SAND2019-3705C

Particle-scale Modeling and Simulation of Powder Processing – Die Compaction

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MACH Conference

April 2019

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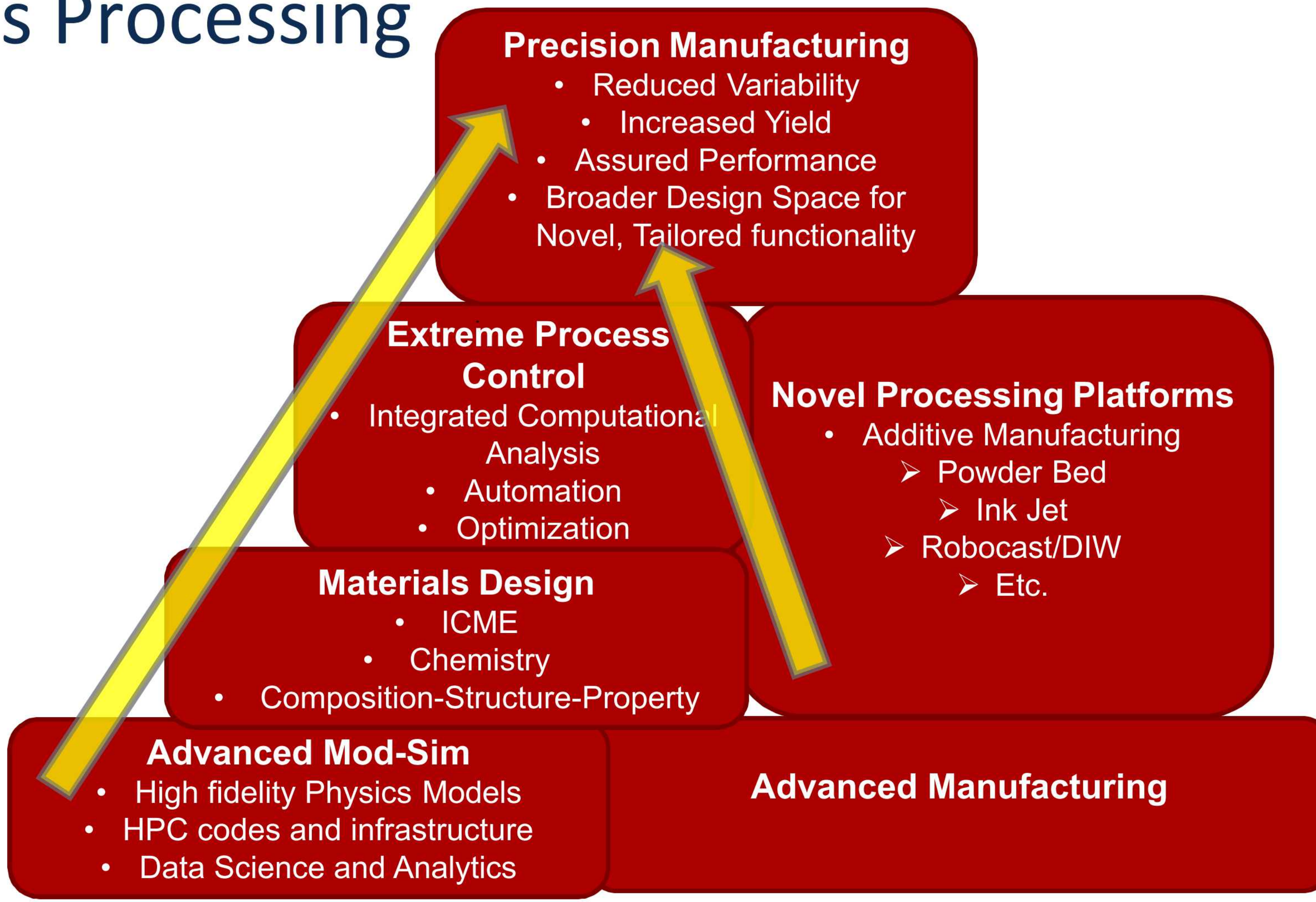
Enabling Precision Manufacturing for High Consequence Small Lot Particulate Materials Processing

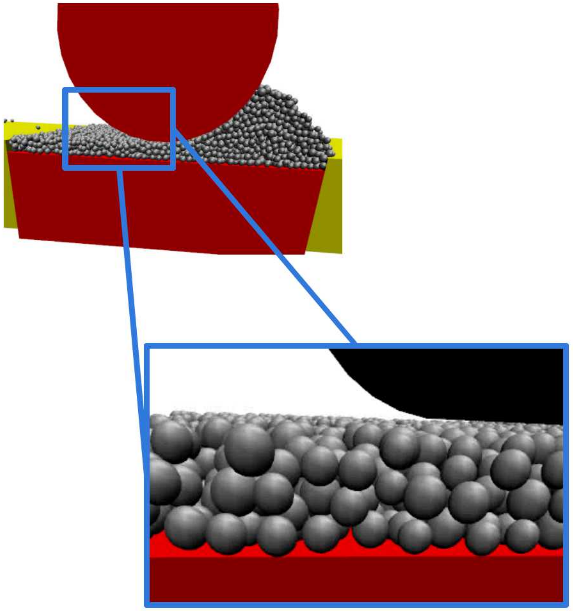


Particulate Materials and Processes in Manufacturing

- Particulate Materials are ubiquitous
  - Complex and highly variable
  - Behavior hard to predict and control → processing is inefficient and energy intensive
    - Nonlinear, dissipative interactions
    - Many nonequilibrium, history dependent, metastable states
  - Manufacturing processes require careful validation (Quality by Design)
    - "Focusing exclusively on qualification efforts without also understanding the manufacturing process and associated variations may not lead to adequate assurance of quality." – FDA guidance to pharma
- Particle dynamics modeling – Newton's equations for each individual particle
  - Provides a framework for analyzing/optimizing process design, controls and validation
  - Links feedstock materials' characteristics to processing conditions to resulting states/properties and performance attributes (FP^3 provides the science basis for QbD)
- Traditional processes
  - Die-filling and compaction
  - Size reduction (crushing, grinding, milling, …)
  - Mixing, blending
  - Extrusion
- AM Processes
  - Powder bed – SLM, SLS
  - Inkjet Binder
  - Robocasting/DIW, …
- Small-lot, intrinsically variable → precision is key for assured performance

