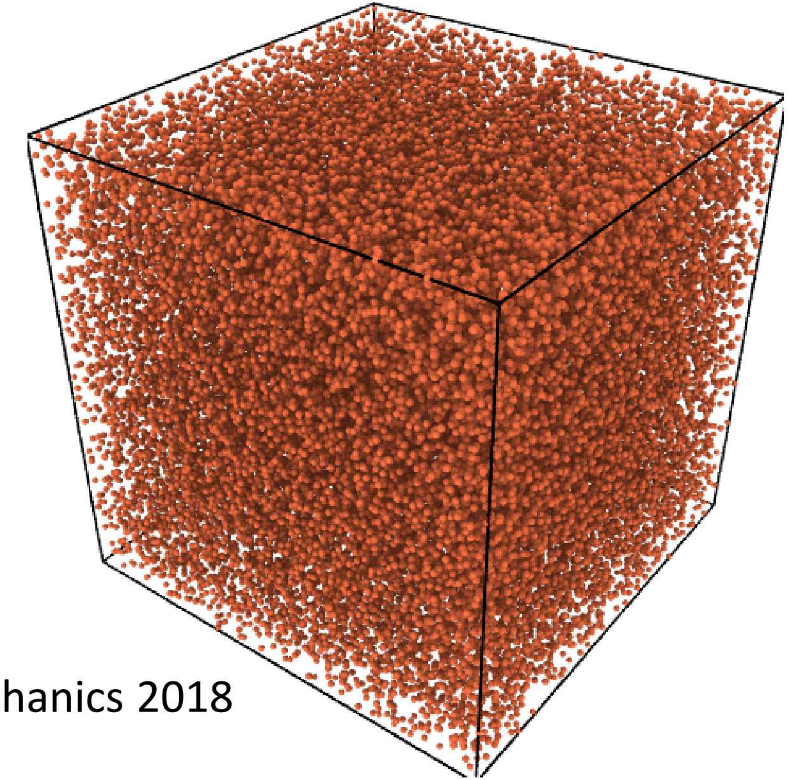
Stress-based simulations: predictions of granular flow-arrest transition and continuum rheology

SAND2018-6932C



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Flow Regimes in Frictional Granular Materials

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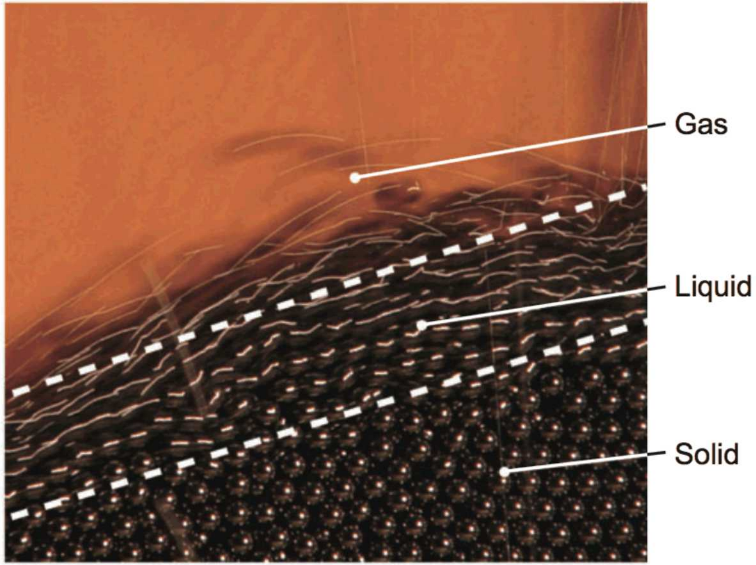
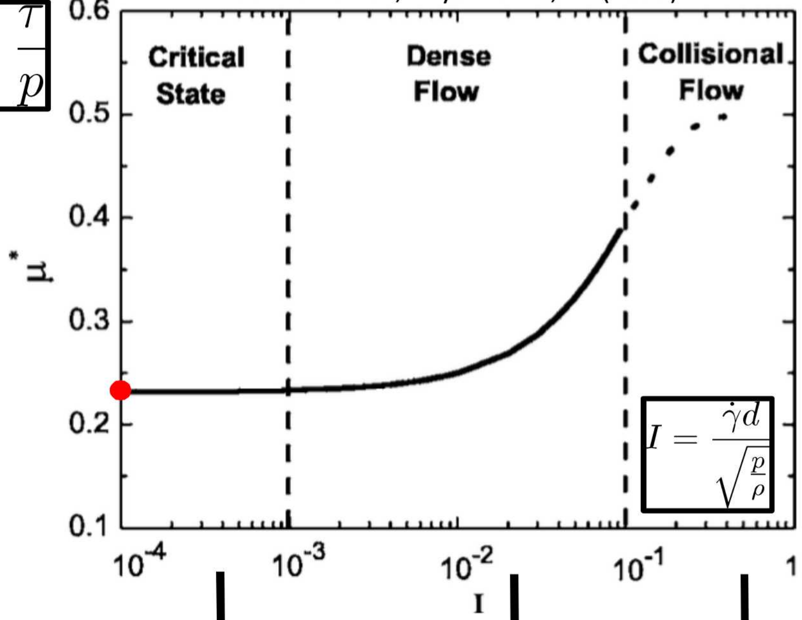
Forterre and Pouliquen, Ann. Rev. Flu. Mech., 40 (2008)



da Cruz et. al., Phys. Rev. E, 72 (2005)

