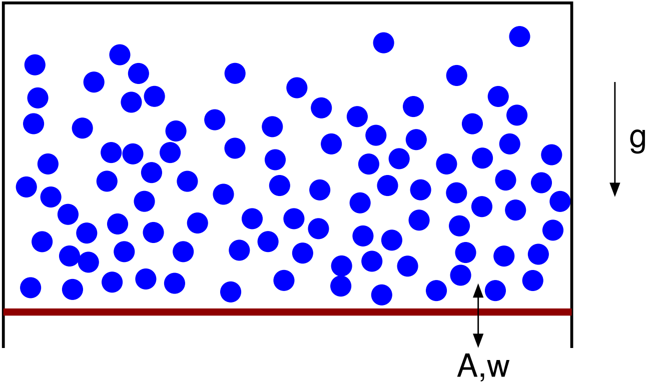
Pressure is uniform $p_0 = nT$, then $n = p_0/T$. Stationary state

$$\frac{d}{dz}\left(\kappa \frac{dT}{dz}\right) - \gamma(1-\alpha^2)\rho^2 T^{3/2} = 0; \quad \kappa = \kappa_0 \sqrt{T}$$

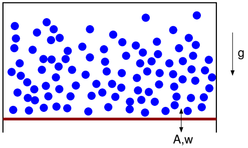
The solution is

$$T^{3/2} = T_0^{3/2} \frac{\cosh(z/L_\alpha)}{\cosh(L/L_\alpha)}$$

Scale of inhomogeneities $L_\alpha \sim 1/(\rho\sqrt{1-\alpha^2})$ can be very small.



At high frequencies, the wall injects energy $Q = Q(\rho, T)$ [Soto 2004].
There is energy dissipation in the bulk.



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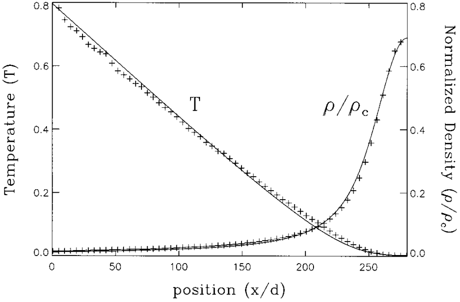
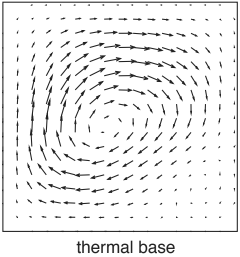
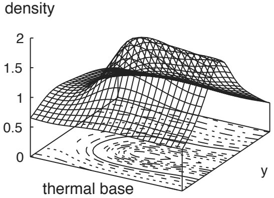
A temperature profile develops, leading a density profile...

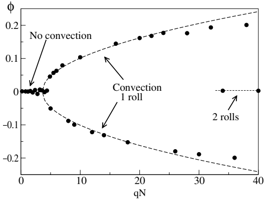


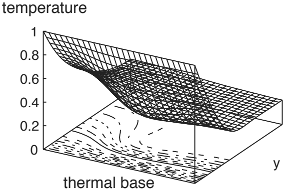
Grossman *et al.* 1997

Temperature and density profiles under gravity induce convection







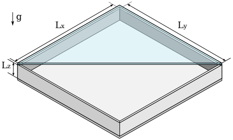


[Ramirez *et al.* 2000, Cordero *et al.* 2003]

Hydrodynamic equations agree with simulations and experiments.

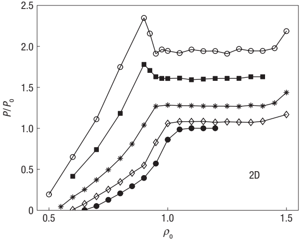
Driven systems

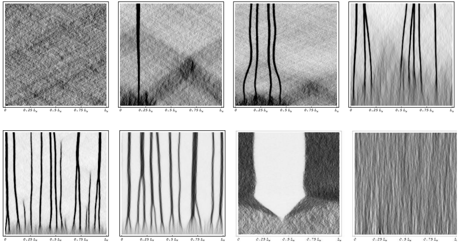
Grains placed in a vibrated shallow box. Energy is injected to the vertical degrees of freedom and transferred to the horizontal ones.