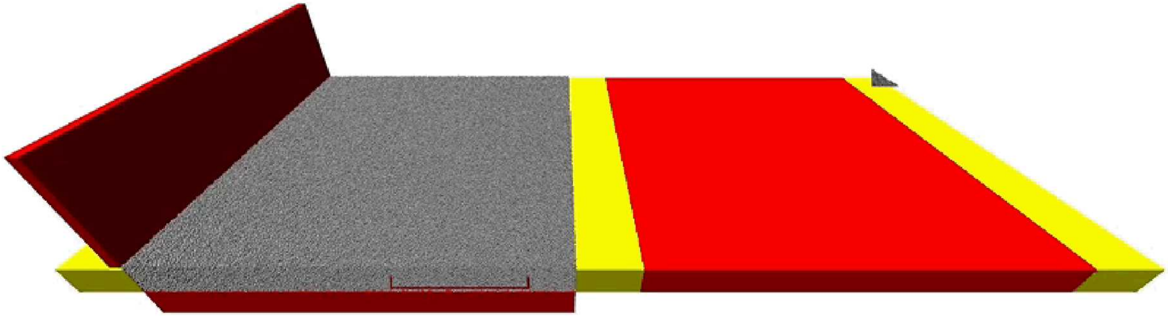
Modeling particle formation, storage/handling, transport, placement, and reuse *at the particle scale* is critical to understanding sources and consequences of variation on both the feedstock and process as well as their interplay

Particle Dynamics Simulation



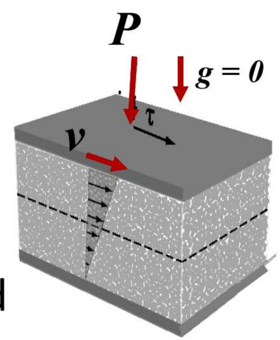
Method of choice: Discrete Element Method (LAMMPS)

- Motion of individual particles numerically simulated
- Particle-Particle interactions: reduced-order contact mechanics models
  - Hertzian elastic and strain-hardening viscoplastic contact forces;
  - Coulomb friction, van der Waals attractions, adhesion
  - Implementing deformable particle capability
- Can account for
  - particle size (100:1), shape variations
  - complex geometries (e.g. moving spreader, partially manufactured part)
  - variations in particle material properties/surface characteristics
- Computationally detailed: leverages high-performance computing resources and next-gen platforms
- **Current challenge: model parameter estimation, calibration, validation and uncertainty quantification**

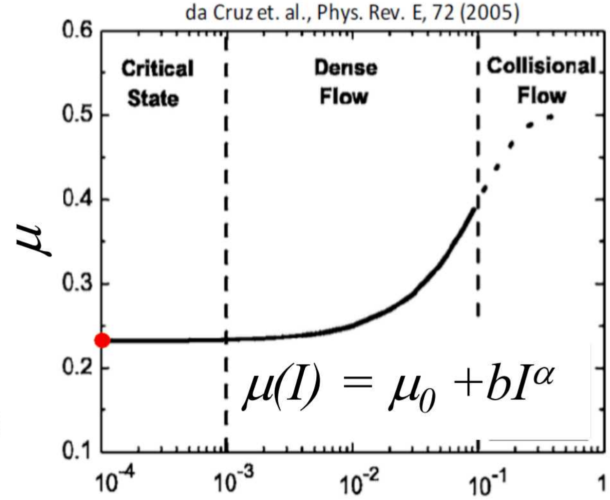


Computational Bulk Rheology

- Rate controlled
  - Flow is always enforced
  - "mu-of-I" rheology proposed
    - Links quasi-static and inertial flow regimes
    - Behaves like a yield stress fluid

