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Flow-Arrest Transition in (Frictional) Granular Materials

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Sandia National Laboratories

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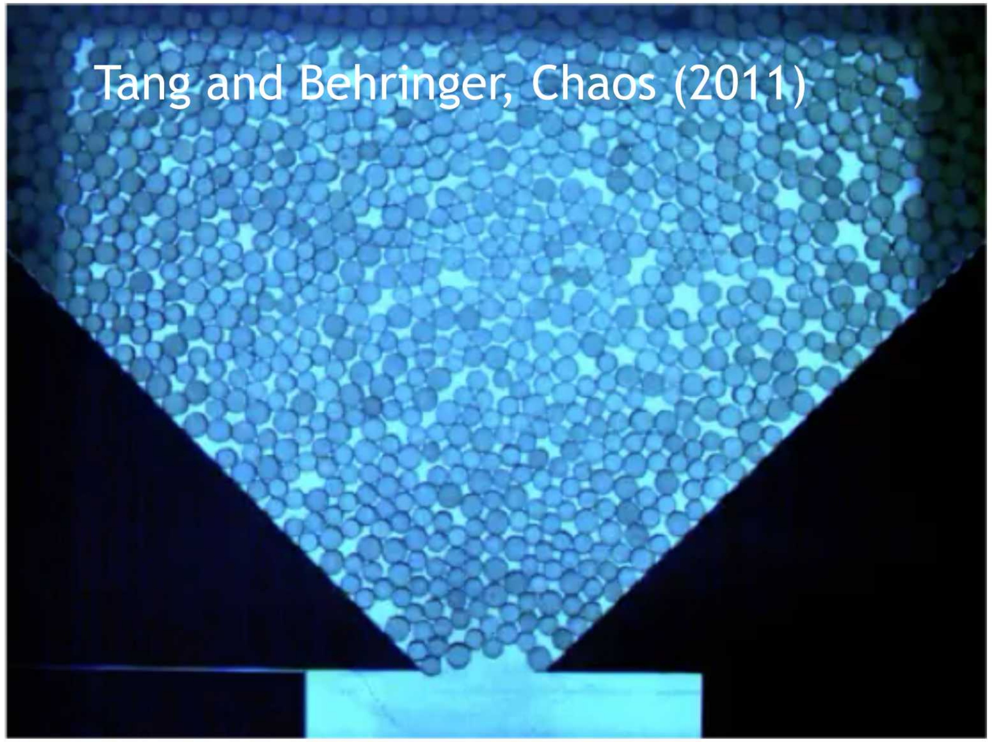
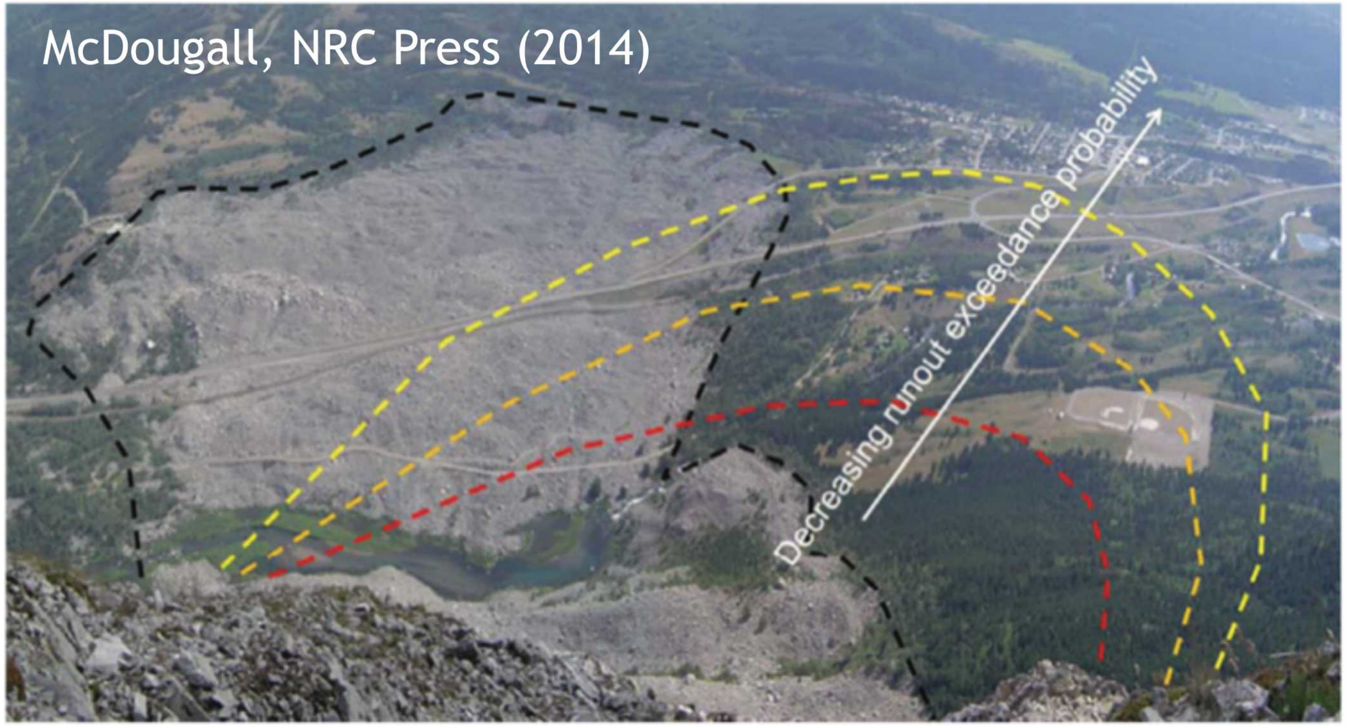
Flow-Arrest Transition in Granular Materials

clogging in hopper

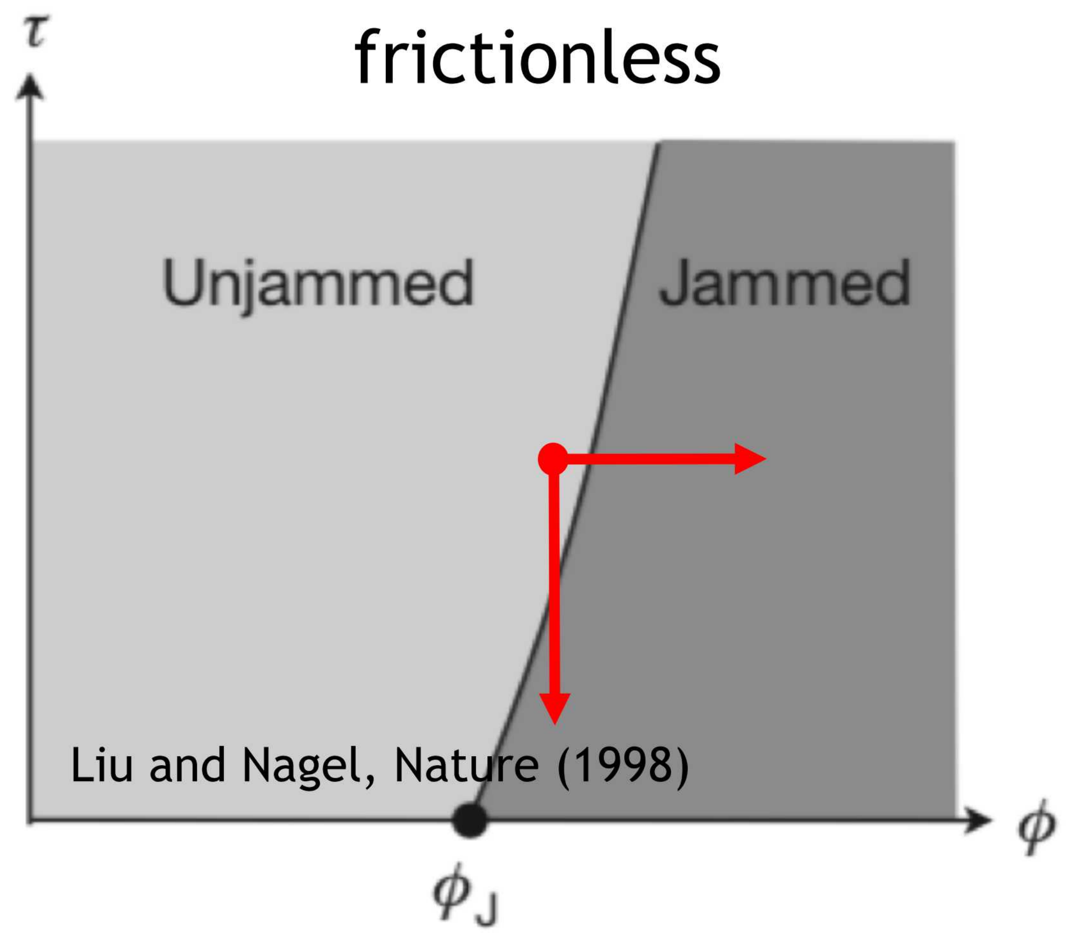


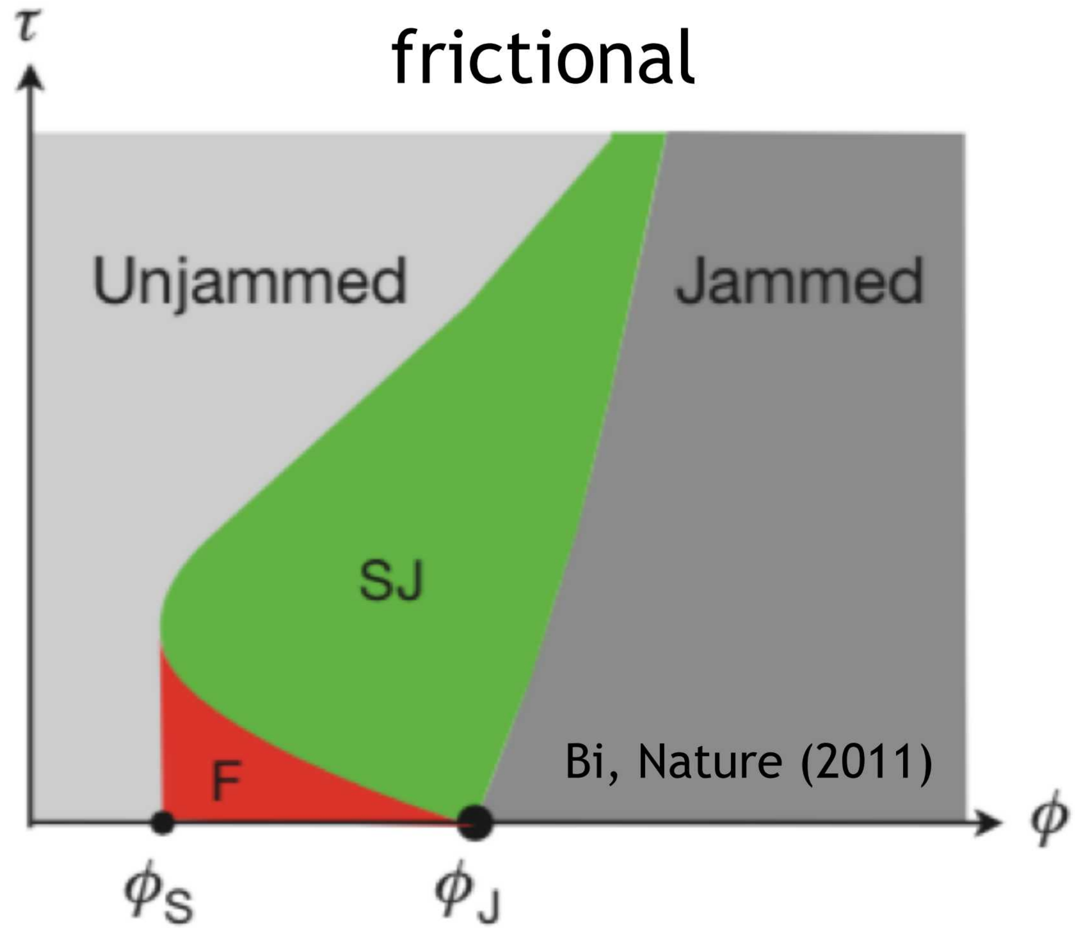
landslide runout probability



1. Will the flow arrest?
2. When will the flow arrest?
3. If it flows, how does it flow?

Will Flowing Granular Material Arrest (Jam)?

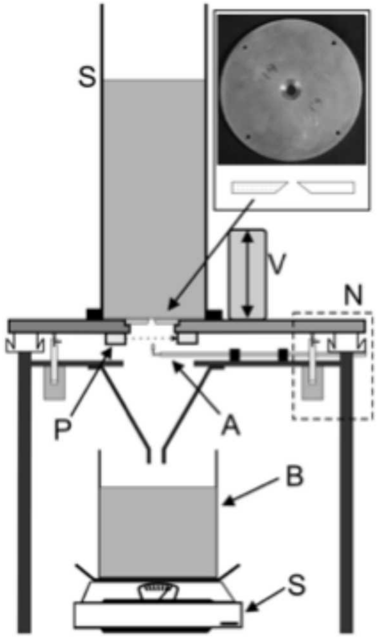


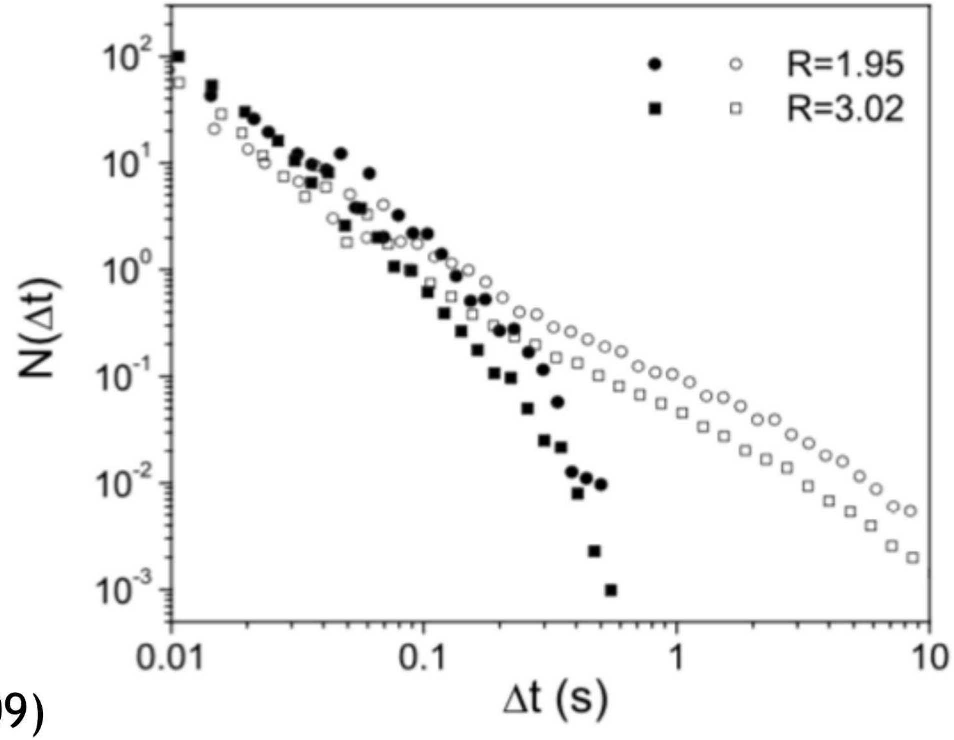


what is the phase diagram under controlled pressure conditions?

When will Flowing Granular Material Arrest?

