# Track 1: Dense Gas-Solid and Granular Flows

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# Track 1 (Expected) Participants

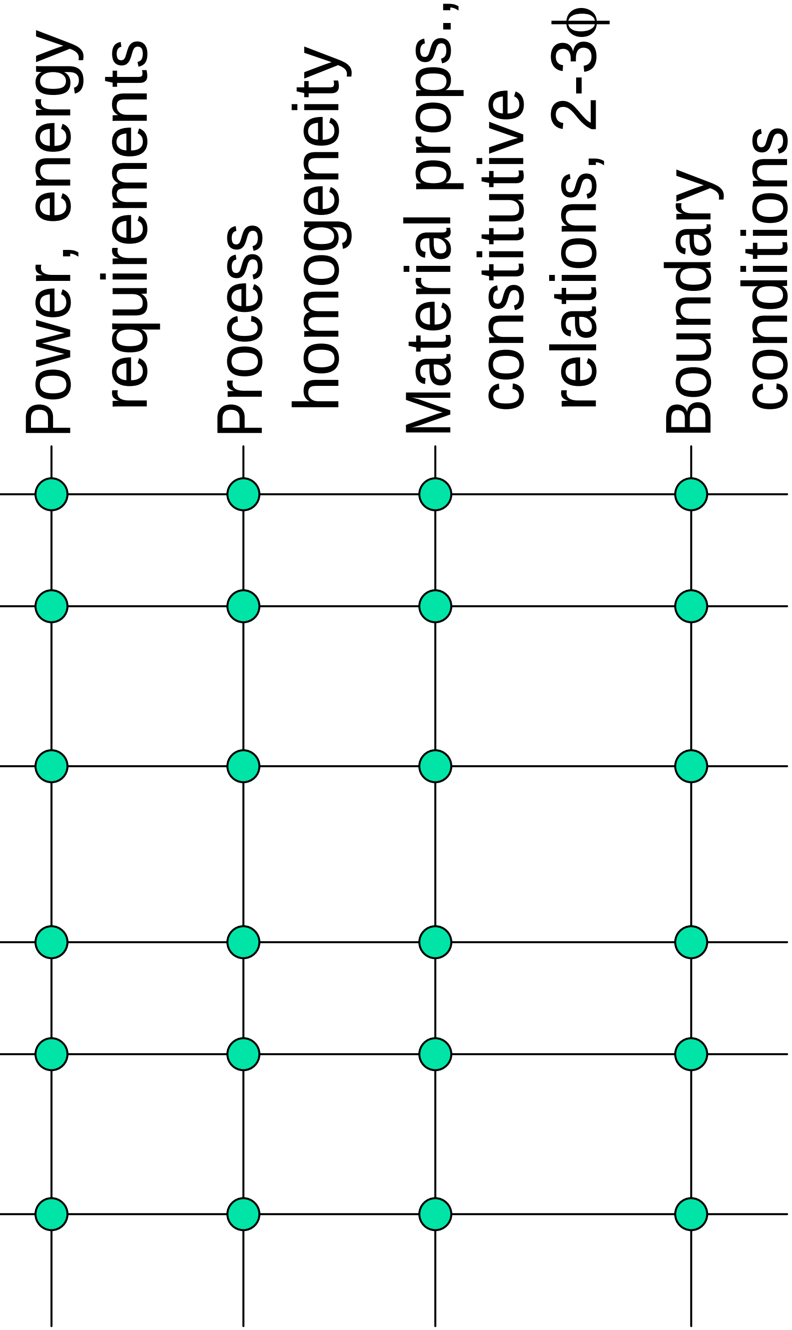
- Losert (Maryland), Mehrabadi (Tulane), Turton (West Virginia), McCarthy (Pittsburgh), Sundaresan (Princeton), Behringer (Duke), O'Hern (Yale), Menon (Massachusetts)
- Banerjee (Millenium Chemical), Mort (P&G), Fiveland (Alstom), Gentzler (Merck), Price (Nova Chemical), Niksa (Niksa Energy)
- O'Brien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



