



Track 1: Dense Gas-Solid and Granular Flows

NETL 2006 Multiphase Flow Workshop
Morgantown, WV
June 6-7, 2006

Paul Mort – P&G, Chair
Joe McCarthy – University of Pittsburgh, Co-Chair
Ron Breault – NETL, Liason



Track 1 (Expected) Participants

- Losert (Maryland), Mehrabadi (Tulane), Turton (West Virginia), McCarthy (Pittsburgh), Sundaresan (Princeton), Behringer (Duke), O'Hern (Yale), Menon (Massachusetts)
- Banerjee (Millenium Chemical), Mort (P&G), Fiveland (Alstom), Gentzler (Merck), Price (Nova Chemical), Niksa (Niksa Energy)
- O'Brien (NETL), Breault (NETL), Rogers (NETL), Massoudi (NETL)

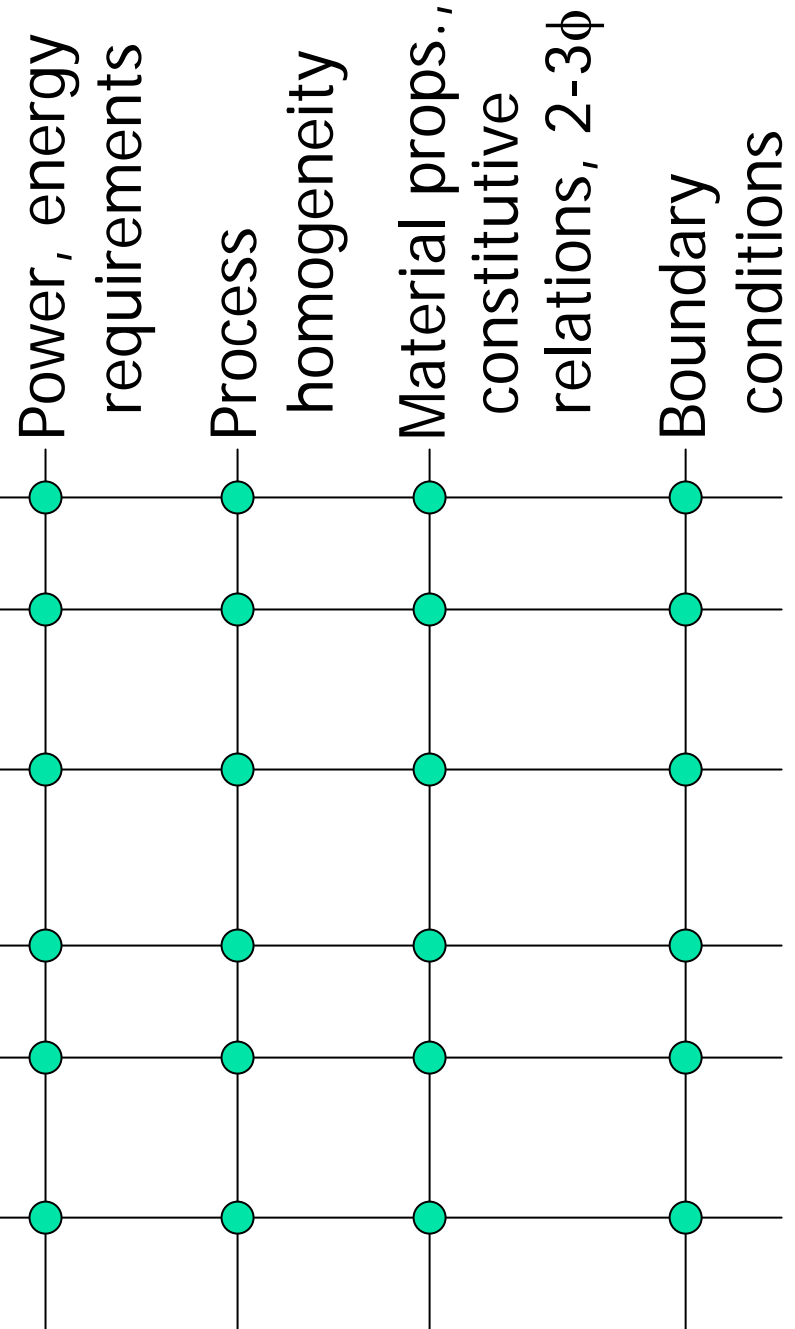


Dense Gas-Solid and Granular Flows

- Characteristics
 - Lasting contacts
 - Fluctuations
 - Clustering and cohesion
 - Compression & dilation → B.C. effects
- Energy-relevant examples
 - Extraction and transport of raw materials
 - Gasifiers and combustions systems
 - Kilns
 - Chemical looping