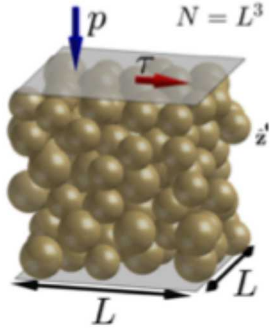
distribution of clog times in silo discharge

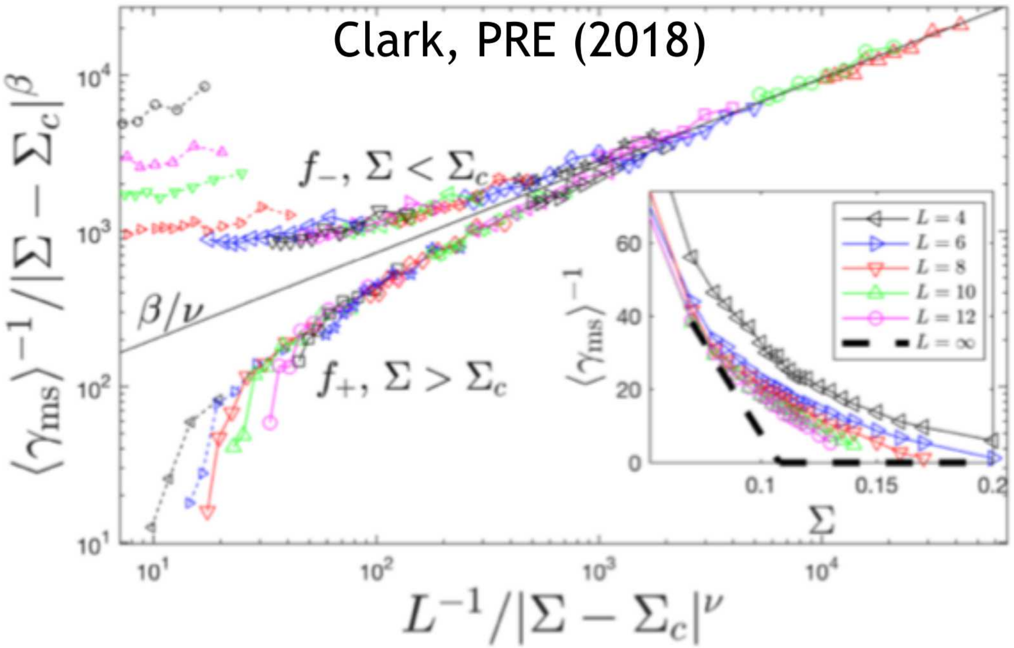




Mankoc, PRE (2009)

diverging shear-jamming strain near yield stress





Clark, PRE (2018)

need a better characterization of transients before arrest

When it does Flow, how does it Flow? (Rheology)

inertial granular rheology

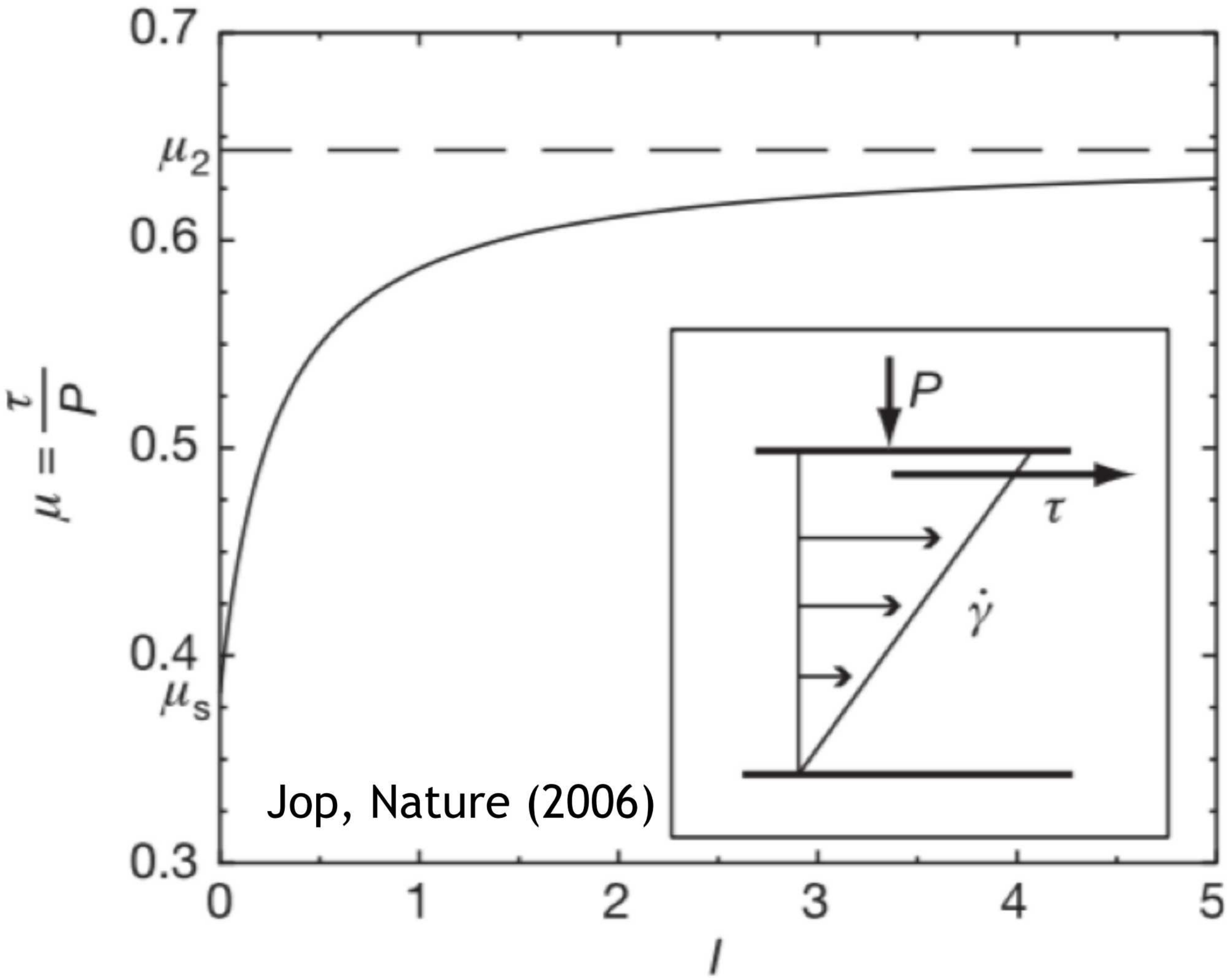
inertial Number: $I = \dot{\gamma} d \sqrt{\frac{\rho}{P}}$

(d : diameter
ρ: density)

stress ratio: $\mu = \frac{\tau}{P}$

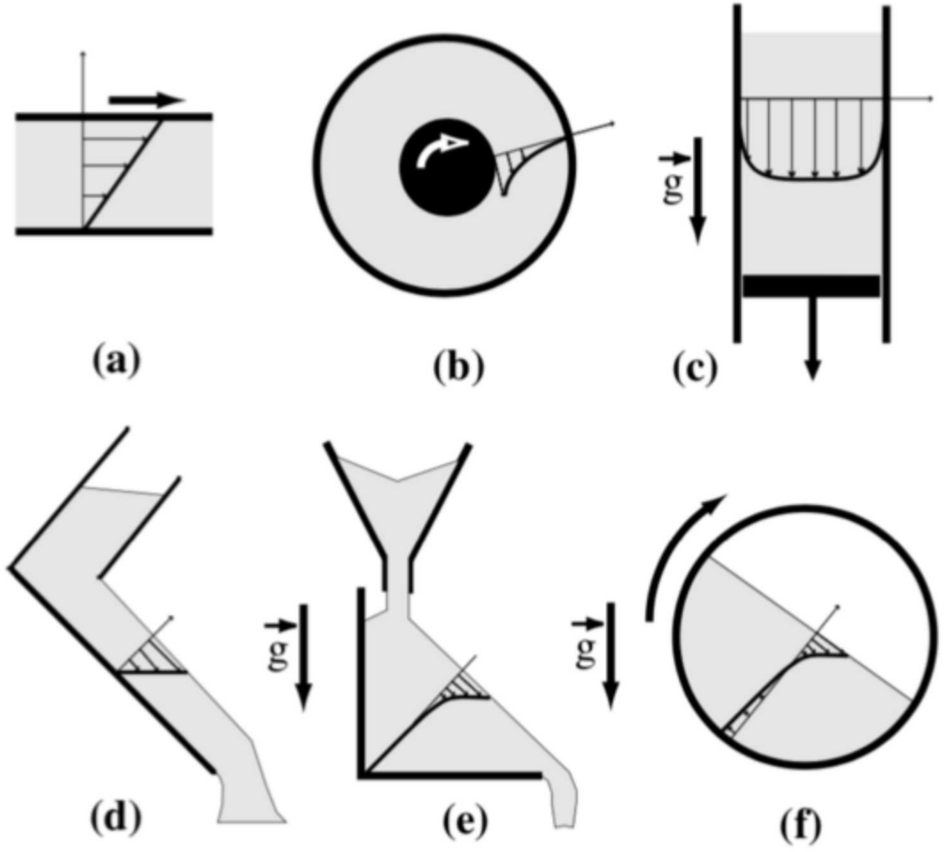
inertial rheology: $\mu(I) = \mu_s + \frac{\mu_s - \mu_s}{I_0/I + 1}$

(monotonic, yield criterion)



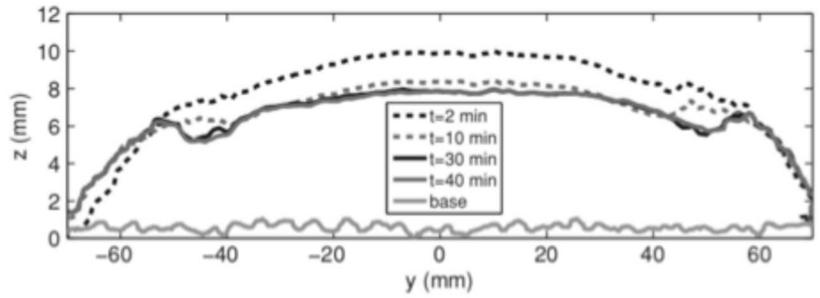
assumes co-directionality of stress and strain rate

Features of 3D Granular Flows

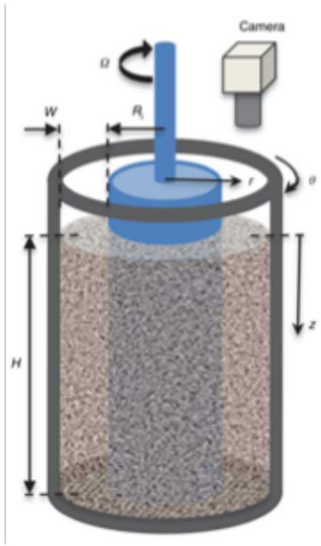


GDR MiDi, EPJ (2004)

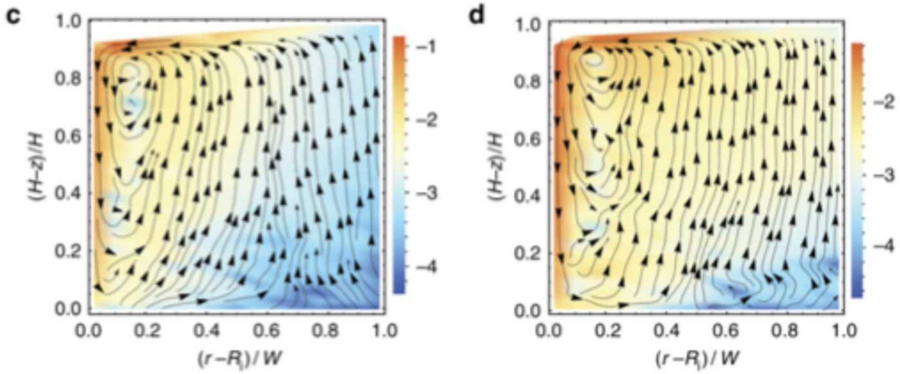
free surface flows



Takagi, PRE (2011)



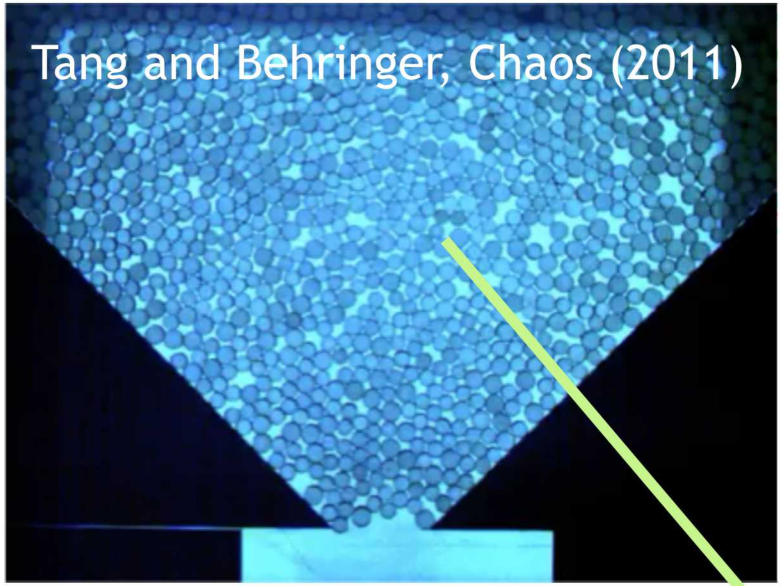
dilation driven vortex flows

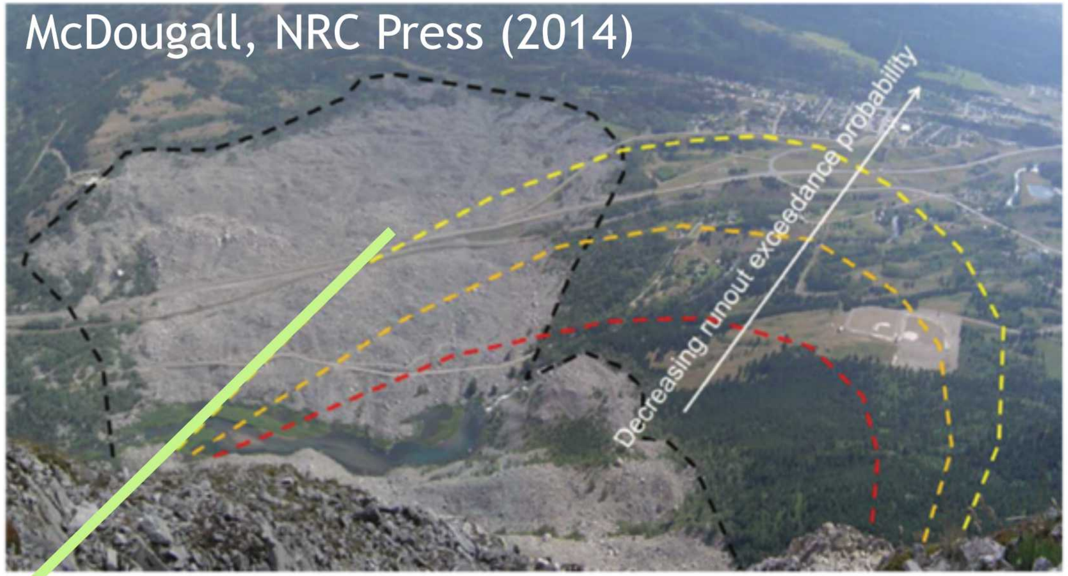


Krishnaraj, Nat. Comm. (2016)

$\mu(I)$ rheology does not completely characterize 3D granular flows

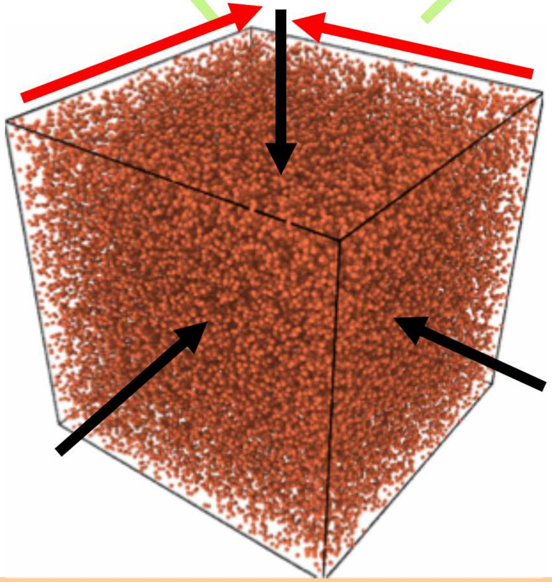
Flow-Arrest Transition: Problem Statement


Tang and Behringer, Chaos (2011)



McDougall, NRC Press (2014)

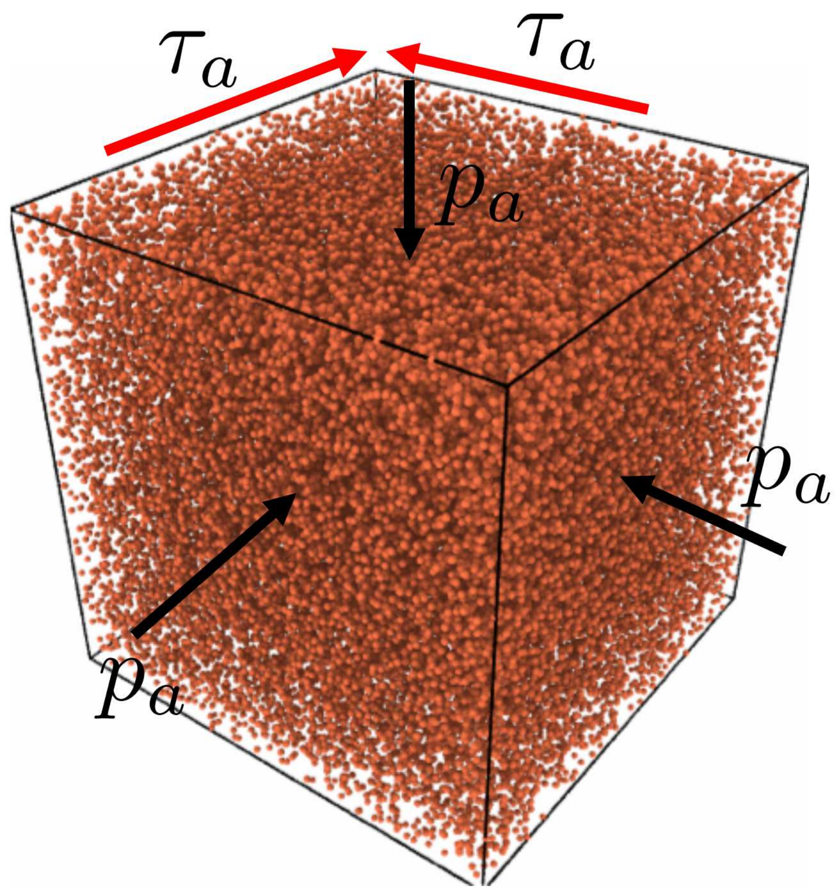
representative volume element under shear & pressure



under prescribed shear and pressure:

1. Will the flow arrest?
2. When will the flow arrest?
3. If it flows, how does it flow?

DEM Simulation Protocol



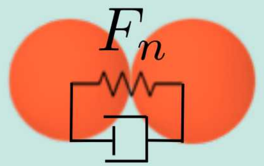
$$\boldsymbol{\sigma}_a = p_a \boldsymbol{I} + \begin{bmatrix} 0 & \tau_a & 0 \\ \tau_a & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Parinello-Rahman dynamics
(isenthalpic-isotension ensemble in MD)

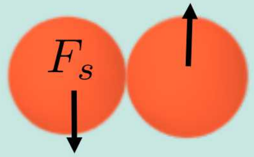
- fully periodic: **no boundary effects**
- uniform surface traction
- homogenous deformation/flow
- no shear bands

contact mechanics

Hookean contacts



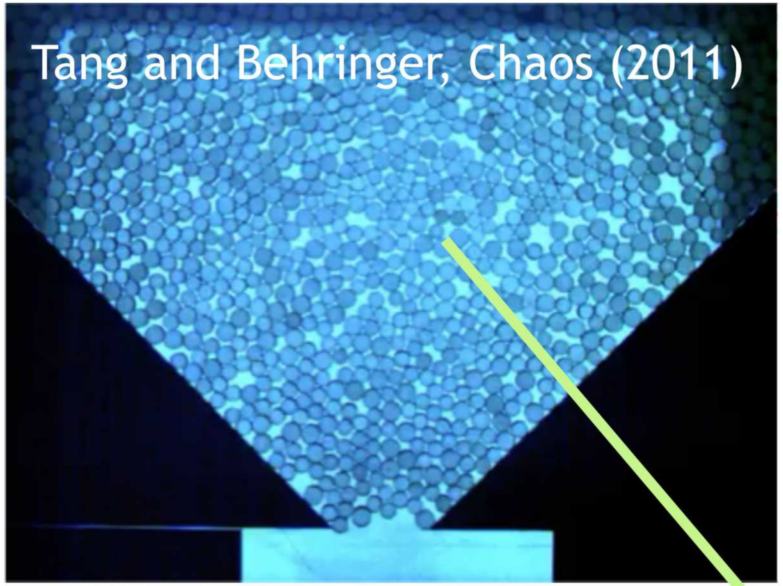
Coulomb surface friction

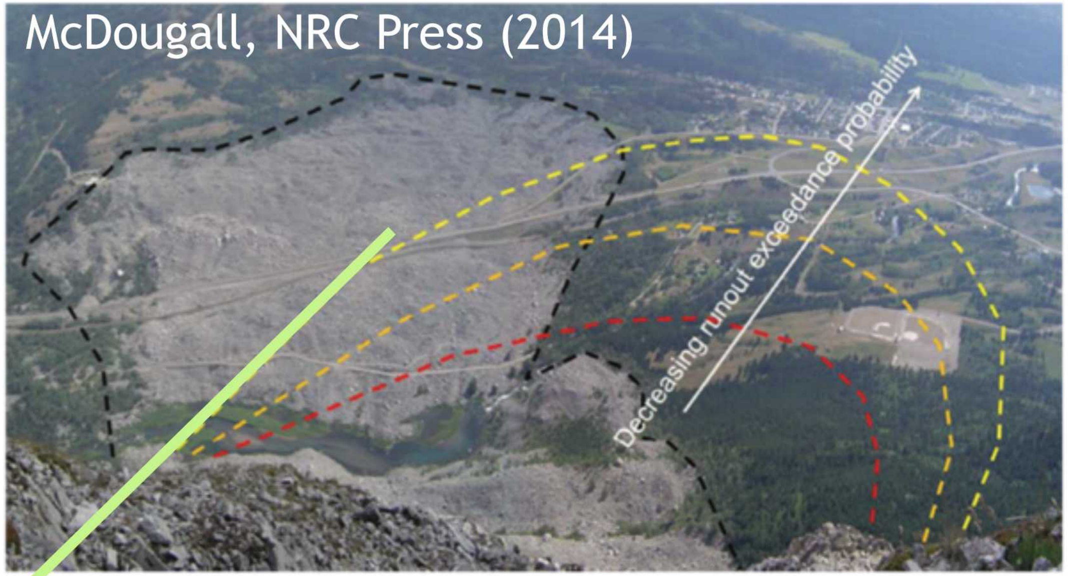


$$||F_s|| < \mu_s ||F_n||$$

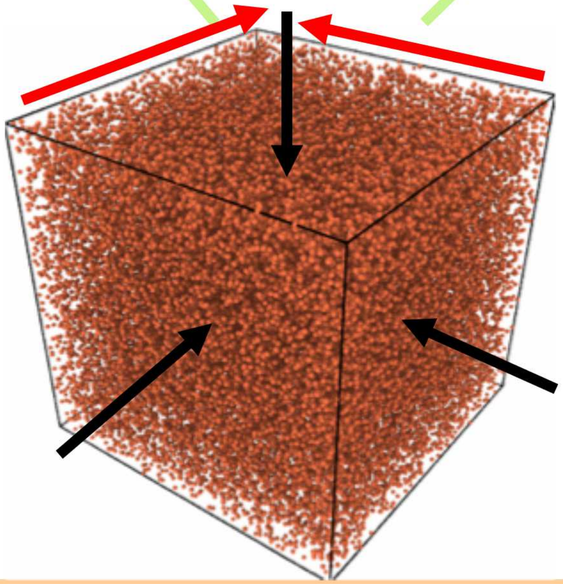
Srivastava et al., PRL, 122 (2019)   **Srivastava** et al., arXiv: 1919.04491

Flow-Arrest Transition: Problem Statement





representative volume element under shear & pressure



under prescribed shear and pressure:

1. Will the flow arrest?
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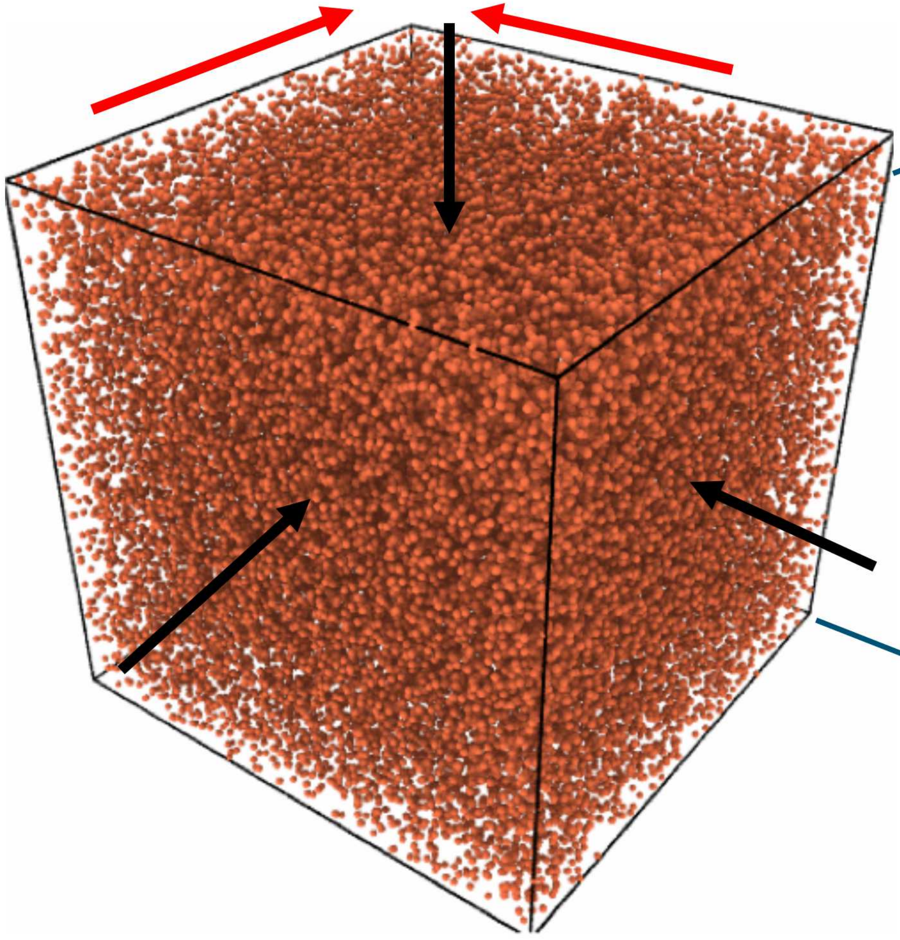
3. If it flows, how does it flow?

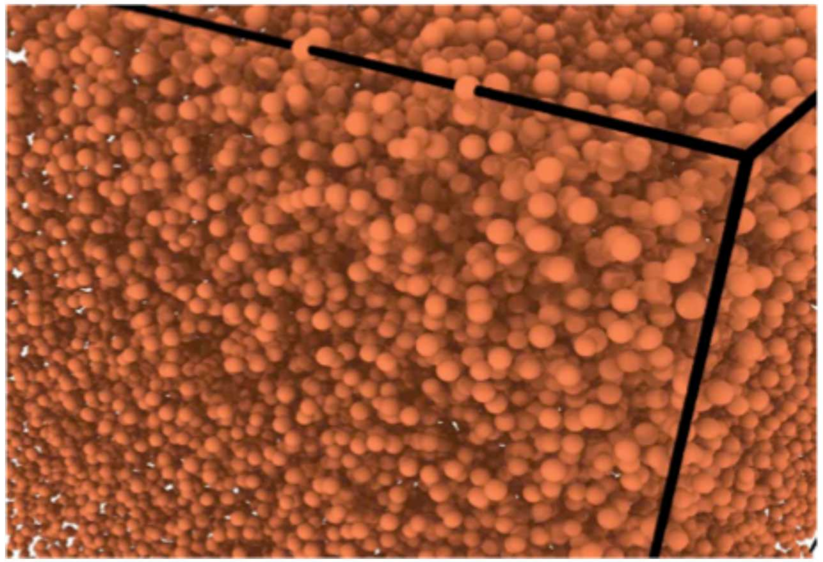
Granular Flow vs. Arrest

initial dilute system: $\phi = 0.05$

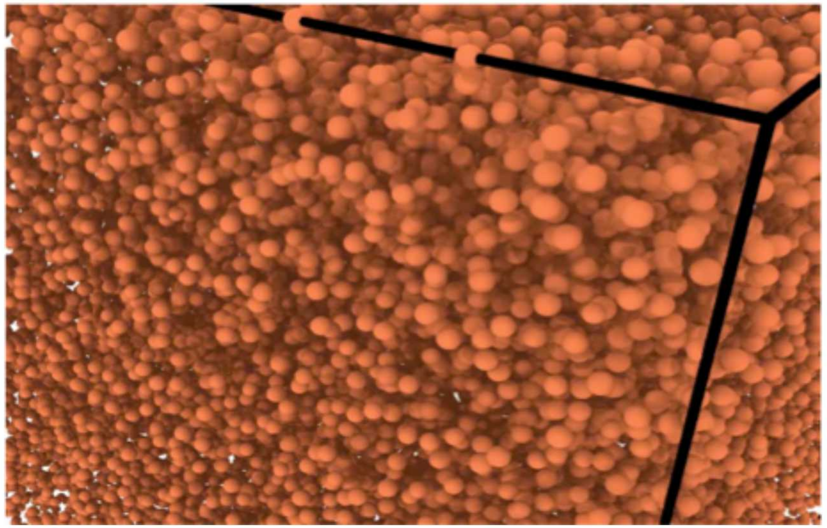


$$\boldsymbol{\sigma}_a = p_a \boldsymbol{I} + \begin{bmatrix} 0 & \tau_a & 0 \\ \tau_a & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