$$\mu = \frac{\tau}{p}$$



rate-independent quasi-static; yield surface concept

Bingham-type visco-plastic rheology

Bagnold regime; kinetic theories

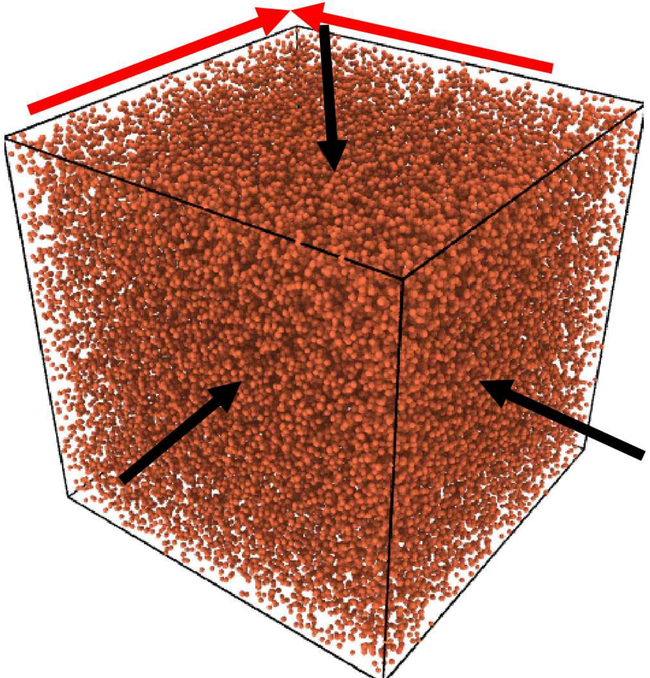
Key aspects analyzed:

- Dynamics of a granular material near the phase transition between flowing and arrest
- Three-dimensional rheology in the flowing state

Stress Boundary Conditions: Granular RVE

second Piola-Kirchhoff stress
(thermodynamic tension)

$$\sigma_a = p_a I + \begin{bmatrix} 0 & \tau_a & 0 \\ \tau_a & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$



Parinello-Rahman dynamics
isenthalpic-isotension ensemble

- fully periodic with no surface effects
- uniform boundary stress state
- homogenous boundary deformation
- stable during jamming and finite-rate flows

Macroscopic Observables:

volume fraction: $\phi(t)$

accumulated strain (3D): $\epsilon(t)$

instantaneous strain rate (3D): $\dot{\epsilon}(t)$

internal stress (3D): $\sigma(t)$

Constant Shear Stress and Pressure Simulations

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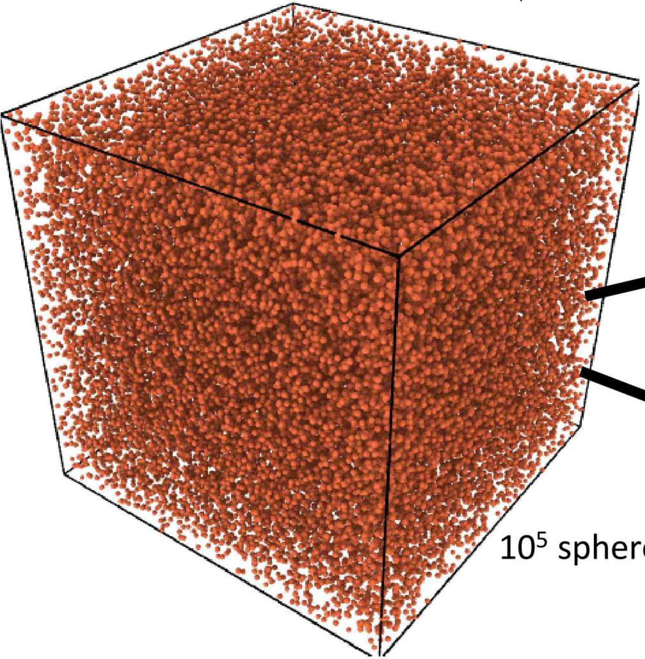
initial low-density assembly: $\phi = 0.05$

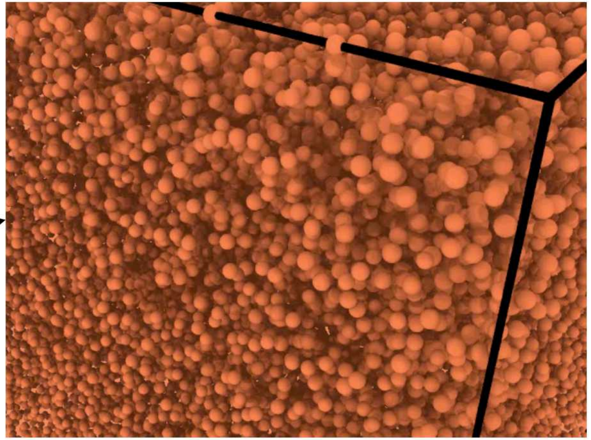


10^5 spheres

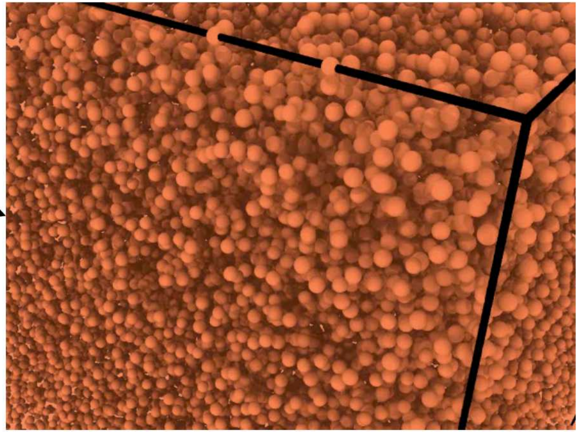
applied stress

$$\sigma_a = p_a I + \begin{bmatrix} 0 & \tau_a & 0 \\ \tau_a & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