Open/Important Issues

- Scaling and scale-up
- Measurement and calculation of flow and stress fields.
- Stress transmission as f (flow rate, material props, BC's, ...)
- Fluctuations (stress and flow)
- Mixed-property and distributed systems
- Multi-scale modeling and simulation





Scaling and Scale-up

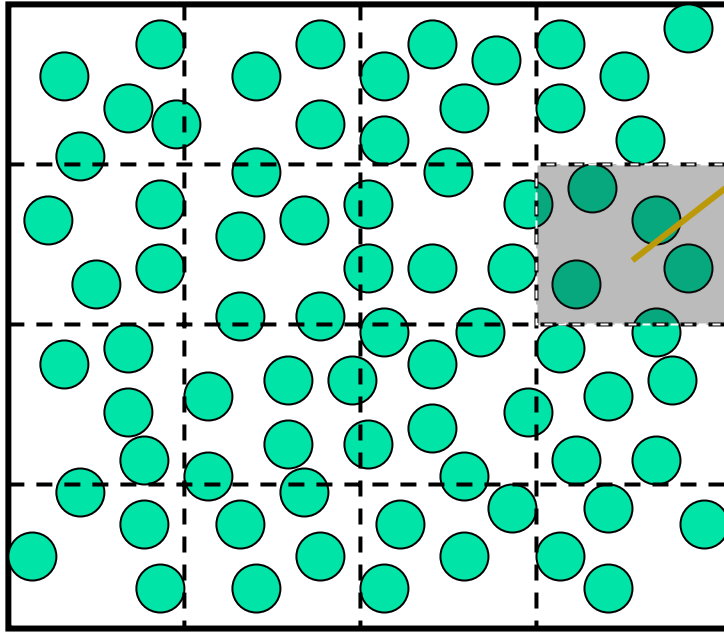
- What are critical controlling groups for scale-up in various flow regimes and/or types of materials?
 - All groups cannot be maintained simultaneously.
- What are relationships between scaling laws and underlying physics?
- Is it possible to coarse-grain for larger scale simulation?



Typical Simulation Techniques

- Discrete Element Modeling (DEM or MD)
 - Soft-sphere – capture contact mechanics
 - Include liquid bridging or adhesion
- Continuum Modeling
 - Lagrangian-Eulerian
 - Eulerian-Eulerian

DEM & volume-averaged equations for the fluid



ϕ_s : particle volume fraction

\mathbf{u}_s : coarse-grained particle velocity

ε : porosity ($= 1 - \phi_s$)

\mathbf{u}_a : gas(air) velocity

p : gas pressure

* Hoomans et al., Chem. Eng. Sci. (1996), Yu and Xu, Chem. Eng. Sci. (1998).

*Works for solid \rightarrow fluid, but will it work for
solid \rightarrow solid coarse-graining?*

Scaling and Controlling Groups

- Stresses

$$\sigma_{xy} = \mu\sigma_{yy} + \sigma_s + v\dot{\gamma}$$

- Controlling groups:

- Number of particles, system scale

$$N = L / d$$

- Froude (chute)

$$Fr = U / \sqrt{gL}$$

- Inertial / confining force

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

- Centripetal / gravitational

$$A = \omega^2 L / g$$

- Reynolds number, solid stress

$$Re = \rho U^2 / \sigma$$

- Reynolds number, viscous

$$Re = \rho UL / \eta$$

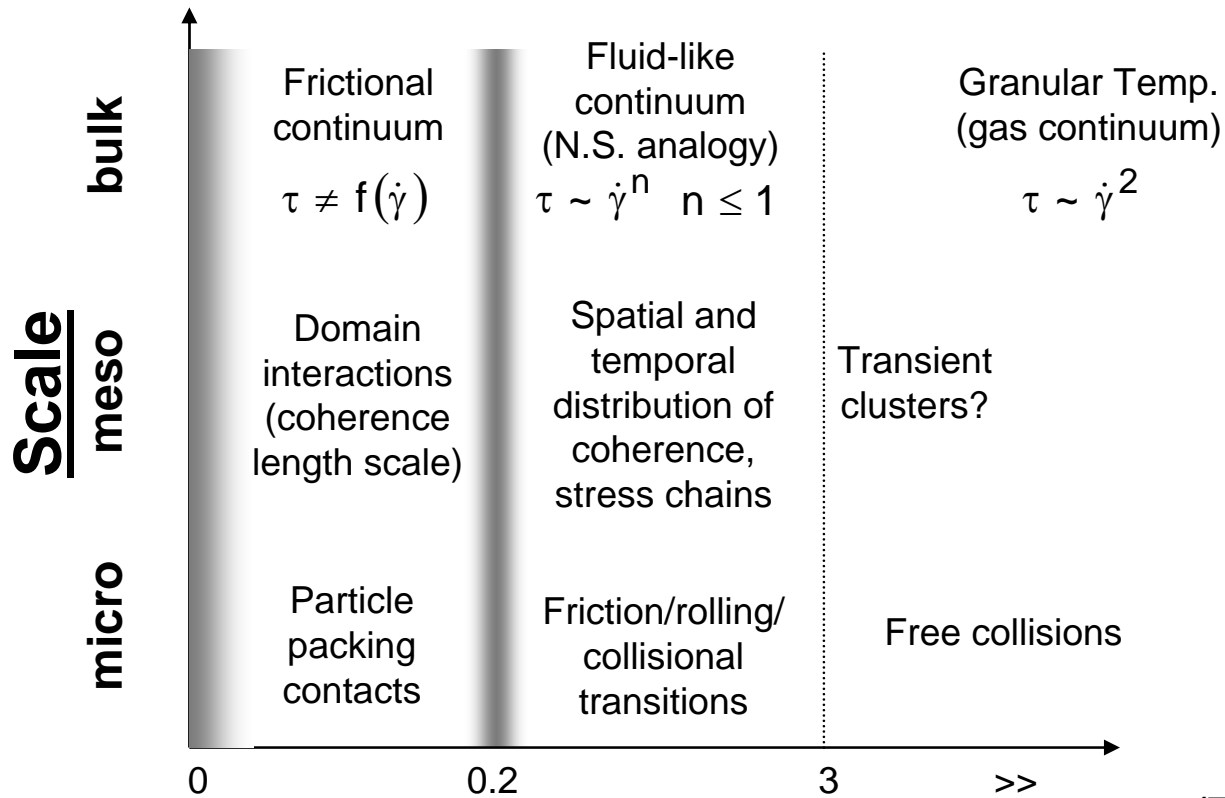
- Swept volume

$$RSV = \omega L^2$$

In general, it is not possible to maintain all groups on scale-up.

Material functions are poorly understood!

Multi-scale Approach



Inertia / confinement,

$$I = \frac{\dot{\gamma} \cdot d_p}{\sqrt{P \cdot \rho_0}}$$

Dimensionless shear rate,

$$\dot{\gamma}^* = \dot{\gamma} \left[\frac{d_p}{g} \right]^{1/2}$$

(Tardos)

(GDR Midi)

Contact time

$$t_c / t_{bc}$$

high

~ 2

1

(Campbell)

Stiffness/shear

$$\frac{k}{\dot{\gamma} \cdot \rho \cdot d^3}$$

high

low

Stokes #

$$\frac{m\dot{\gamma}}{6\pi\eta d}$$

0

~ 10

high

(Brady)