The vertical scale is fast. The granular temperature adapts to the local density: $T(\rho)$ is a decreasing function.
The pressure is $p = p(\rho, T) = p(\rho, T(\rho)) = \hat{p}(\rho)$.

Presents a van der Waals loop triggering a mechanical instability





[Clerc *et al.* 2008]

[Argentina *et al.* 2003]

Part II: Granular hydrodynamics of dense granular liquids

- Usual geometries
- Dimensional analysis
- The inertial number rheology
- Application of the local rheology to avalanches
- Extensions: tensorial form, hysteresis, non-locality
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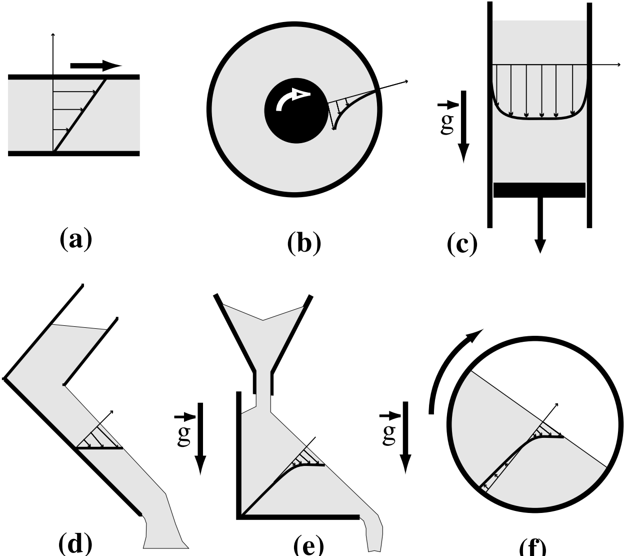
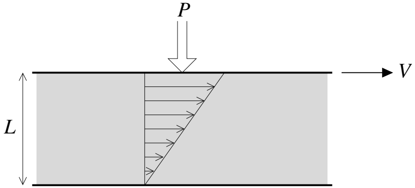
Usual geometries



GDR MiDi 2004

Consider a simple shear at constant pressure.



The input data are:

- pressure P
- shear rate $\dot\gamma = du_x/dy$
- plate separation L
- particle diameter d
- particle density ρ_p.

We measure: shear stress τ, volume fraction ϕ

In the limit of impenetrable particles, their elastic properties are irrelevant.

In the limit of large boxes ($L \gg d$), L is irrelevant for a local rheology.

Dimensional analysis. Only dimensionless input quantity

$$I = \frac{\dot\gamma d}{\sqrt{P/\rho_p}} \quad \text{inertial number}$$

[GDR MiDi, 2004, da Cruz *et al.* 2005, Jop *et al.* 2008]

Inertial number

$$I = \frac{\dot{\gamma} d}{\sqrt{P/\rho_p}}$$

Can be written as

$I = t_{\mathrm{micro}}/t_{\mathrm{macro}}$

$t_{\mathrm{micro}} = d/\sqrt{P/\rho_p}$ Time to arrange one grain by pressure

$t_{\mathrm{macro}} = 1/\dot{\gamma}$ Time to move a grain its diameter by the flow

Regimes:

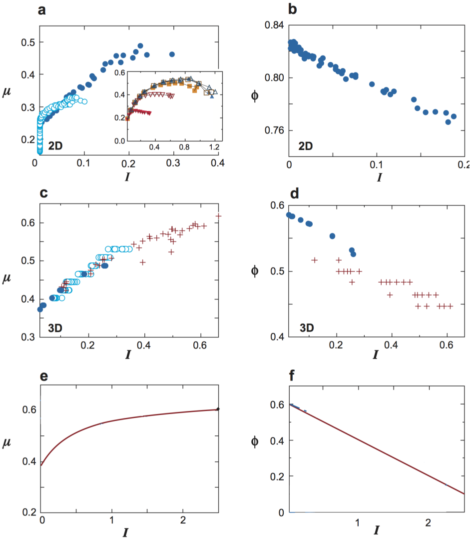
$I = 0$ solid

$I \ll 1$ quasistatic

$I \gtrsim 1$ fluid (kinetic theory)

By dimensional analysis, the measured quantities must be

$$\tau = P\,\mu(I)$$
$$\phi = \phi(I)$$

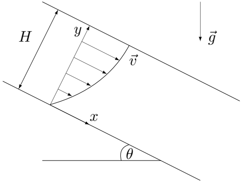


[Forterre *et al.* 2008]