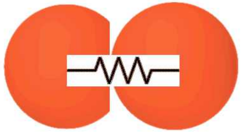
arrest



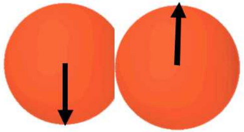
steady flow



harmonic contacts

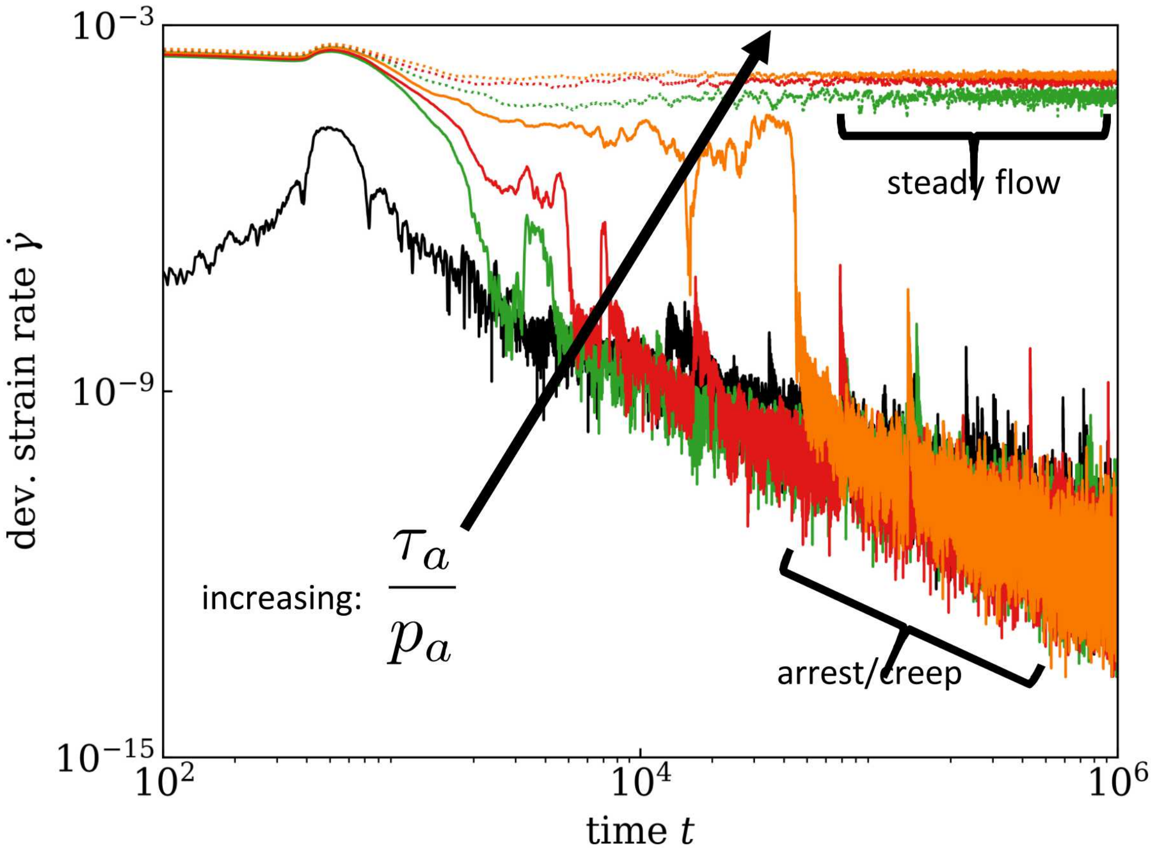


Coulomb microscopic friction



$||F_s|| < \mu_s ||F_n||$

Strain-rate Evolution: Arrest (creep) vs. Steady Flow



shear rate

$$\dot{\gamma} = \sqrt{0.5\dot{\gamma}_{ij}\dot{\gamma}_{ij}}$$

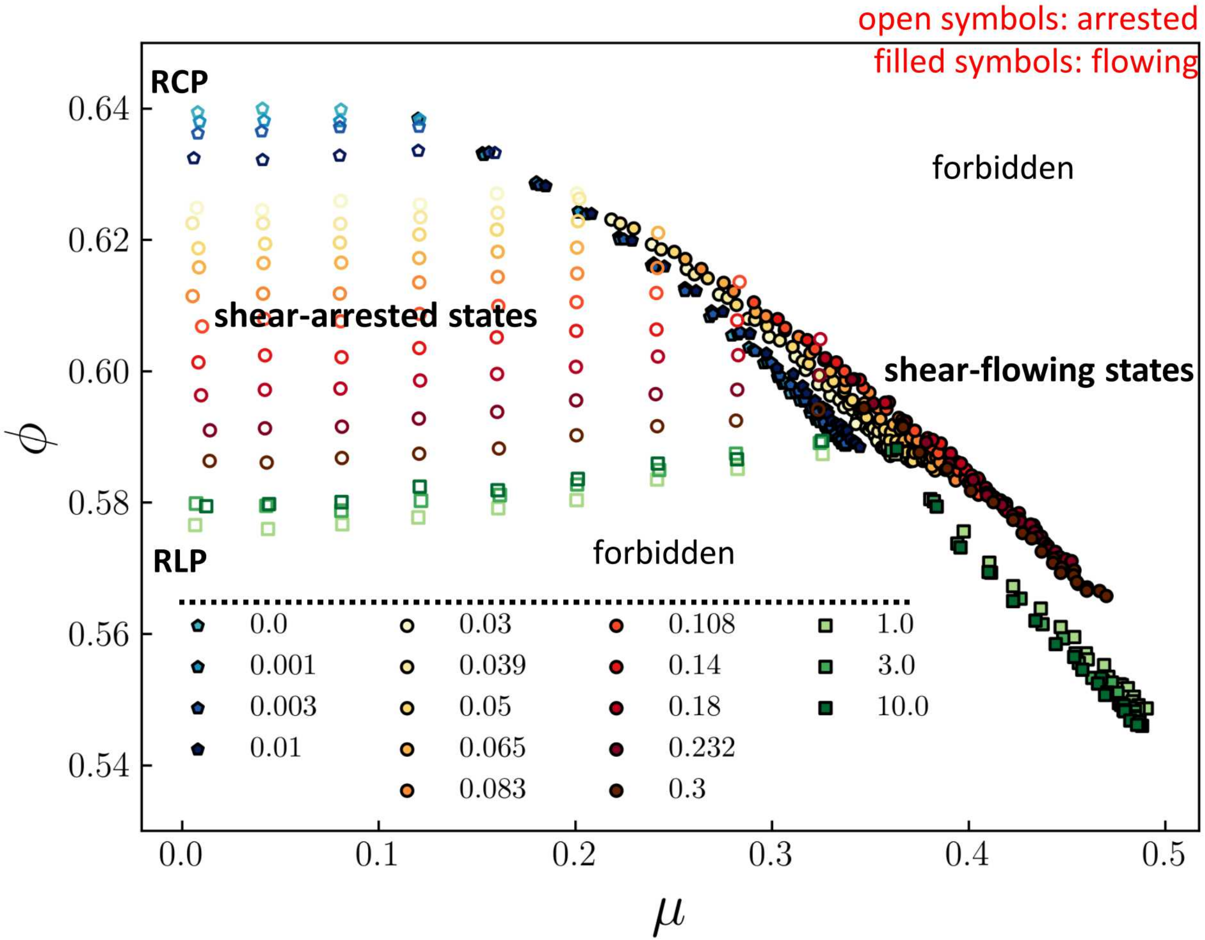
Steady Flow:

- constant strain rates at long times
- strain rate is shear stress dependent (monotonically increasing)

Arrest/Creep:

- orders of magnitude drop in strain rate during creep towards an arrested state

Steady-State Flow-Arrest Phase Diagram



$$p = \frac{1}{3}\mathrm{tr}[\sigma] \qquad \sigma_d = \sigma - pI$$

$$\mu = |\sigma_d|/p\sqrt{2}$$

Drucker-Prager

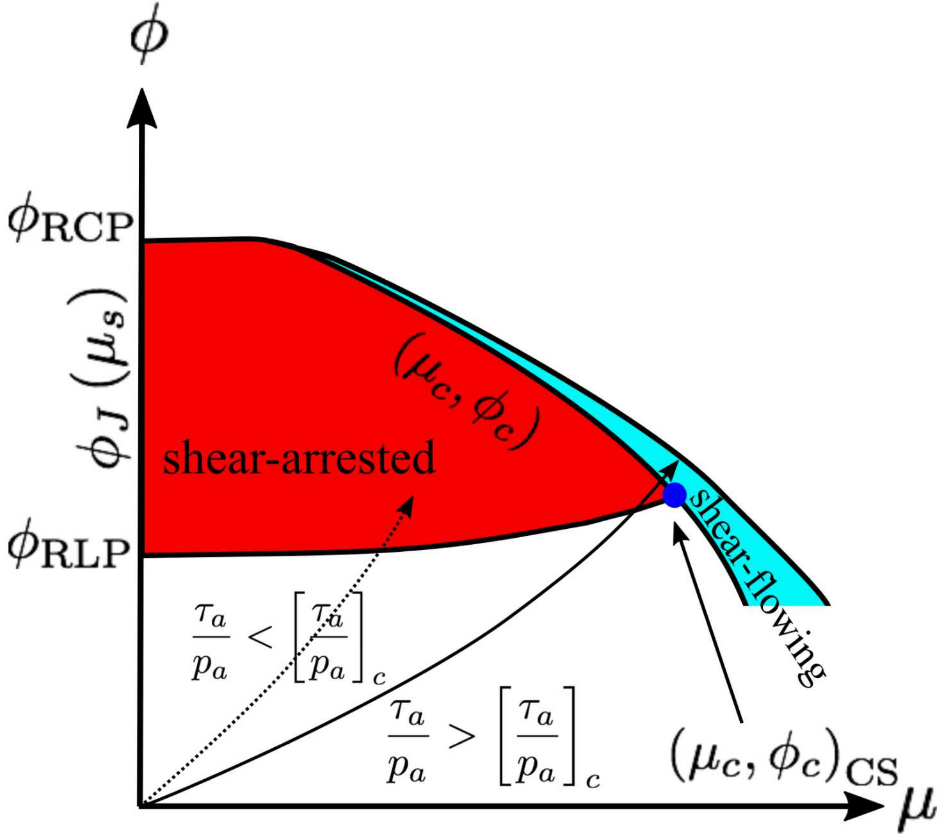
Steady Flow:

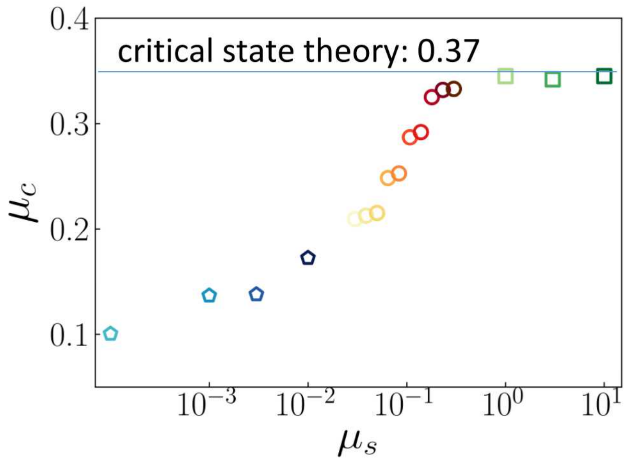
- significant ***dilation*** as shear stress is increased for all microscopic friction
- ***static yield stress*** strongly depends on microscopic friction (increases)

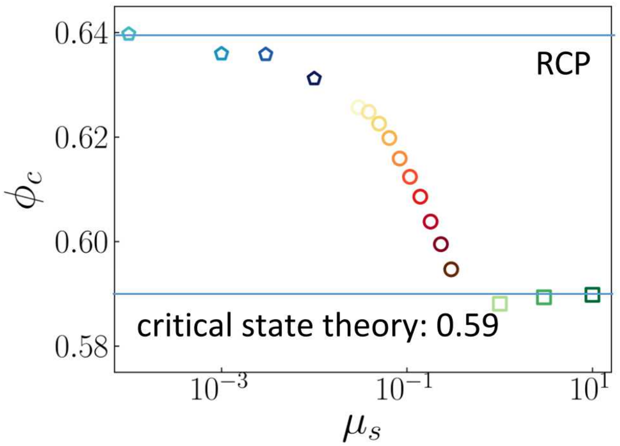
Arrest/Creep:

- shear-arrested states show increased ***compaction*** as the flow-arrest phase boundary is approached
- relative magnitude of compaction increases with increasing microscopic friction

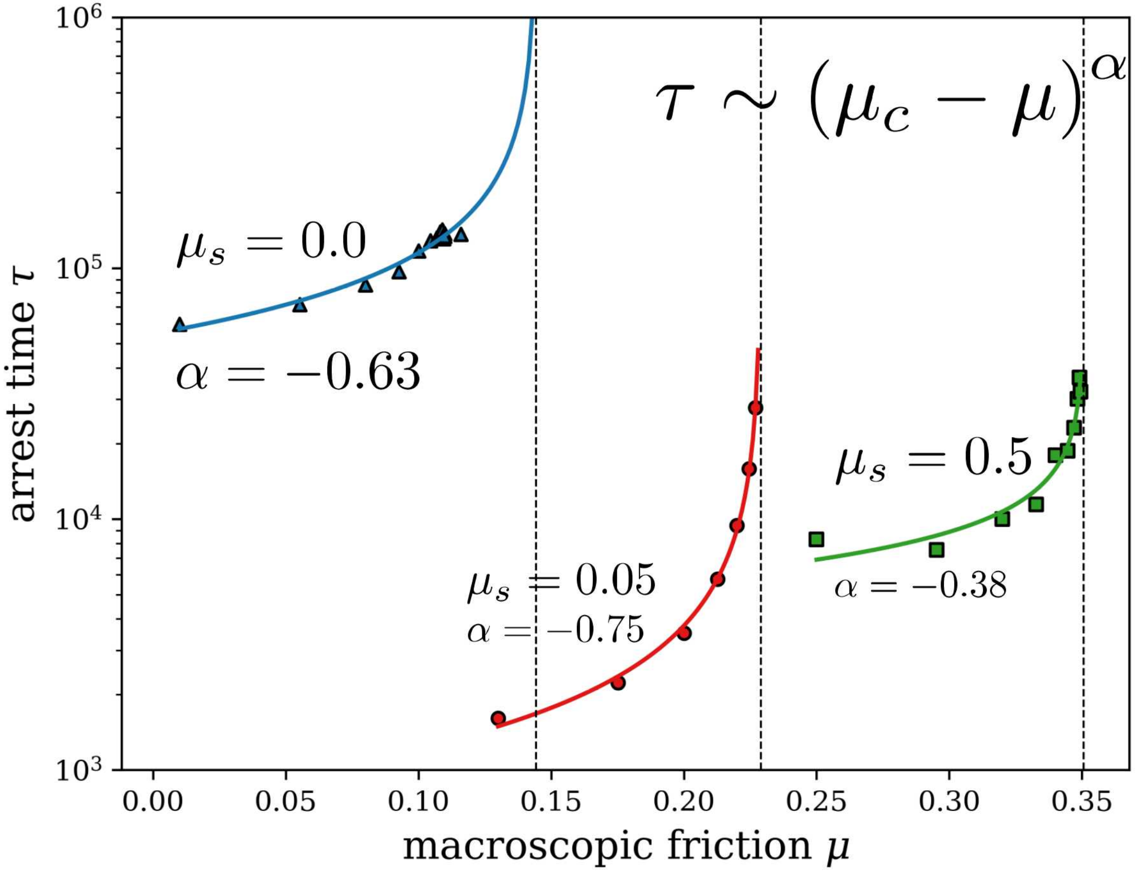
Steady-State Flow-Arrest Phase Diagram: Critical Points