steady flow

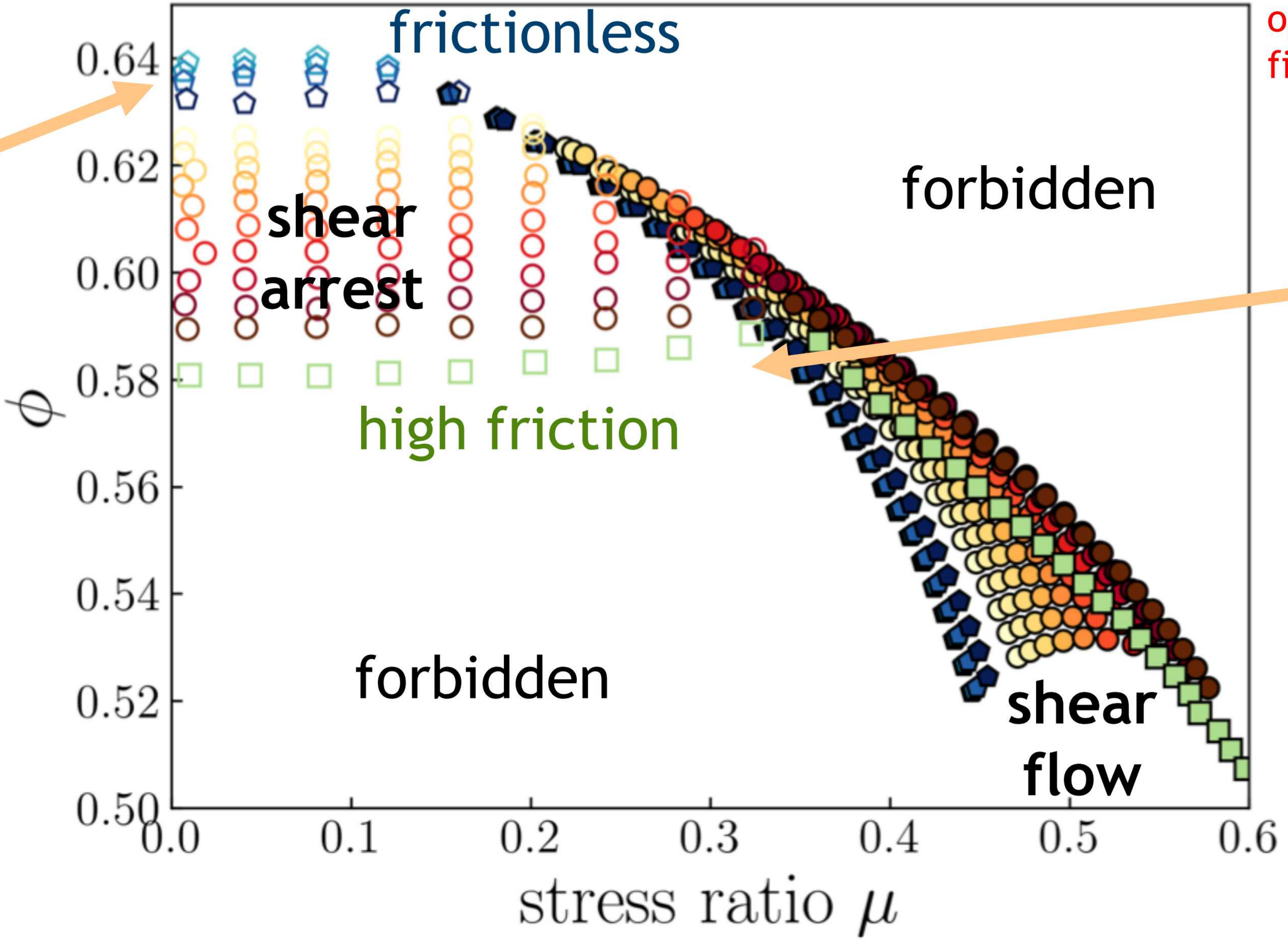


shear arrest



Srivastava et al., PRL, 122 (2019)   **Srivastava** et al., arXiv: 1919.04491

Flow-Arrest Phase Diagram



open symbols: arrest
filled symbols: flow

random close packing

critical state soil mechanics

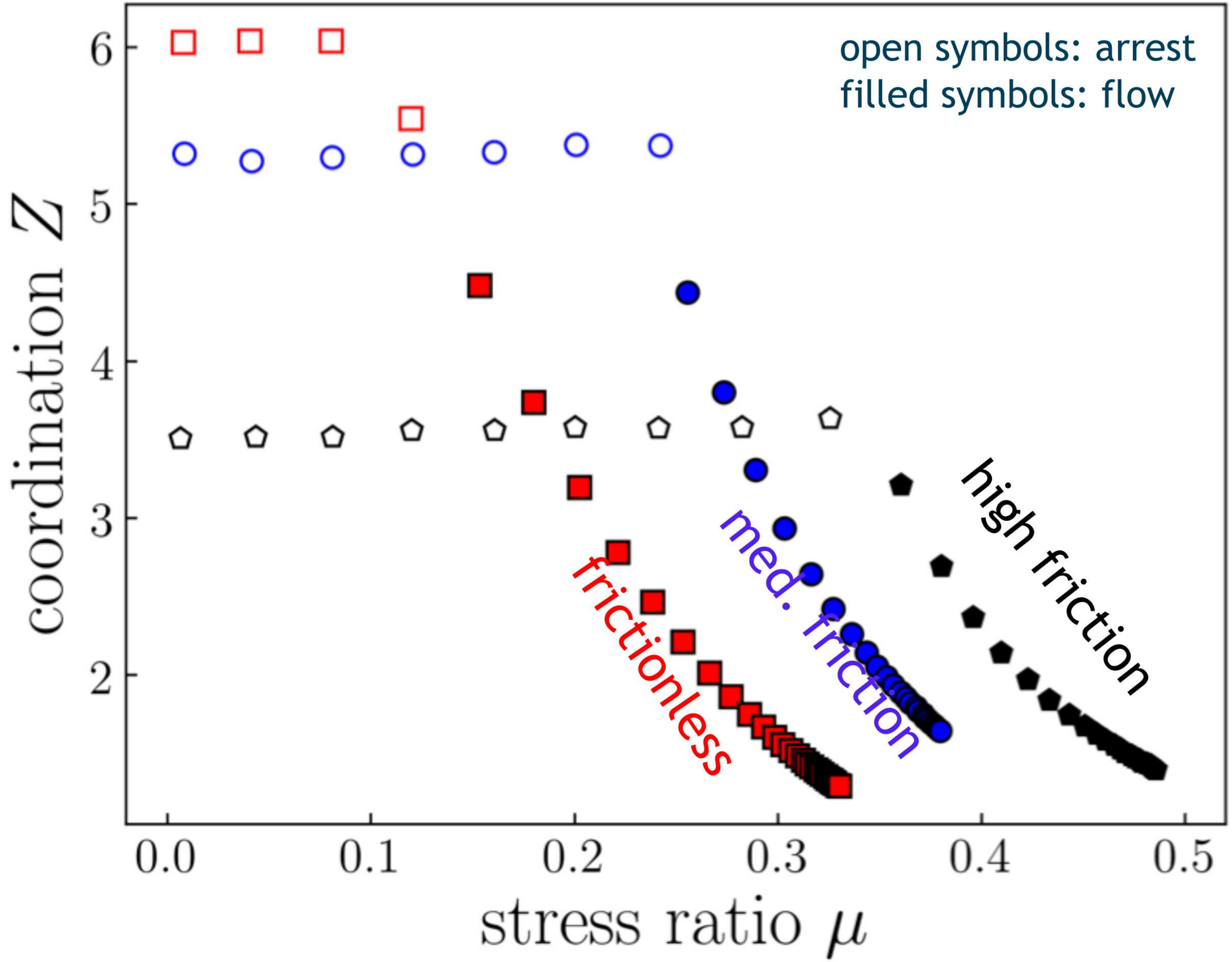
$\mu = 0.36$

$\phi = 0.59$

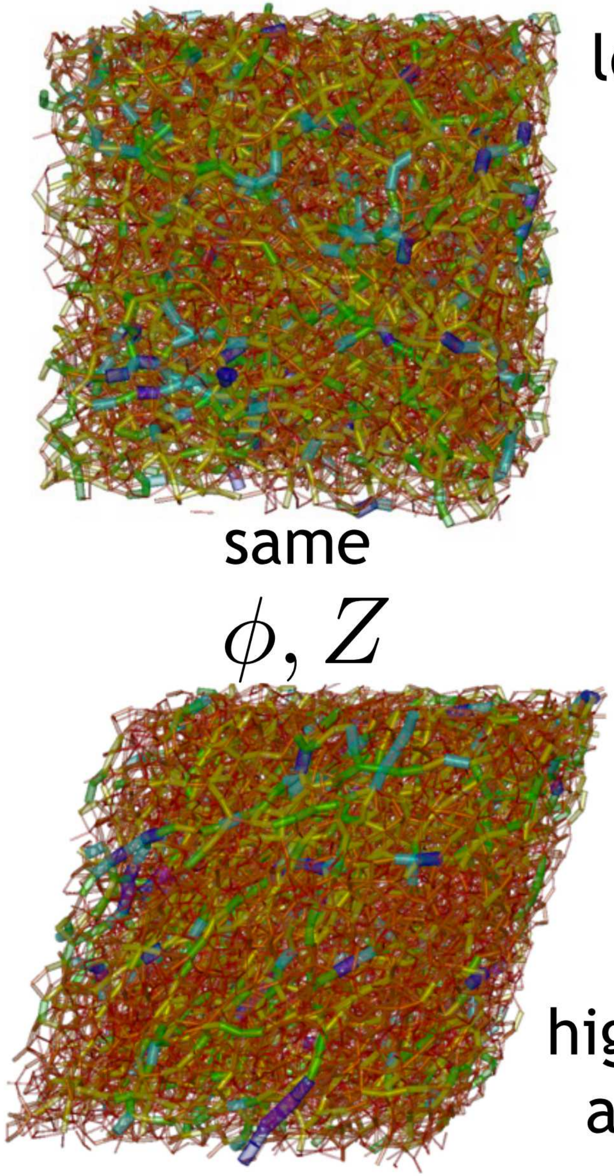
Coordination at Flow-Arrest Transition

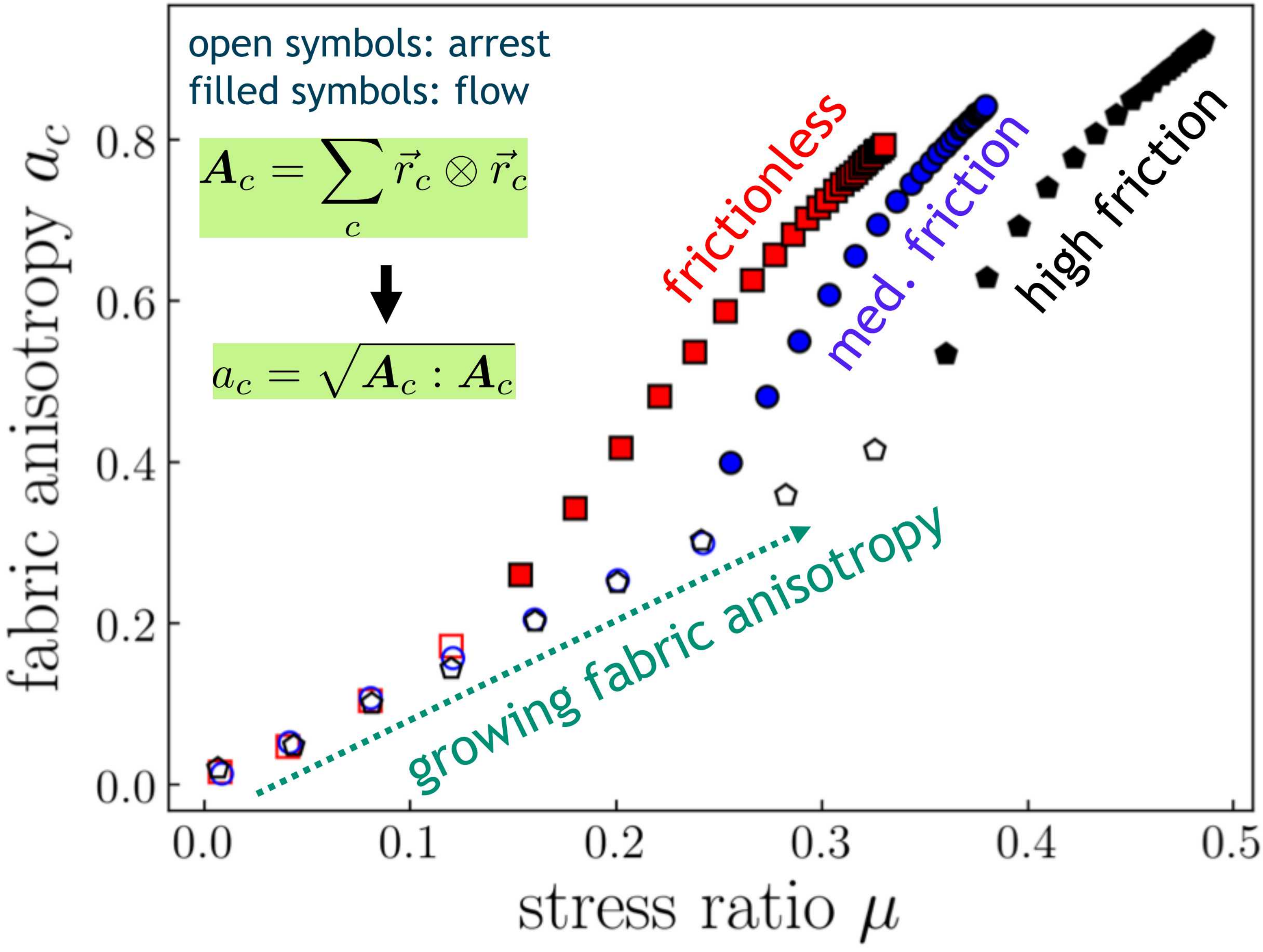
well-defined coordination at arrest for every friction

low coordination for high shear flows



Granular Fabric at Flow-Arrest: Stress-Dependent





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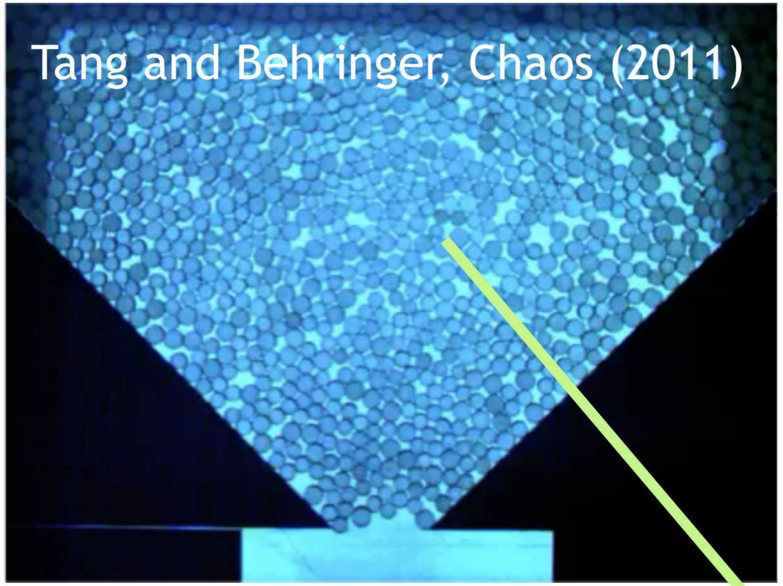

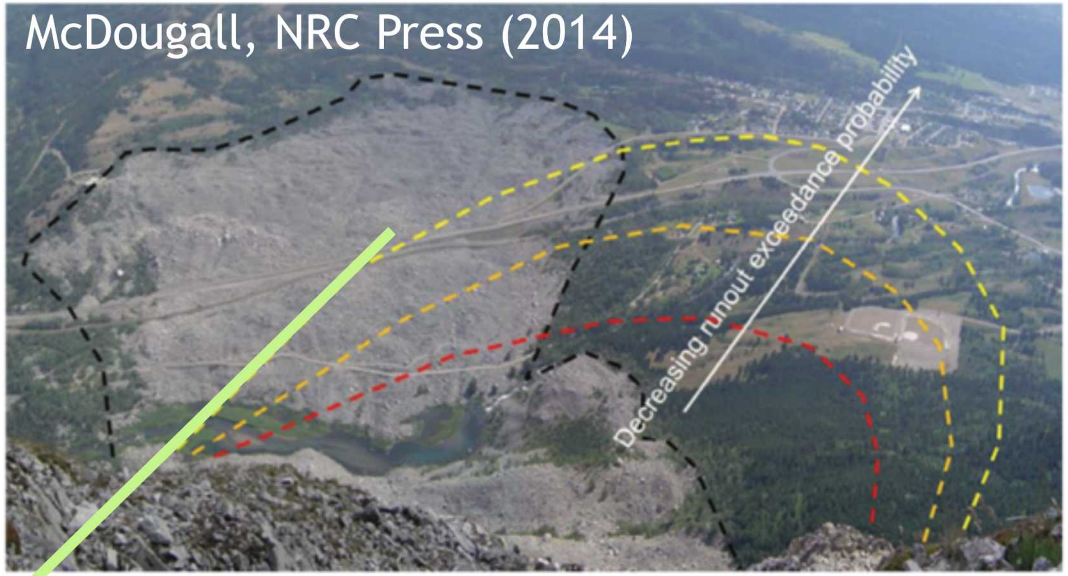

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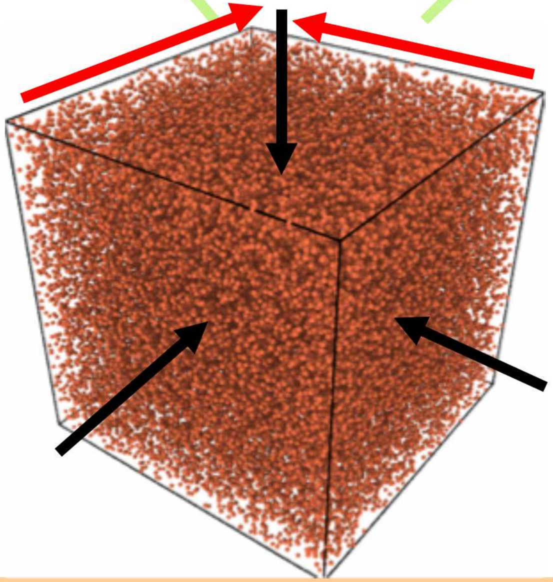

under prescribed shear and pressure:

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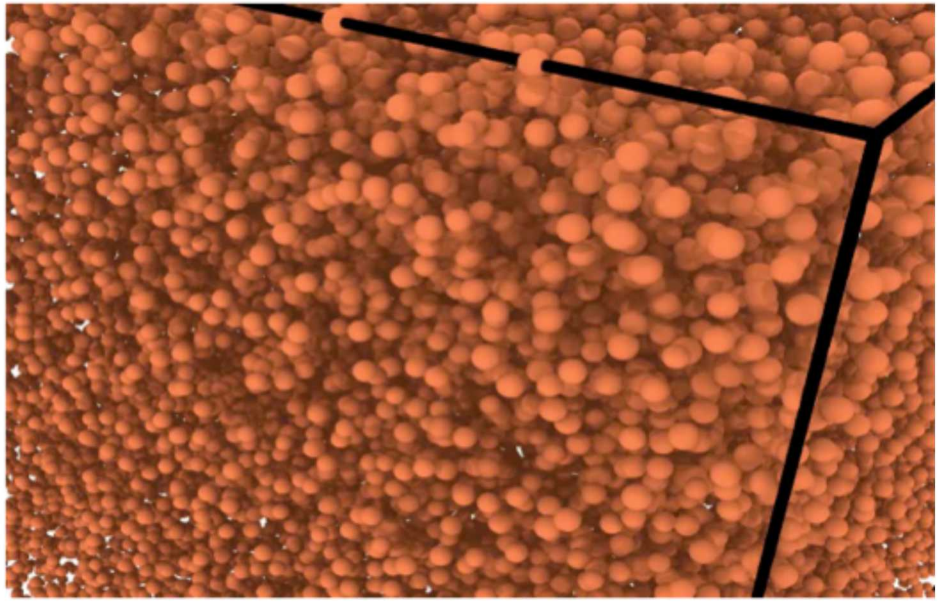
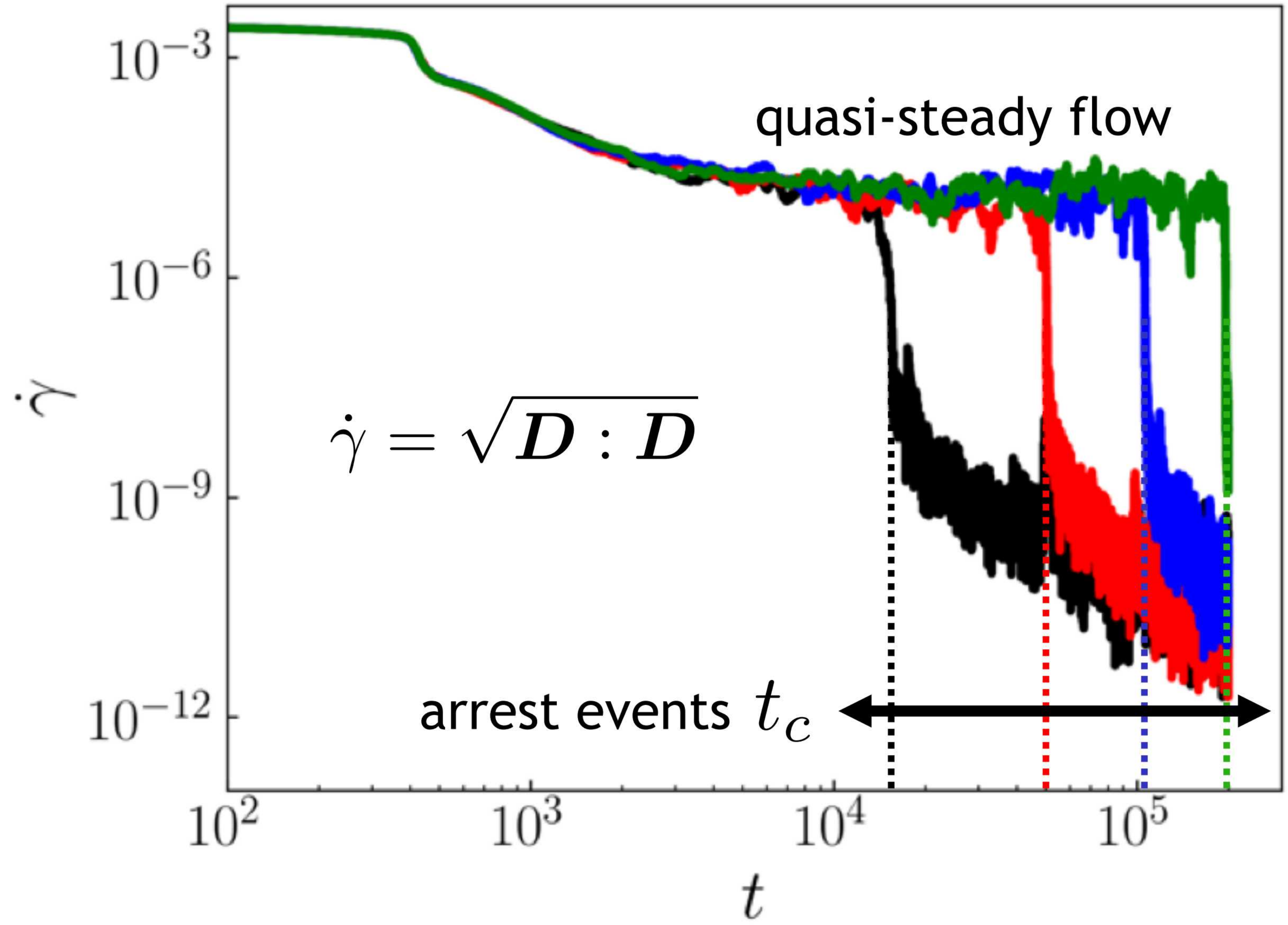
Time to Arrest is Stochastic