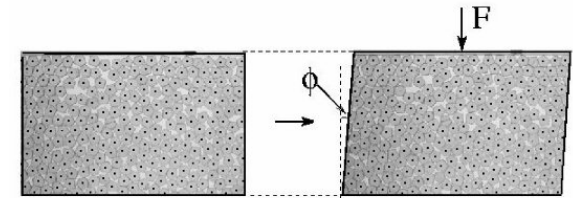


Stress calculation, fluctuations, and transmission

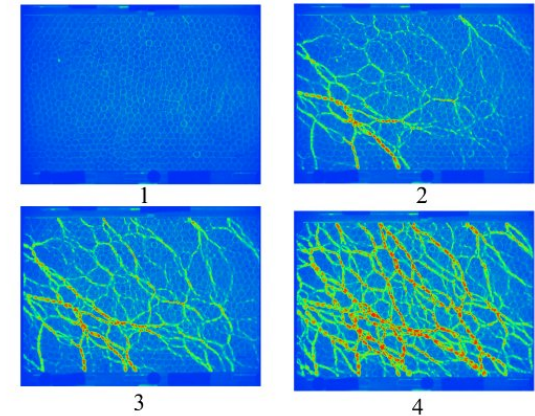
- How is stress (and other quantities) transmitted through bulk? What is effect of BCs?
- How do we quantify (and understand) fluctuations?
- How do we quantify the transition from quasi-static to intermediate to rapid flows?
- What experimental (or computational, DEM?) methodologies are best suited?
- How do we build [and use] rheological models?

Stress and Flow Fields

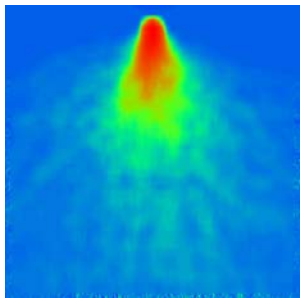
- Flow paradigms: Couette, mixer, orifice flow
- Questions
 - Stress transmission
 - Material heterogeneity
 - States and boundary conditions
 - Fluctuations
 - Transitions between states
 - Measurement tools



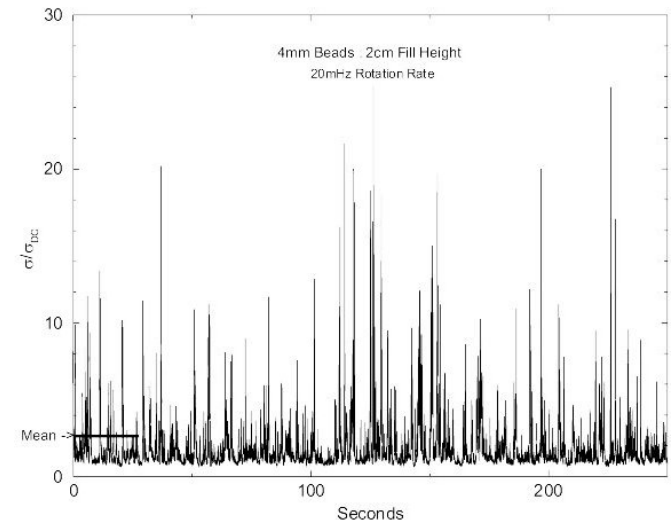
(a)



(b)



