Is accurate continuum modelling of granular/ powder flow an achievable target?

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Continuum modelling – why bother?

The rise in power (and reduction in cost) of computations – leading to efficient particle dynamics simutations (DEM and all its variants) have made it seem that continuum descriptions are not necessary – **but good continuum descriptions are indispensible.**

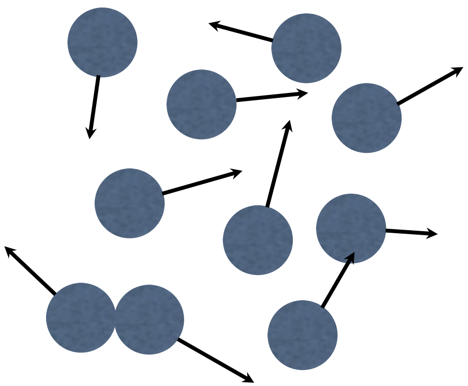
> *However discrete may be nature itself, the mathematics of a very numerous discrete system remains even today beyond anyone's capacity. To analyze the large, we replace it by the infinite, because the properties of the infinite are simpler and easier to manage. And understanding the infinite is more insightful, and elegant!*
>
> Truesdell and Muncaster (1980)

But DEM is an extremely very valuable tool – a "clean" controllable experiment, that can provide microstructural understanding.

A combination of continuum modelling, targeted experiments, and DEM can uncover new phenomena of practical interest, and explain them.

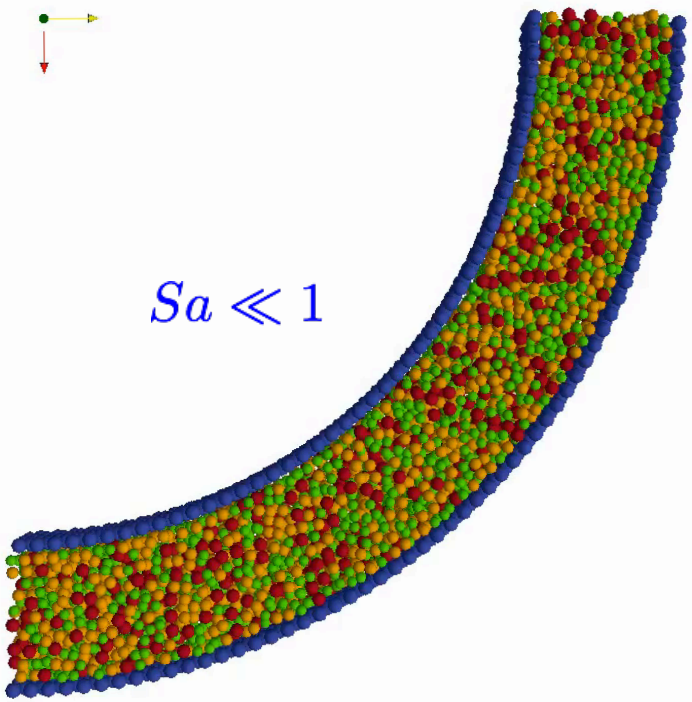
Regimes of granular flow: ‘gases’ and ‘liquids’

Rapid flow (grain inertia)



$Sa \sim O(1)$

Slow (quasistatic) flow



$Sa \ll 1$

Savage number

$$Sa \equiv \frac{\rho_p d_p^2 \dot{\gamma}^2}{\sigma}$$

Savage & Hutter (1989)

$$I = Sa^{1/2}$$

Stress quadratic in shear rate: $Sa \gtrsim 10^{-1}$

Haff (1983), Jenkins & Savage (1983), Lun et al (1984)

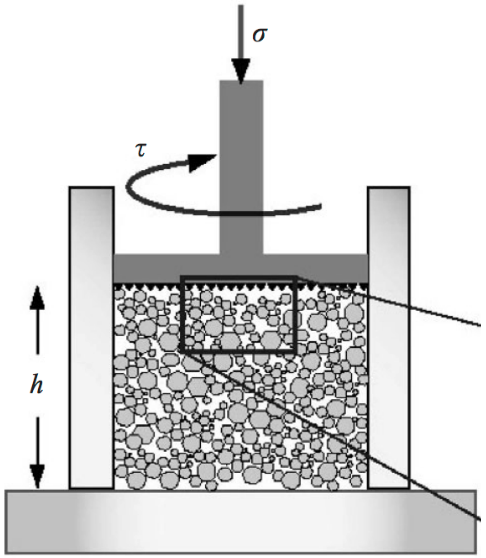
Kinetic theory-based analyses reasonably accurate, but several challenges remain

Stress rate independent: $Sa \lesssim 10^{-6}$

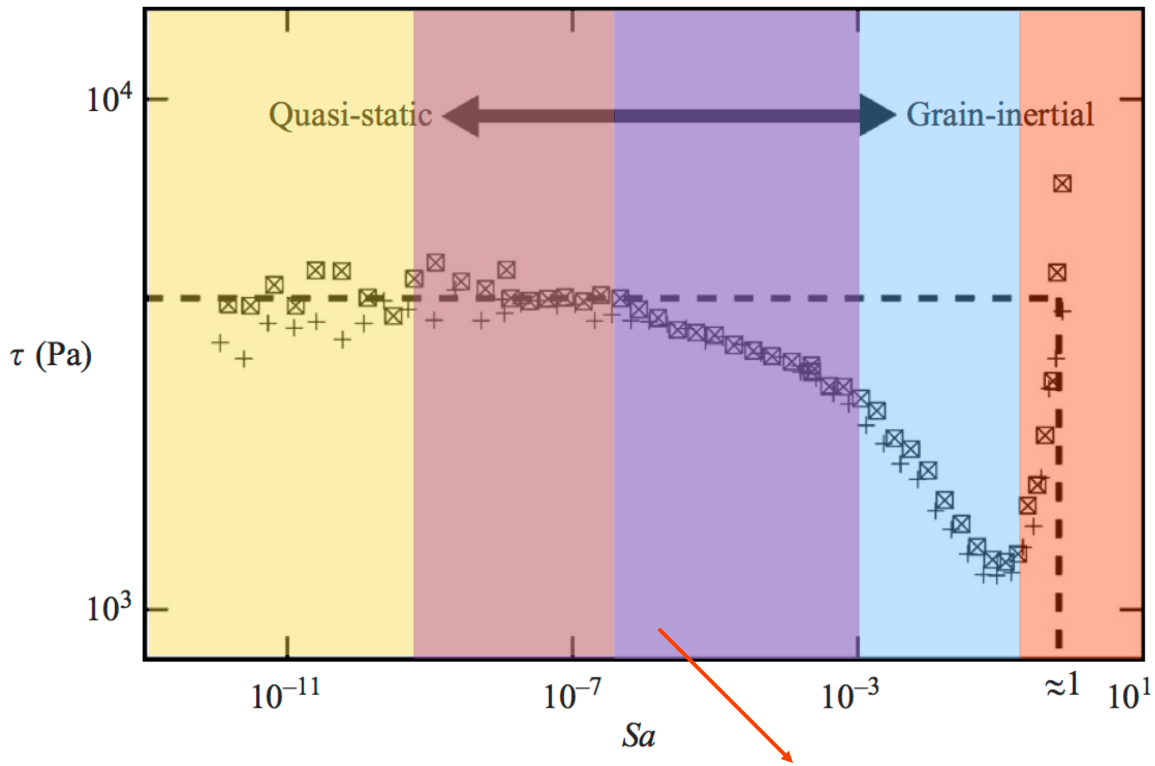
Lu, Brodsky & Kavehpour (2007)

Plasticity theories: moderate successes, but huge challenges remain

But there is a vast span between the two limiting regimes



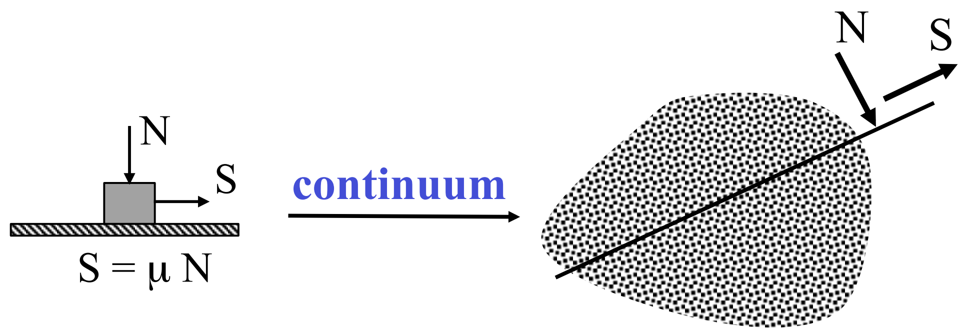
Lu, Brodsky & Kavehpour (2007)



Today's talk

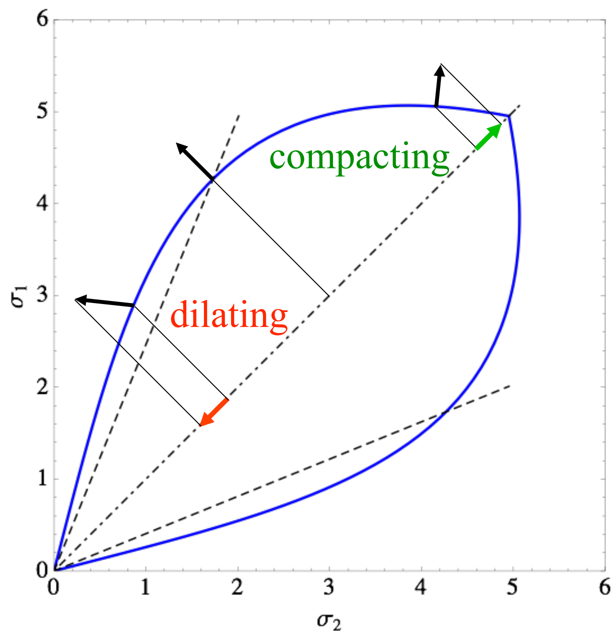
A few phenomenological models proposed for the intermediate regime, the $\mu(I)$ model of GDR Midi being the most popular.