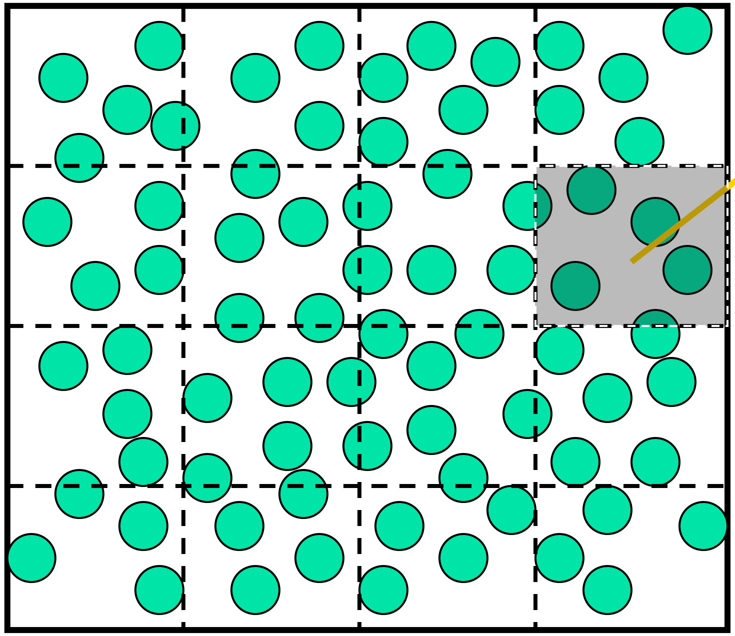
# Scaling and Scale-up

- 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



- $\phi_s$ : particle volume fraction
- $\mathbf{u}_s$ : coarse-grained particle velocity
- $\varepsilon$ : 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 -> fluid, but will it work for solid -> solid coarse-graining?*

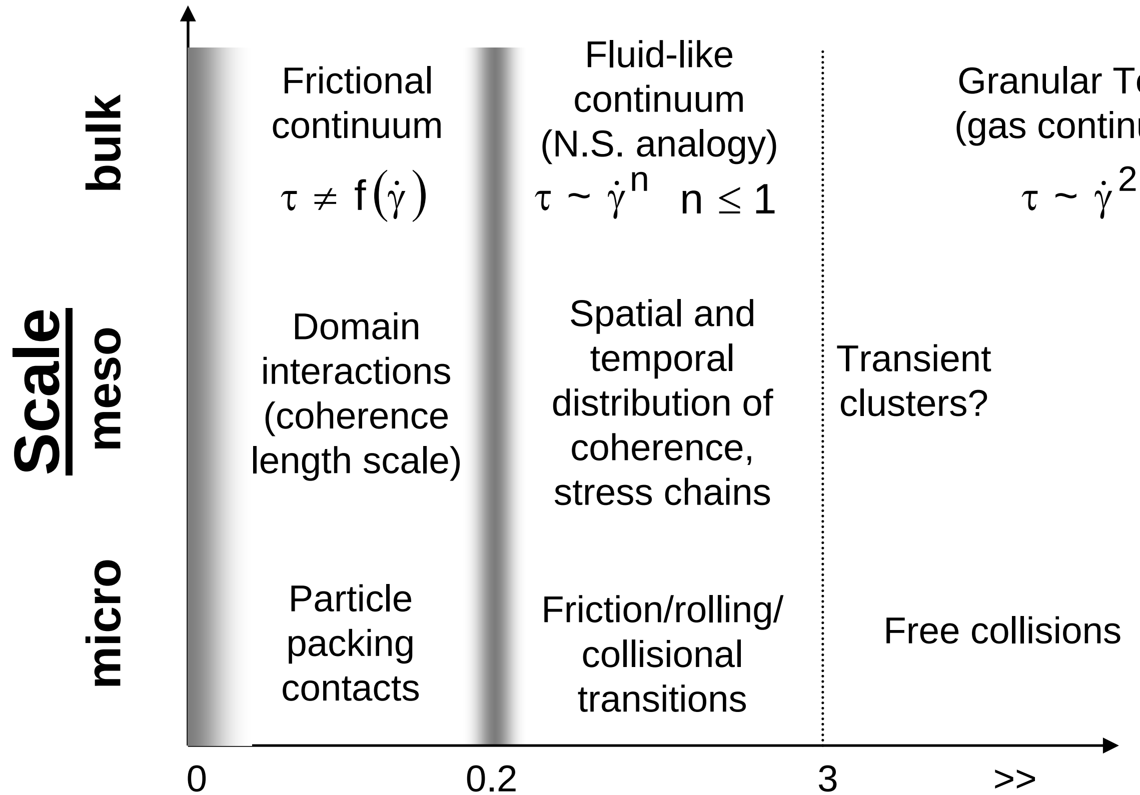
# Scaling and Controlling Groups

- Stresses $\sigma_{xy} = \mu\sigma_{yy} + \sigma_s + \nu\dot{\gamma}$
- 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