Figures from Behringer's group



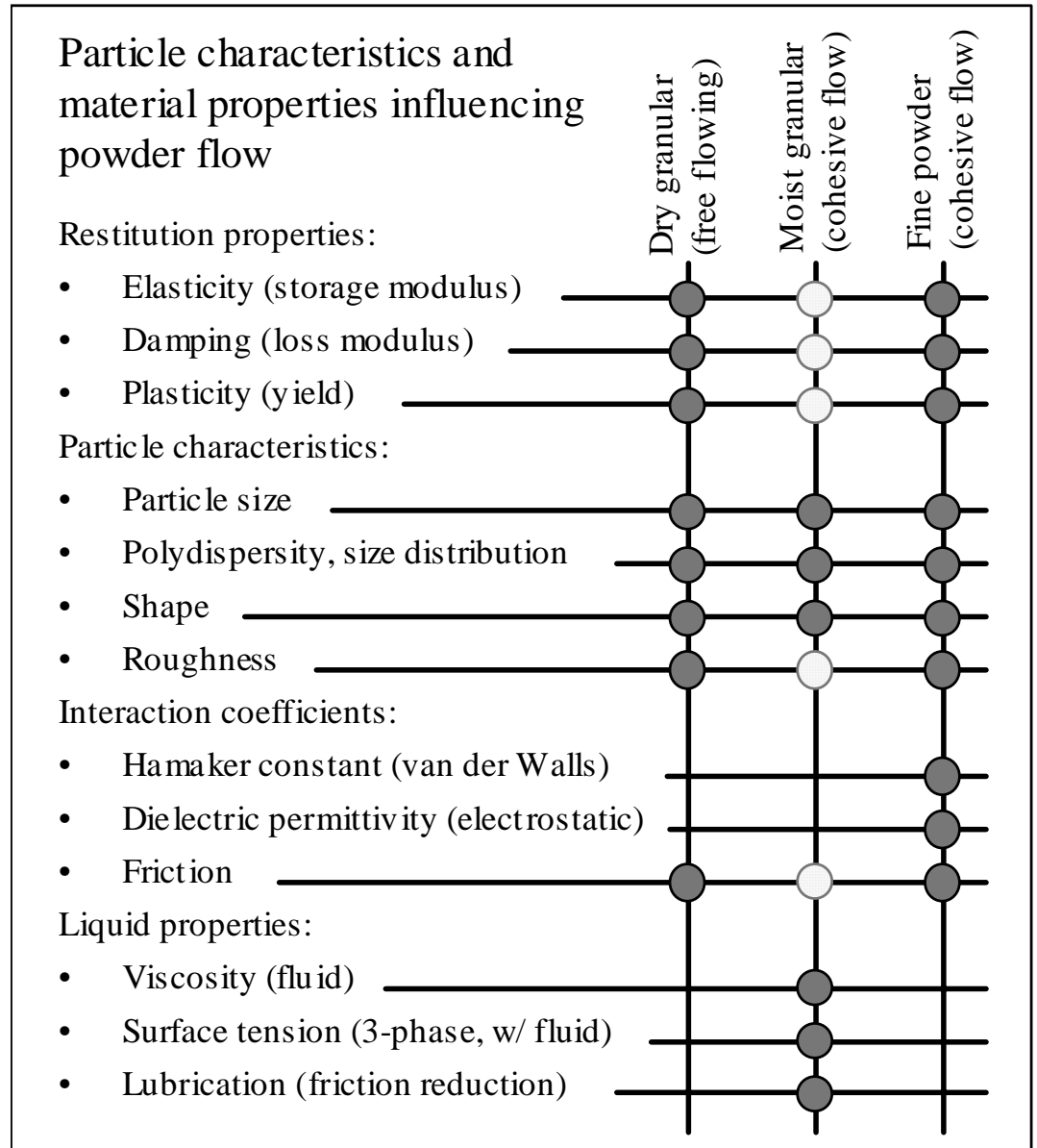


Mixtures and distributed systems

- How do we capture ranges and distributions of material properties like size, shape, etc?
- How do we incorporate this info into models?
- Is there a way to examine only a subset of the parameter space and still be accurate?
- How does mixing and segregation impact flow and vice versa?

Effect of particle characteristics and material properties on bulk flow

- Dark connection points indicate significant relationships.
- Solid restitution and frictional interactions (light connections) may be eclipsed by viscous dissipation, lubrication and/or dampening effects in a 3-phase granular material.





Fluctuations

- How do we reconcile the range of possible states that are observed for a given set of (boundary) conditions? Is there a connection to the range of fluctuation strengths?
- How do fluctuations affect repeatability? Uniqueness?
- What mathematical descriptions can handle fluctuations explicitly?
- Given that dissipation (athermal behavior) is prevalent, is the granular temperature the correct quantity for modeling?

Fluctuations in Dense Granular Flows

Corey S. O'Hern (Department of Mechanical Engineering, Department of Physics, Yale)
Narayanan Menon (Department of Physics, University of Massachusetts-Amherst)

Large fluctuations in dense granular flows can affect performance of granular-processing devices.