Critical state plasticity theory



Yield condition

$$F(\boldsymbol{\sigma}, \nu) \equiv \tau(\boldsymbol{\sigma}') - Y(p, \nu) = 0$$



Flow rule

$$D_{ij} = \dot{\lambda} \frac{\partial F}{\partial \sigma_{ji}}$$

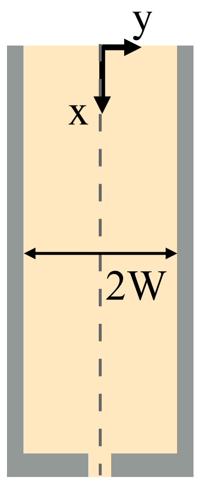
Writing the above in stress-explicit form,

$$\sigma_{ij} = p\,\delta_{ij} + \sigma'_{ij}$$

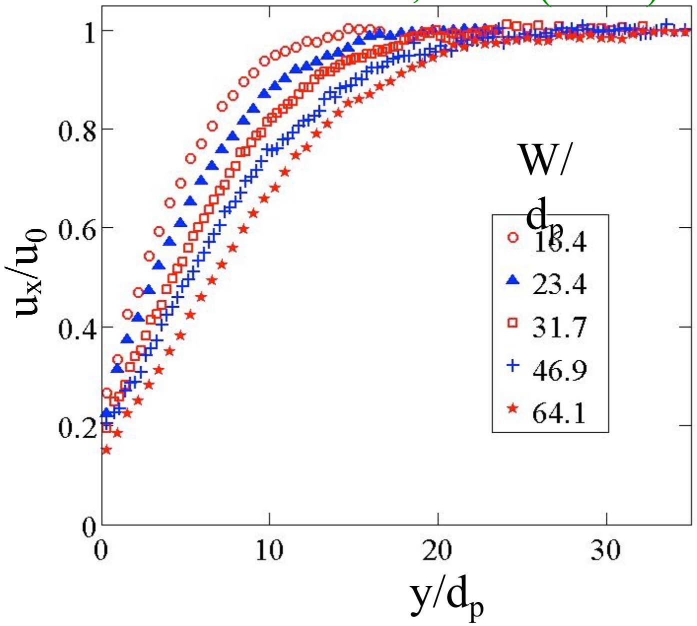
$$\sigma'_{ij} = -2 \boxed{\frac{Y}{\dot{\gamma}}} D'_{ij}, \quad p = p_c(\nu)\left(1 - \frac{1}{n \sin\phi} \frac{\nabla \cdot \boldsymbol{u}}{\dot{\gamma}}\right)^{n-1}$$

But classical plasticity has deficiencies

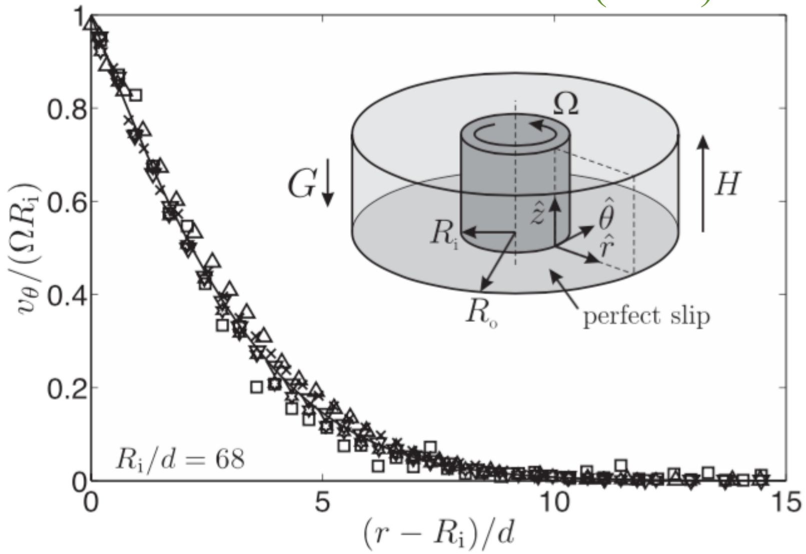
It cannot predict the velocity fields and dilatancy in simple shear flows

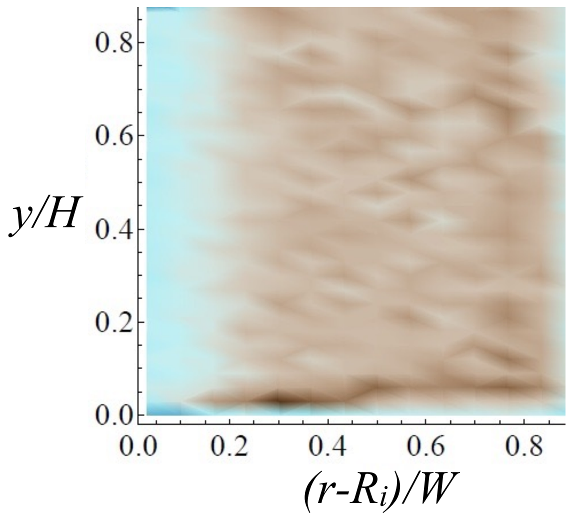


Ananda *et al, JFM* (2008)



Henann & Kamrin *PRL* (2013)





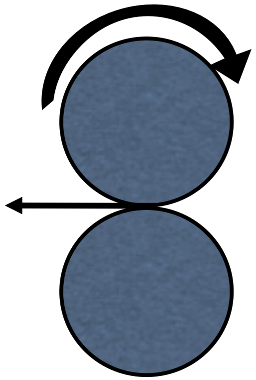
Colour map of volume fraction

No length scale in classical plasticity

Extensions of classical plasticity (that introduce a length scale)

Cosserat plasticity model

Mohan, Rao & Nott, *JFM* (1999, 2002)
Tejchman & Wu, *Acta Mech.* (1994);



Surface couples arise from tangential forces between grains (friction).

linear momentum $D(\nu \mathbf{u})/Dt + \nabla \bullet \boldsymbol{\sigma} - \rho\, \mathbf{g} = 0$

angular momentum $D(\rho\, \boxed{\omega})/Dt + \nabla \bullet \boxed{M} - \boxed{\varepsilon : \sigma} = 0$

M – Couple stress, **ω** – mean particle spin

Non-local fluidity model

Henann & Kamrin, *PRL* (2013)

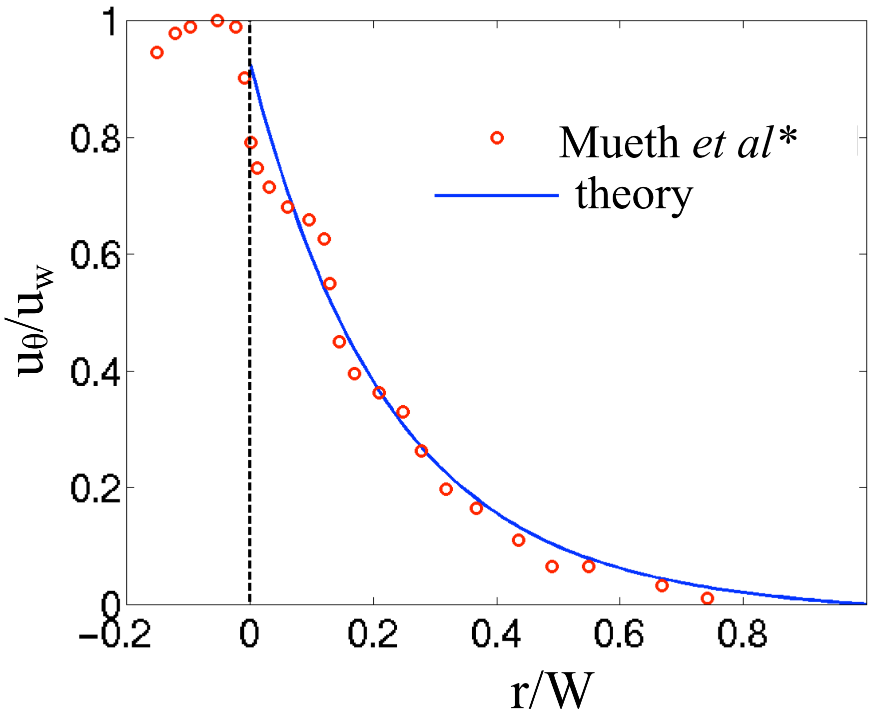
$$\sigma'_{ij} = p\,\delta_{ij} + \frac{p}{\dot{\lambda}} D'_{ij}, \qquad \boxed{\dot{\lambda} = \dot{\gamma} + \ell^2 \nabla^2 \dot{\lambda}}$$

