SAND2005-7369C

Discrete Element Simulation of Granular Flow in a Modified Couette Cell

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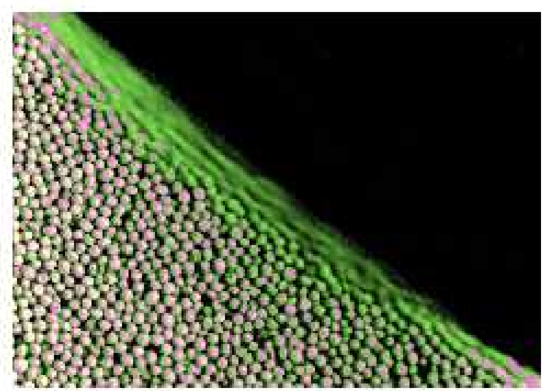
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.

Dense Granular Flow

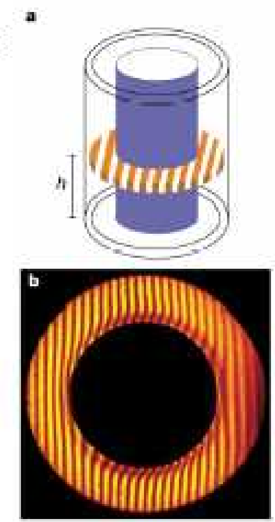
- Shear bands: narrow and distinct bands of high rates of shear deformation (localization of energy dissipation)
  - Phenomenon plays an important role in many applications
    - ballistic impact
    - explosive fragmentation
    - high speed machining
    - metal forming
    - interfacial friction
    - powder compaction
    - soil failure
    - seismic events
    - **granular flow**
- typically W ~ 3-5d
- Non-universality
- What gives rise to them?

Free surface granular flow:



H.M. Jaeger et al, Rev. Mod. Phys. 68, 1259 (1996).

Couette Cell:



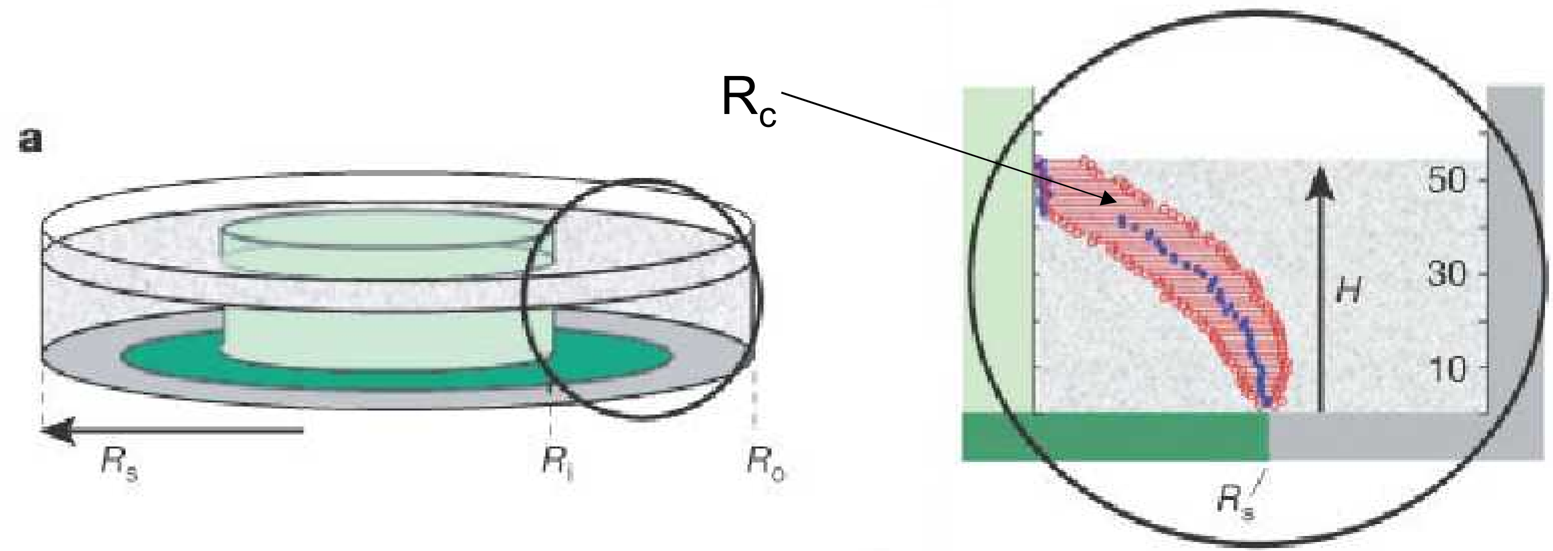
D.M. Mueth, et al, Nature 406, 385 (2000).

exponential velocity profiles

Shape of Universal and Wide Shear Zones

- Parameters involved in rescaling **$R_c = f(R_s, H)$** and $W = f$(H,particle) appear to have separate length scales.

- Theoretical description/predictions for shape of shear zone, $R_c(r,h)$. [$H > 0.5R_s$]



Fenistein et al. (Nature **425**, 256; PRL **92**, 094301)

Discrete Element Simulations

- Allows observation of bulk behavior away from influence of side walls without the use special techniques (e.g., MRI)
- Allows detailed measurements of microscopic quantities (e.g., inter-particle forces)
- Observe bulk behavior, go beyond “shallow” regime, test theory

Integrate Newton’s equations-translational and rotational d.o.f.

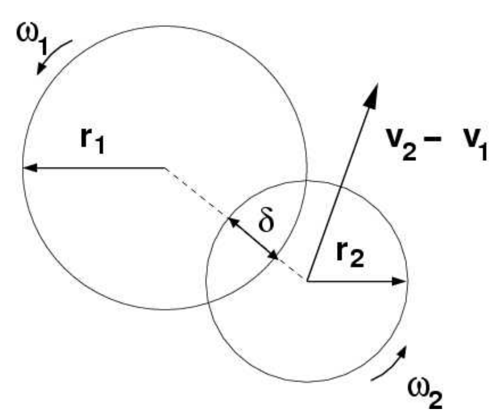
$$\mathbf{F}_n = f(\delta / d)(k_n \delta \mathbf{n}_{ij} - \frac{m}{2}\gamma_n \mathbf{v}_n)$$

$$\mathbf{F}_t = f(\delta / d)(-k_t \Delta \mathbf{s}_t - \frac{m}{2}\gamma_t \mathbf{v}_t)$$