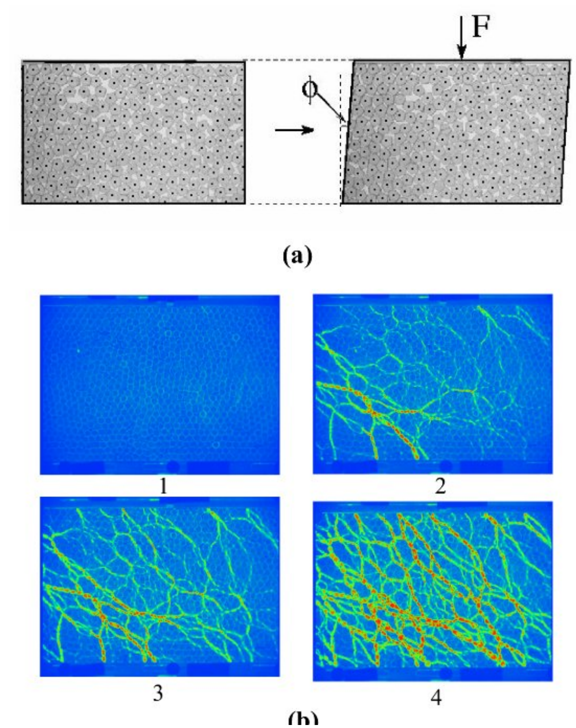



| | | | | | |
|---|---|---|---|---|---|
| Inertia / confinement, $I = \frac{\dot{\gamma} \cdot d_p}{\sqrt{P \cdot \rho_0}}$ | Dimensionless shear rate, $\dot{\gamma}^* = \dot{\gamma}\left[\frac{d_p}{g}\right]^{1/2}$ | | | | (Tardos) (GDR Midi) |
| Contact time $t_c / t_{bc}$ | high | ~2 | | 1 | (Campbell) |
| 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) |

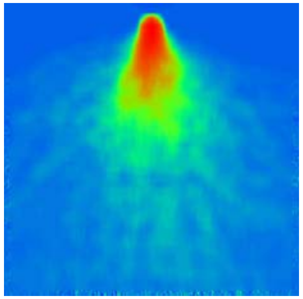
# Stress calculation, fluctuations, and transmission

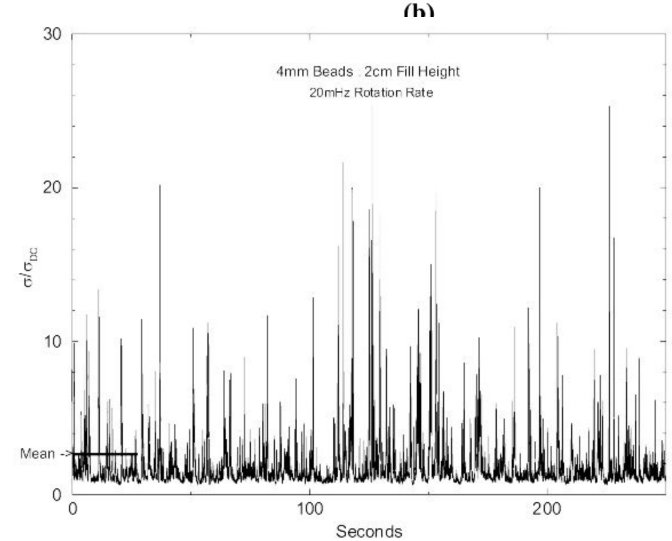
- How is stress (and other quantites) transmitted through bulk? What is effect of BCs?
- How do we quantify (and understand) fluctuations?
- How do we quantify the transition from quasi-static to intermediate to rapid flows?
- What experimental (or computational, DEM?) methodologies are best suited?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






*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.