The fluidity diffuses

Results of the extensions of classical plasticity

Both models

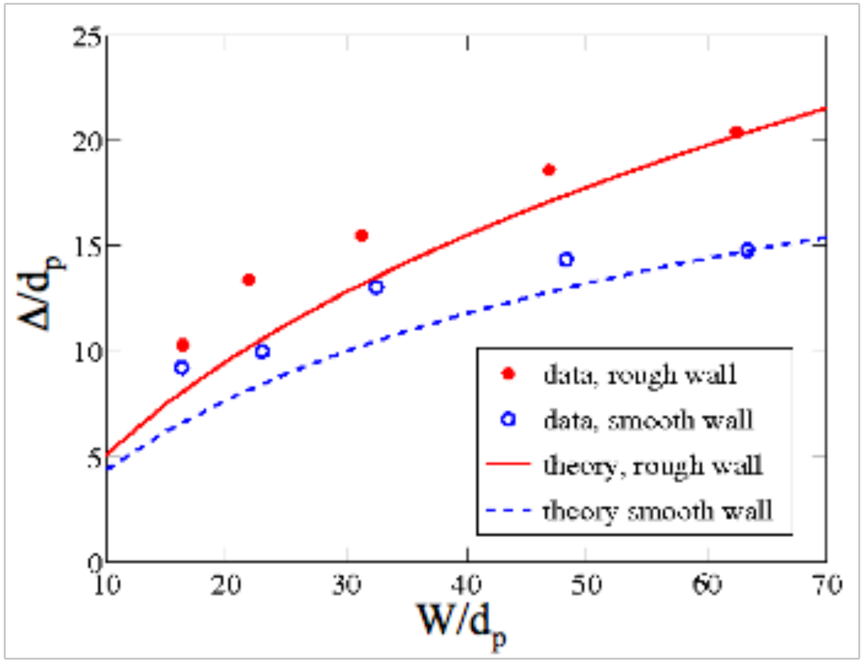
Velocity profile for mustard seeds in cylindrical Couette flow



Mueth *et al, Nature* (2000)

Cosserat model

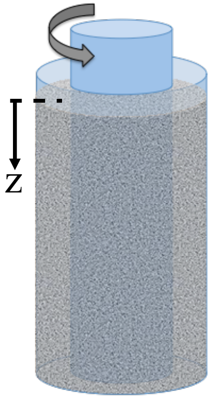
Shear layer thickness in a vertical channel, as a function of channel width



Ananda *et al, JFM* (2008)

Both these models cannot predict constant pressure dilatancy

Stress in a cylindrical Couette device: how a combination of continuum modelling, experiments and DEM solved a puzzle



$u_\theta = u_\theta(r), \;\; u_r = u_z = 0$

$\sigma_{rr} = \sigma_{\theta\theta} = \sigma_{zz} = \rho g z$

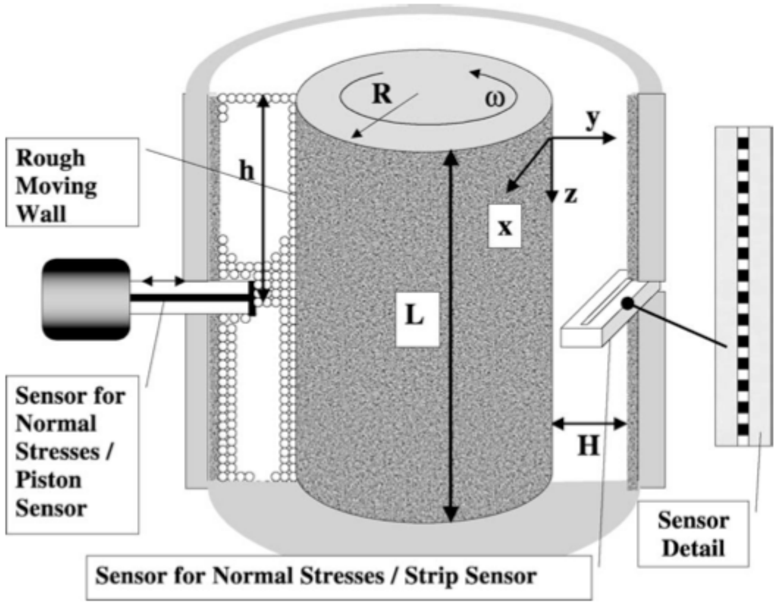
$\sigma_{rz} = \sigma_{\theta z} = 0$

All plasticity theories (including extensions) predict a fluid-like stress!

Previous experiments: Tardos and coworkers (1998, 2003)

Shear and normal stress vary linearly with distance from the free surface

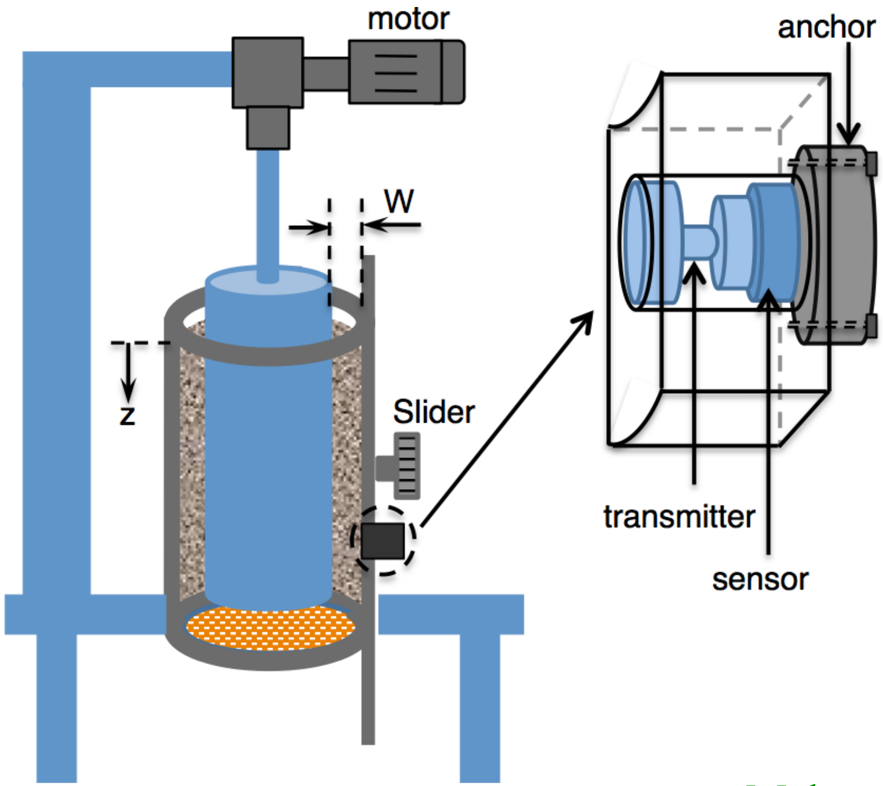
Fluid-like stress.

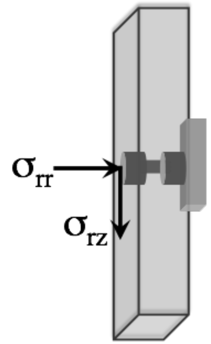


Tardos *et al, Powder Tech.* (1998, 2003)

But several inaccuracies in experiments

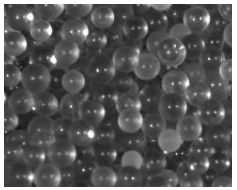
Stress in a sheared column: our recent experiments





Mehandia, Gutam & Nott, *PRL* (2012)

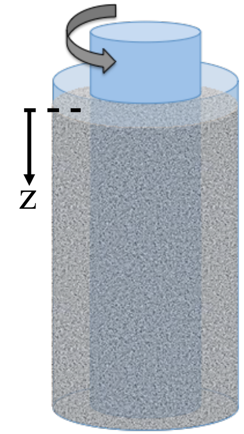
Gutam, Mehandia & Nott, *Phys. Fluids* (2013)