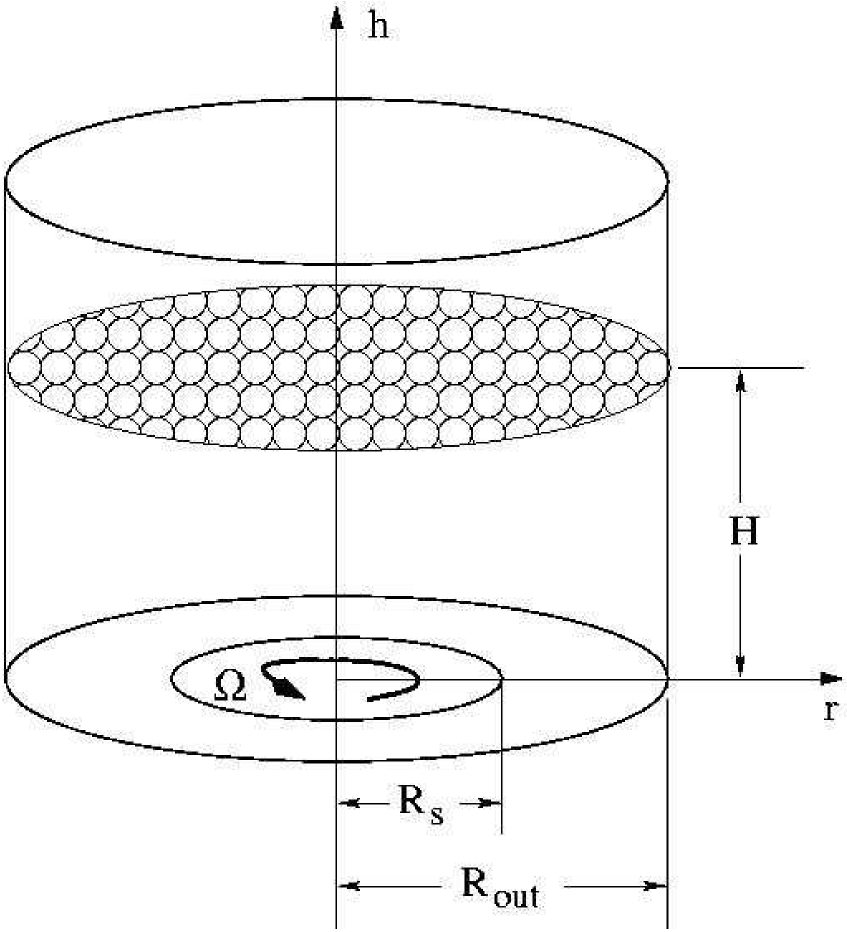
$f(x) = \sqrt{x}$ **Hertzian springs**

Δs_t **Elastic tangential displacement**

$F_t \le \mu F_n$ **Coulomb Failure Criterion**



System Parameters



$R_s = 30.0d$

$R_{out} = 37.8d$

$\Omega = 0.014 \text{ rad}/\tau \quad \text{where} \quad \tau = \sqrt{d/g}$

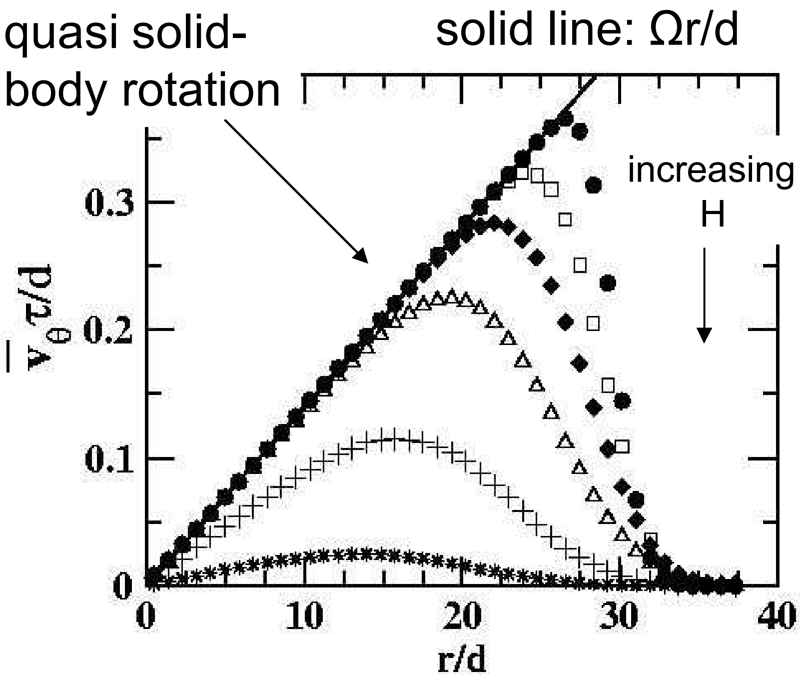
$5.4d \leq H \leq 34.2d$

20,000 – 180,000 particles

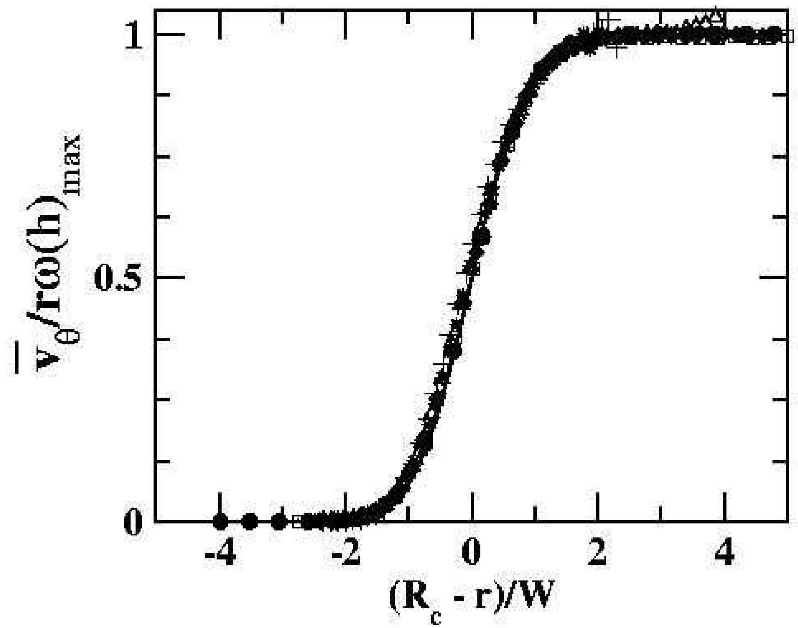
rough bottom composed of layer of glued particles

- Values picked to exactly match experimental system at The University of Chicago

Simulation Surface Velocity Profiles

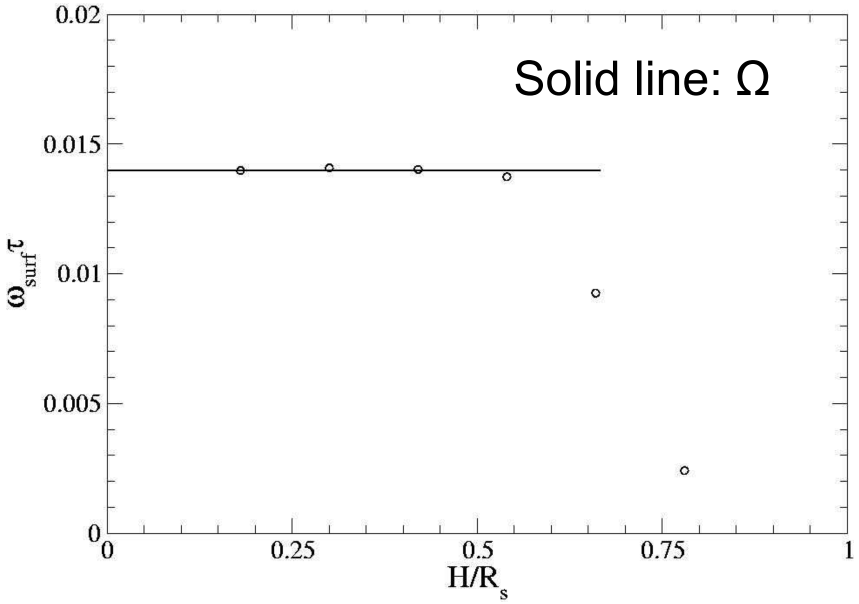


Azimuthal velocity profiles for varying pack heights



Rescaled velocity profiles

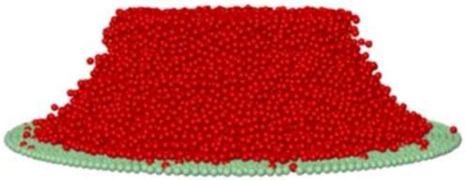
Shallow vs. Deep Packs

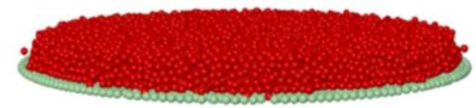


- As observed from the surface: qualitative change at $H/R_s > 0.5$ in agreement with previous work

What happens in the bulk?