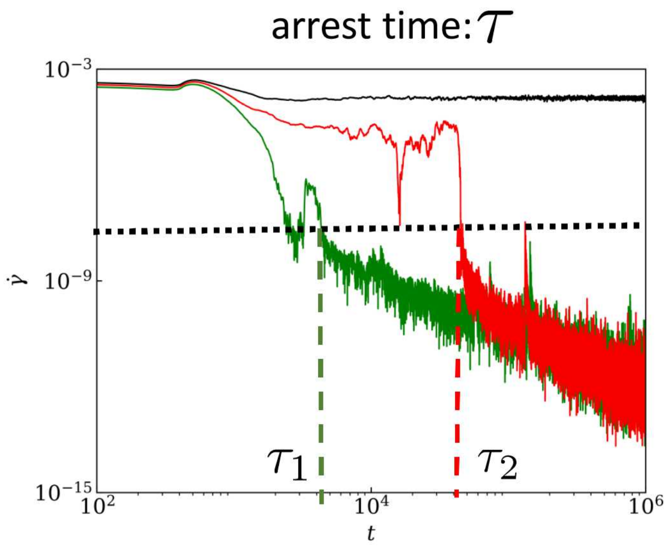






Flow-Arrest Phase Transition: Power-law Scaling

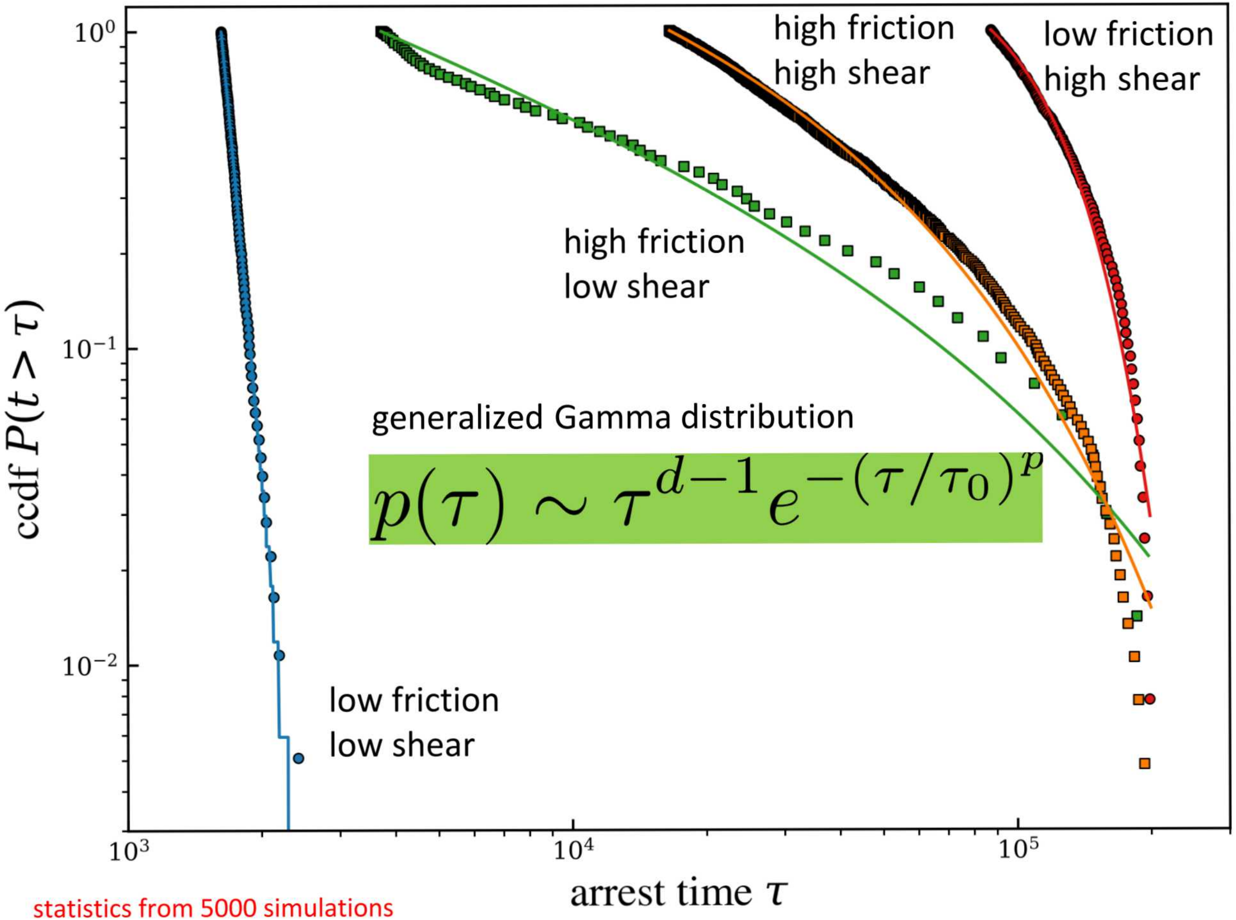




- power law scaling enables precise computation of the ***critical yield stress***
- time to arrest below yield diverges at the critical yield stress as a power law
- sensitivity of the arrest time to the distance to critical yield stress increases with decreasing microscopic friction

averaged over 100 simulations

Arrest Times Distribution



statistics from 5000 simulations

applied stress:
distance from yield stress

$$\mu_c - \mu = 10^{-3}, 10^{-1}$$

microscopic friction

$$\mu_s = 0.05, 0.5$$

- **long-tailed** distribution**:** generalized Gamma distribution
- **large variance** near critical yield stress
- variance more sensitive to shear for smaller microscopic friction: could be because of increased fluctuations (noise) at particle-particle contacts (DeGiuli and Wyart, PNAS 2017)

Stress States at Yielding and Flow

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$$\Delta E(t) = \int_{\Gamma} f_i \Delta u_i \mathrm{d}S - \int_{V} \sigma_{ij} \frac{\partial \left(\Delta u_i\right)}{\partial x_j} \mathrm{d}V$$

change in kinetic energy — boundary traction work — second order work (constitutive)

Arrest (Jammed): $$\int_{\Gamma} f_i \Delta u_i \mathrm{d}S = \int_{V} \sigma_{ij} \frac{\partial \left(\Delta u_i\right)}{\partial x_j} \mathrm{d}V$$

equilibrium: balance of internal and external stress

Yielding: $$\int_{\Gamma} f_i \Delta u_i \mathrm{d}S > \int_{V} \sigma_{ij} \frac{\partial \left(\Delta u_i\right)}{\partial x_j} \mathrm{d}V$$

