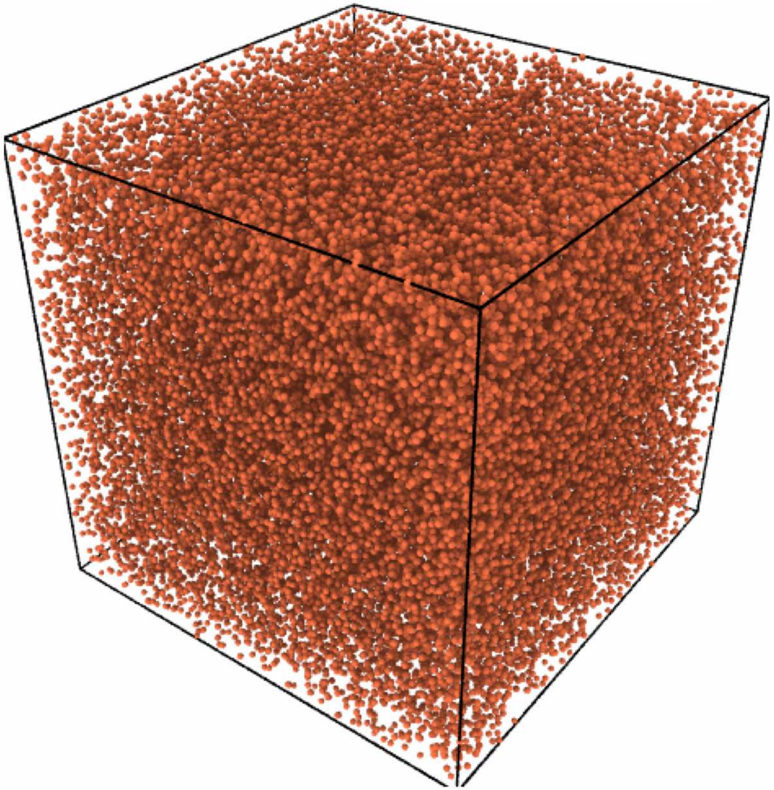
# Flow-Arrest Transitions and Frictional Rheology of Dense Granular Matter

SAND2018-11755PE



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Dr. Scott Roberts (Sandia)


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# Granular Matter: Definition

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**collection of hard, non-Brownian, and frictional particles**

images: www.wikipedia.org

# Granular Matter in the Industry

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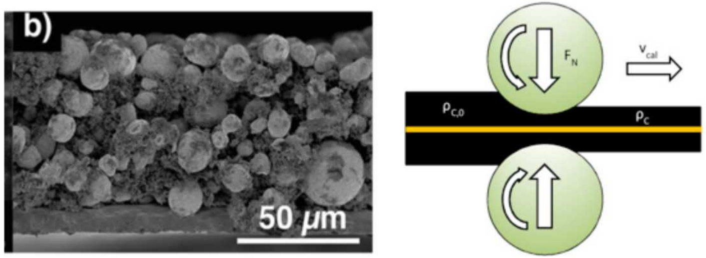
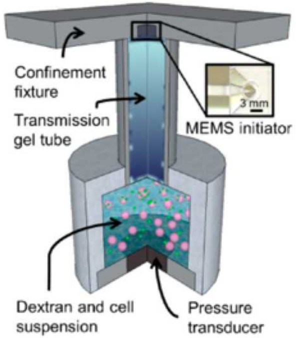


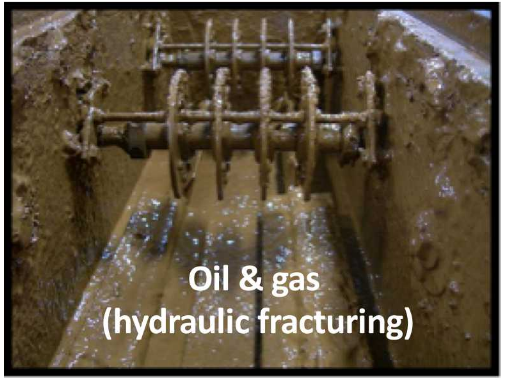

**Li-ion electrode processing**
(Ebner et al., Adv. Ener. Mater., 2013)


- second most widely used material in industry after water
- processing consumes 10% of world's energy


(Zhou et al., App. Mater. Inter., 6, 2014)