Shape of Inner Core and Shear Zone for Shallow Packs



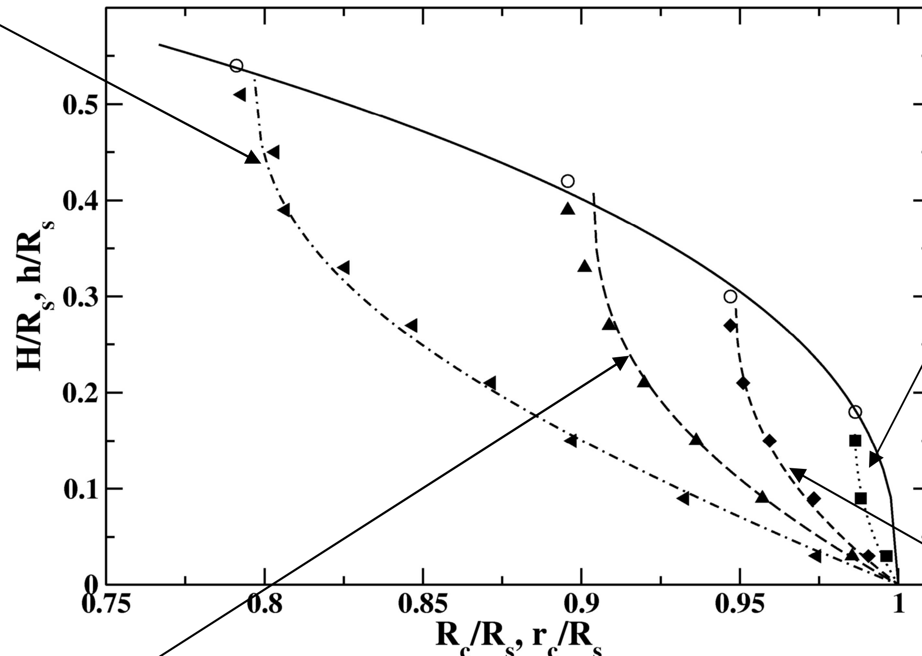


$H/R_s = 0.54$

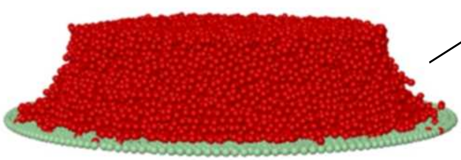
surface data (solid line):

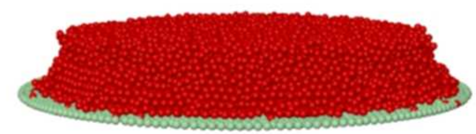
$$1 - \frac{R_c}{R_s} = \left(\frac{H}{R_s}\right)^{\alpha}$$

Fenistein et al. PRL **92**, 094301



$\alpha \approx 2.5$





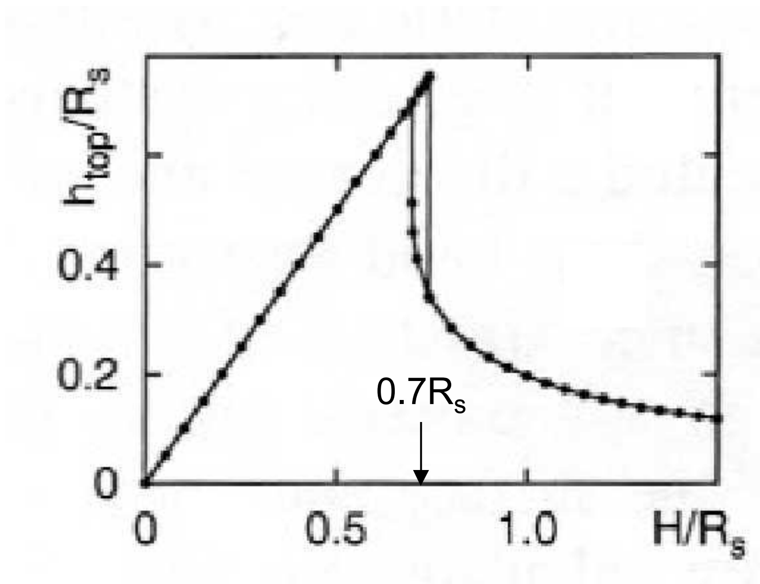
bulk data (broken lines):

$$\frac{h}{R_s} = \frac{H}{R_s} - \frac{r}{R_s}\left[1 - \frac{R_s}{r}\left(1 - \left(\frac{H}{R_s}\right)^{\alpha}\right)\right]^{1/\alpha}$$

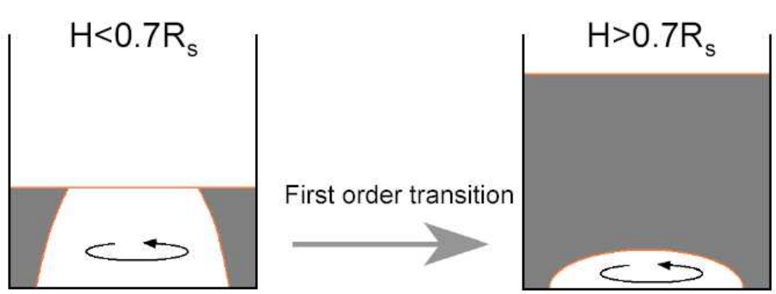
Unger et al. PRL **92**, 214301

Proposed Theory

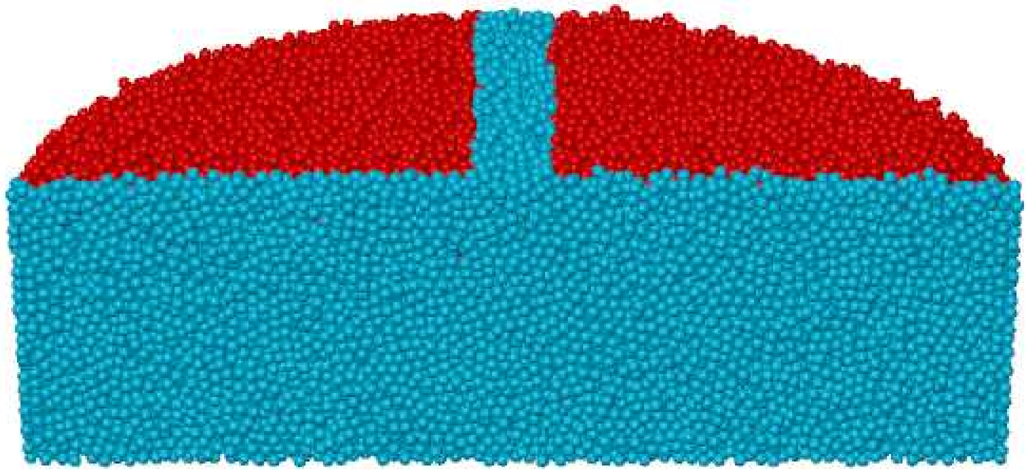
- Least dissipation (minimum torque)
  - Assumes:
    - infinitely thin shear surface between two bulk solid regions
    - hydrostatic pressure
    - coulomb friction between solid regions
- Describes shape of shear zone for shallow packs based on bulk stress state
- Predicts for tall packs:
    - transition in shape of shear zone (open → closed)
    - first order accompanied by hysteresis
    - beyond transition, height of the shear zone, h_{top} is proportional to R_s/H.