shear arrest



four random cases, same stress

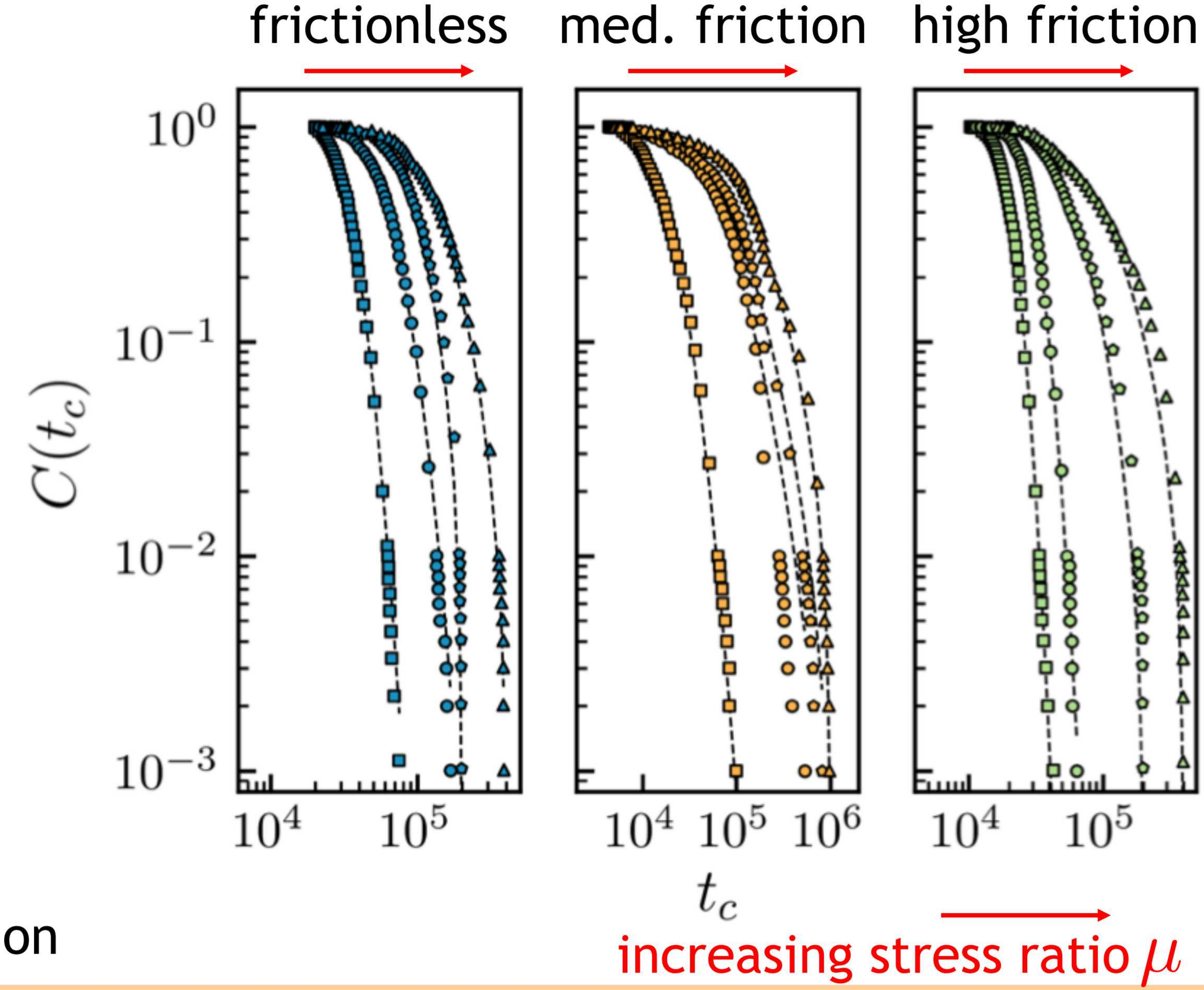


Srivastava et al., PRL, 122 (2019)

Time to Arrest: Long-tailed Distributions

long-tailed *log-normal* distribution of arrest times

longer tails at higher stress ratio



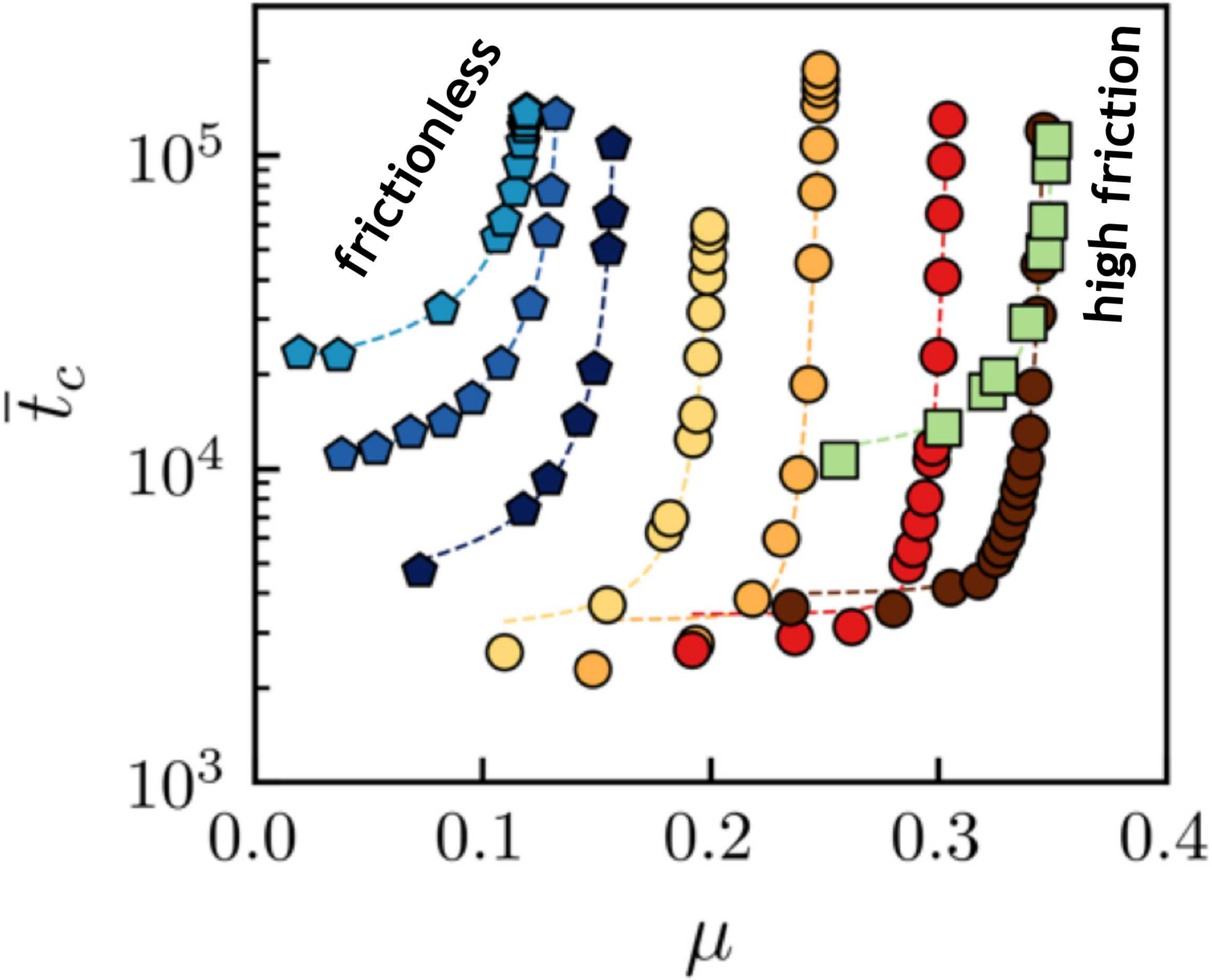
arrest times:
complementary cumulative distribution

Divergence of Mean Arrest Times

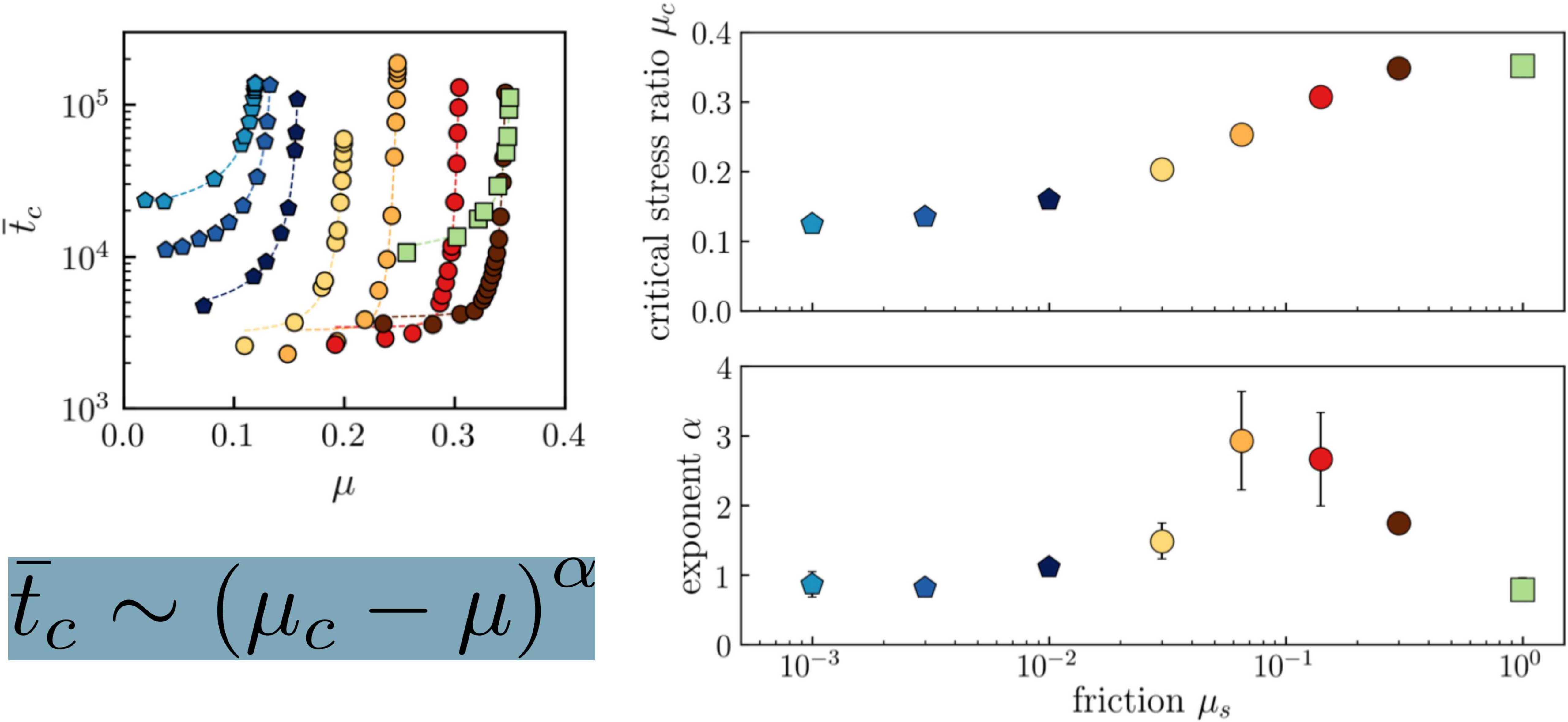
$$\bar{t}_c \sim (\mu_c - \mu)^{\alpha}$$

power-law divergence of mean arrest times at a critical stress ratio

averaged over 10^3 simulations per data

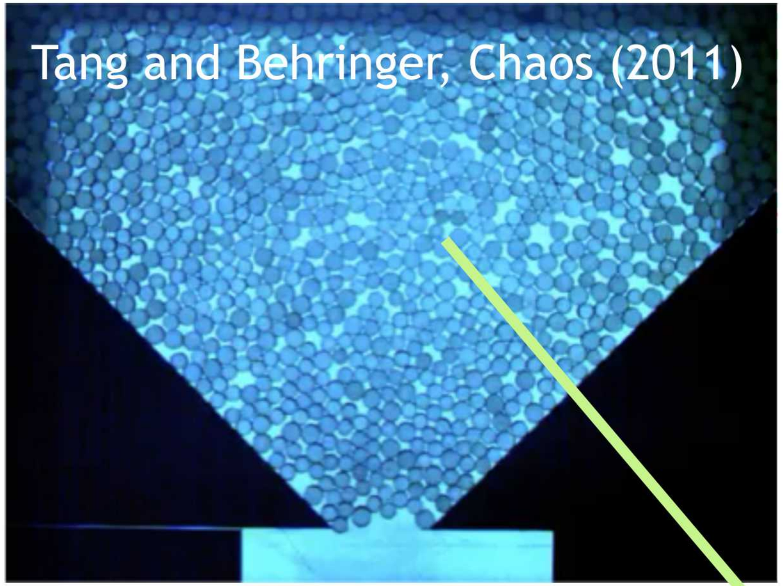


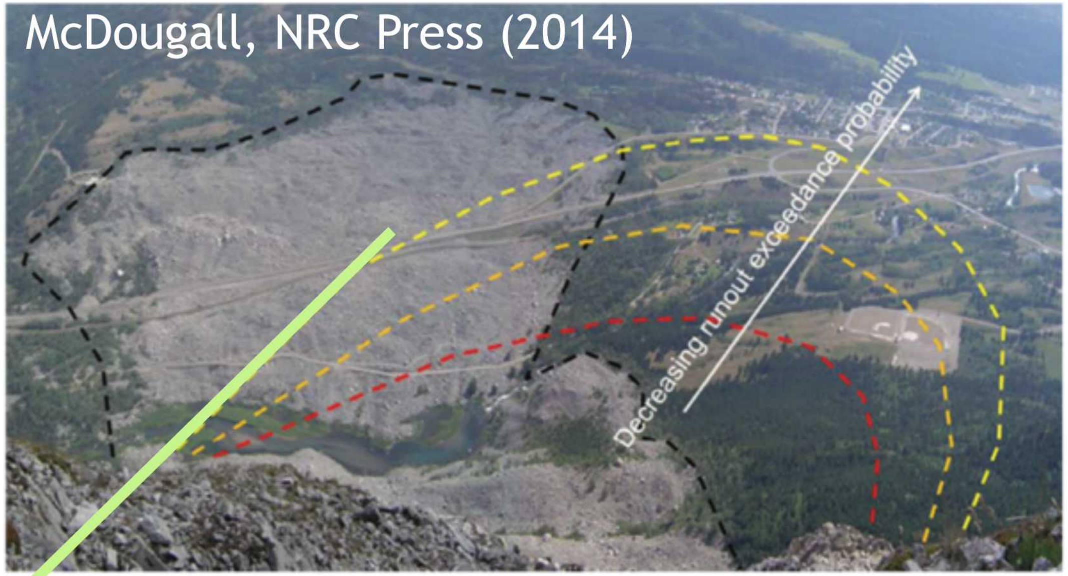
Power-law Divergence: Critical Exponents



$$\bar{t}_c \sim (\mu_c - \mu)^{\alpha}$$

Flow-Arrest Transition: Problem Statement





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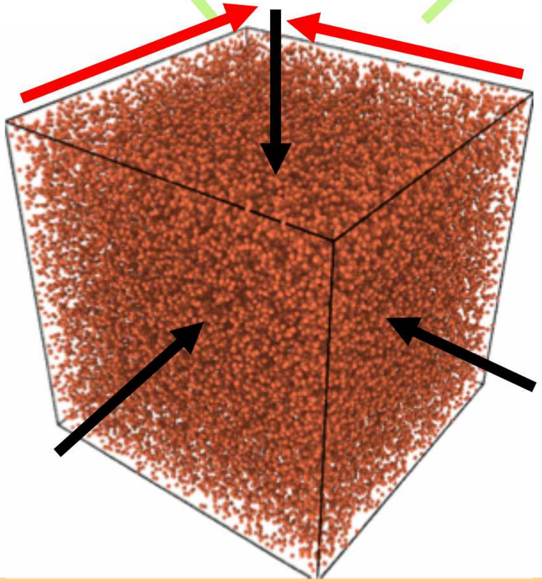

under prescribed shear and pressure:

1. Will the flow arrest?
2. When will the flow arrest?
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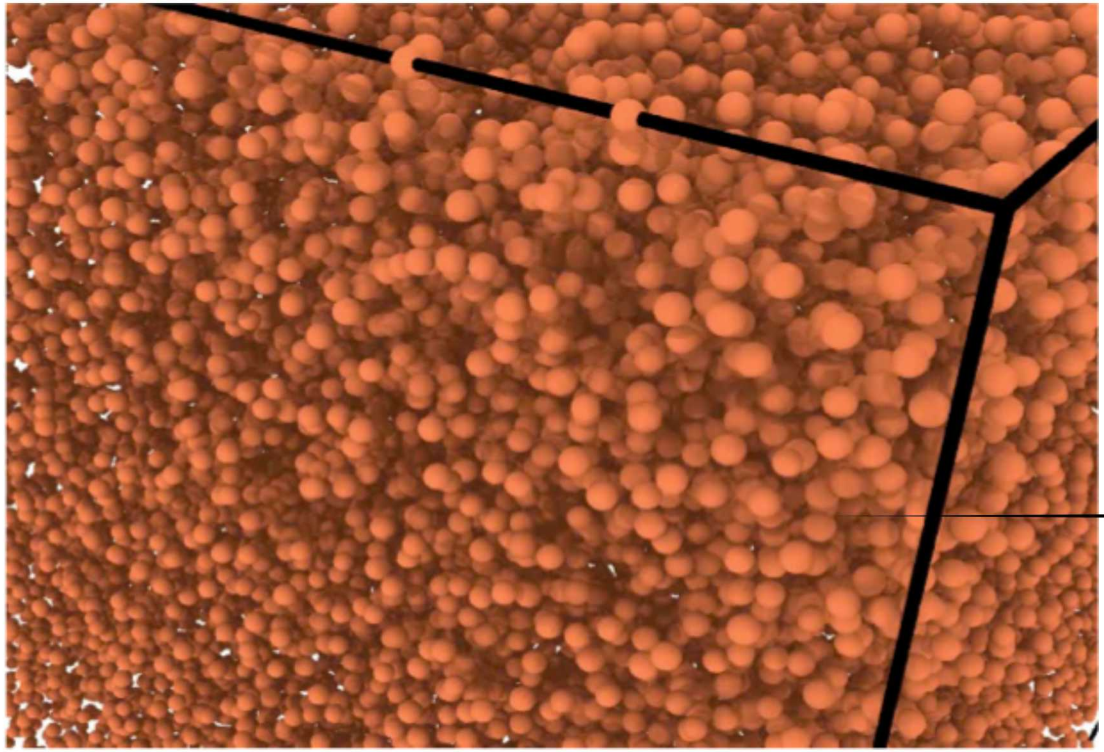
Planar Shear Rheology



after appropriate coordinate transformation

vel. gradient

$$\nabla u = \begin{bmatrix} 0 & \dot{\gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

strain rate

$$\boldsymbol{D} = \begin{bmatrix} 0 & \dot{\gamma}/2 & 0 \\ \dot{\gamma}/2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

spin

$$\boldsymbol{W} = \begin{bmatrix} 0 & \dot{\gamma}/2 & 0 \\ -\dot{\gamma}/2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

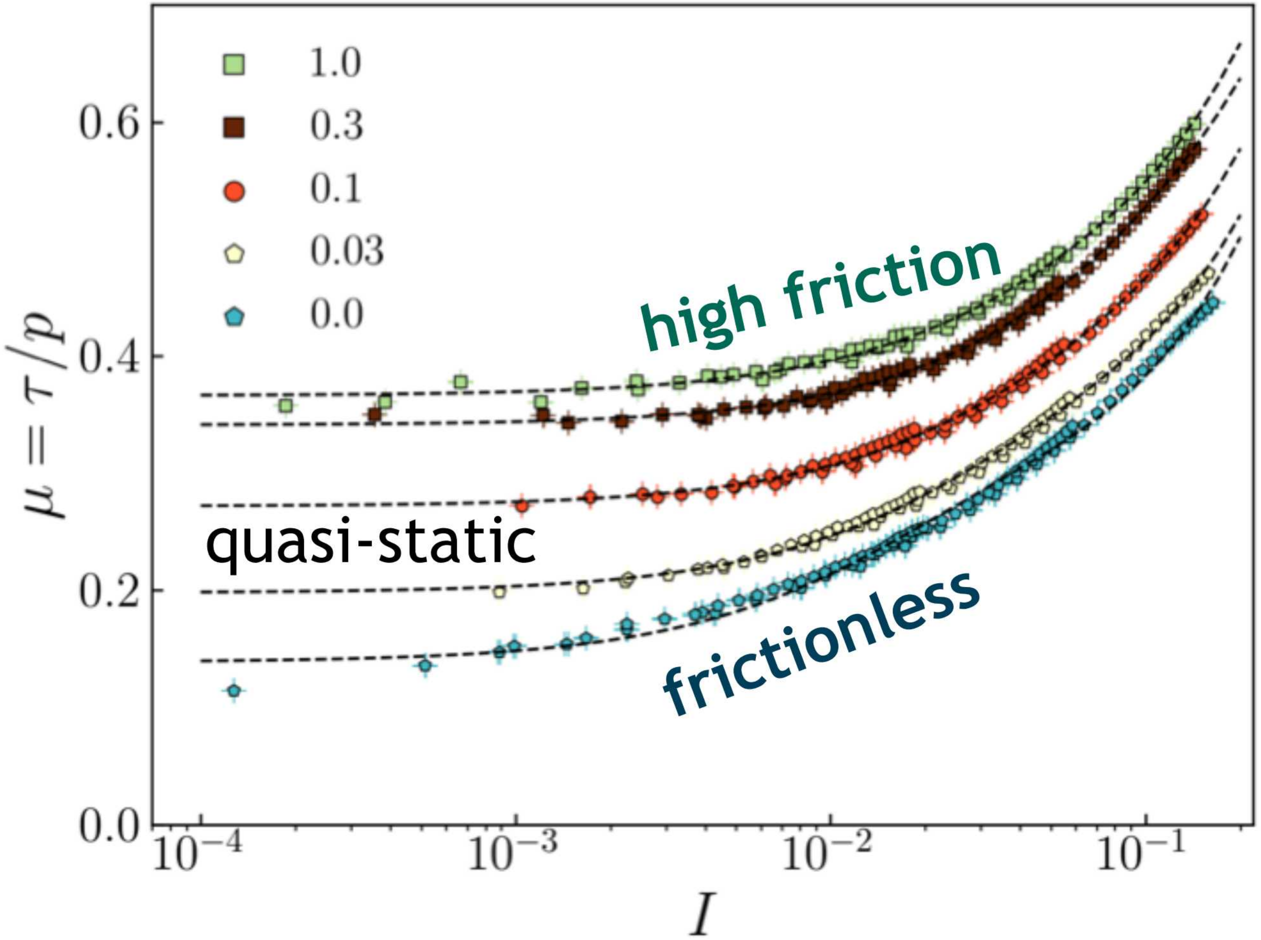
Cauchy stress

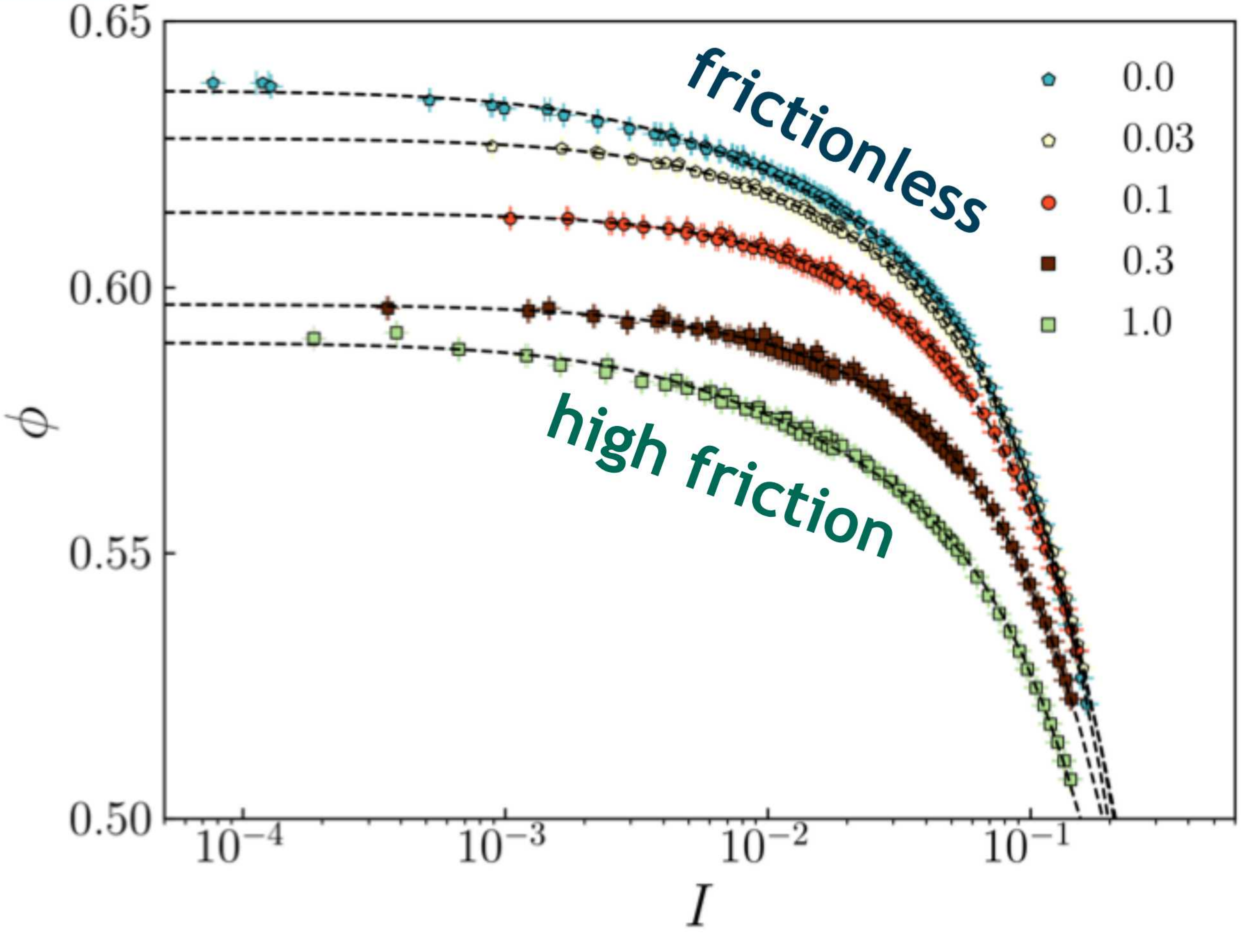
$$\boldsymbol{\sigma} = \sum_c \vec{r}_c \otimes \vec{F}_c$$

Rheology: $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{D})?$

Srivastava et al., arXiv: 1919.04491

Shear $\mu(I)$ and Dilation $\phi(I)$ laws





$$\boldsymbol{\sigma} = -p\boldsymbol{I} + \boldsymbol{\sigma}_D$$

$$\tau = \sqrt{\frac{1}{2}\boldsymbol{\sigma}_D : \boldsymbol{\sigma}_D}$$

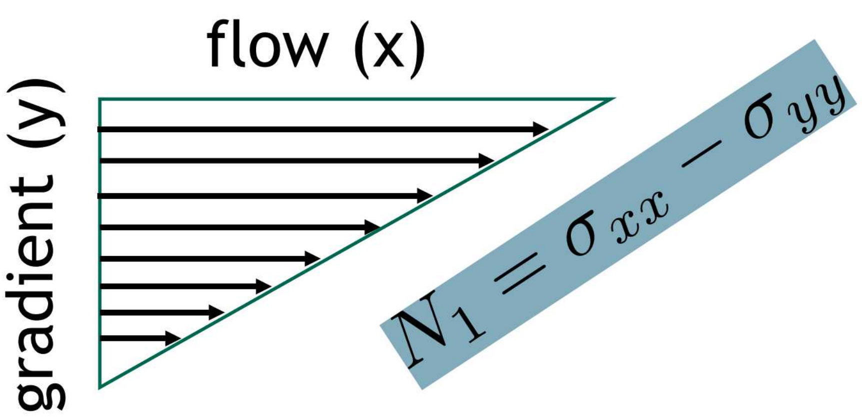
$$\mu = \mu_1 + aI + (\mu_0 - \mu_1)\, e^{-I/b}$$

$$\phi = \phi_1 - pI + (\phi_0 - \phi_1)\, e^{-I/q}$$

Srivastava et al., arXiv: 1919.04491

First Normal Stress Difference

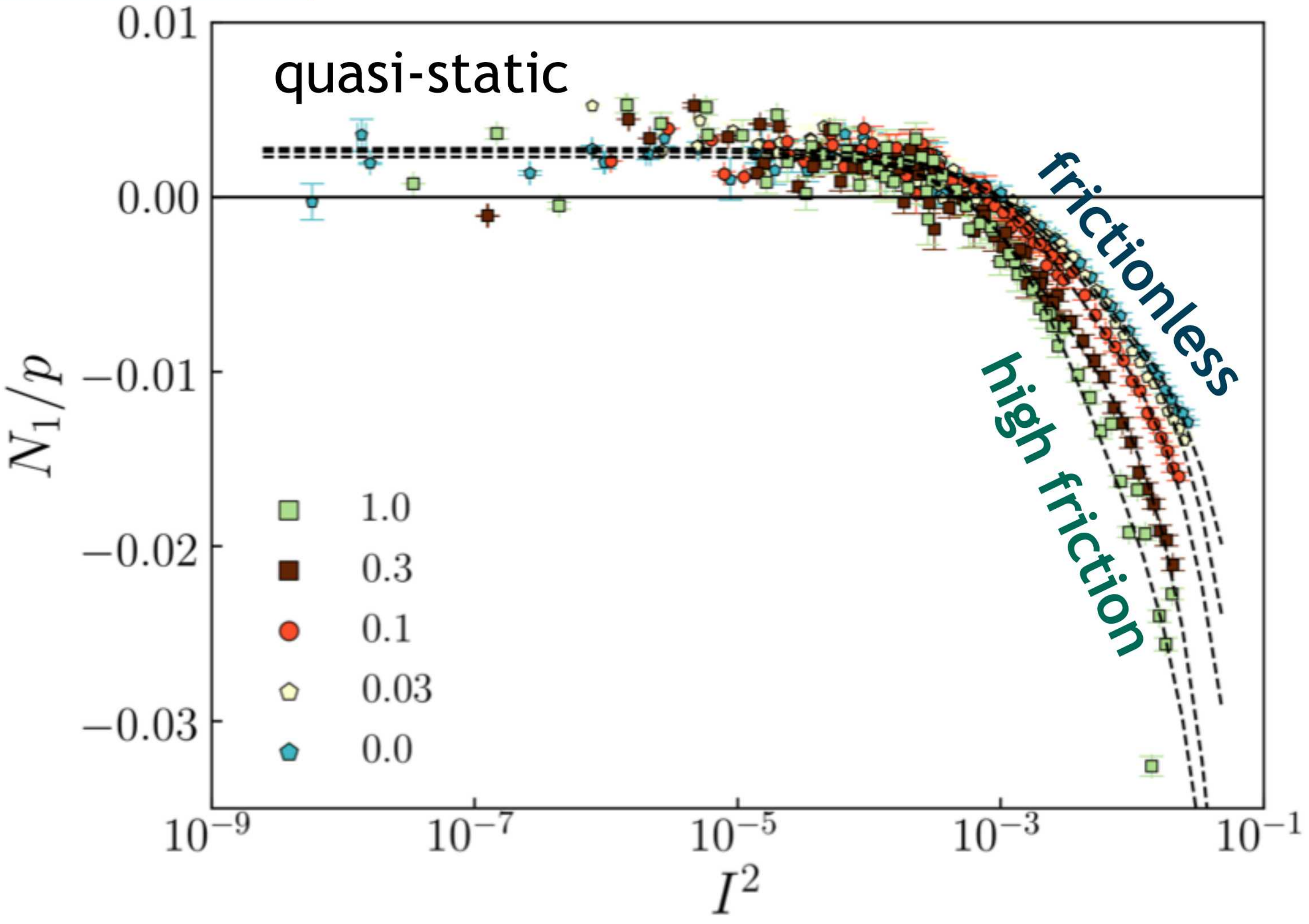
flow plane



N_1 is negative in the inertial regime

N_1 is slightly positive in quasi-static regime

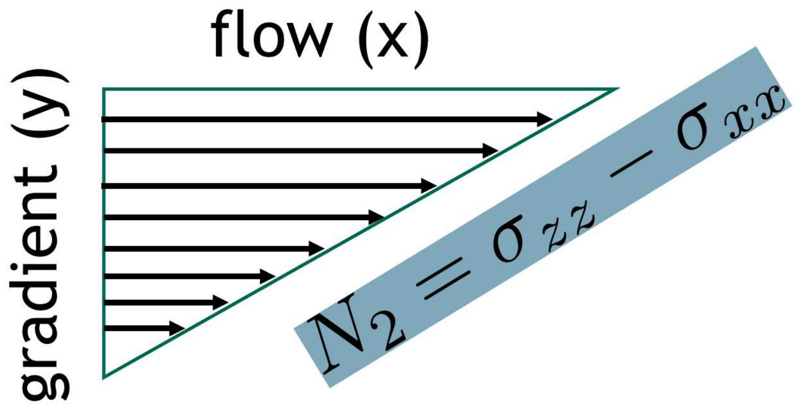
microstructure-induced anisotropy in flow plane