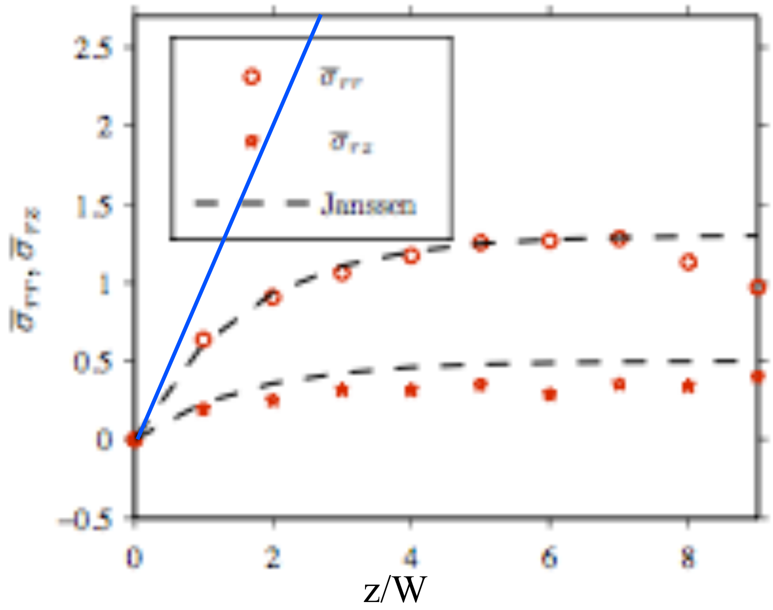
glass beads

mustard seeds

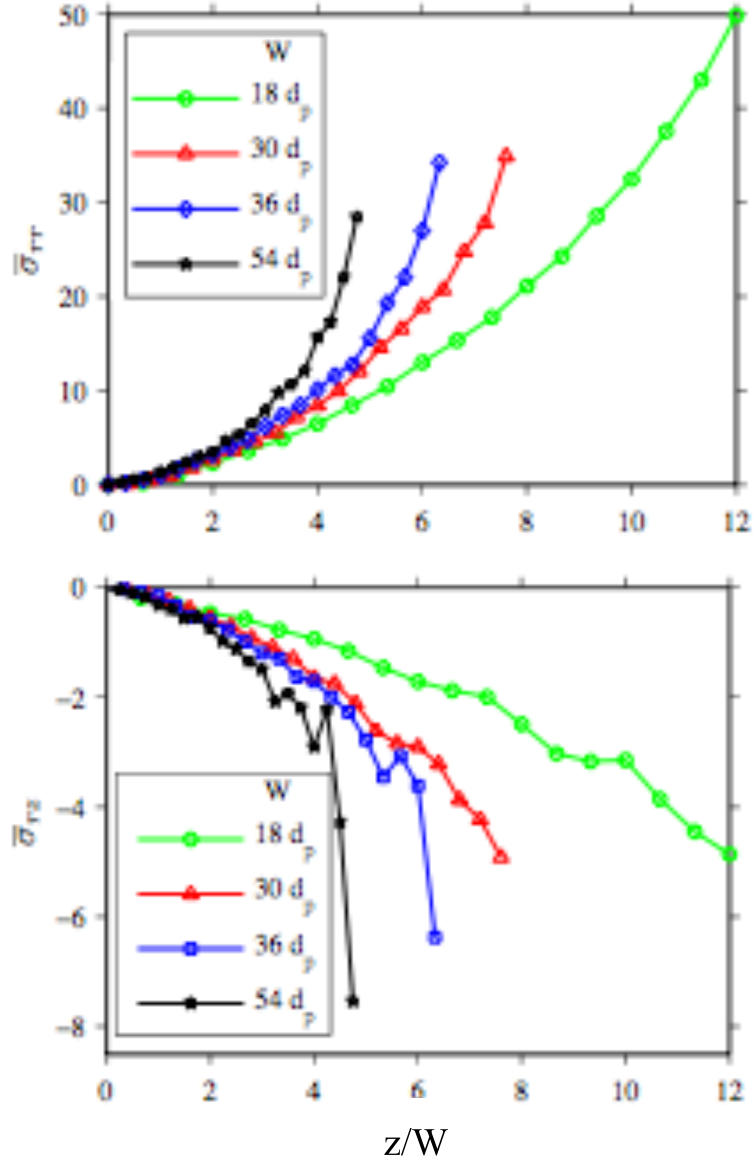
Anomalous stress profile upon shearing



Static column: Janssen saturation



Sheared column: exponential rise



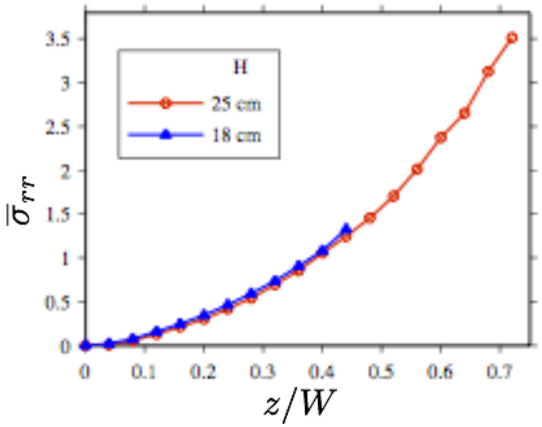
Stress profile qualitatively similar for all Couette gaps, fill heights, and shear rates.

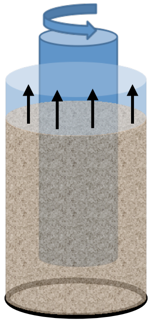
Mehandia, Gutam & Nott, *PRL* (2012);
Gutam, Mehandia & Nott, *Phys. Fluids* (2013)

What causes the anomalous stress – our earlier conjectures

Impenetrable, frictional base?

No

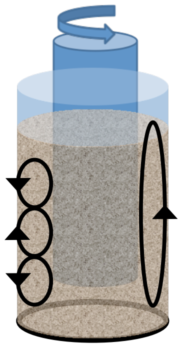




Shear-induced dilation?

No, because:

- Free surface drops during the experiment.
- Vertical shear stress remains constant in time.



Secondary flow?

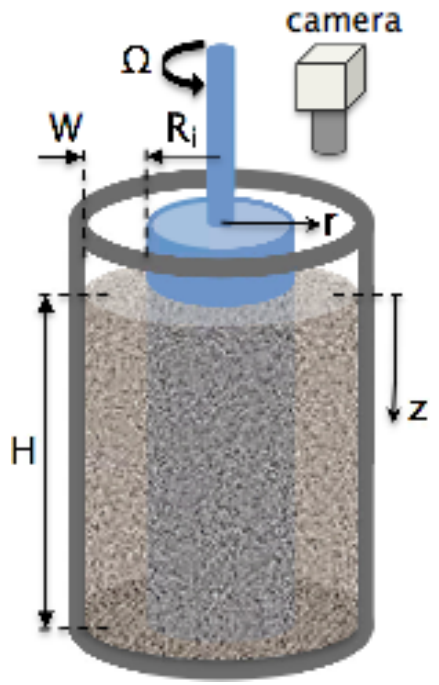
Unlikely, because

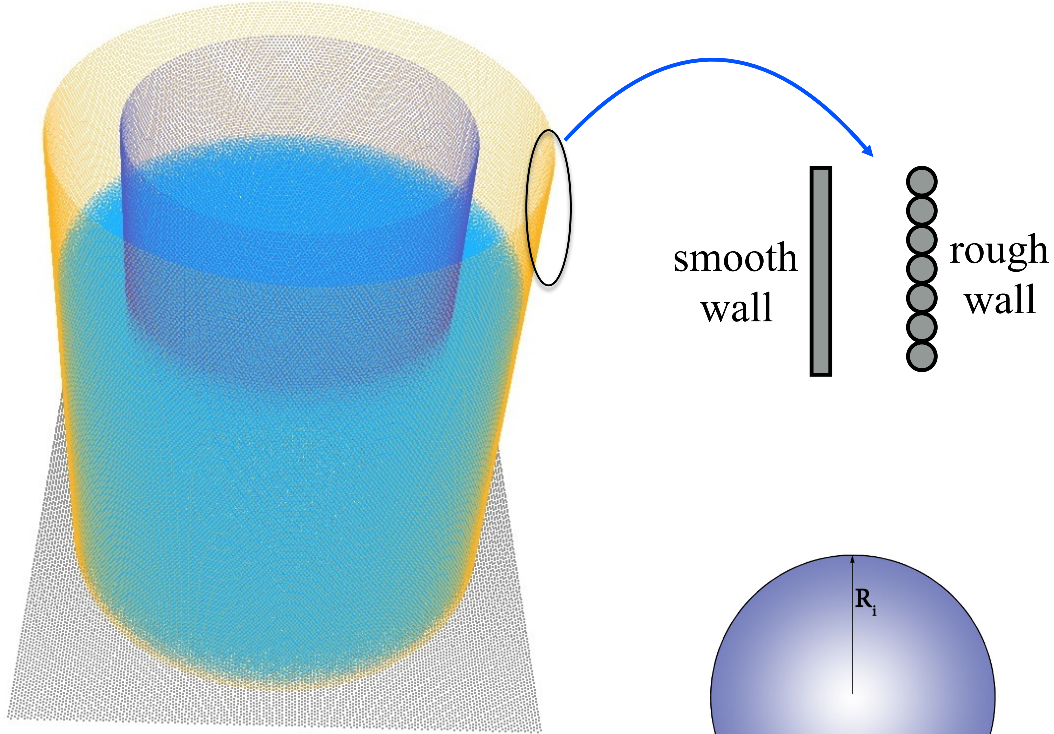
- It requires a single column-spanning vortex, regardless of the fill height!

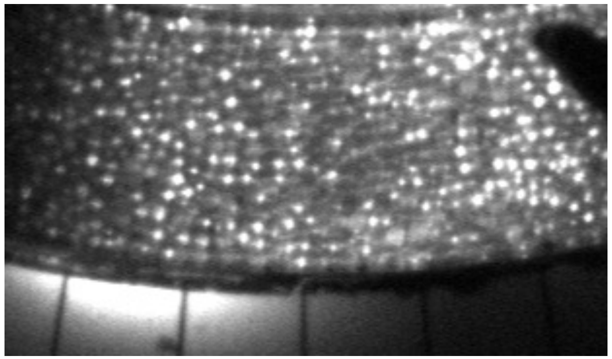
Right and wrong on all counts!

Probably caused by anisotropic fabric

Cause of anomalous stress: Investigations using DEM simulations and video imaging