Unger et al. PRL **92**, 214301



Bulk Shear Zones in Deep Packs



$H/R_s = 0.78$

Shallow vs. Deep Packs (normalized angular velocities)

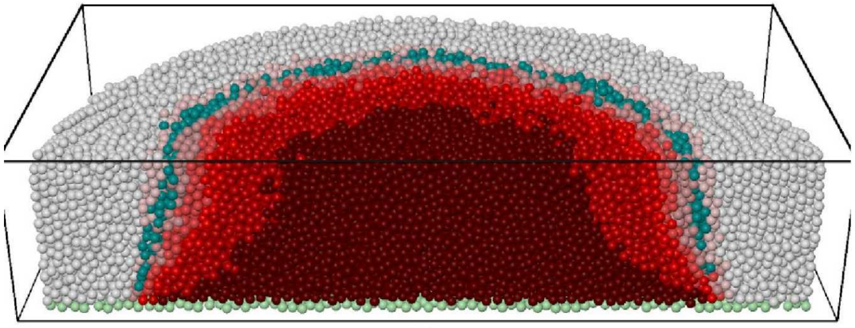
“open” shape

$$\frac{\omega}{\Omega} \geq 0.95 \quad \textbf{dark red}$$

$$0.45 \leq \frac{\omega}{\Omega} < 0.55 \quad \textbf{teal}$$

$$\frac{\omega}{\Omega} < 0.35 \quad \textbf{white}$$

“closed” shape



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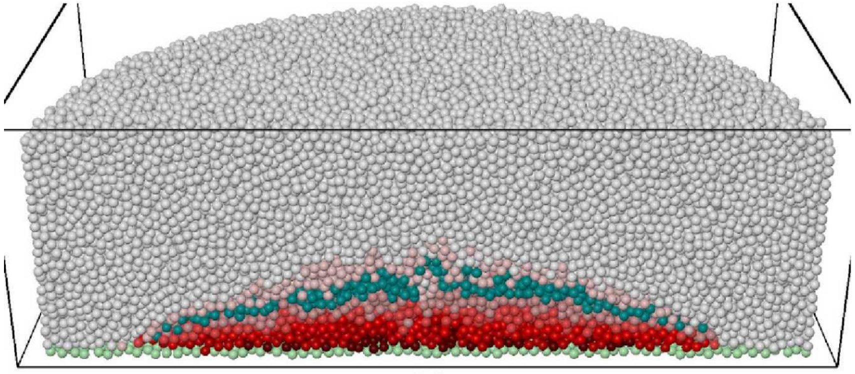
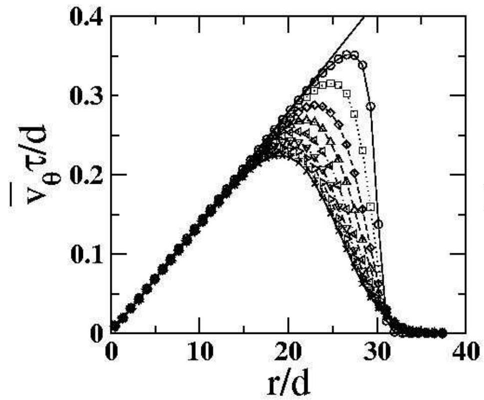
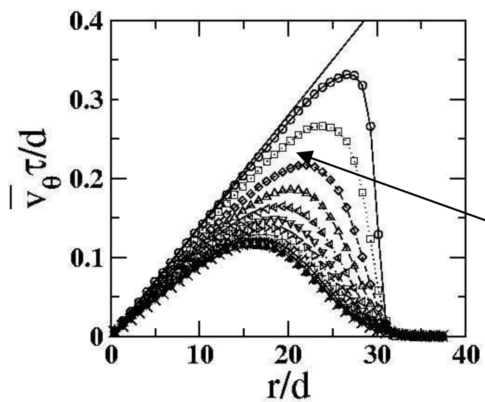


$H/R_s = 0.78$

Bulk Azimuthal Velocity Profiles

$H/R_s = 0.54$

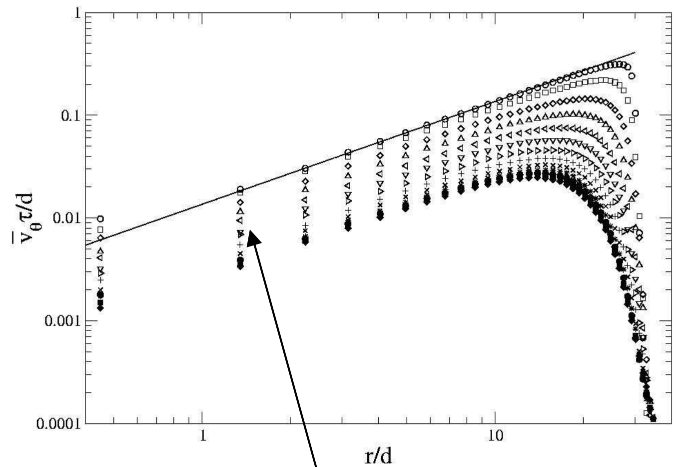




$H/R_s = 0.66$

solid lines: $v_\theta = \Omega r/d$

$H/R_s = 0.78$

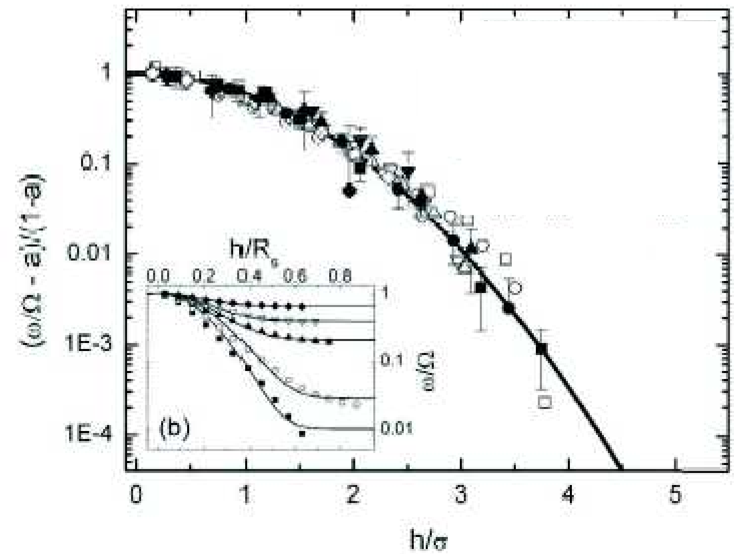


slip between layers related to torsion failure of inner core

Also, loss of universal collapse of data with in the bulk for deep packs.