$$\frac{N_1}{p} = \mu_2 - cI^2 + (\mu_2 - \mu_3)\, e^{-I^2/d}$$

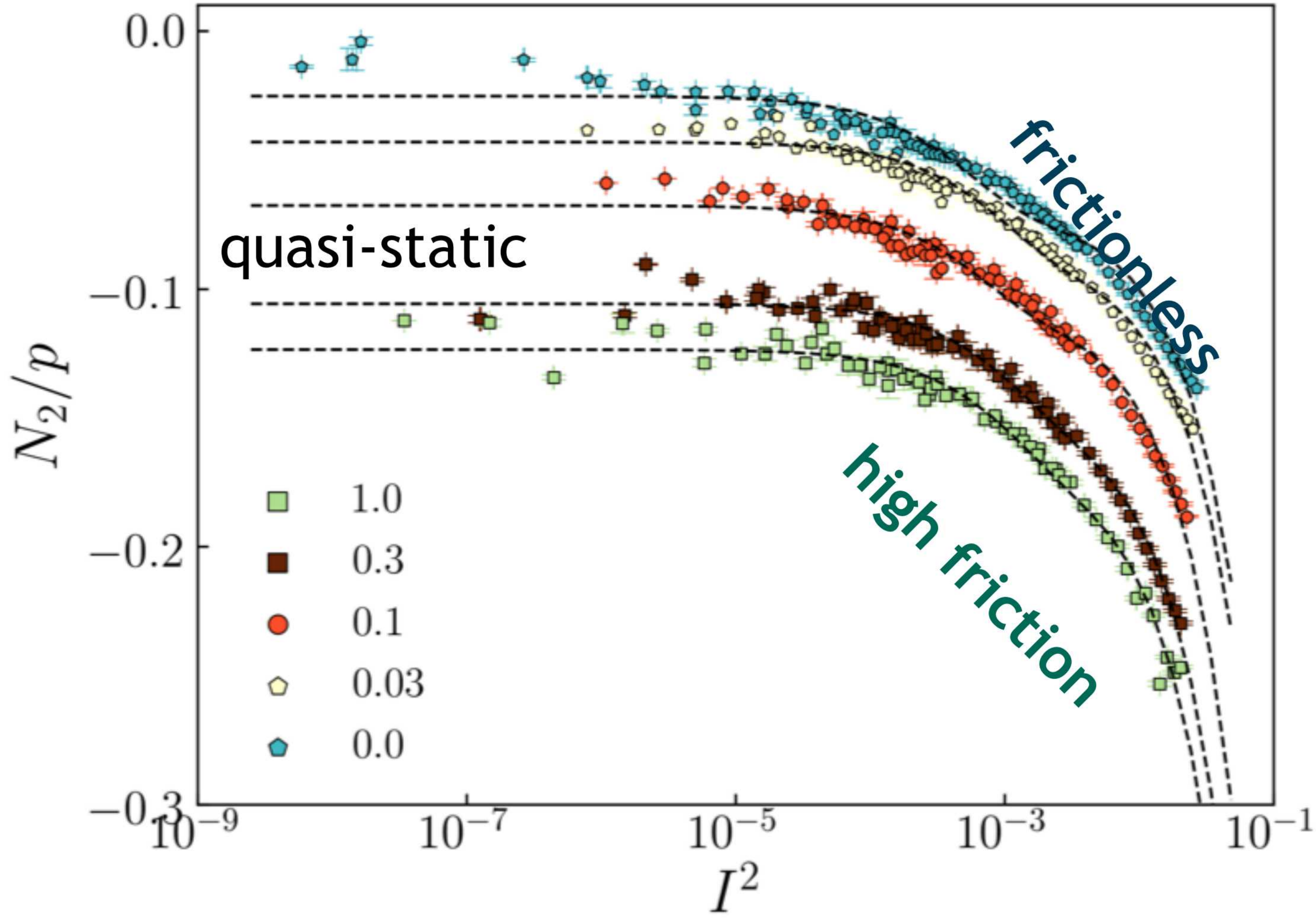
Second Normal Stress Difference

flow plane



second normal stress is always negative

frictionless particles show zero normal stress difference at RCP



$$\frac{N_2}{p} = \mu_4 - eI^2 + (\mu_4 - \mu_5)\, e^{-I^2/f}$$

3D Constitutive Model for Granular Rheology

purely dissipative rheological framework: Goddard (1984,1986)

$$\boldsymbol{\sigma} = p\boldsymbol{I} + \eta_1 \boldsymbol{D} + \eta_2 \left[\boldsymbol{D}^2 - \frac{\mathrm{tr}\left(\boldsymbol{D}^2\right)}{3}\boldsymbol{I}\right] + \eta_3 \left[\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}\right]$$

hydrostatic — shear — second normal stress diff. — first normal stress diff.

$$+\kappa_1 \frac{\boldsymbol{D}}{|\boldsymbol{D}|} + \kappa_2 \left[\frac{\boldsymbol{D}^2}{|\boldsymbol{D}|^2} - \frac{\mathrm{tr}\left(\boldsymbol{D}^2\right)}{3|\boldsymbol{D}|^2}\boldsymbol{I}\right] + \kappa_3 \left[\frac{\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}}{|\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}|}\right]$$

shear (rate-independent) — second normal stress diff. (rate-independent) — first normal stress diff. (rate-independent)

Srivastava et al., arXiv: 1919.04491

Extensions to Complex Flow Scenarios

$$\boldsymbol{\sigma} = p\boldsymbol{I} + \eta_1 \boldsymbol{D} + \eta_2 \left[\boldsymbol{D}^2 - \frac{\mathrm{tr}\left(\boldsymbol{D}^2\right)}{3} \boldsymbol{I} \right] + \eta_3 \left[\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W} \right]$$

$$+ \kappa_1 \frac{\boldsymbol{D}}{|\boldsymbol{D}|} + \kappa_2 \left[\frac{\boldsymbol{D}^2}{|\boldsymbol{D}|^2} - \frac{\mathrm{tr}\left(\boldsymbol{D}^2\right)}{3|\boldsymbol{D}|^2} \boldsymbol{I} \right] + \kappa_3 \left[\frac{\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}}{|\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}|} \right]$$

$$\eta_{1,2,3} = \eta_{1,2,3} \left(\mathrm{tr}\left(\boldsymbol{D}^2\right), \mathrm{tr}\left(\boldsymbol{D}^3\right) \right)$$

… shear vs. extensional vs. complex flows

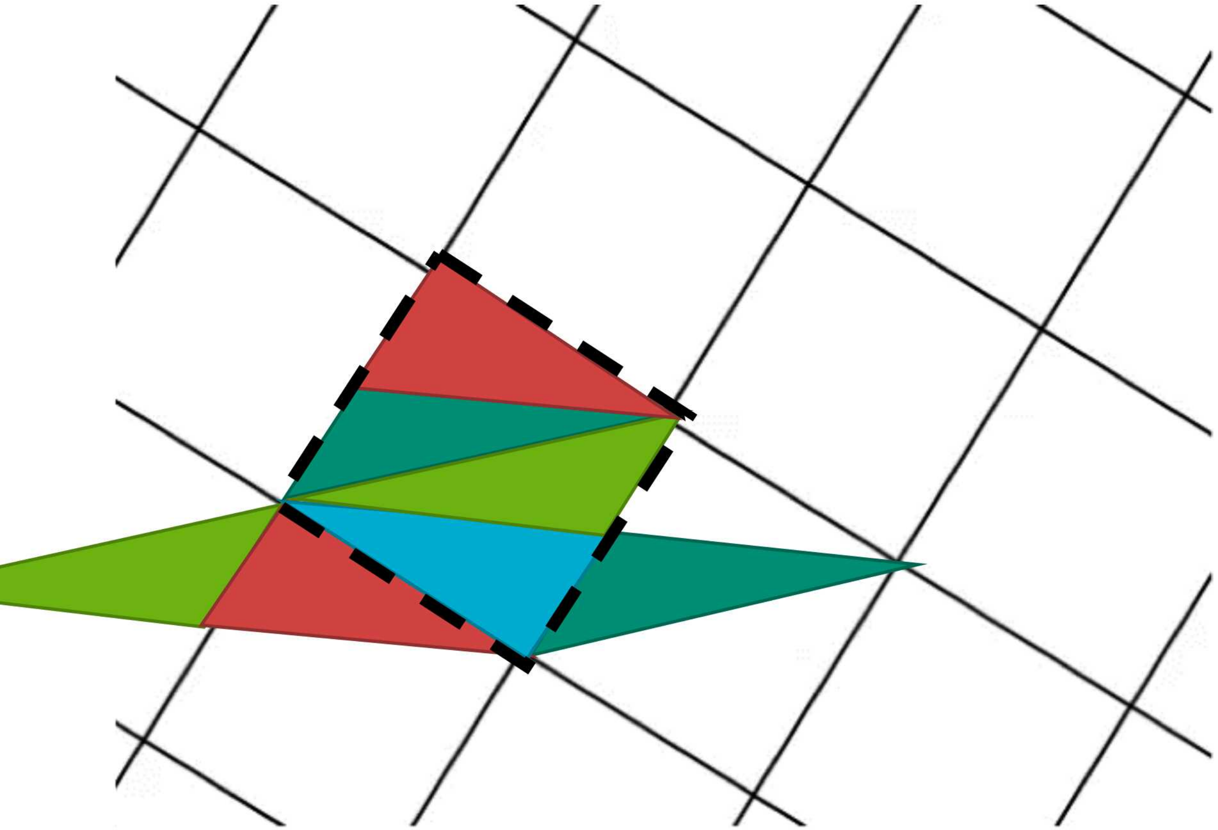
$$\kappa_{1,2,3} = \kappa_{1,2,3} \left(\frac{\mathrm{tr}\left(\boldsymbol{D}^2\right)}{|\mathrm{tr}\left(\boldsymbol{D}^2\right)|}, \frac{\mathrm{tr}\left(\boldsymbol{D}^3\right)}{|\mathrm{tr}\left(\boldsymbol{D}^3\right)|} \right)$$

… direction-dependent deformation - soil plasticity (Lode angle)

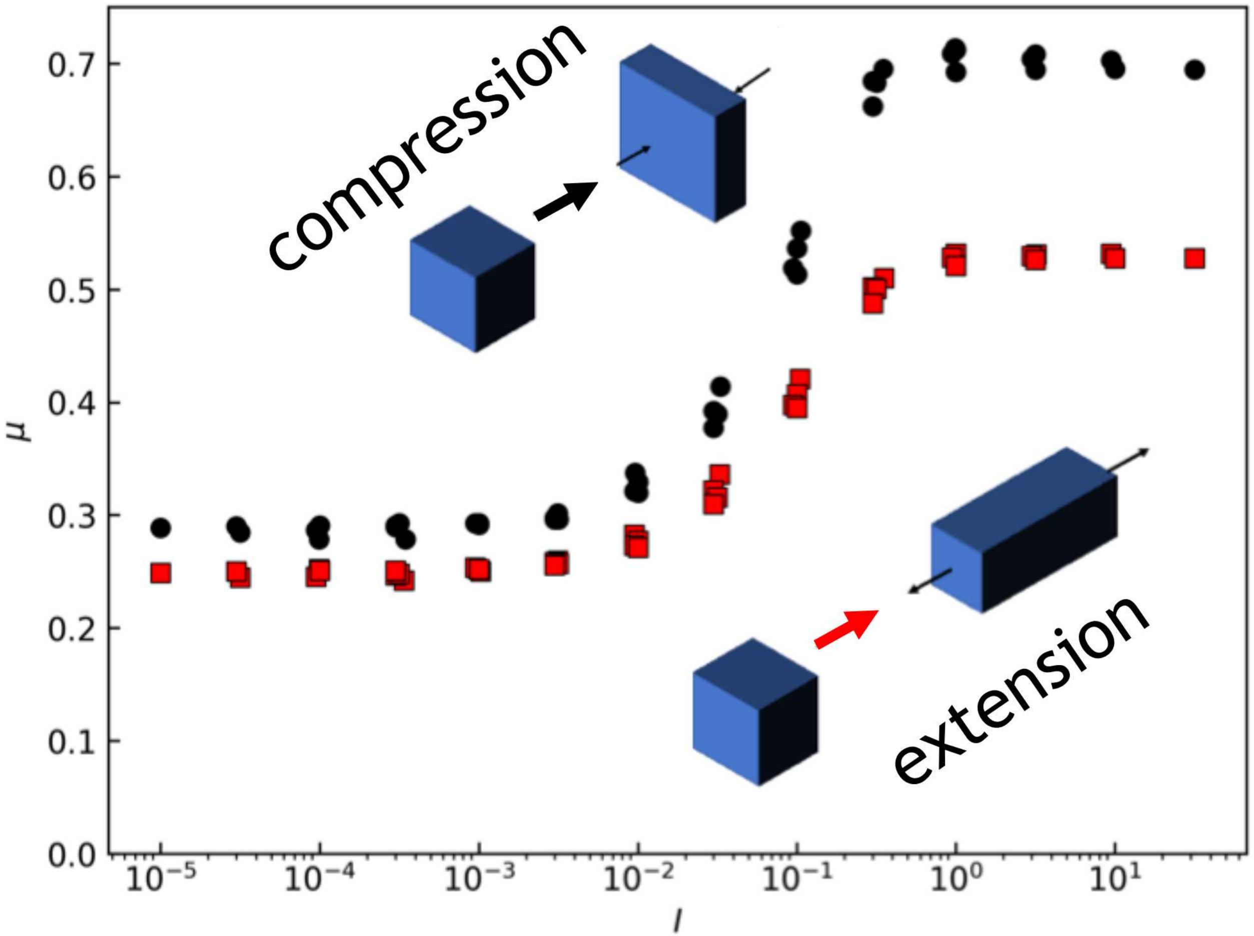
Srivastava et al., arXiv: 1919.04491

Compressional and Extensional Flows

compressional and extensional flows



Kraynik-Reinelt boundary conditions

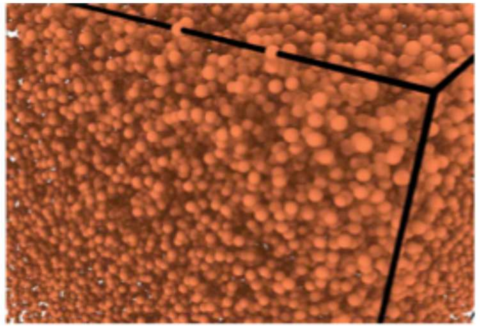


Conclusions & Outlook

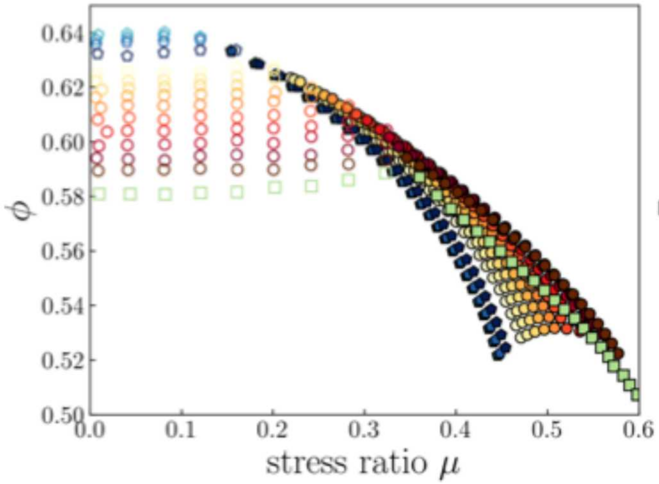
Email: isriva@sandia.gov

CONCLUSIONS

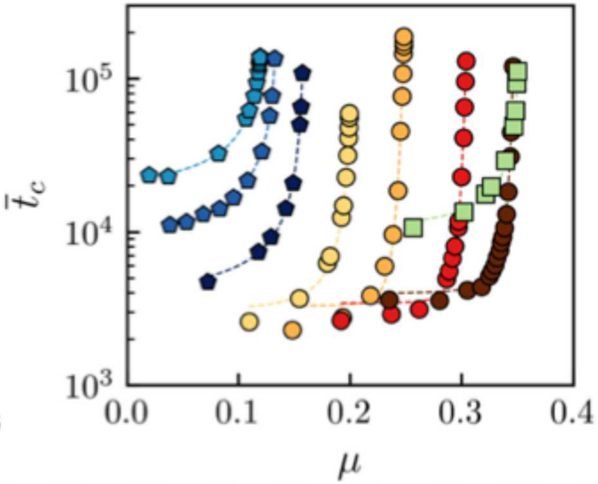
stress-driven simulations



IF: flow-arrest diagram

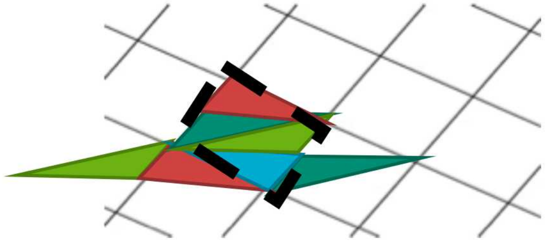


WHEN: diverging arrest times



HOW: beyond $\mu(I)$ rheology

$$\boldsymbol{\sigma} = p\boldsymbol{I} + \eta_1 \boldsymbol{D} + \eta_2 \left[\boldsymbol{D}^2 - \frac{\mathrm{tr}\,(\boldsymbol{D}^2)}{3}\boldsymbol{I}\right] + \eta_3 \left[\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}\right] + \kappa_1 \frac{\boldsymbol{D}}{|\boldsymbol{D}|} + \kappa_2 \left[\frac{\boldsymbol{D}^2}{|\boldsymbol{D}|^2} - \frac{\mathrm{tr}\,(\boldsymbol{D}^2)}{3|\boldsymbol{D}|^2}\boldsymbol{I}\right] + \kappa_3 \left[\frac{\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}}{|\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}|}\right]$$