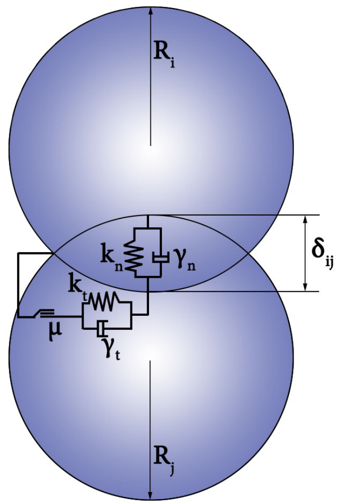


~10^6 particles tracked for several rotation of the cylinder **using LAMPPS**

Mixture of diameters 0.9 d_p, d_p, 1.1 d_p

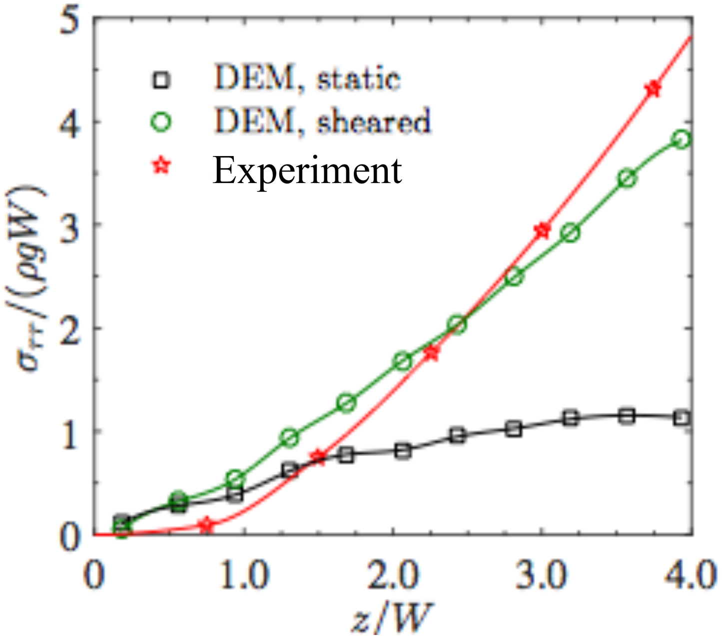
$R_i = 37\ d_p$, $W = 16\ d_p$,

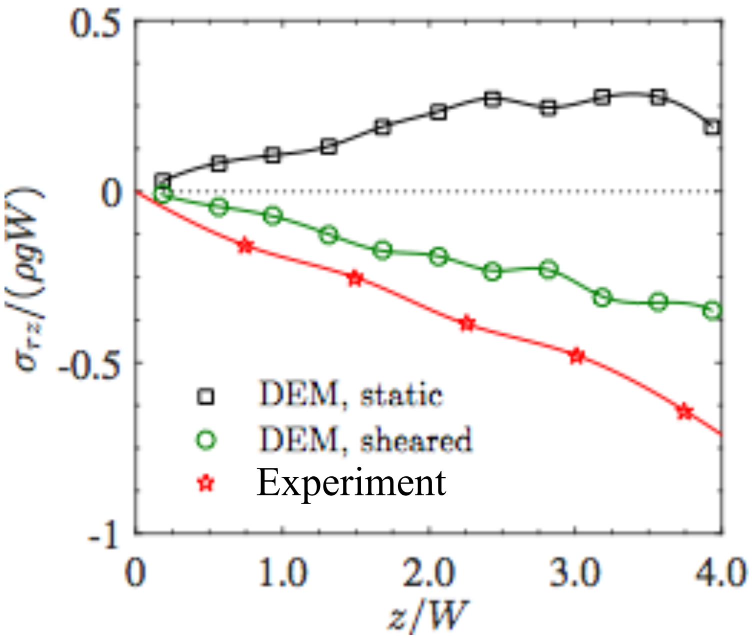
$H = 30, 60, 90\ d_p$

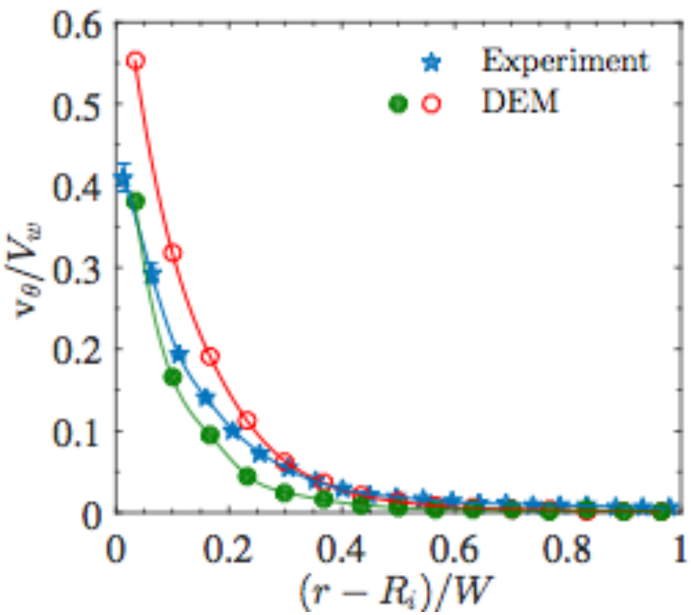


Cundall-Strack-Walton

Validation: wall stress and azimuthal velocity profiles

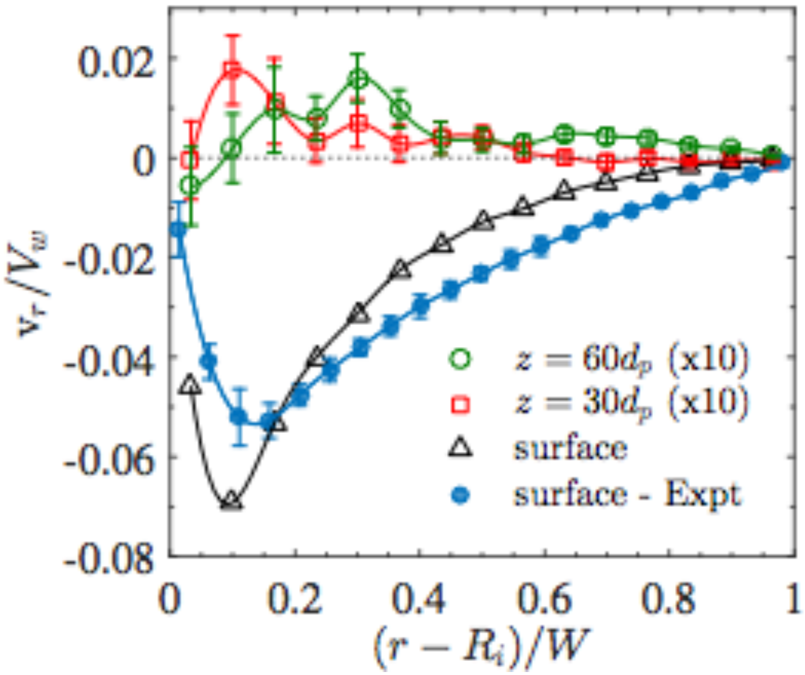


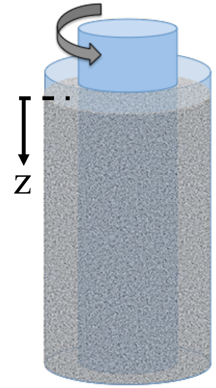


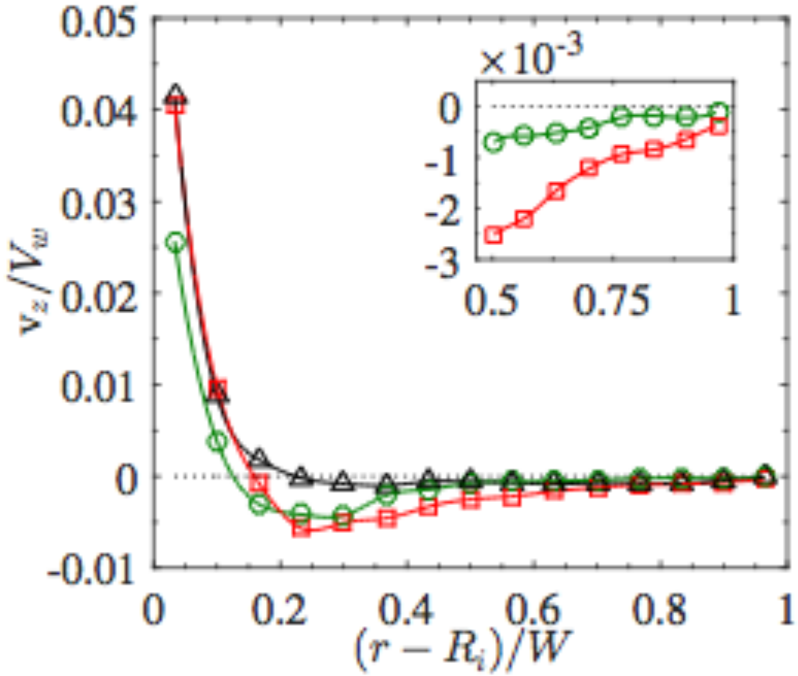


Good qualitative agreement
with experiments

Interrogating the kinematics reveals a secondary flow

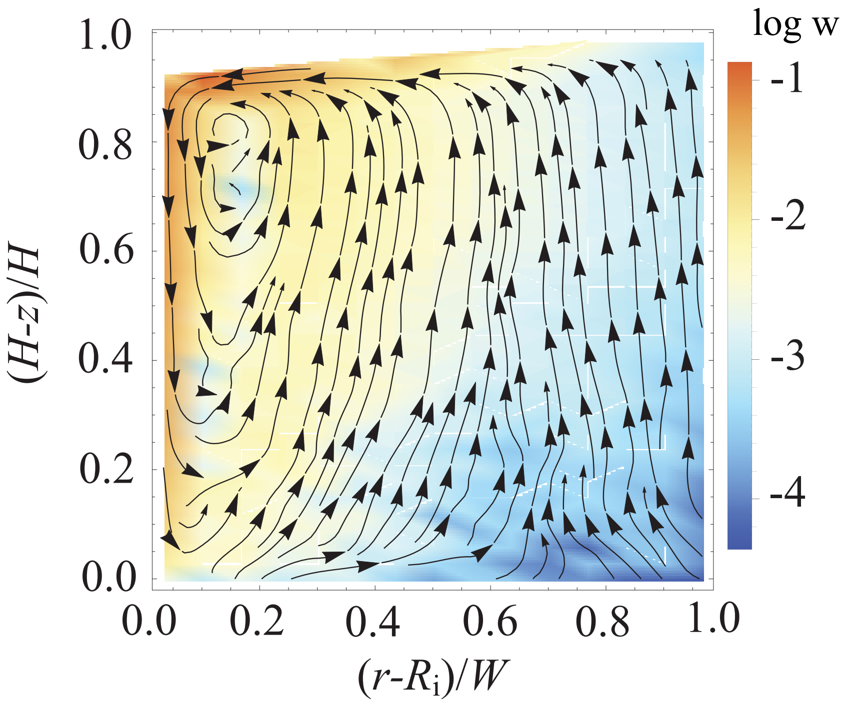






The secondary vortex

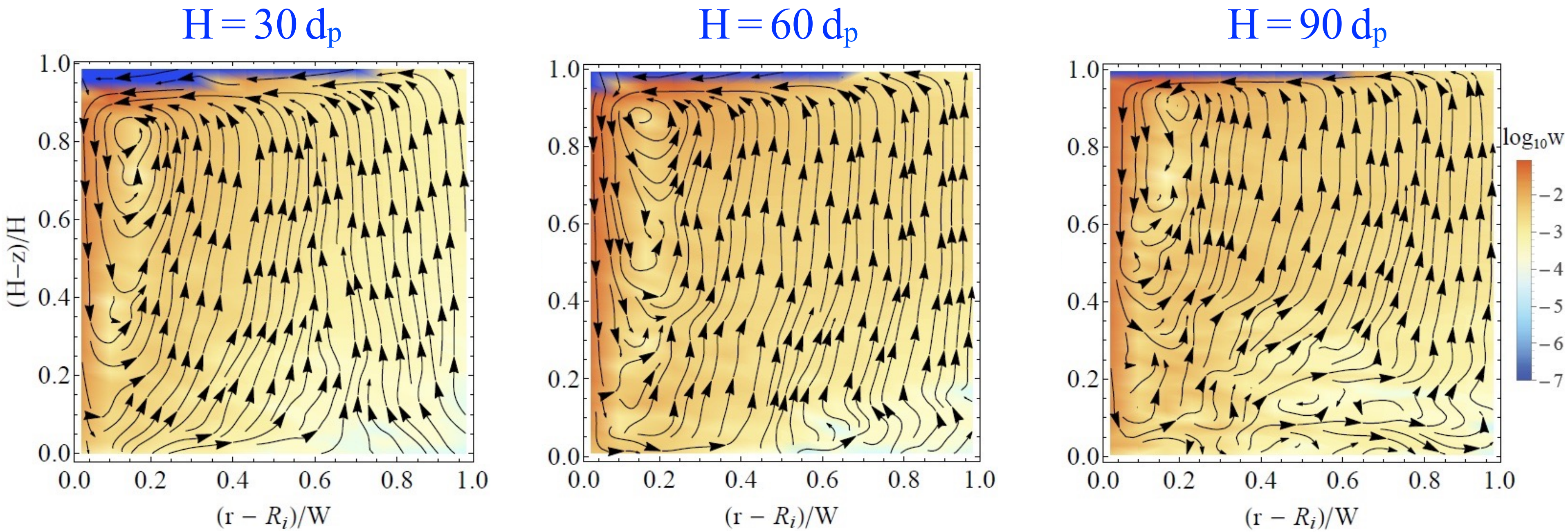
$H = 30\, d_p$, $W = 16\, d_p$

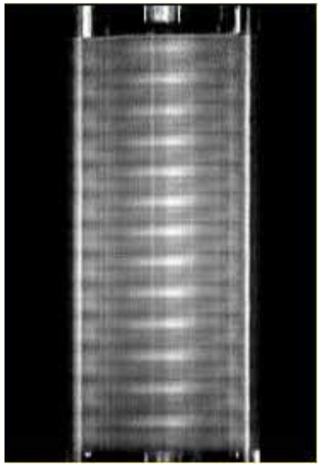


$w \equiv (v_r^2 + v_z^2)^{1/2}$