rapid increase in kinetic energy: imbalance of internal and external stresses

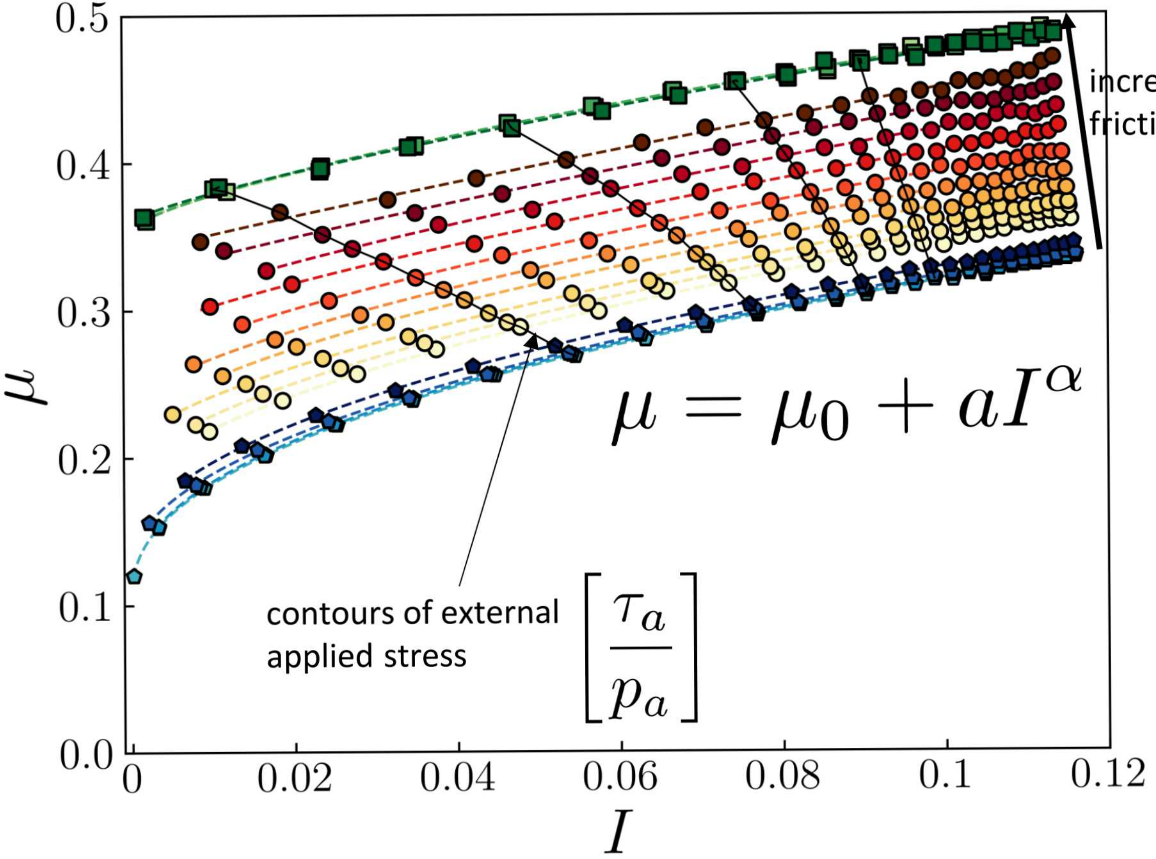
Nicot et. al., IJP, 29 (2012)
Hill, J. Mech. Phys. Sol., 6, 1958