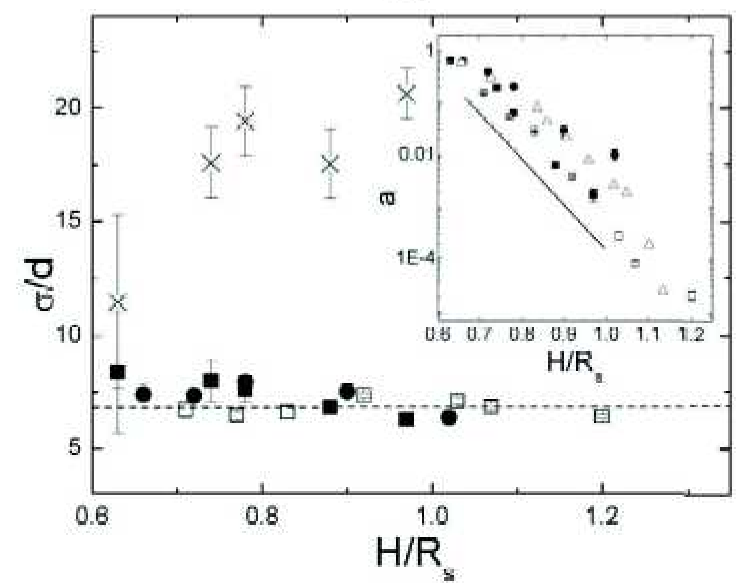
Onset of Axial Shear: slipping layers

- ω/Ω along h-axis of cell
  - fit $a+(1-a)*\exp(-x^b/(2\sigma)^b)$
  - gaussian (b = 2) fits well
    - simulation best fit: $b \approx 1.4$



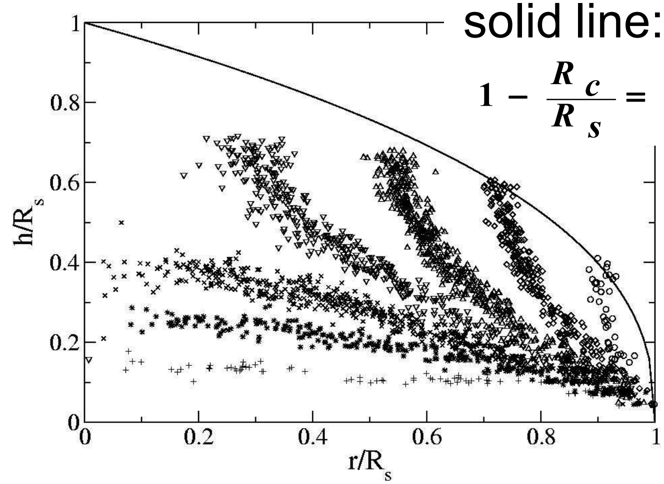
- Offset, a
  - exponential in H
  - goes to 1 as $H \rightarrow H^*$
  - extrapolating, $H^* \approx 0.6$

- Width, σ
  - ~7d, for $H>H^*$



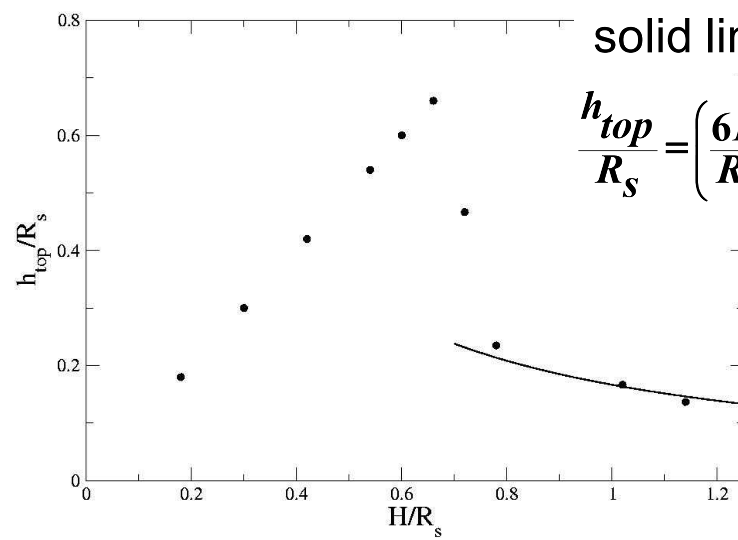
“Unger Transition”?

- Basic assumptions violated
  - Shear zone has finite width
  - Smooth transition between moving and stationary regions
  - Slip between layers
- Direct test: How to define top of shear zone?
  - Choose $\dfrac{\omega}{\Omega} = 0.5$?



solid line:

$$1 - \frac{R_c}{R_s} = \left(\frac{H}{R_s}\right)^{\alpha}$$

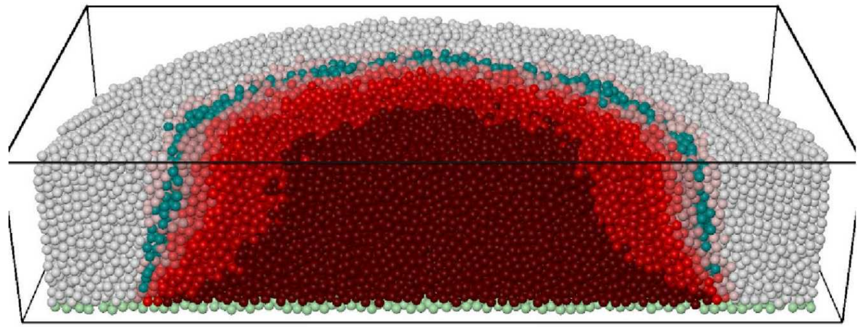


solid line:

$$\frac{h_{top}}{R_S} = \left(\frac{6H}{R_S}\right)^{-1}$$

Normalized Angular Velocity

"open" shape



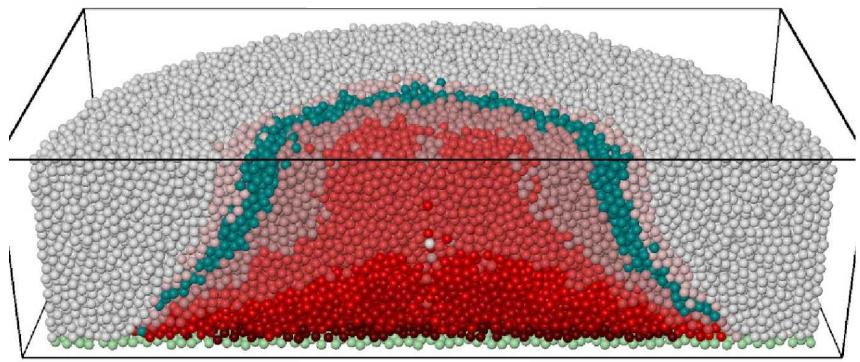
$H/R_s \leq 0.5$

$H/R_s = 0.54$

$\frac{\omega}{\Omega} \geq 0.95$ **dark red**

$0.45 \leq \frac{\omega}{\Omega} < 0.55$ **teal**

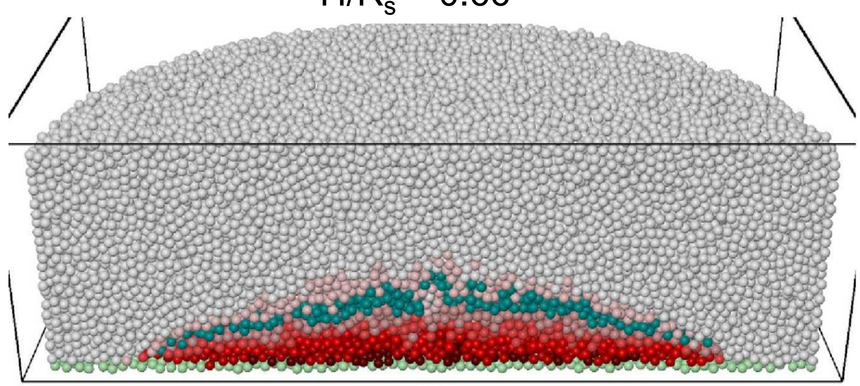
$\frac{\omega}{\Omega} < 0.35$ **white**