Krishnaraj & Nott, *Nature Comm.* (2016)

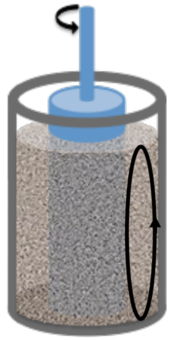
Only one system-spanning vortex, no matter how tall the Couette cell

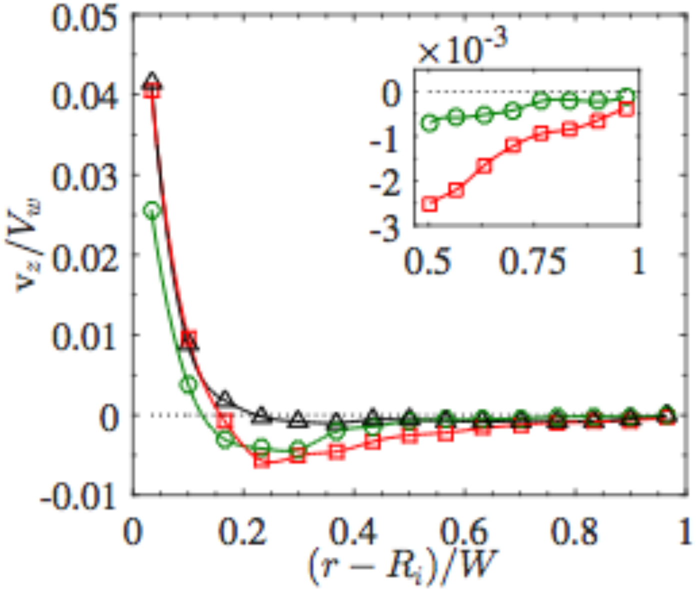




In contrast to the vertical stack of Taylor-Couette vortices in fluids

The vortex explains the anomalous stress





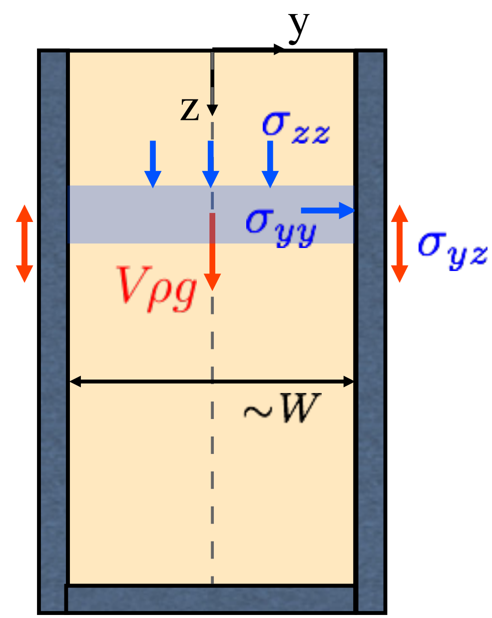
Simplest plasticity model:

$$\boldsymbol{\sigma} = p_c(\phi)(1-\mu_b \nabla\cdot\mathbf{v}/\dot{\gamma})^m\,\boldsymbol{\delta} - 2\mu_s\, p_c(\phi)\boldsymbol{D}/\dot{\gamma}$$

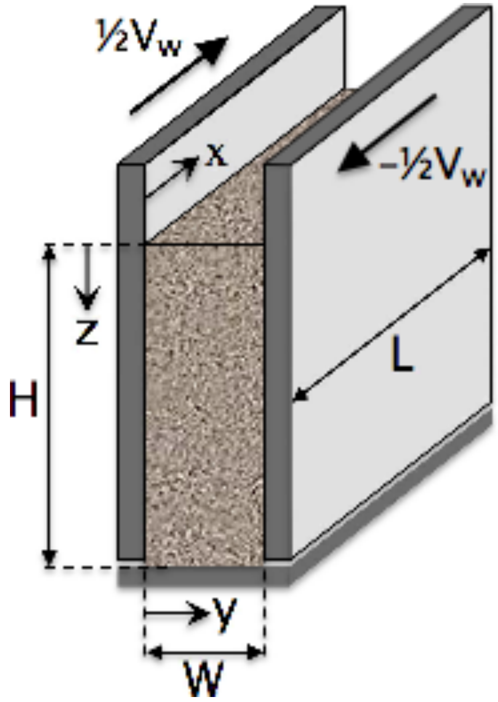
At the outer cylinder, $\mathrm{v}_r = 0$, whence $D_{rz} = \dfrac{1}{2}\dfrac{\partial \mathrm{v}_z}{\partial r}$

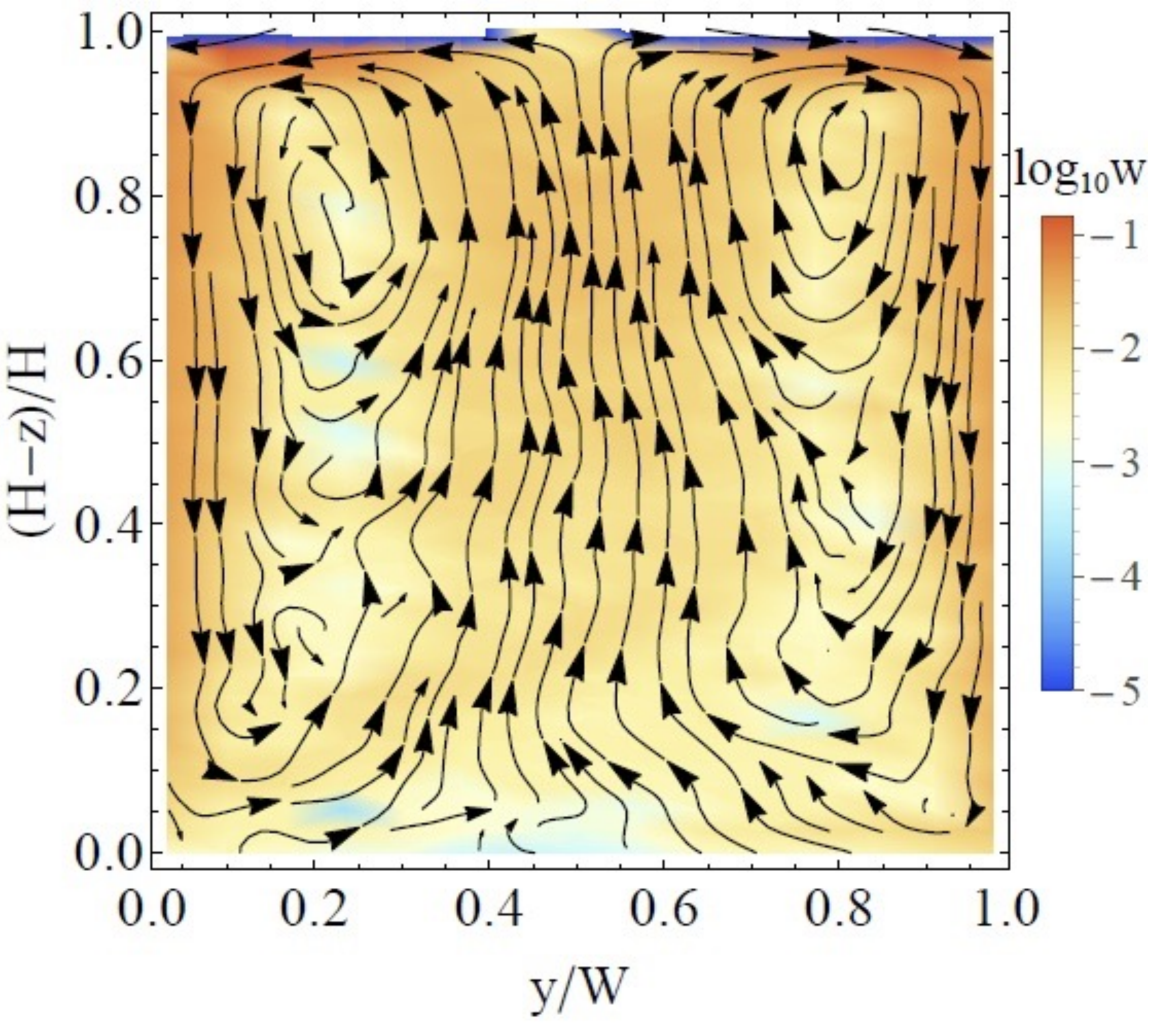
$$\therefore\ \sigma_{rz} = -\frac{\mu_s\, p_c(\phi)}{\dot{\gamma}}\frac{\partial \mathrm{v}_z}{\partial r} < 0$$