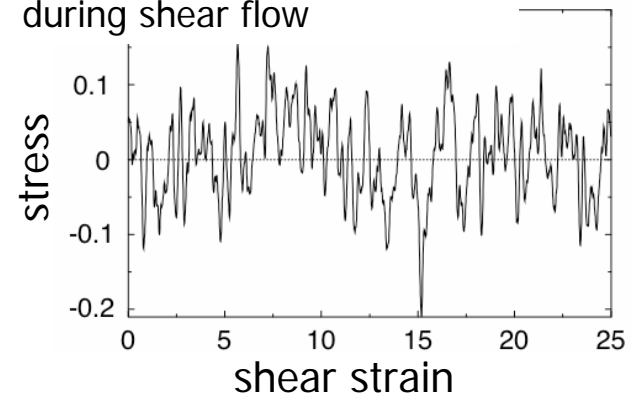
Important Questions:

- Can we predict the size of these fluctuations?
- Can we understand fluctuations using the response to a small perturbation?

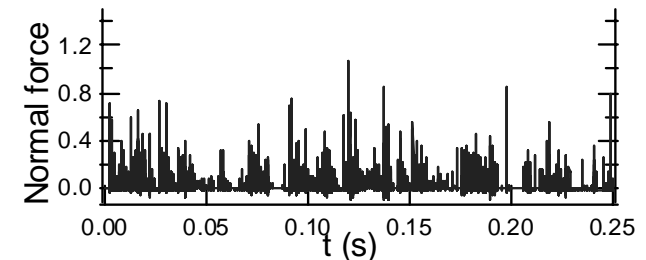
In analogy with fluctuation-dissipation relations from equilibrium statistical mechanics

- Are fluctuations induced by external driving forces similar to thermal fluctuations?

Simulation of fluctuations during shear flow

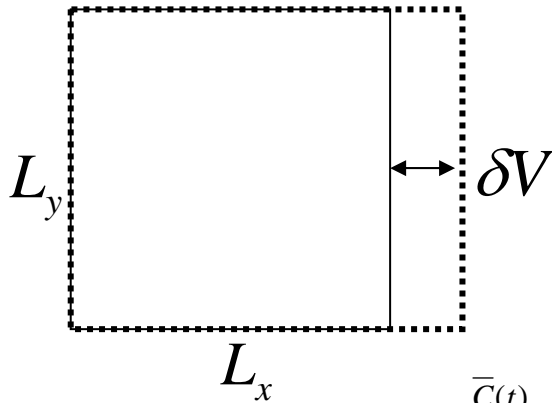


Experimentally measured pressure fluctuations in rapid channel flow



Equilibrium Fluctuation-Dissipation Relations

Linear response to small perturbation proportional to fluctuations at all times



Pressure fluctuations $\bar{C}(t) = \langle P(t)P(0) \rangle - \langle P \rangle^2$

Response to small change in volume $\bar{R}(t) = \frac{\langle P(t) \rangle - \langle P(0) \rangle}{\delta V}$

T=temperature

$$C(t) = \frac{\bar{C}(t)}{\bar{C}(0)}$$

$$R(t) = \frac{\bar{R}(t)}{\bar{C}(0)}$$

$$R(t) = \frac{1 - C(t)}{T}$$

Other examples of fluctuation-dissipation relations

Response	Fluctuations	Perturbation
Translational mobility	Translational diffusion	force
Rotational mobility	Rotational diffusion	torque
Compressibility	Volume fluctuations	Pressure change
Density at wavenumber \vec{k}	Density fluctuations	Spatially-modulated force

References:

- J. Chem. Phys. 116 (2002) 6228.
- Phys. Rev. E 55 (1997) 3898.
- Nature 415 (2002) 614.
- PNAS 102 (2005) 2299.
- Phys. Rev. Lett. 94 (2005) 055701.