[GDR MiDi, 2004, da Cruz *et al.* 2005, Jop *et al.* 2008]

Application of the local rheology to avalanches

In a stationary avalanche the momentum equation reads



$$\rho \cancelto{0}{\frac{\partial u_x}{\partial t}} = \frac{\partial \tau}{\partial y} + \rho g \sin\theta$$

$$0 = -\frac{\partial P}{\partial y} - \rho g \cos\theta$$

The solution is

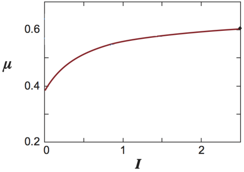
$$P = \rho g \cos\theta (H - y)$$

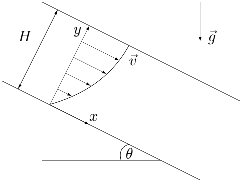
$$\tau = \rho g \sin\theta (H - y)$$

Notably $\tau / P = \tan\theta$. According to the local rheology $\tan\theta = \mu(I)$. Both μ and I are uniform and given only by the geometry.

Application of the local rheology to avalanches

We have $\mu = \tan\theta$ uniform in the avalanche.





Case 1: $\tan\theta < \mu_c$. The solution is $I = 0$, static pile.

Case 2: $\tan\theta > \mu_c$. The solution is $I \neq 0$ uniform. But $I = \frac{\frac{du_x}{dy} d}{\sqrt{P/\rho_p}}$ and $P = \rho g(H - y)$, then

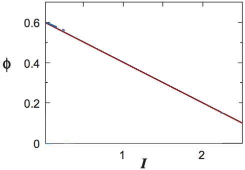
$$u_x = \frac{2IH^{3/2}}{3d}\sqrt{\frac{\rho_0 g\cos\theta}{\rho}}\left[1 - (1 - y/H)^{3/2}\right]$$

In this regime, the granular temperature is not a relevant field. It is completely enslaved to the flow (Bagnold scaling).

In a shear flow at fixed volume, ϕ is fixed.
From the definition of $I = \frac{\dot{\gamma} d}{\sqrt{P/\rho_p}}$
The pressure is

$$P = \frac{\rho_p d^2 \dot{\gamma}^2}{I^2}$$

Close to the jamming transition $\phi = \phi_c - aI$, then $I = (\phi_c - \phi)/a$.



Back in the pressure

$$P = \frac{\rho_p d^2 \dot{\gamma}^2 a^2}{(\phi_c - \phi)^2}$$

The confining pressure diverges at jamming.

Extensions: tensorial form, hysteresis, non-locality

The local rheology derived for planar shear flows $\mathbf{u} = u_x(y)\hat{\mathbf{x}}$.

What happens in more complex (2D or 3D) flows?
It was proposed that the shear rate and shear stress tensors are parallel. [Jop *et al.* 2006]