Exponential saturation of stress changes to exponential rise

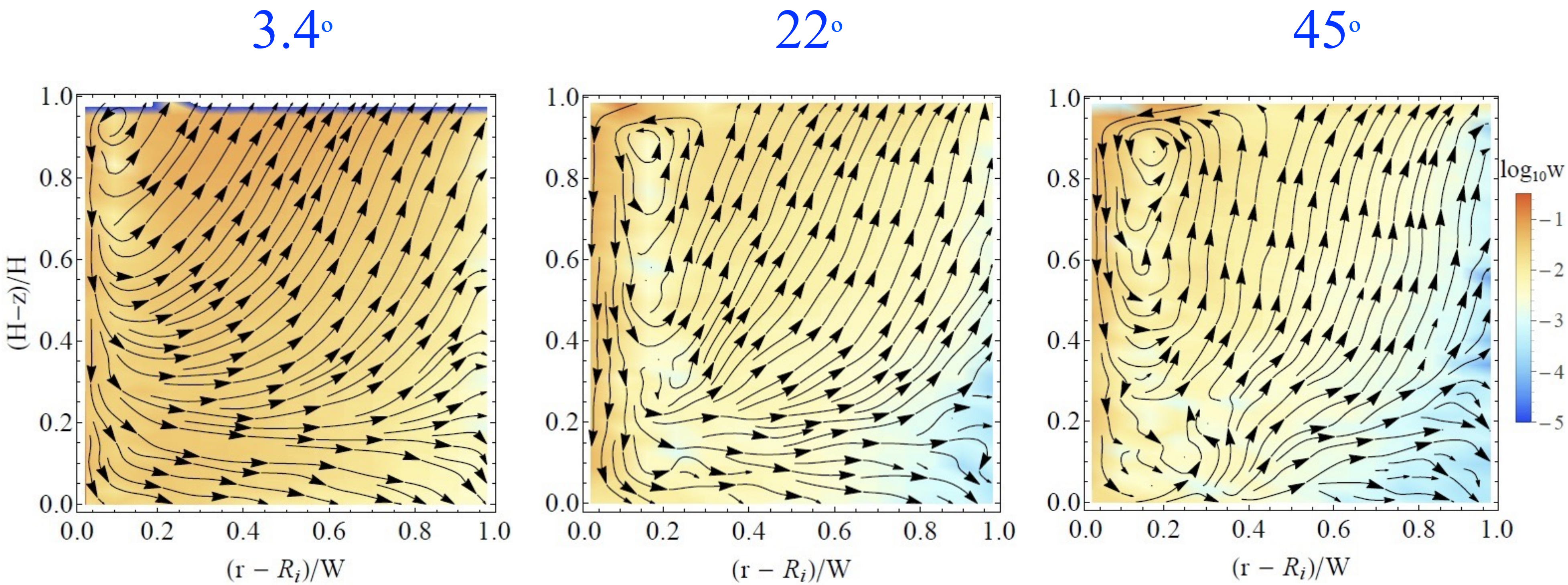


What causes the secondary vortex? Not the centrifugal force.





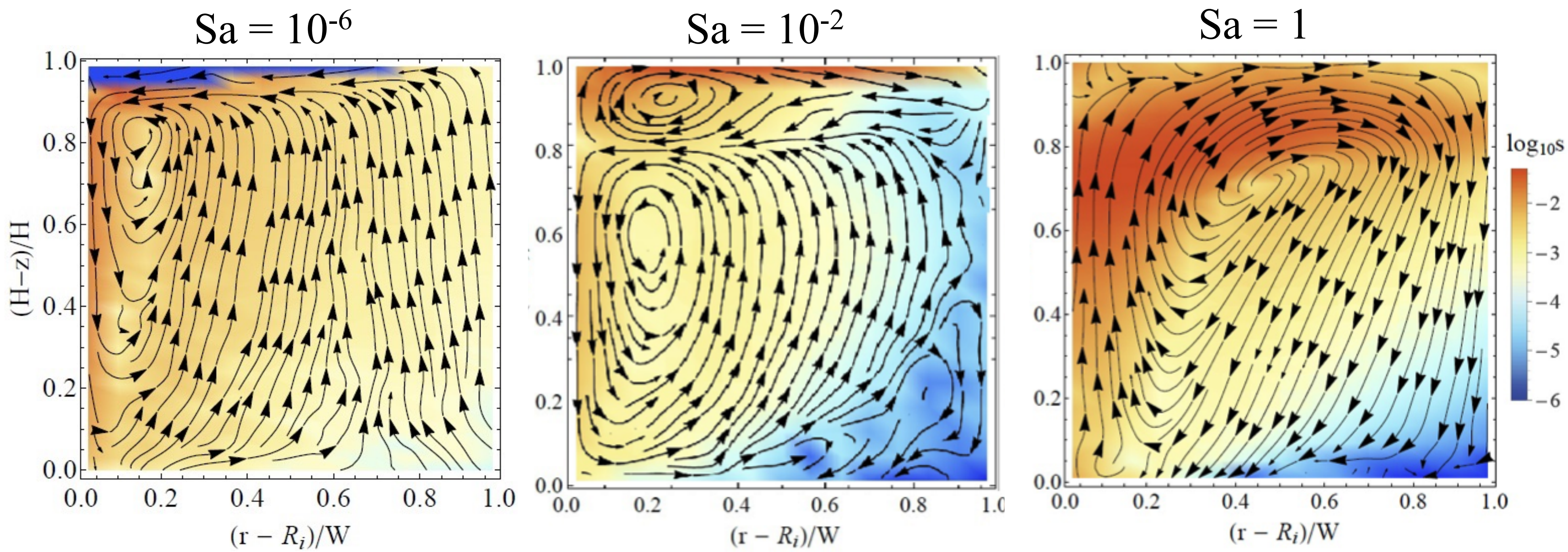
What causes the secondary vortex? Early evolution of the flow provides the answer.



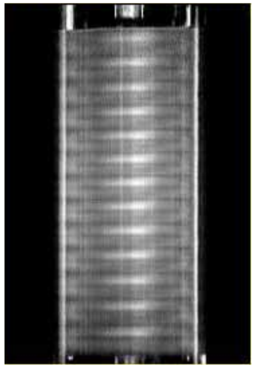
Dilatancy

How does the vortex change with increasing grain intertia?

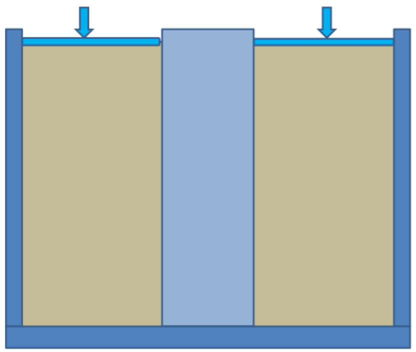
$$\mathrm{Sa} = \rho\, d_p^2\, \dot{\gamma}^2 / N$$