$\sim 0.6 < H/R_s < \sim 0.7$

$H/R_s = 0.66$

"closed" shape



$H/R_s > 0.7$

$H/R_s = 0.78$

Conclusions

- Theory captures shape transition due to bulk stress state, but misses other features of the flow.
  - A “shape transition” is present
  - For deep packs, shear is increasingly localized at the bottom (h_{top} α R_s/H)

- Slip between layers has an increasingly significant effect on the flow for packs of $H > \sim 0.6R_s$
  - related to torsional failure mode of the inner core
  - continuous transition in the shape of the shear zone due to slip
  - axial and radial shear have different character
    - significance of boundary conditions for shear localization

- Can theory be extended to account for these?
  - Finite width of radial shear zone, axial shear band, continuous transition

Acknowledgements

- D. Fenistein

- Collaborators at The University of Chicago: X. Cheng, A. F. Barbero, M. Möbius, H. M. Jaeger, S. R. Nagel

- This collaboration was performed under the auspices of the DOE Center of Excellence for the Synthesis and Processing of Advanced Materials.

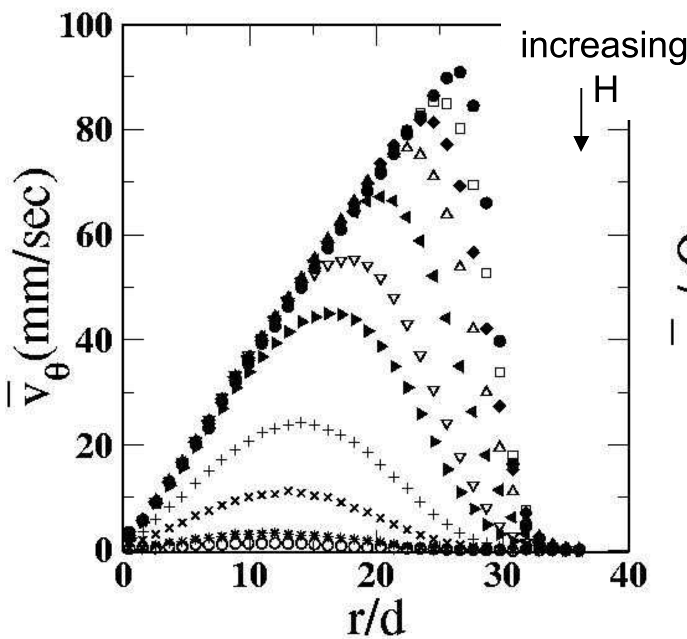
- Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories

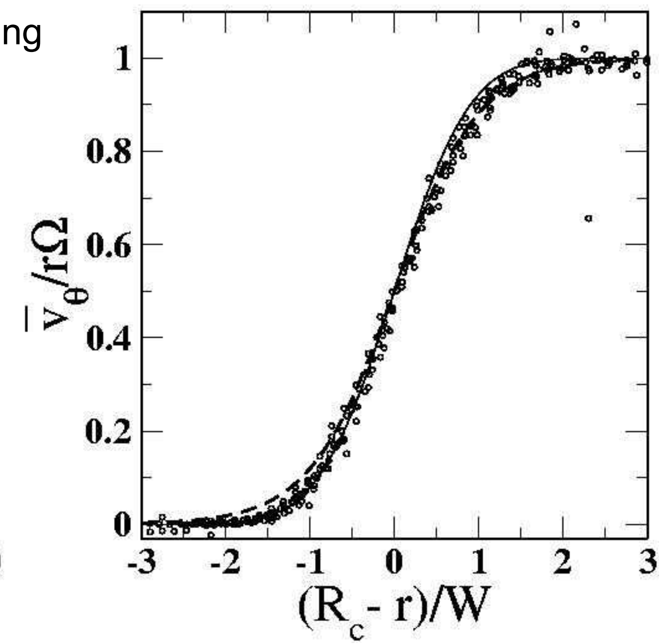
Outline

- What is the interest in granular materials?
  - Where are they found?
  - What are the issues related to the understanding of their behavior?
    - In particular, how do we begin to understand dense granular flows?
- Onset of 3-dimensional flow in a split-bottom Couette cell.

Experimental Surface Velocity Profiles



azimuthal velocities

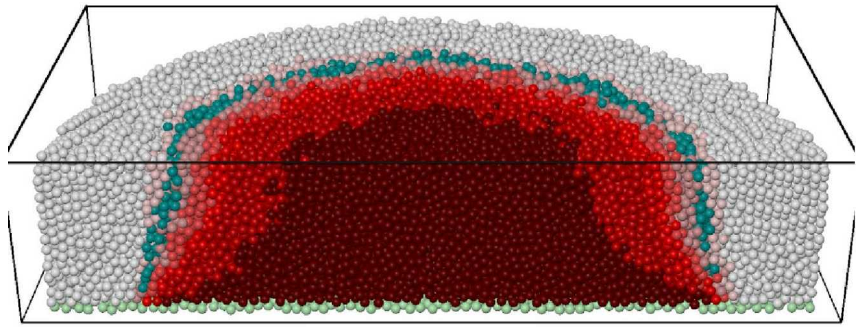


rescaled velocities

- Linear azimuthal velocity profile near center for shallow packs (regime of previous work)
- Slight asymmetry in the rescaled velocities