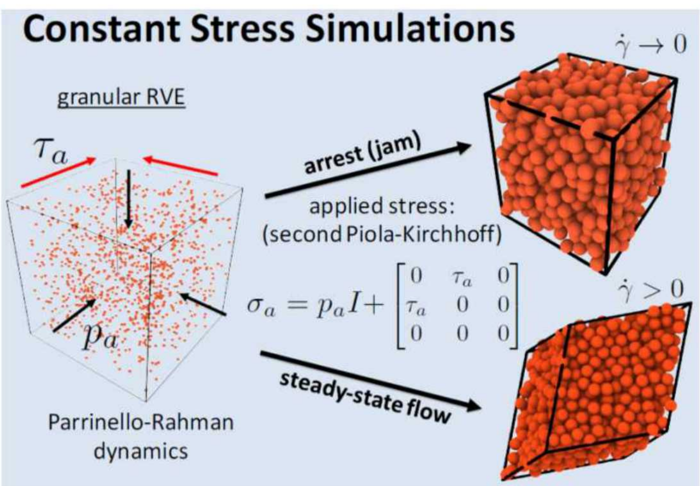


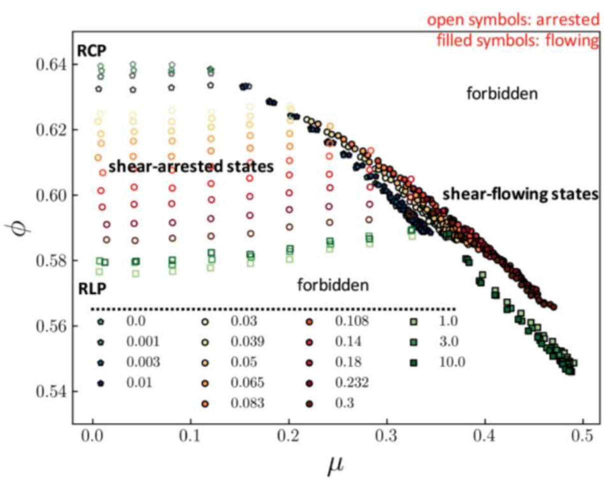
$$\mu = \tau/P$$



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

- Stress controlled
  - May or may not flow…

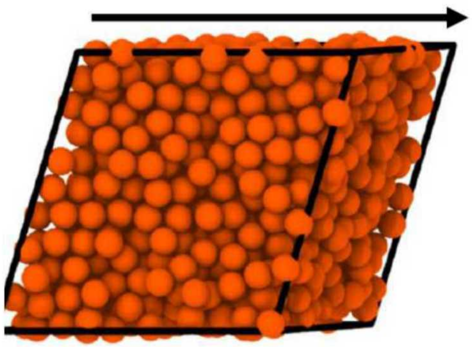




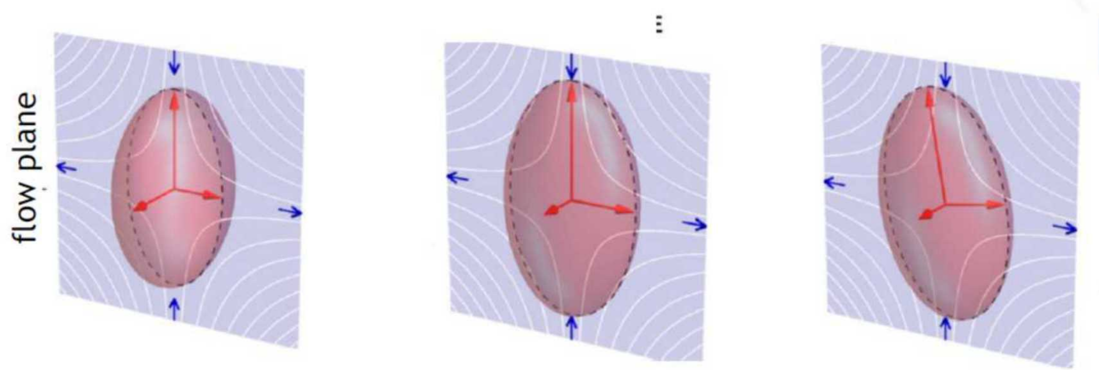
μ_c, ϕ_c

General Decomposition of Steady Shear Flow

$$\mathbf{L} = \mathbf{D} + \mathbf{W}$$



co-directional flow | co-axial flow | complex flow



$$\boldsymbol{\sigma}_a = p_a I + \begin{bmatrix} 0 & \tau_a & 0 \\ \tau_a & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

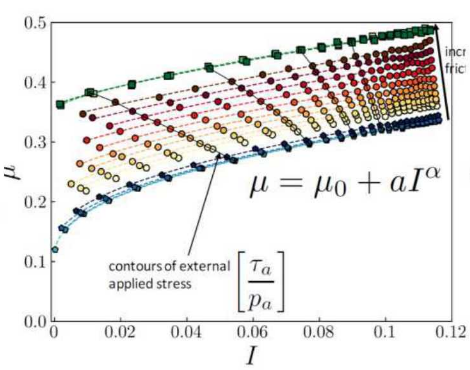
$$\frac{\boldsymbol{\sigma}}{|\boldsymbol{\sigma}|} = \frac{\mathbf{D}}{|\mathbf{D}|}$$

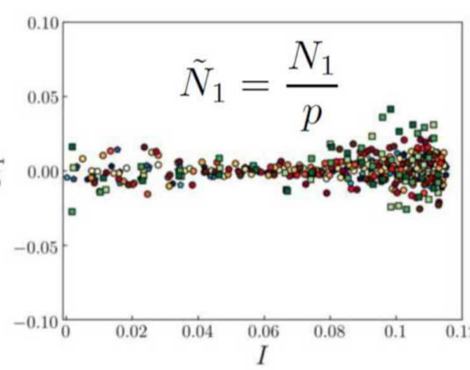
principal directions of stress and strain rate tensors coincide

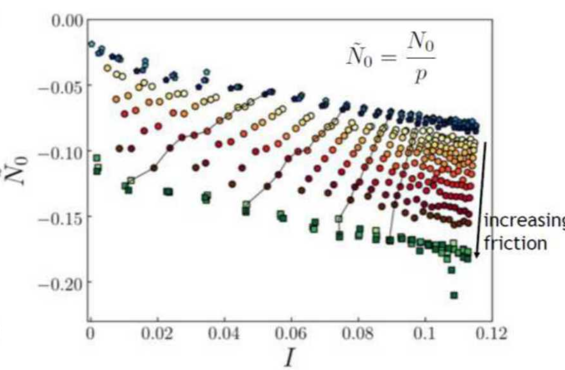
principal directions of stress and strain rate tensors do not coincide

stress tensor in planar xy-shear

$$\boldsymbol{\sigma} = \begin{pmatrix} p & \tau & 0 \\ \tau & p & 0 \\ 0 & 0 & p' \end{pmatrix} p' < p$$

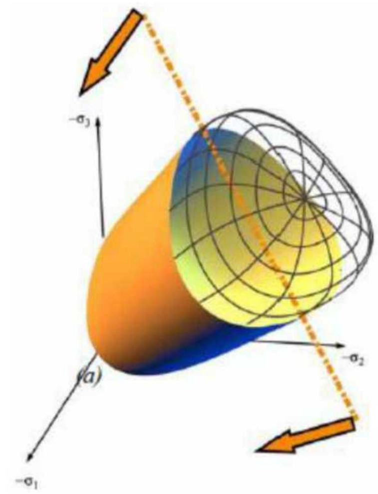


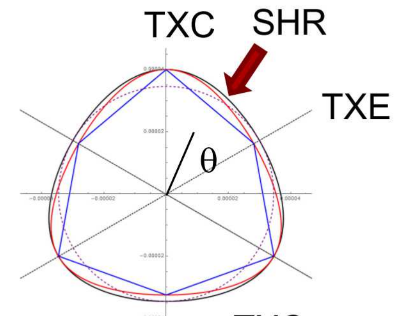


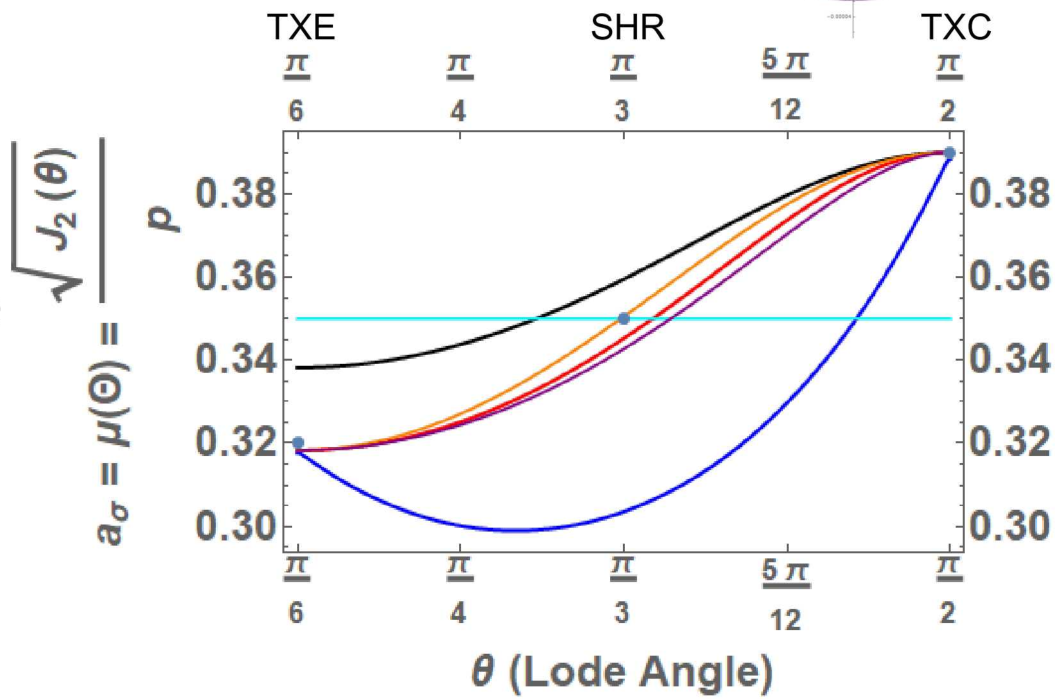


3D Stress Dependence of Flow (Arrest/Yield)