OUTLOOK:

- are shear-arrested states fragile/stable? mechanical properties?
  à la [Bi, Behringer, Nature (2011)]
- is there a diverging length scale at shear-arrest near critical yield?
- calibrate the constitutive model for complex flow scenarios

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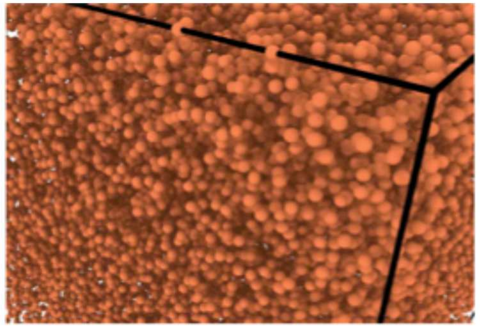
Center for Integrated Nanotechnologies,
Sandia National Laboratory

Conclusions & Outlook

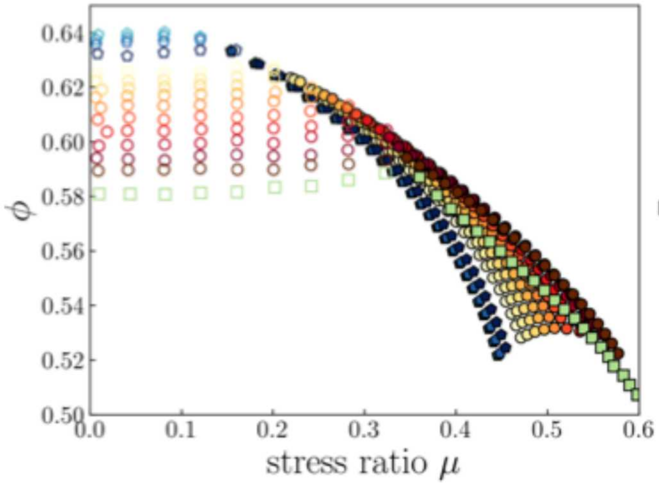
Email: isriva@sandia.gov

CONCLUSIONS

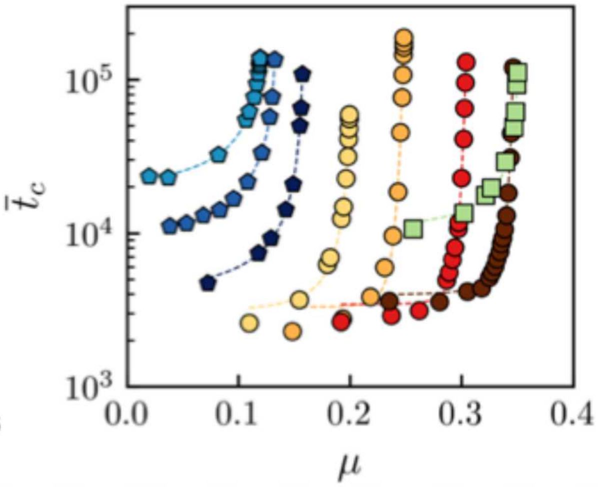
stress-driven simulations



IF: flow-arrest diagram

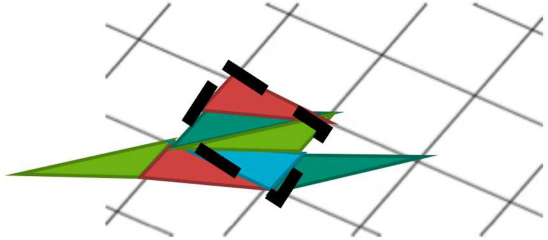


WHEN: diverging arrest times



HOW: beyond $\mu(I)$ rheology

$$\boldsymbol{\sigma} = p\boldsymbol{I} + \eta_1 \boldsymbol{D} + \eta_2 \left[\boldsymbol{D}^2 - \frac{\mathrm{tr}\,(\boldsymbol{D}^2)}{3}\boldsymbol{I}\right] + \eta_3 \left[\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}\right] + \kappa_1 \frac{\boldsymbol{D}}{|\boldsymbol{D}|} + \kappa_2 \left[\frac{\boldsymbol{D}^2}{|\boldsymbol{D}|^2} - \frac{\mathrm{tr}\,(\boldsymbol{D}^2)}{3|\boldsymbol{D}|^2}\boldsymbol{I}\right] + \kappa_3 \left[\frac{\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}}{|\dot{\boldsymbol{D}} - \boldsymbol{W}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{W}|}\right]$$



OUTLOOK:

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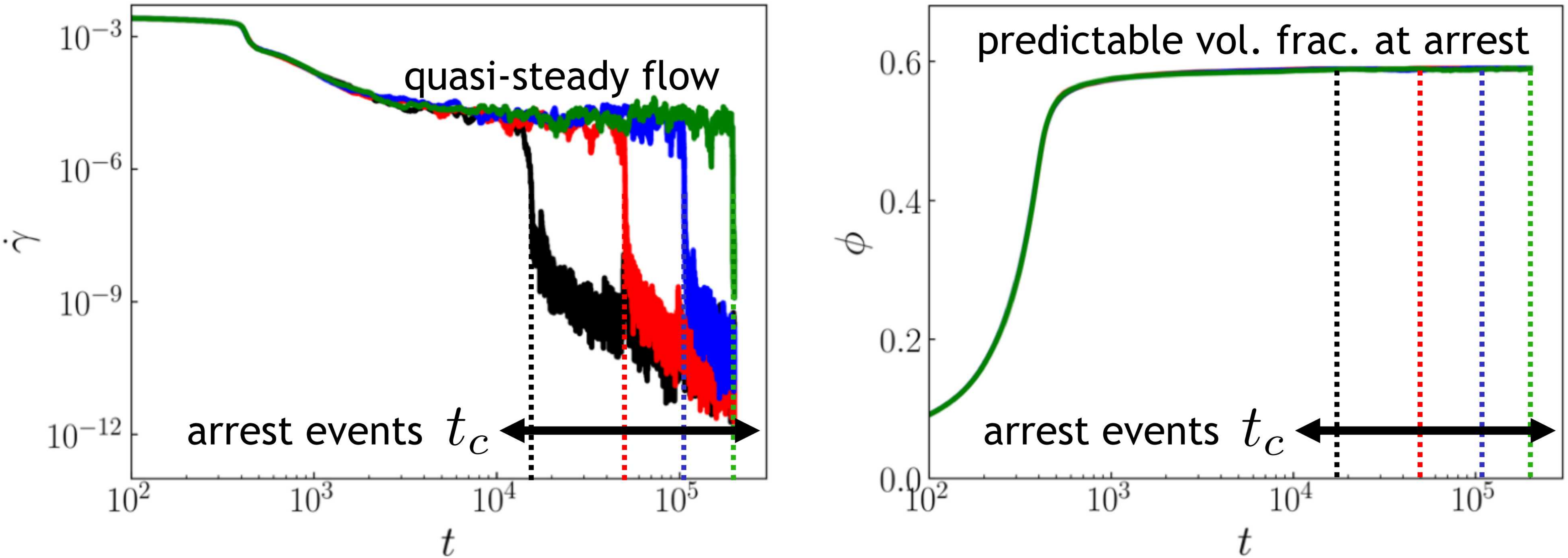
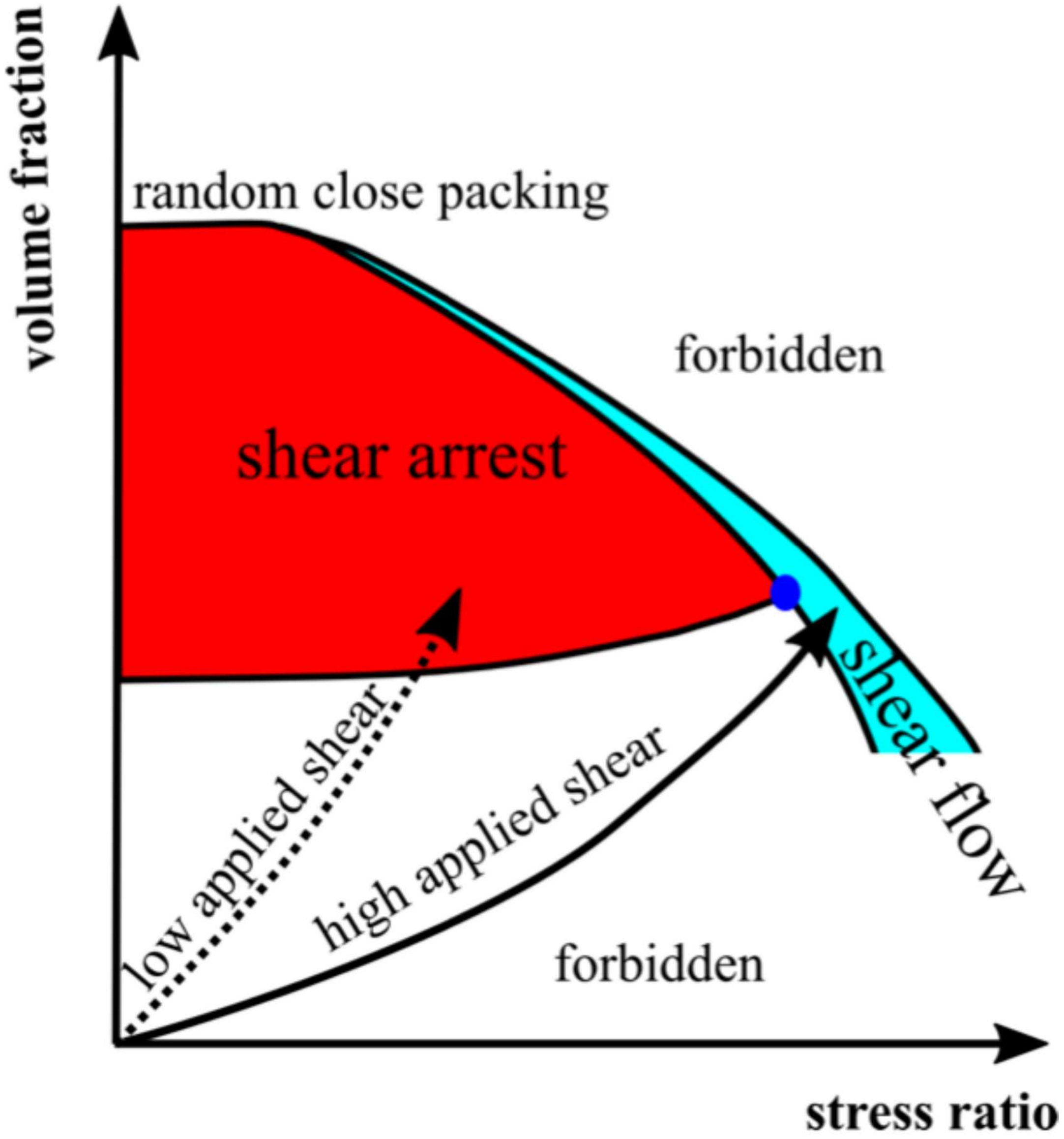
Volume Fraction at Arrest is Deterministic

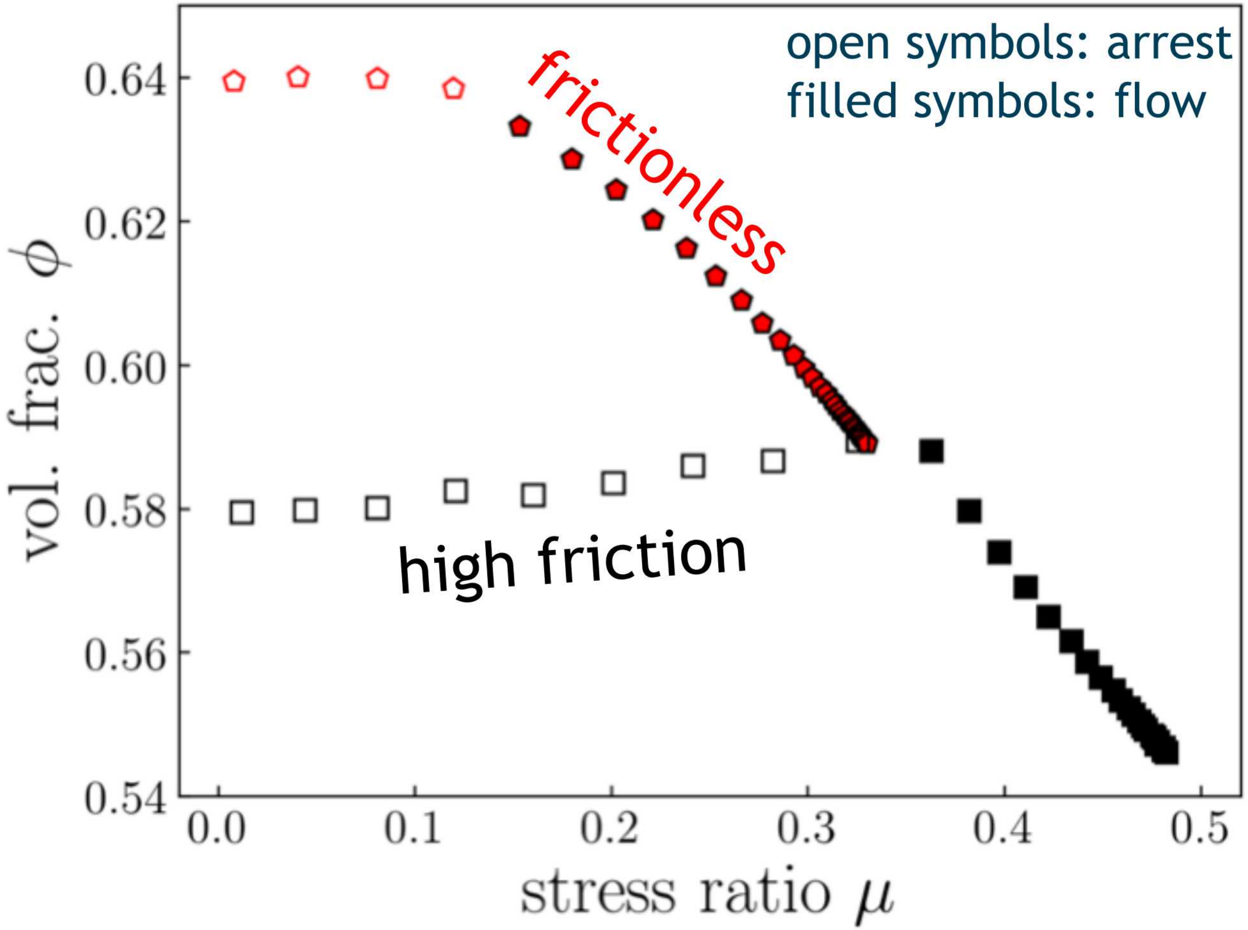


difficult to predict when a flow will arrest,
but sure of volume fraction & coordination upon arrest

Paths to Flow or Arrest



well-defined flow & arrest states for every friction



Srivastava et al., *in prep.*

Stress States at Yielding and Flow

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

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