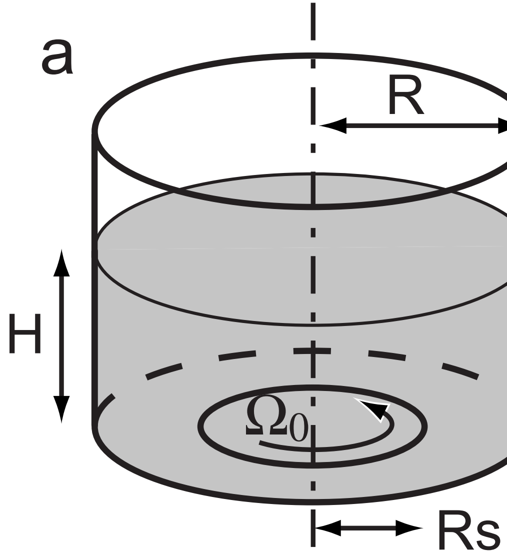
$$\mathbb{P} = P\mathbb{I} - \tau$$

$$\tau_{ik} = P\mu(I)\frac{\dot{\gamma}_{ik}}{|\dot{\gamma}|}$$

$$I = \frac{|\dot{\gamma}|d}{\sqrt{P/\rho_p}}$$

$$\dot{\gamma}_{ik} = \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}$$

$$|\dot{\gamma}| = \sqrt{\dot{\gamma}_{ik}\dot{\gamma}_{ik}/2}$$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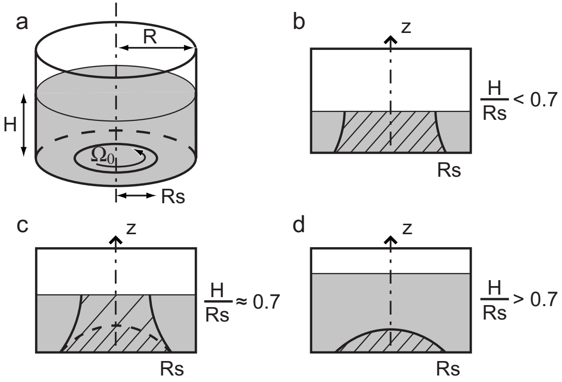
Extensions: tensorial form, hysteresis, non-locality



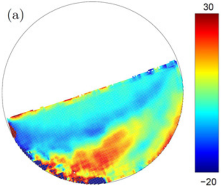
[Cheng *et al.* 2006, Fenistein *et al.* 2006, Jop 2008]

Shear bands develop.

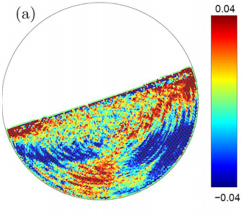
Qualitatively well captured by the continuous model.

But simulacion rotating drum

The tensors τ_{ik} and $\dot{\gamma}_{ik}$ are not parallel.



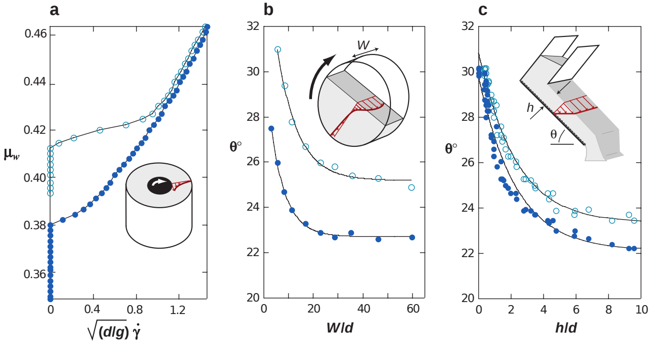
However, the invariants do follow the local rheology.



[Cortet *et al.* 2009]

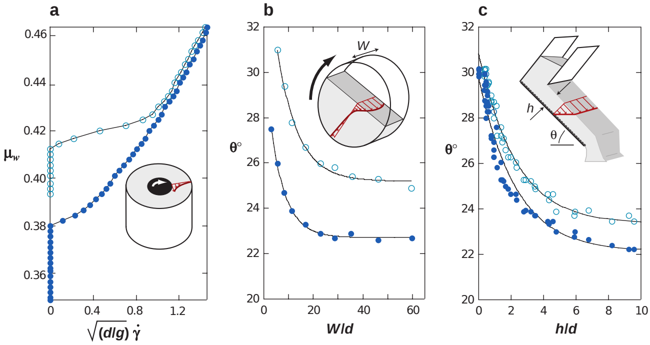
Extensions: tensorial form, hysteresis, non-locality

We predicted that μ_c gives the critical avalanche angle
But experiments and simulations indicate that there are stop and start angles: $\theta_{\text{stop}} < \theta_{\text{start}}$.



[Forterre and Pouliquen 2008]

Needs hysteresis: two fluid model [Aranson *et al.* 2008]



The critical angles depend on the thickness height $\theta_{\rm stop}(H)$ and $\theta_{\rm start}(H)$.

This effect cannot be described by the local-rheology.

Force chains?

Both the hydrodynamic and kinetic equations need boundary conditions.

Free surface:

There is no stress $\tau = 0$. But $\tau = P\mu(I)$. However, $P = 0$ at the surface!! So, there is nothing imposed on I.

But, $I = \frac{\dot{\gamma} d}{\sqrt{P/\rho_p}}$. Vanishing P implies vanishing $\dot{\gamma}$.

In summary: $P = 0$ and $\frac{\partial u_x}{\partial y} = 0$.

Solid boundary:

If it is rough enough, then $\mathbf{u} = 0$.

Vibrating beds:

At high frequencies, the wall injects energy $Q = Q(\rho, T)$ [Soto 2004].

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