- Rheology will also depend on Lode angle
    - Black: Duncan-Lade
    - Orange: Gudehus
    - Red: Matsuoka-Nakai
    - Purple: William-Warnke
    - Blue: Mohr-Coulomb
    - Cyan: Drucker-Prager

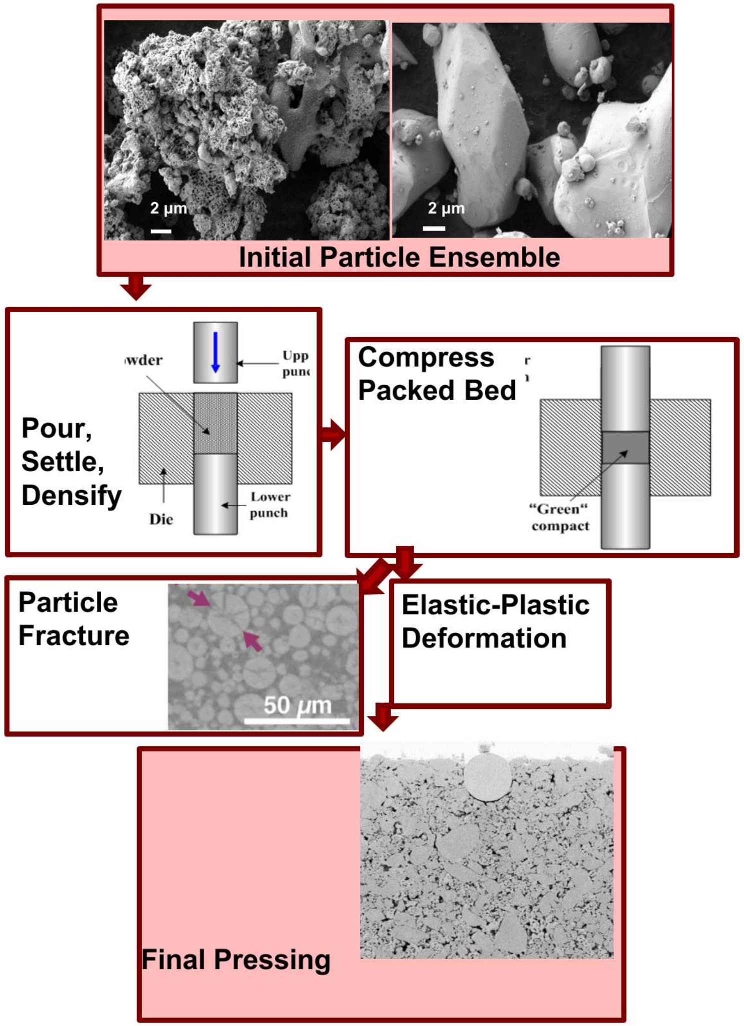






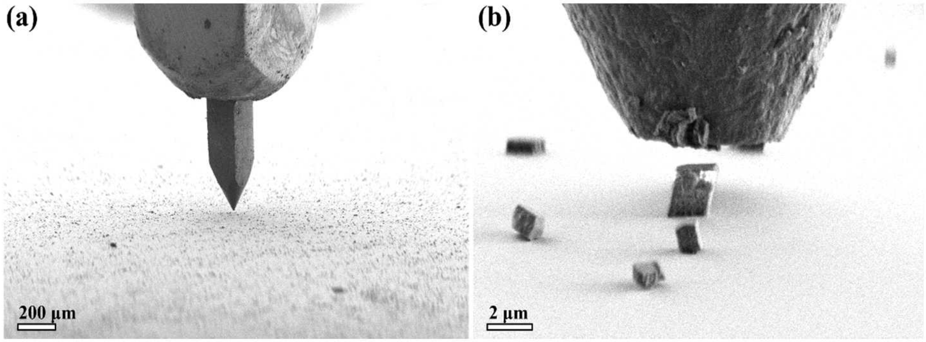
Traditional Process – Die Compaction

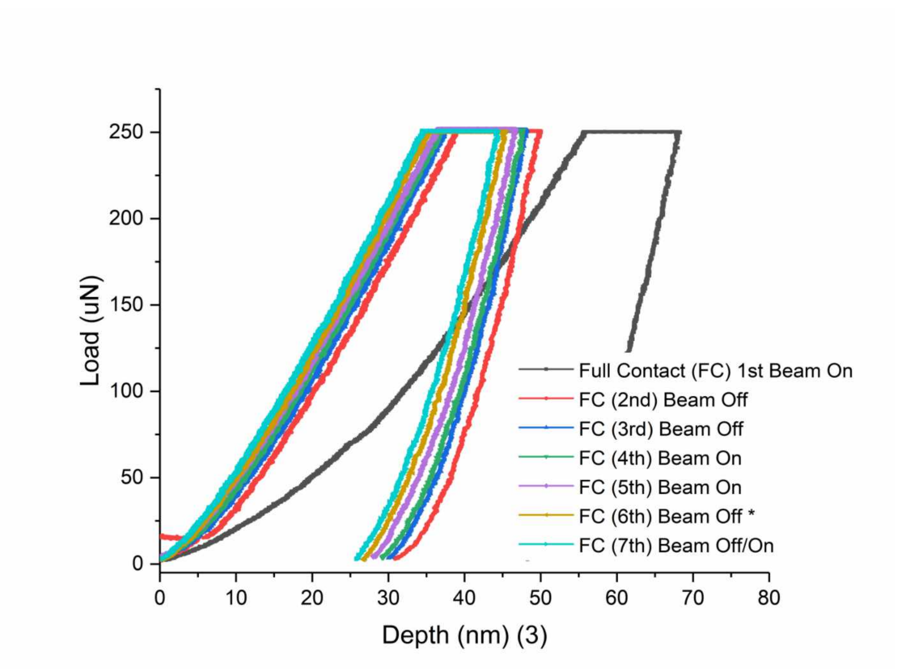
- Low porosity particle packings manufactured by simple die compaction
- Particle characteristics and manufacturing methods determine the morphology of the resulting packing
- The microstructure of low-porosity packings of energetic powders is influenced by particles' deformation, strength, and fracture behavior
  - Particles vary in size/shape distribution, material type (ductile, brittle, quasi-brittle) and surface characteristics
- Must discover complex-shaped energetic particle deformation and fracture
- Measure particle strength using nanoindentation with imaging at the microscale