| Particle characteristics and material properties influencing powder flow | Dry granular (free flowing) | Moist granular (cohesive flow) | Fine powder (cohesive flow) |
|---|---|---|---|
| **Restitution properties:** | | | |
| • Elasticity (storage modulus) | ● | ○ | ● |
| • Damping (loss modulus) | ● | ○ | ● |
| • Plasticity (yield) | ● | ○ | ● |
| **Particle characteristics:** | | | |
| • Particle size | ● | ● | ● |
| • Polydispersity, size distribution | ● | ● | ● |
| • Shape | ● | ● | ● |
| • Roughness | ● | ○ | ● |
| **Interaction coefficients:** | | | |
| • Hamaker constant (van der Walls) | | | ● |
| • Dielectric permittivity (electrostatic) | | | ● |
| • Friction | ● | ○ | ● |
| **Liquid properties:** | | | |
| • Viscosity (fluid) | | ● | |
| • Surface tension (3-phase, w/ fluid) | | ● | |
| • Lubrication (friction reduction) | | ● | |

# 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 prevelent, is the granular temperature the correct quantity for modeling?

# Fluctuations in Dense Granular Flows

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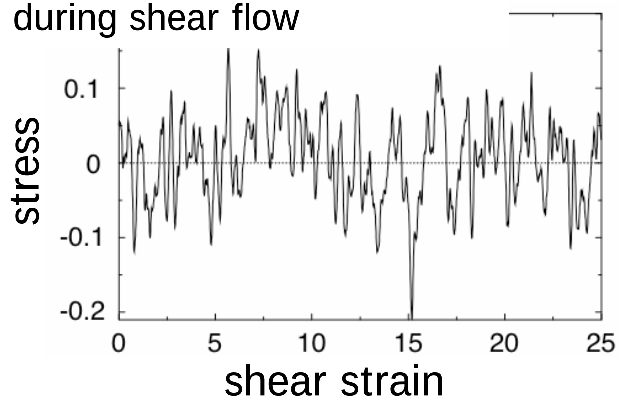
Narayanan Menon (Department of Physics, University of Massachusetts-Amherst)

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

Simulation of fluctuations during shear flow



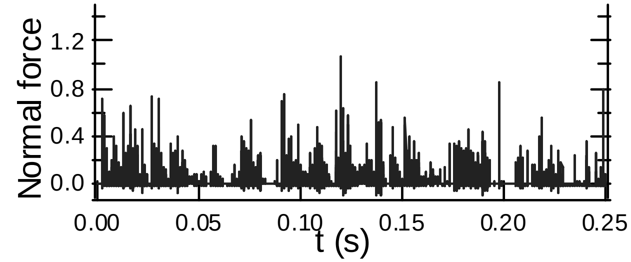

## Important Questions:

- 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

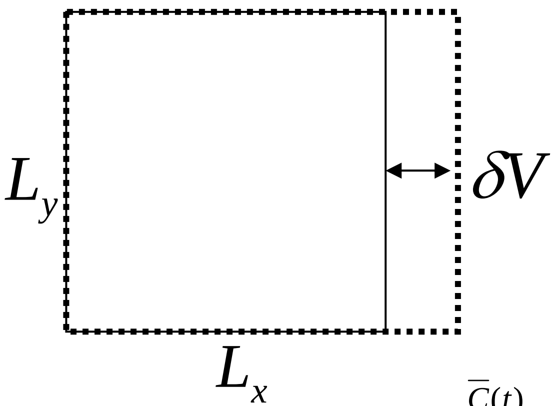
- Are fluctuations induced by external driving forces similar to thermal fluctuations?

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

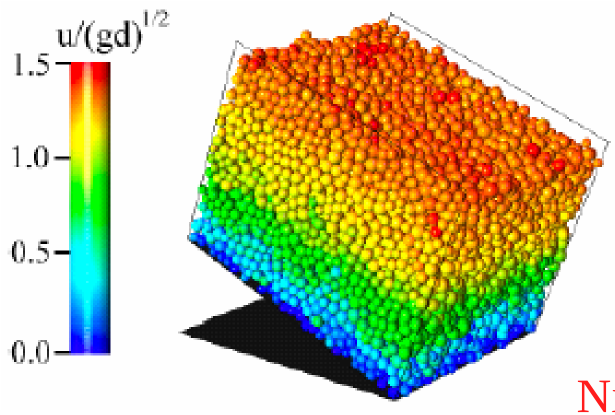
- How much do changes in boundary conditions affect everything else?
- Is there a simple [useful] way to incorporate cohesive and other interparticle forces?
- Compression and dilation as functions of BC's.
- How do we account for stick-slip motion?
- Process history, flow and stress pathways.
- The 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.*