Normalized Angular Velocity

"open" shape



$H/R_s = 0.54$

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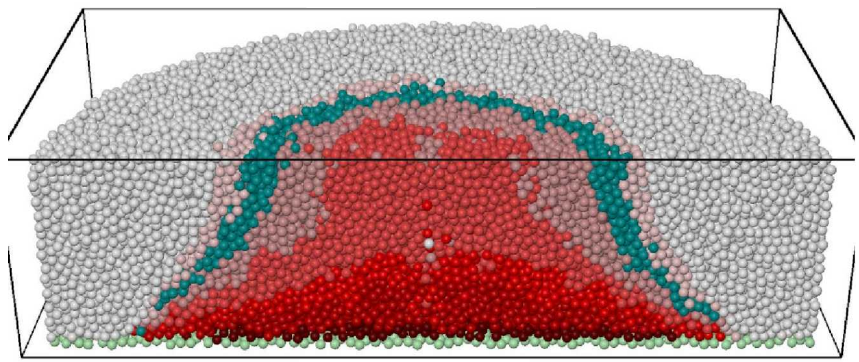
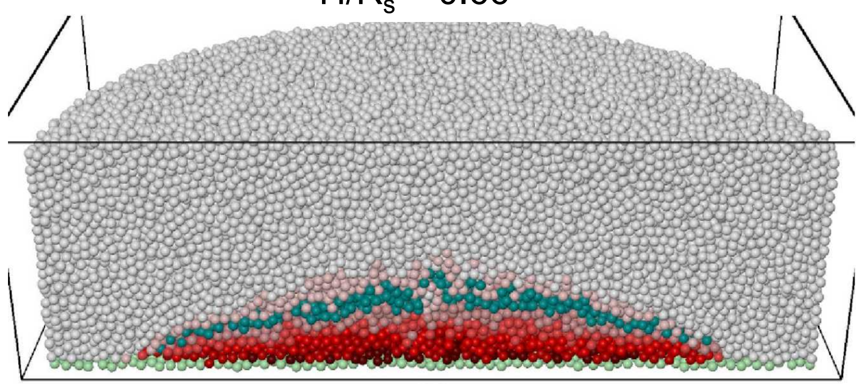


$H/R_s = 0.66$

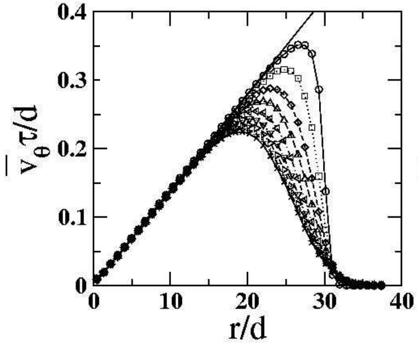
"closed" shape



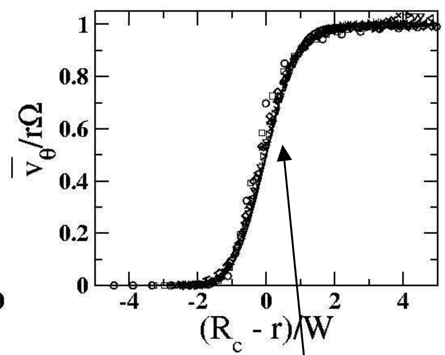
$H/R_s = 0.78$

Bulk Velocity Profiles

azimuthal velocities

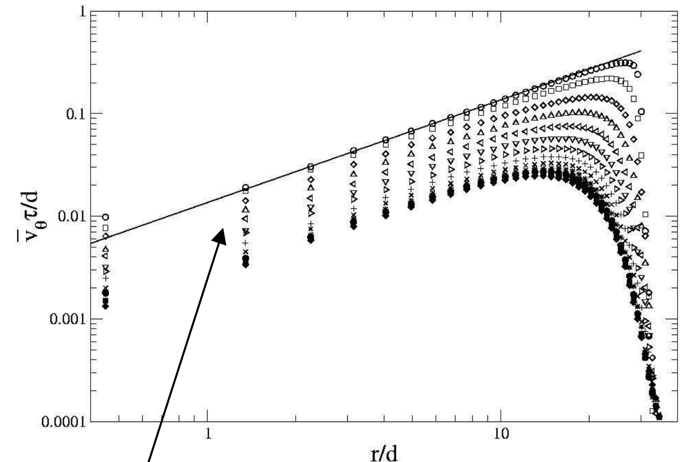


rescaled velocities



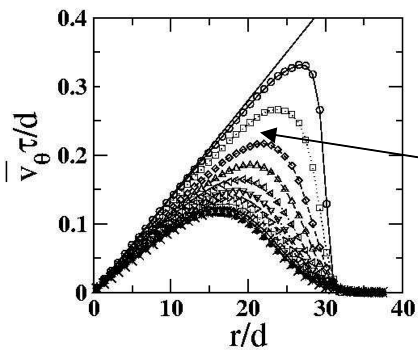
$H/R_s = 0.54$

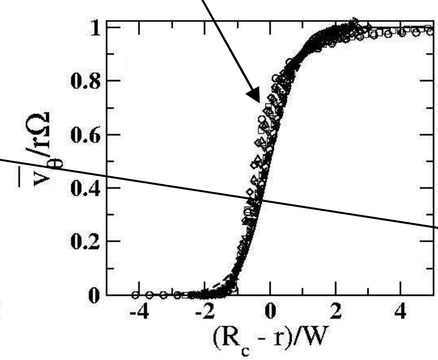
azimuthal velocities



deviation from erf

$H/R_s = 0.78$





slip between layers

$H/R_s = 0.66$

Note: solid lines in azimuthal plots are $v_\theta = \Omega r/d$

Torsion Failure

$$T = \int_A r\tau dA = 2\pi \frac{\tau_{\max}}{R_s} \int_0^{R_s} r^3 dr$$

$$T_b = \frac{\pi}{2} \tau_{\max} R_s^3$$

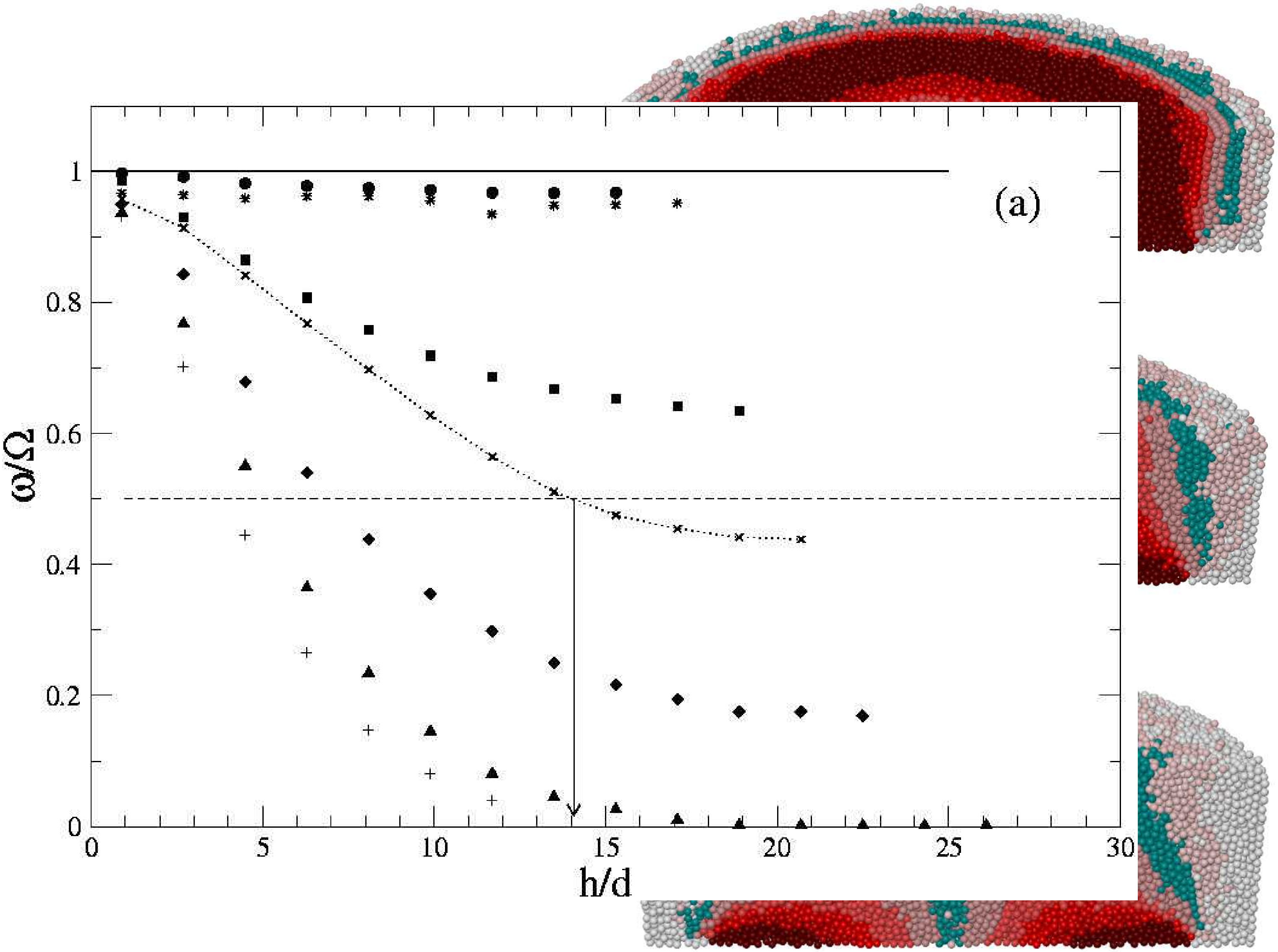
$$\text{where } \frac{\tau_{\max}}{R_s} = \frac{\tau}{r} \text{ from proportionality of triangles}$$