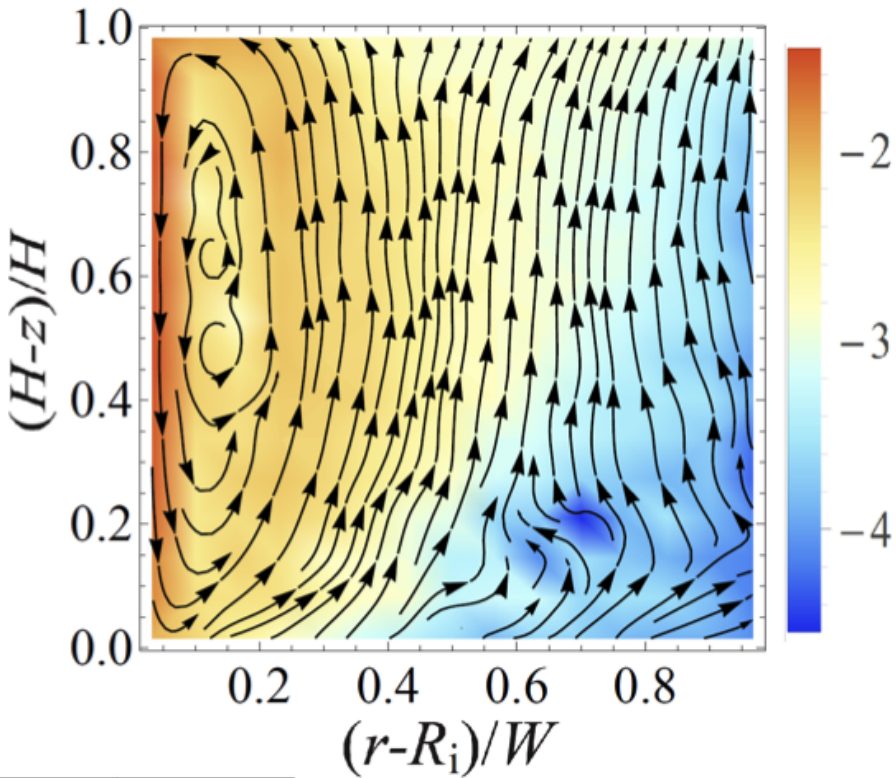


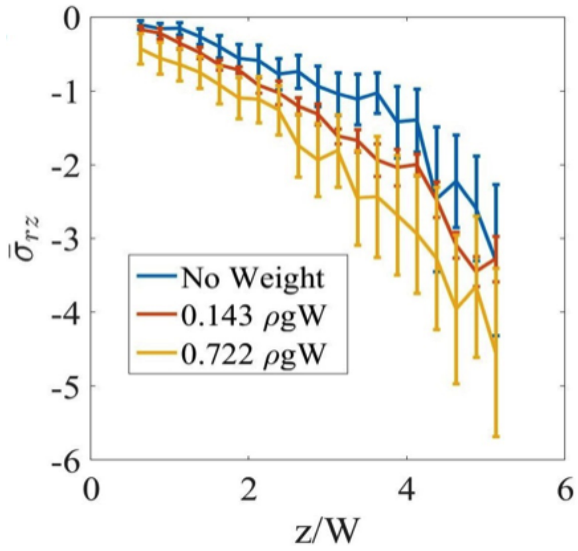
It transitions from dilatancy-driven to centrifugally-driven

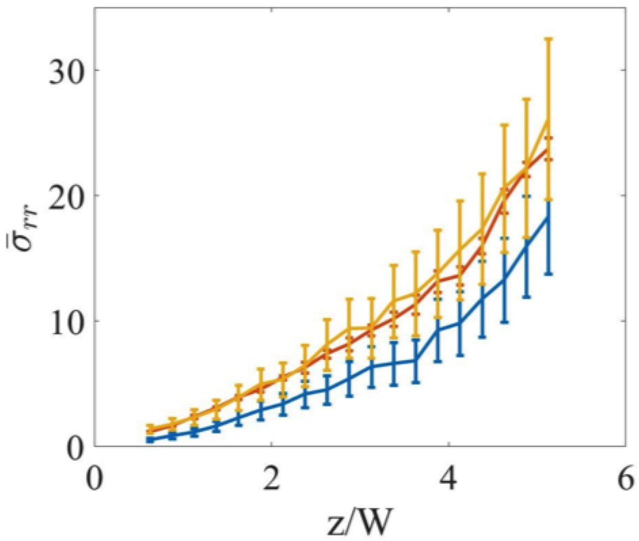


How does confinement at the top affect the behaviour?







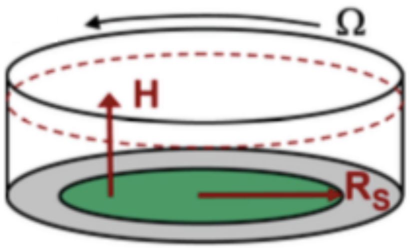


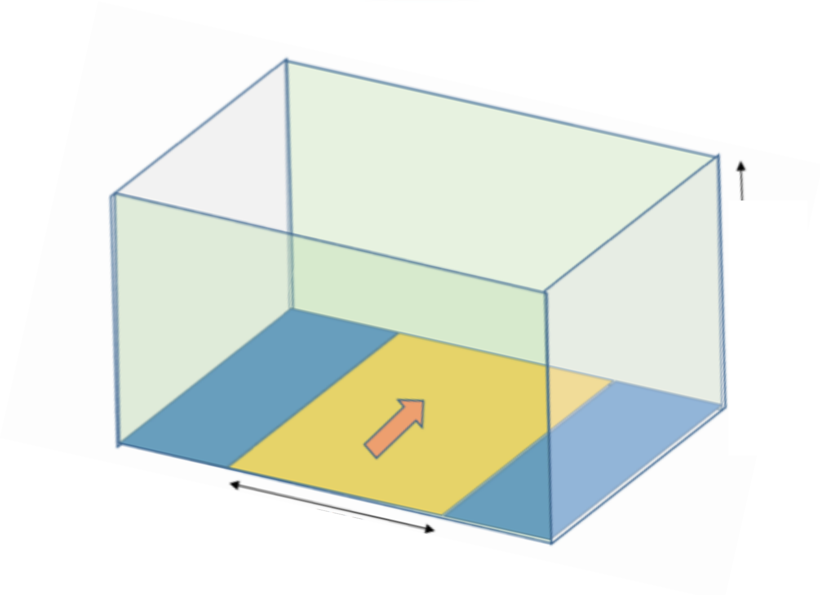
It doesn't!
The entire column need not dilate.

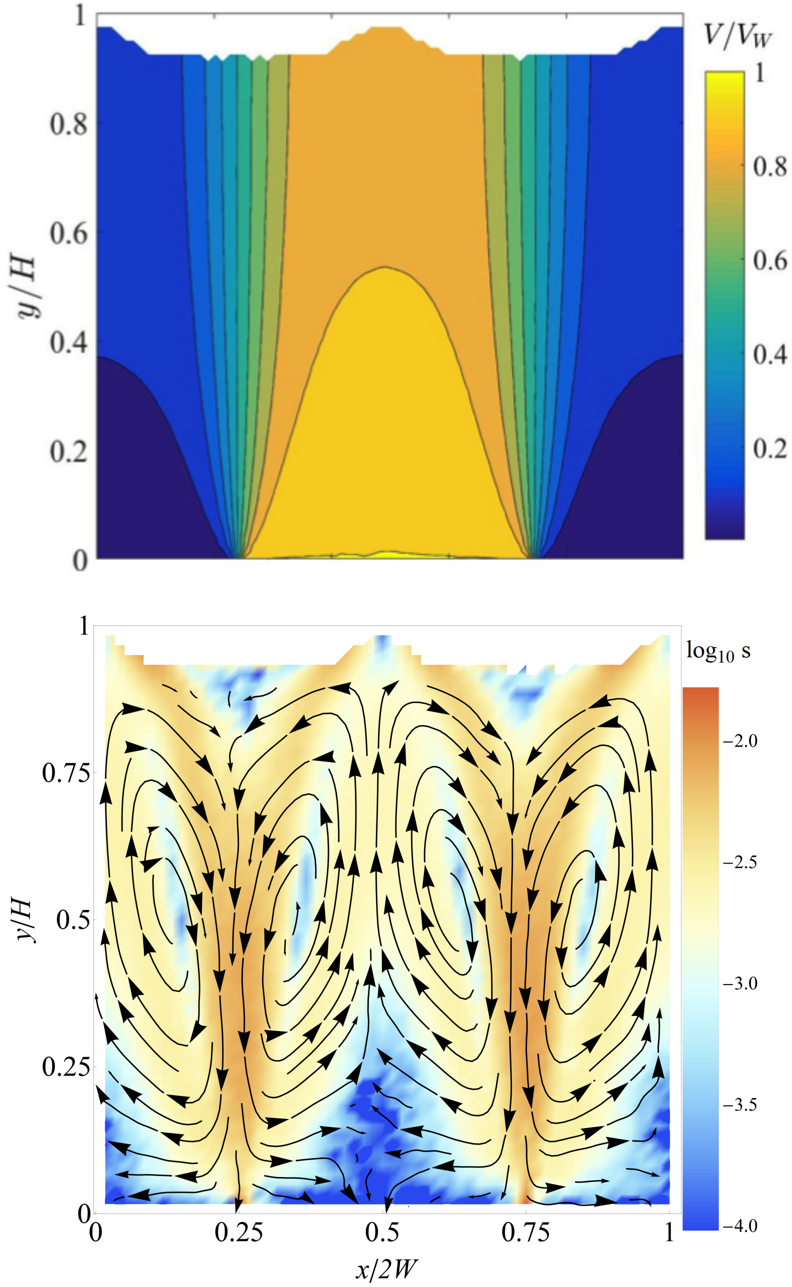
How general is this dilation-induced secondary flow?

Split-bottom Couette cell

van Hecke and coworkers







Probably present in all flows where shear is perpendicular to gravity

Conclusions

- A system spanning vortex forms spontaneously when a dense granular material is sheared perpendicular to gravity

- A novel vortex, driven by dilatancy.

- The vortex explains anomalous variation of stress with depth – **crucial for rheometry**.

- Further refinements of plasticity theories necessary to capture constant pressure dilatancy.

Suggestions of scientific questions that IFPRI should promote

- **Build better continuum plasticity model for granular/powder flows**
  - Incorporate dilation at constant pressure
  - Refine non-local effects to address deficiencies (Hadamard ill-posedness)
  - Incorporate microstructural anisotropy (force chains)
  - Extend models to cohesive powders – a major challenge
- **Develop well-instrumented experiments for simple flows to validate models**
- **A combination of experiments, DEM and continuum modelling, to answer questions on powder processing**

Huge challenges: Cohesion, mixing, segregation, …. but I'm optimistic