Micromechanics of Particles

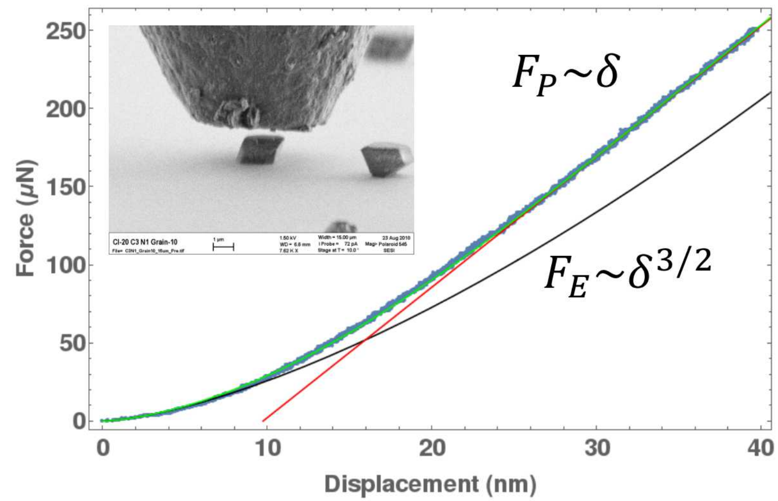
- 1.6 micron (light scattering) CL-20 particles
- Nanoindenter with SEM imaging
- Electron beam effects were determined to be negligible
- Load – displacement curves were found to be very reproducible



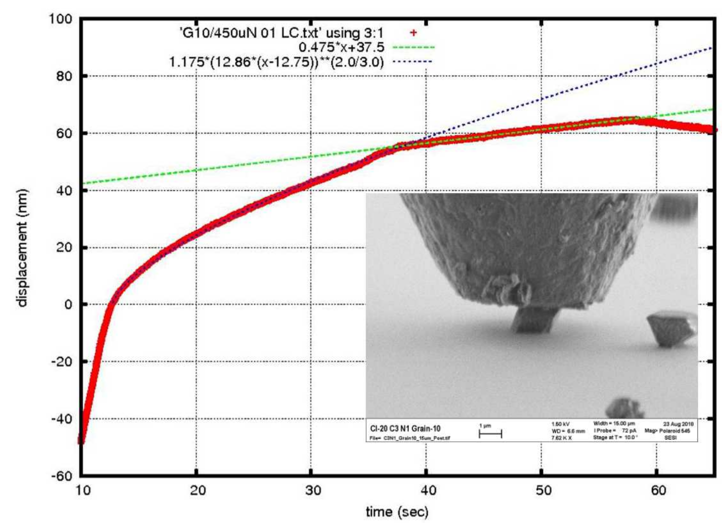


Force-Controlled Experiments

- Data is clean
- Clear linear elastic type response for early time in force ramp
  - Hertzian contact theory models this region well
    - Force vs. displacement
    - Displacement vs. time
- Later force-displacement data is linear
  - Could be indicative of yield?
- Force hold indicates plastic fluid-like flow consistent with yield noted previously
  - Force constant while displacement increases linearly in time
  - No clear bound seen – rate of increase small and hold time was short
- Model for loading response: Brake (2015) Int. J. Solid. Struct., 62, 104-123

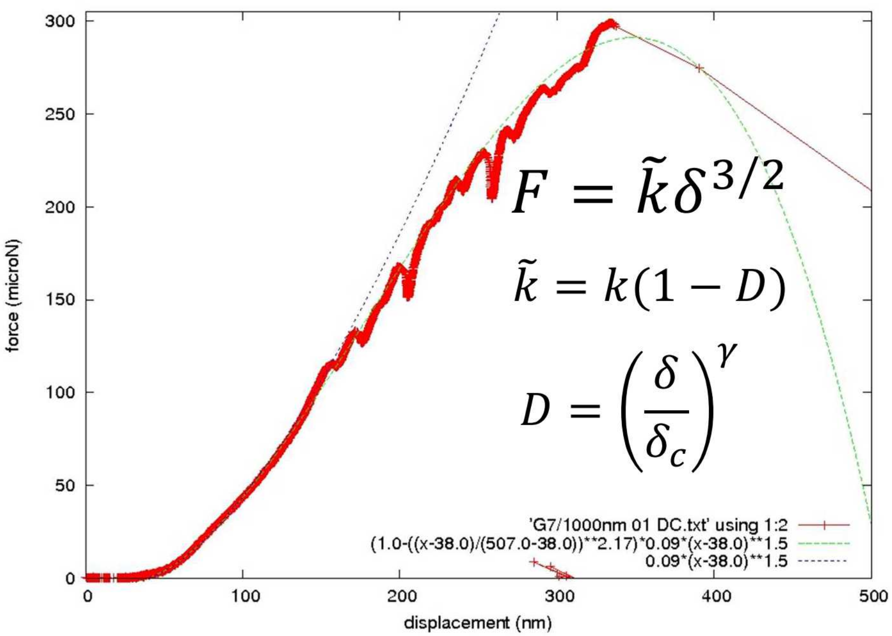


$$F_{tot}(\delta) = \varphi_1(\delta) F_E(\delta) + \varphi_2(\delta) F_P(\delta)$$



Displacement-Controlled Experiments

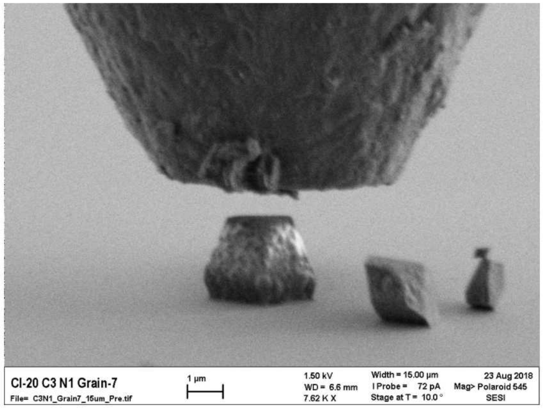
- Quasi-brittle behavior with damage accumulation
- Complicated load displacement response…