$$\tau_{\max} \leq \mu\rho g H \quad \text{from Mohr - Coulomb}$$

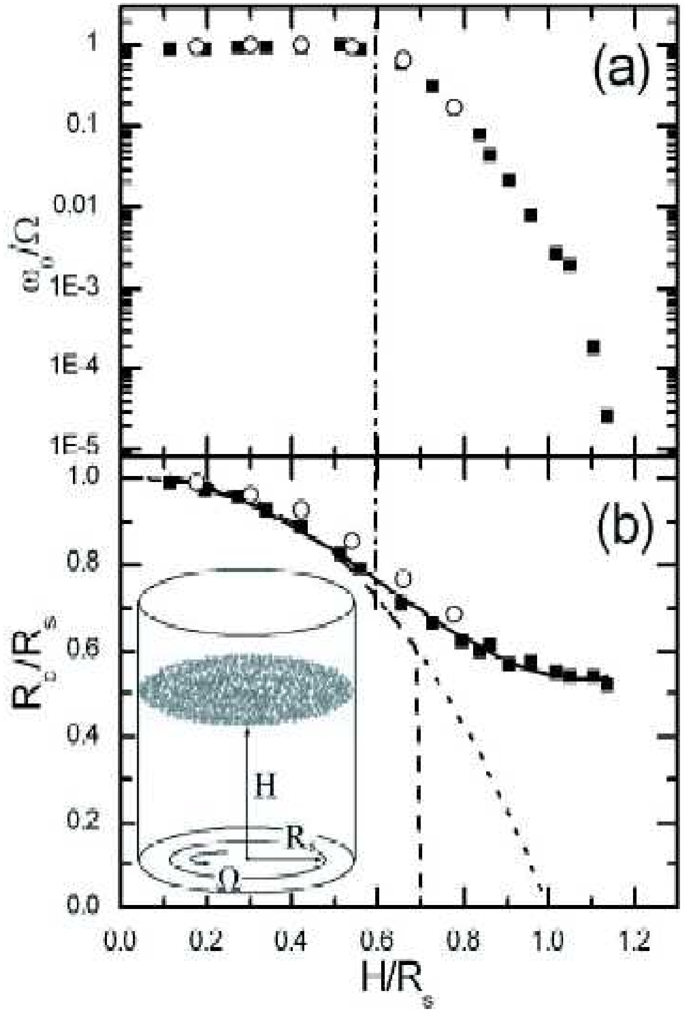
$$T_z = 2\pi\mu\rho g \int_0^H r^2 \sqrt{1 + (dr/dh)^2}\,(H - h)dh$$

$$T_z \leq T_b \ \text{ for no slip at the base}$$

$$\frac{4\Theta}{HR_s^3} \leq 1$$



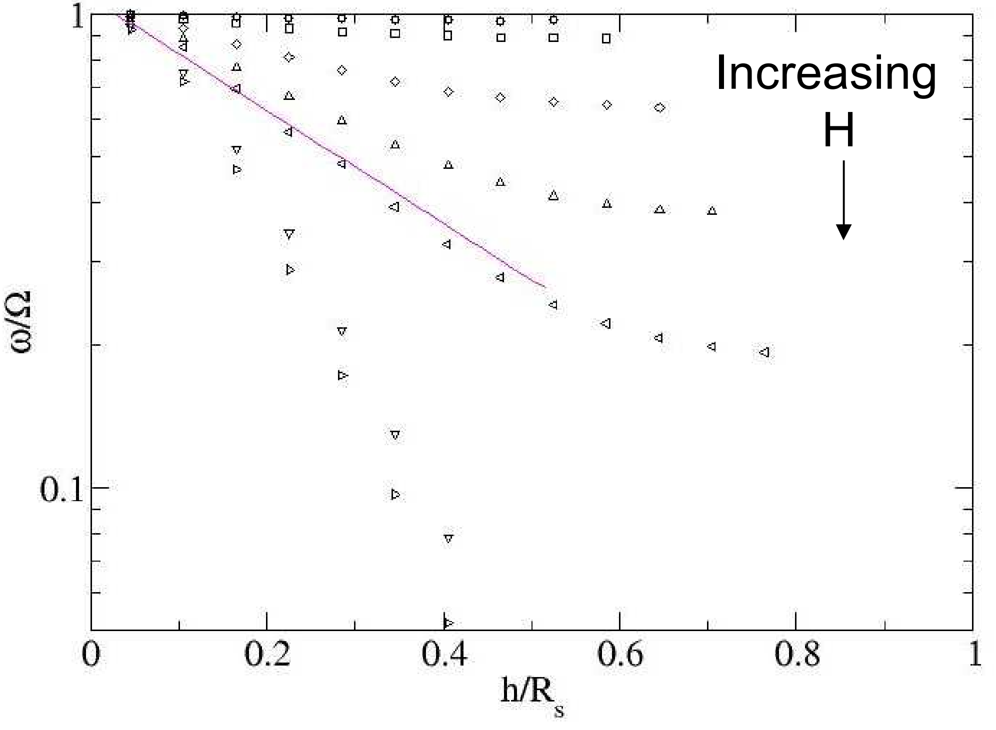
(a)
ω/Ω
h/d
0
0.2
0.4
0.6
0.8
1
0
5
10
15
20
25
30



(a)
(b)
1
0.1
0.01
1E-3
1E-4
1E-5
ω_o/Ω
1.0
0.8
0.6
0.4
0.2
0.0
R_c/R_s
0.0
0.2
0.4
0.6
0.8
1.0
1.2
H/R_s
H
R_s
Ω

Slip Between Layers

- For $H/R_s > 0.5$ slip between layers increases with H
- MRI give good data for deep packs and longer times.
- Can we rule out slip for shallower packs?



Slip Transition?

- From w(h) ~ exp(-H/ξ)
- ξ gives characteristic length scale
- ξ diverges with decreasing H