Other Considerations

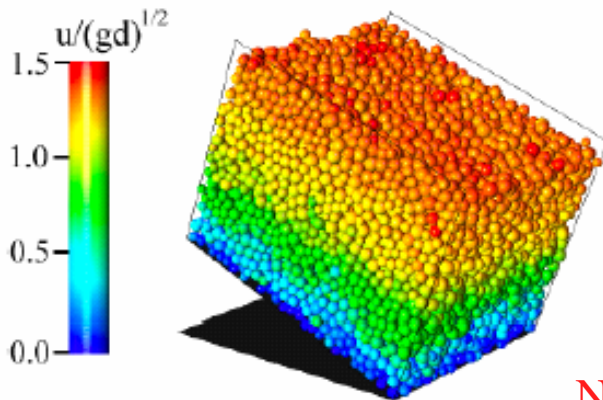
- How much do changes in boundary conditions affect everything else?
- Is there a simple [useful] way to incorporate cohesive and other interparticle forces?
- Compression and dilation as functions of BC's.
- How do we account for stick-slip motion?
- Process history, flow and stress pathways.
- The effect of interstitial fluids (3-phase systems): bridging cohesion, lubricity, dampening?

Example 1: Flows down Inclines

Multiple flow states.

Different behavior with bottom boundary condition.

bumpy base

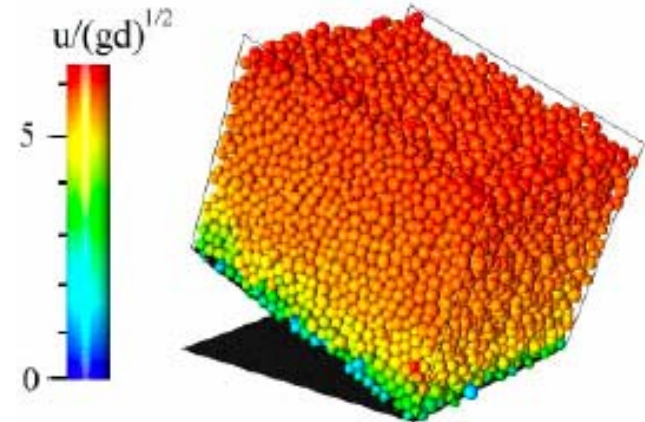


$$\bar{u} \propto h^{3/2}$$

Nicolas Taberlet's
DEM simulations

sheared through the depth

flat, frictional



$$\bar{u} \propto h^{1/2}$$

high shear rate in basal layer

Currently, rapid theoretical progress for cohesionless systems

Addition of cohesion?

Example 2: Power scaling

How to predict and optimize power and energy consumption as a function of process requirements, material properties, scale of production?

To what extent can this be done using small-scale experiments?

Continuous mixer-agglomerator



Detergent granulation process:

- Agglomerate mixture of surfactant and inorganic particulates
- Up to $\sim 60 \text{ m}^3/\text{hr}$.
- High shear, $Fr > \sim 20$
- Shaft drive $\sim 250 \text{ kW}$

“Cyrus” the bucketwheel excavator



Oil sand surface excavation:

- Mixture of sand and bitumen
- Up to $\sim 6000 \text{ m}^3/\text{hr}$.
- Lower speed, $Fr \sim 0.3$
- 560 kW bucketwheel drive.

Forward look worksheet 1 –

How to address issues for energy relevant handling and processing of powders and granular materials?

	NETL	CMFR	Other (CMFR leverage)
• Size-scaling (unit-op / particle) is critical to industrially-relevant case studies.			
• What sets the stress and flow fields for the relevant flow regimes? How are stress changes or changes in other quantities transmitted throughout the sample?			
• How are these related to boundary conditions, particle properties, and process control parameters?			
• How should one characterize a granular mixture, particularly one where the particles have a continuous range of sizes, shapes and/or surface properties?			
• Given that real granular materials may require a very large number of parameters for a complete physical description, what are the most useful truncations of such a parameter space that give reasonably accurate characterization?			
• What is the range of states that is compatible with a given set of (boundary) control parameters? The answer to these will address the repeatability issue.			
• What is the character of fluctuations that occur in stresses/forces and flow fields?			
• What mathematical approach can be used to incorporate these fluctuations into a suitable theory (e.g. Langevin approach for random uncorrelated fluctuations, extended granular temperature...).			
• Is there a connection between the possible states consistent with control/boundary conditions, and the range of fluctuations seen? What is the nature of repeatability tied to fluctuations?			
• What is the response of a system to a change at the boundaries?			
• In a dynamical process, what is the relation between energy input [power] and flow?			