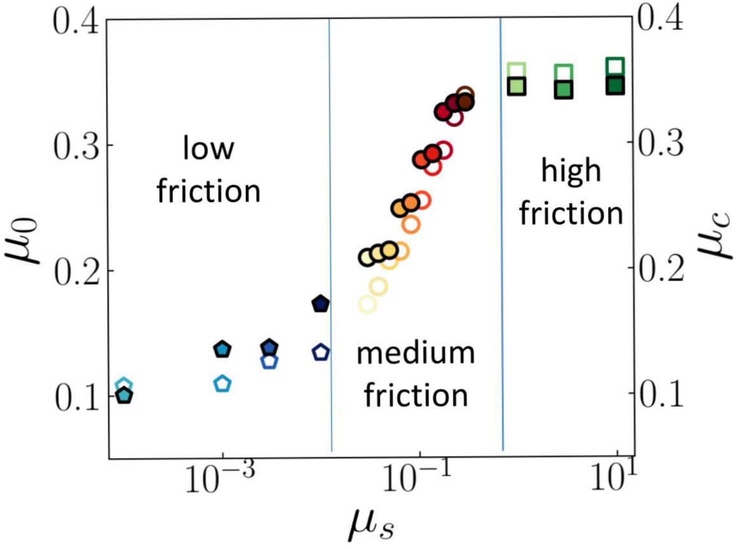
Steady State Flow: Rheology

$$\mu = |\sigma_d|/p\sqrt{2}$$

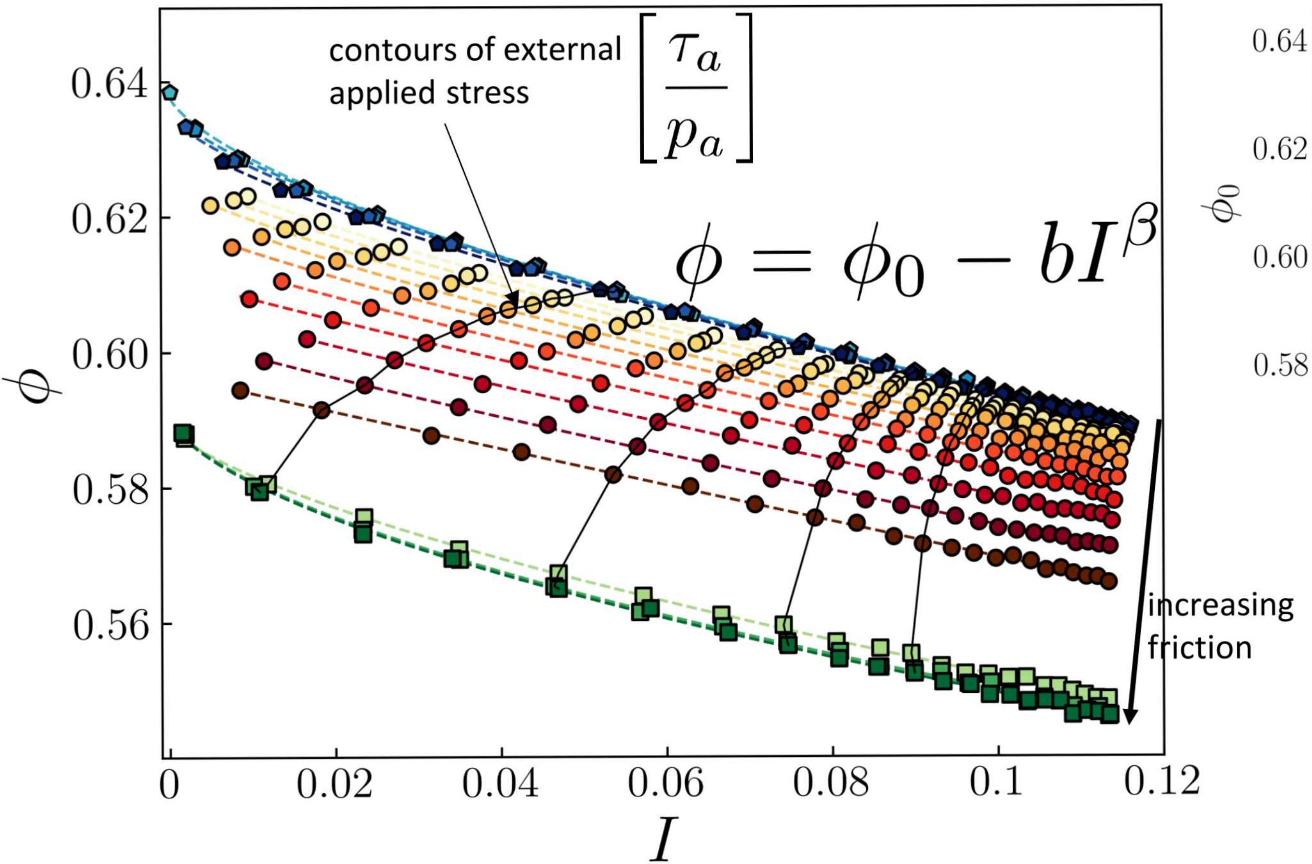
$$I = |\dot{\gamma}|d/\sqrt{p/\rho}$$

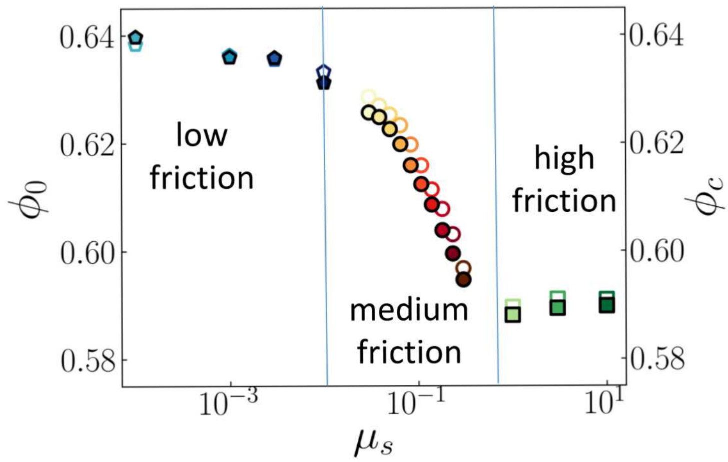
Jop et. al., Nature, 441, 2008



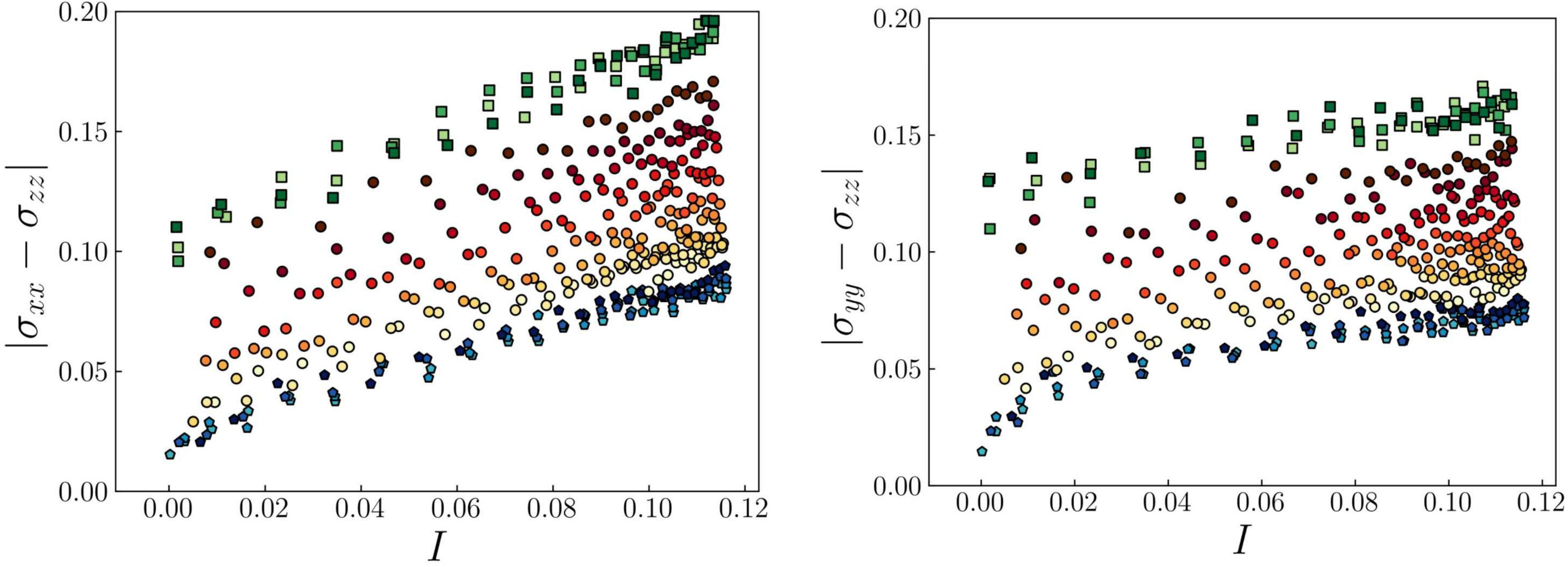


Steady State Flow: Dilation





Steady State Flow: Normal Stress Differences



- although granular materials dilate to flow, they're incompressible in steady state
- rheology, however, can not be described by a shear viscosity function alone
- systematic variations in the two normal stress differences are observed
- is this an example of viscometric flow characterized by viscosity and normal stress difference functions?
- need to check co-axiality/co-directionality of the flows to probe any non-viscometric behavior

Conclusions

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- a homogenous stress-based method enables probing flow-arrest transition and three-dimensional granular rheology
- power-law divergence at the transition and critical phase transition line is identified; shows correspondence with known results from soil mechanics and jamming literature
- granular rheology (three-dimensional) is more complicated than predicted by \mu(I) rheology; existence of normal stress difference functions indicate possibility of viscometric flows

Future Work

- subject frictional granular materials to more ***complex stress loading paths*** to predict 3D rheology; check for non-viscometric flows

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