<u>*bumpy base*</u>

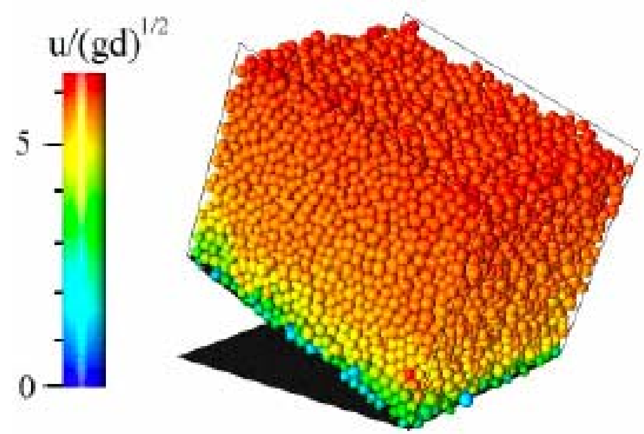



$\bar{u} \propto h^{3/2}$

sheared through the depth

Nicolas Taberlet's DEM simulations

<u>*flat, frictional*</u>




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

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 ~60 $m^3$/hr.
- High shear, Fr > ~20
- Shaft drive ~250 kW

**"Cyrus" the bucketwheel excavator**

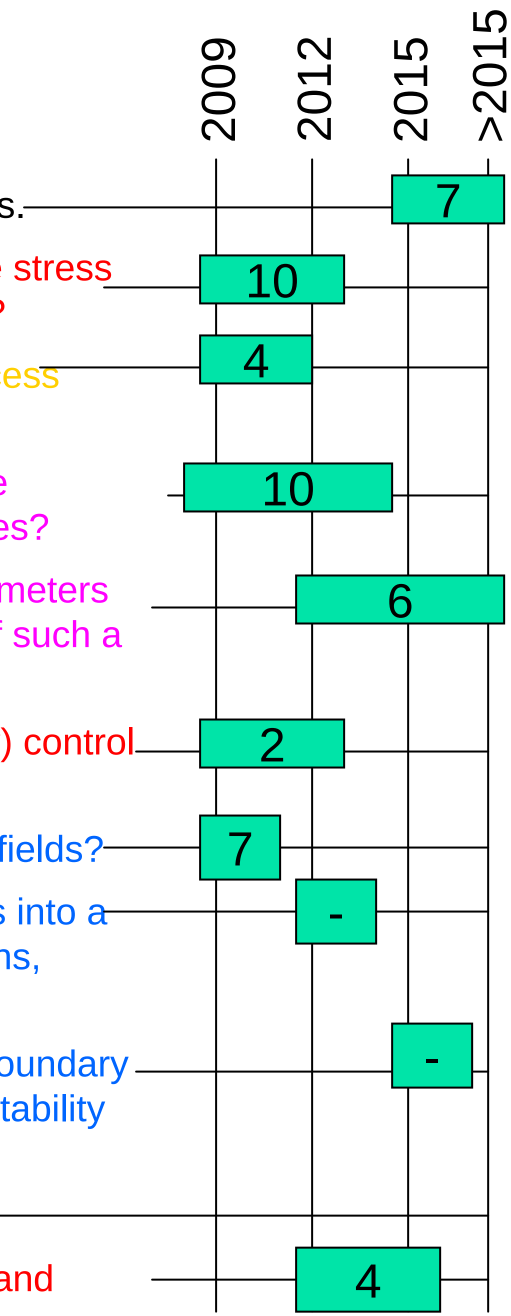

Oil sand surface excavation:

- Mixture of sand and bitumen
- Up to ~6000 $m^3$/hr.
- Lower speed, Fr ~ 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?*

1. Size-scaling (unit-op / particle) is critical to industrially-relevant case studies.
2. 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?
3. How are these related to boundary conditions, particle properties, and process control parameters?
4. How should one characterize a granular mixture, particularly one where the particles have a continuous range of sizes, shapes and/or surface properties?
5. 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?
6. 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.
7. What is the character of fluctuations that occur in stresses/forces and flow fields?
8. 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…).
9. 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?
10. What is the response of a system to a change at the boundaries?
11. In a dynamical process, what is the relation between energy input [power] and flow?