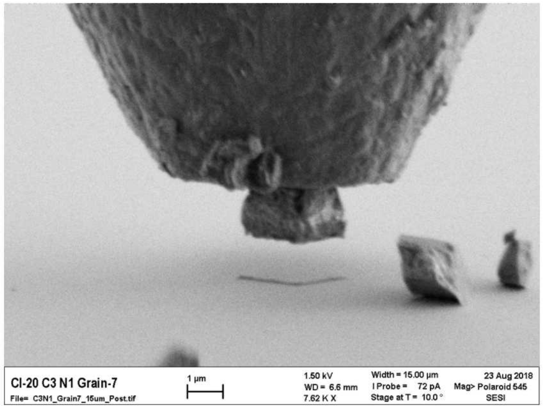


$$F = \tilde{k}\delta^{3/2}$$

$$\tilde{k} = k(1 - D)$$

$$D = \left(\frac{\delta}{\delta_c}\right)^{\gamma}$$





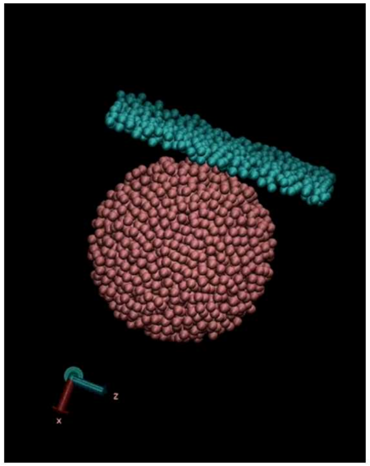
Deformable Particles via beam-bonded DEM

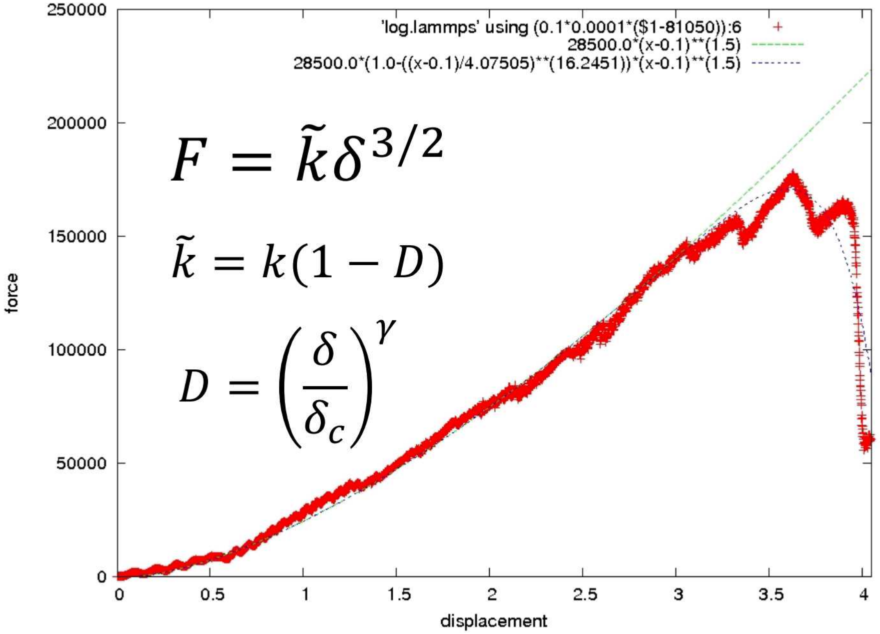
- Construct large particle from many smaller particles bonded by beam-like springs

Bonded-DEM model based on Carmona et al. (2008) Phys Rev E, 77, 051302-1-10

- Force response consistent with LE mechanics with damage – continuum damage mechanics type phenomenology

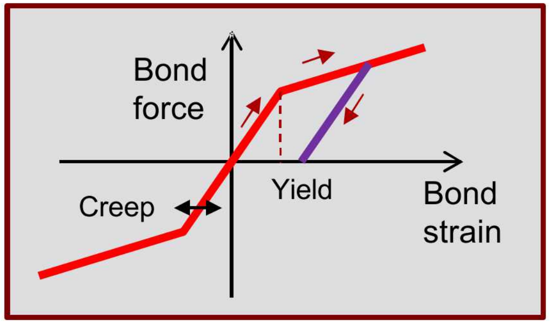
L.M. Tavares, R.P. King, Powder Technology 123(2) (2002) 138-146

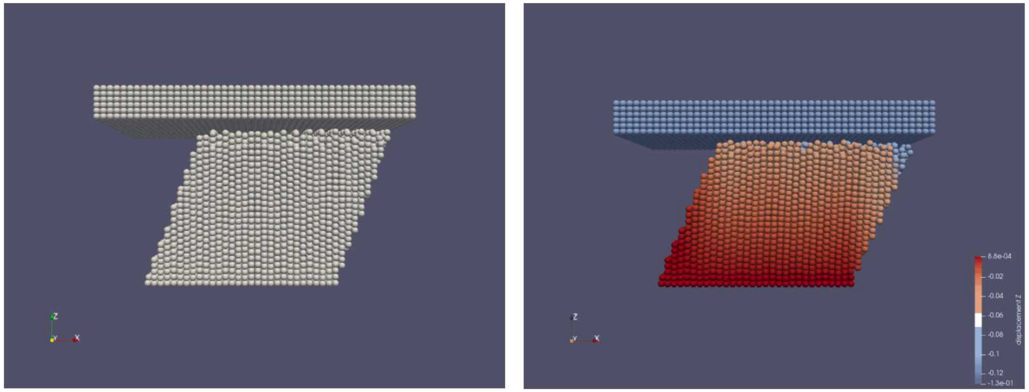




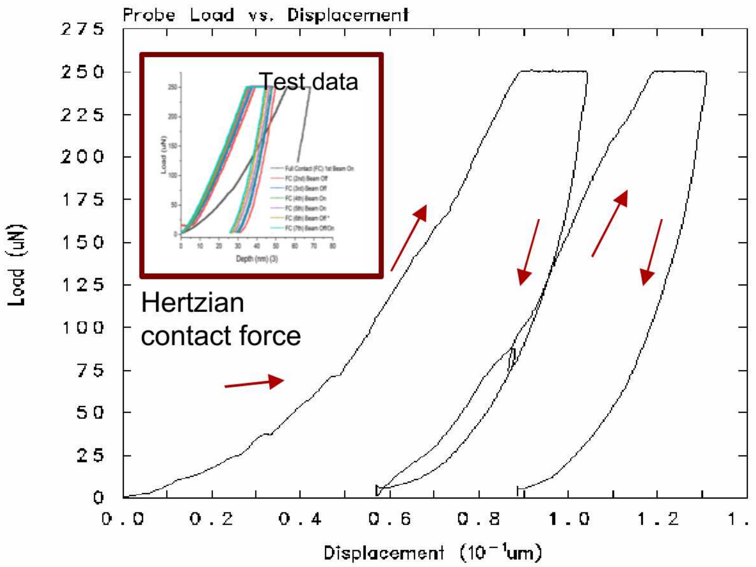
Peridynamic material model for particle mechanics

- Key features: Includes permanent deformation from
  - Plasticity (instantaneous)
  - Creep (time dependent)