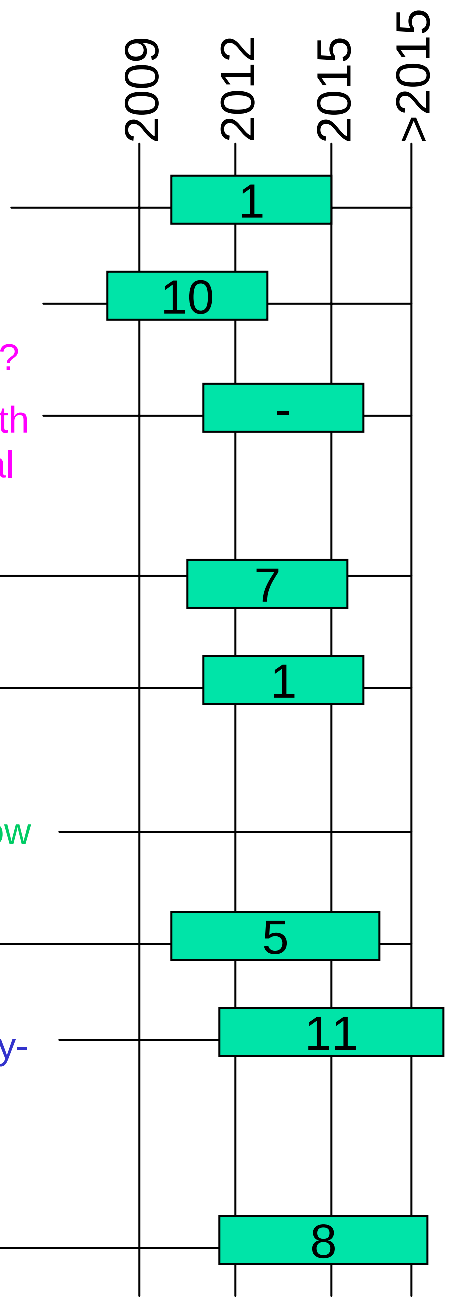


# Forward look worksheet 2 –

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

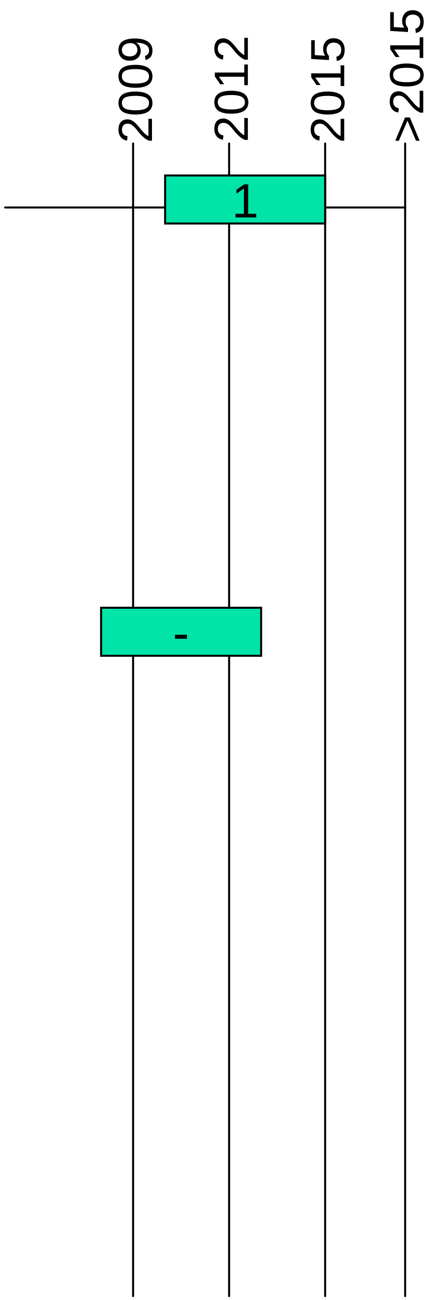
12. What parameters control the transitions between different granular states, e.g. quasi-static vs. intermediate? What is the nature of these transitions?
13. What experimental [and simulation] methods are most useful in a) addressing basic physical questions, and b) providing key insights for practical applications?
14. What diagnostics can be used to infer information of flow fields and stresses both internally and at the boundaries? Develop criteria to expose when the interstitial fluid flow is important in a given problem involving powder flow.