Two loading cycles in an irregularly shaped crystal

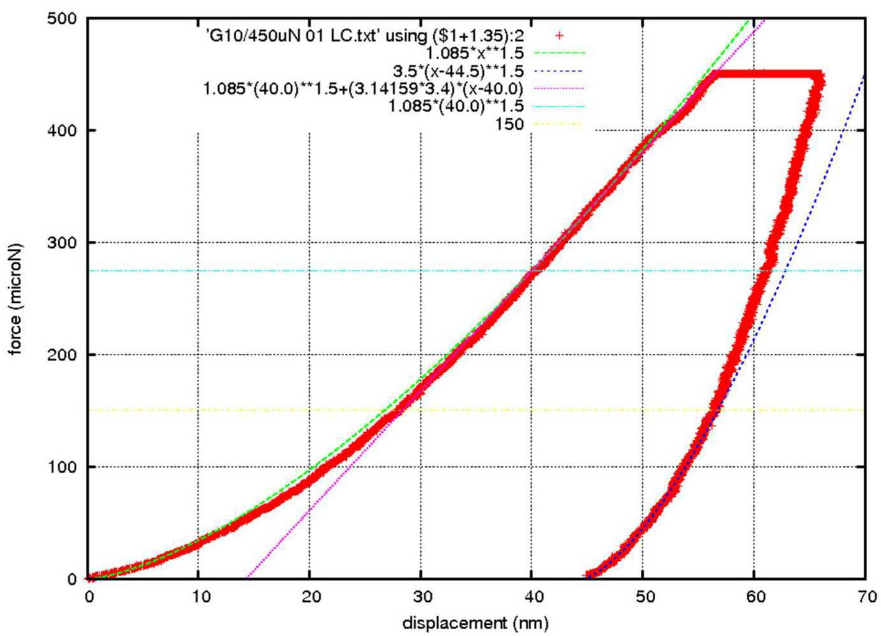


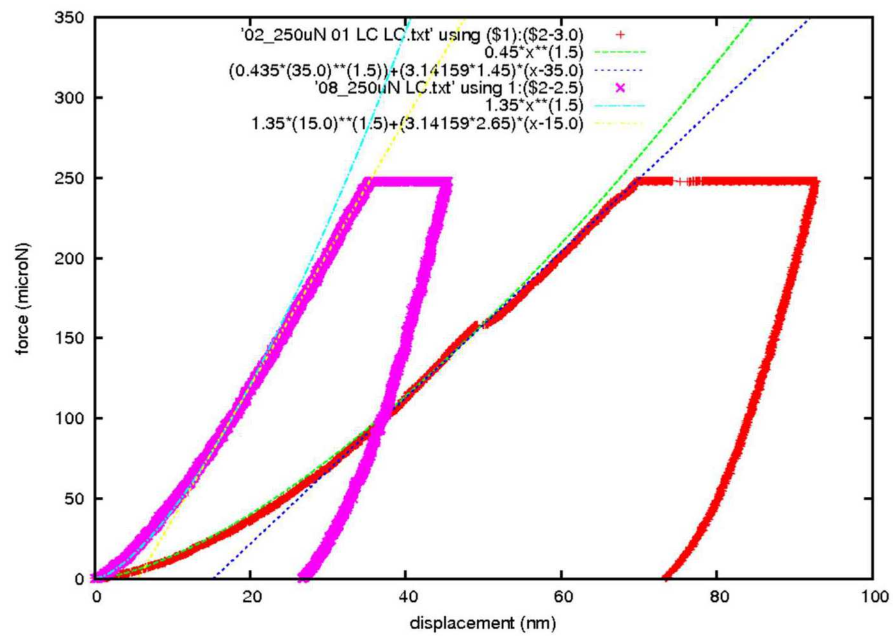
Conclusions and Outlook

- DEM becoming predictive for powder rheology under low pressures
- Many applications involve high pressure – die compaction
- Micromechanics of particles can be characterized
- Phenomenology of particle micromechanics can be captured in reduced-order and robust particle-type models
- Ongoing work is focused on coupling these methods in HPC code

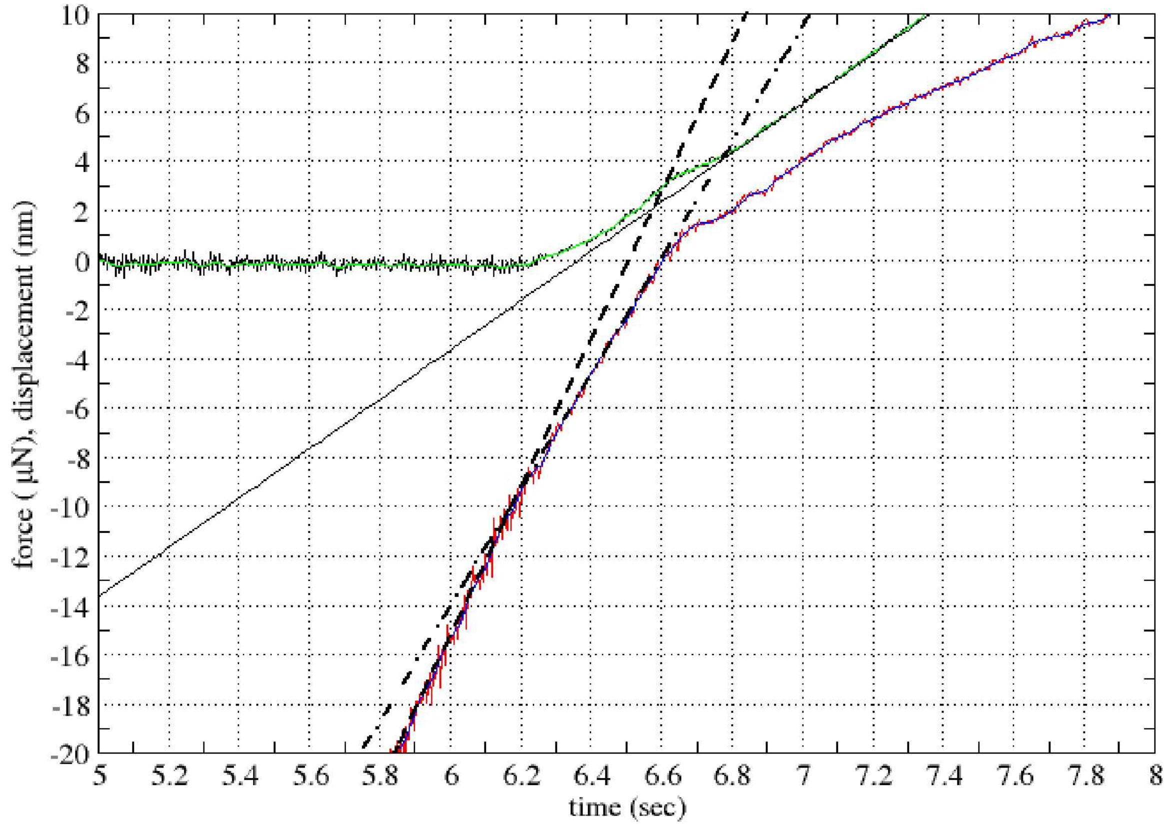
Thank you.