- Develop a physical understanding of the effect of interparticle forces on the hierarchy of flow-induced inhomogeneous structures.
- Develop quantitative models for the effects of vibration and pressure pulsations generated through a microphone – either by themselves or in conjunction with fluidizing gas flow – on the dynamics of particle agglomerates.
- Develop a better understanding of stick-slip motion of cohesive powders and how it can be manipulated to get optimum flow and mixing characteristics
- Probe the effect of microstructure on the drag coefficient.
- Develop continuum rheological models for assemblies of particles [2 and 3 phase] – from quasi-static to rapid flow regimes, bringing in the path- and history-dependence [compression, dilation] manifested by cohesive systems. Use experiments, simulations, statistical frameworks.
- Develop equations of motion and associated closures by coarse-graining over meso-scale structures (such as collections of agglomerates).



# Forward look worksheet 3 –

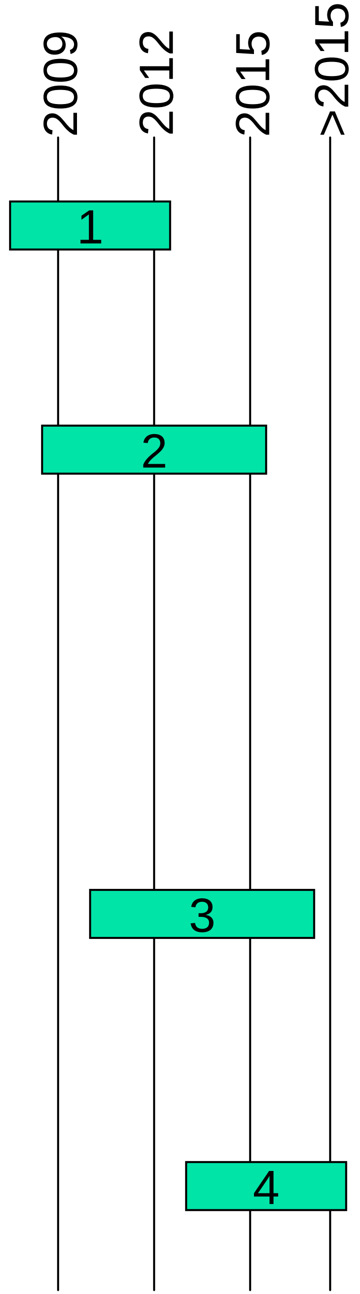
*How to address issues for energy relevant handling and processing of powders and granular materials?*




21. Heat transfer, reactive flows (experimental and simulation, DNS→continuum)
22. Energy based systems, how to use what is available, e.g., scale-up?
    1. Fluidization
    2. Coal gasification, predict carbon utilization as f (operating conditions)
    3. System integration models, steady state vs. transient
    4. Dry feeding into high T, P environments; a-priori simulation followed by [costly] experimental validation
23. There is a key need to define relevant material properties on a particle scale, and efficient ways to include thiese properties into models. How to establish standards for material properties, methods (NIST, ASTM, etc…)
    1. Need to define key material parameters
    2. Reported conditions, environmental, boundary conditions…
    3. Table of metadata
    4. Collaboratory round robin or grand challenge
        1. Experimental
        2. Simulation (DEM, continuum…)
24. Continuum models are used now. What are the limitations, what more can we do, and how to proceed forward? Connect with soil mechanics on use of finite element models ← → translate to other modeling approaches (numerical methods).

# Forward look worksheet Summary: Dense Flows

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




A. What defines the stress and flow fields for the relevant flow regimes? How is stress transmitted throughout the material? How are these related to boundary conditions, particle properties, and process control parameters?
   - What is the character of fluctuations that occur in stresses/forces and flow fields?

B. Define relevant material properties on relevant scales. Develop efficient ways to represent properties in models. How to establish standards for material properties, methods (NIST, ASTM, etc…)
   - Need to define key material parameters (interparticle forces…)
   - Reported conditions, environmental, boundary conditions…
   - Table of metadata
   - Collaboratory round robin or grand challenge
     - Experimental
     - Simulation (DEM, continuum, constitutive…)

C. Continuum models are used now. What are the limitations, what more can we do, and how to proceed forward, e.g., hybrid models? Connect with other models for finer resolution (DNS, DEM, finite element, stochastic, etc.).
   - Continuum strategy
   - Hybrid strategy (define continuum → high-resolution criteria, e.g., based on structural inhomogeneities and/or discontinuities).

D. Size-scaling (unit-op / particle) is critical to industrially-relevant case studies. System integration models, steady state vs. transient