Comparison to Thornton Elastic-plastic Contact Model



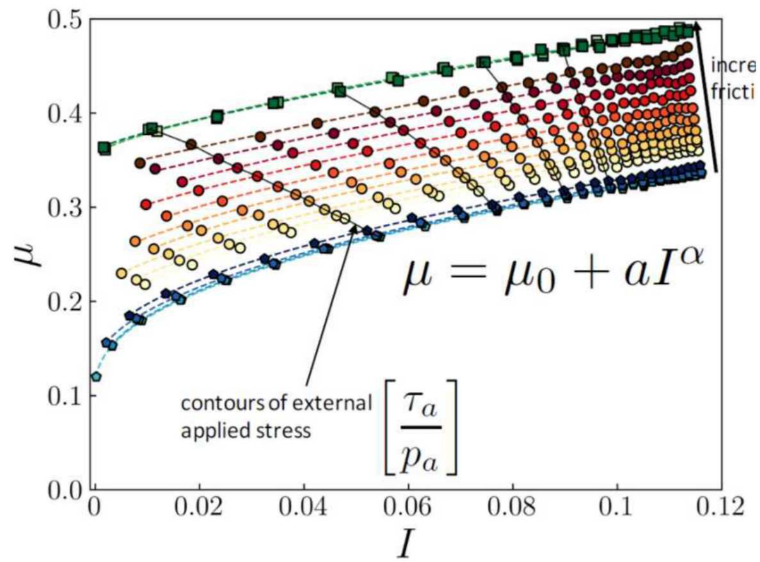


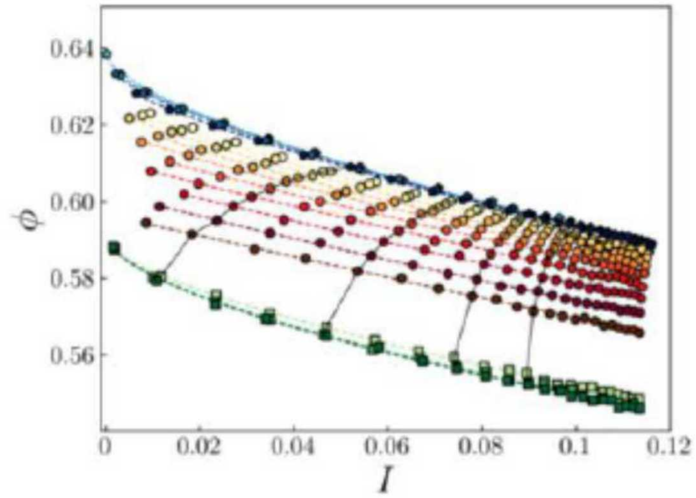
Early time details – where's the zer ?



How Does Powder Flow?

- Apply stress state consistent with viscometric flow
- Decompose macroscopic/bulk flow
  - Homogeneous
  - Planar → viscometric
- For incompressible simple fluid, three viscometric functions necessary for full rheological description
  - Shear viscosity
  - Two normal stress differences





Normal Stresses in Steady Granular Flows

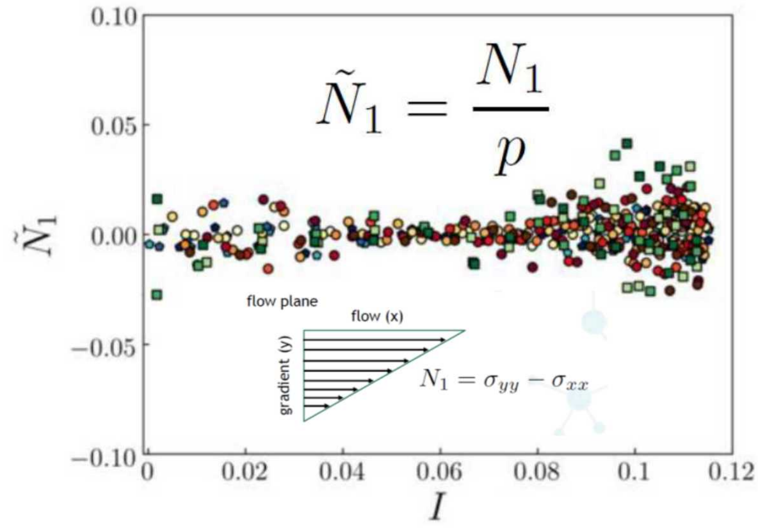
- Steady-state flows of isotropic granular particles are
  - Not complex
    - Stress and strain-rate tensors are aligned
  - Not co-directional
    - Magnitudes of stress and strain-rate in principle directions are different
  - Coaxial

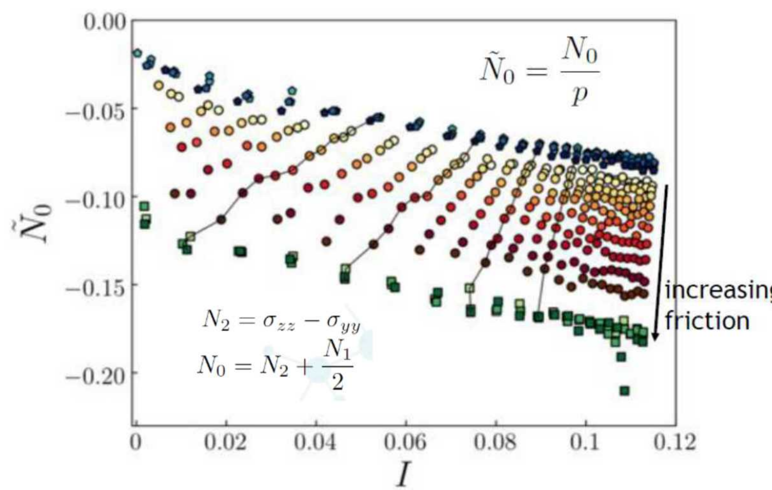
stress tensor in planar xy-shear

$$\boldsymbol{\sigma} = \begin{pmatrix} p & \tau & 0 \\ \tau & p & 0 \\ 0 & 0 & p' \end{pmatrix} p' < p$$

flow functions in dense granular flows

$$\mu(I) \quad \phi(I) \quad \tilde{N}_0(I)$$





Statistical Analysis and Optimization for Control of Heterogeneous Materials