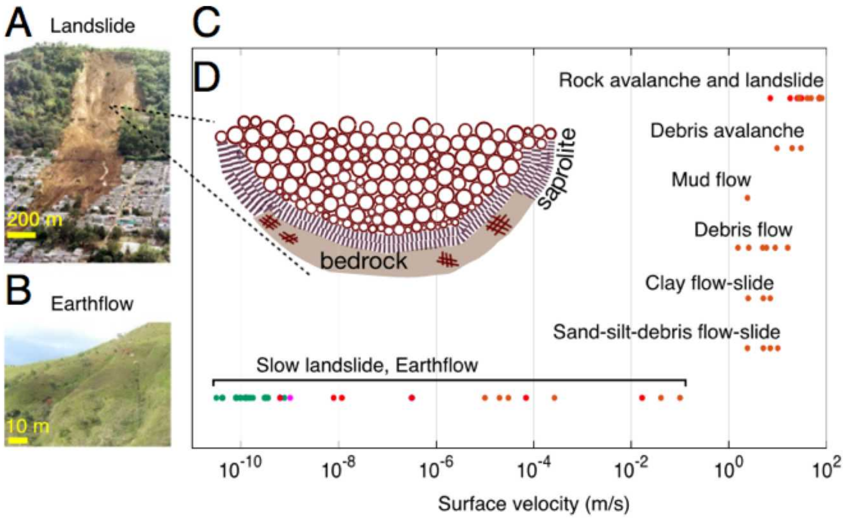
**energetic materials: powder packing**




all other images: www.wikipedia.org

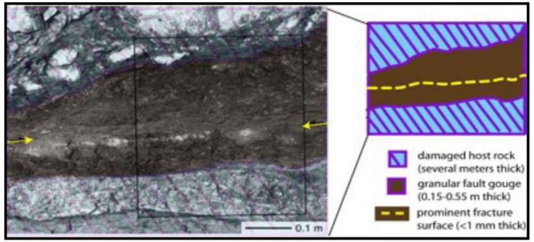
# Granular Matter in Nature

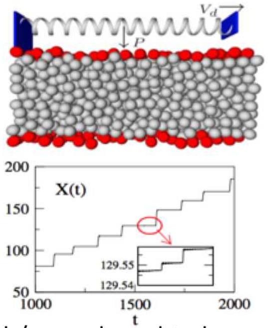
### evolution of landscapes: creep earthflow vs. landslides




(Ferdowsi et al., PNAS, 2018)

### gouge failure in earthquakes

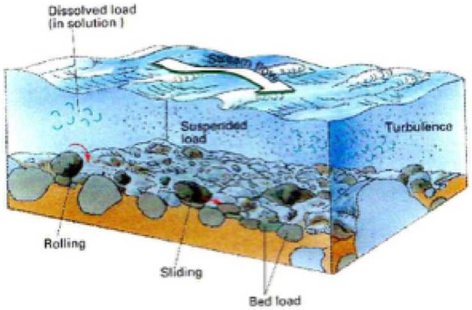


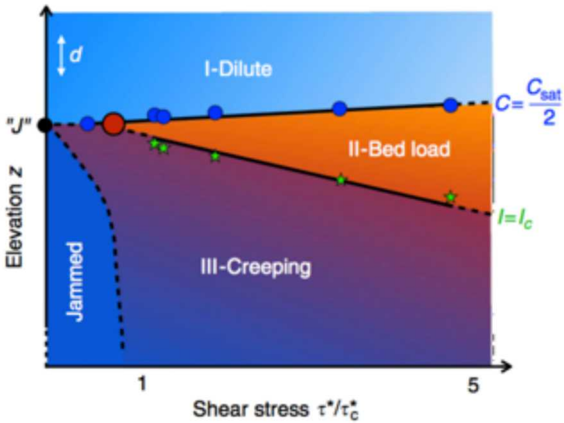




[1]http://web.physics.ucsb.edu/~complex/research/amorphous.html

[2]Ciamarra et al., Phys. Rev. Lett., 104, 238001, 2010

### river bed sediment transport: bed load vs. creep

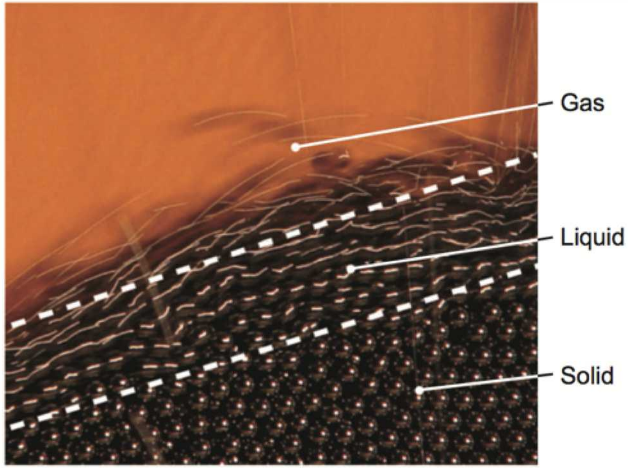


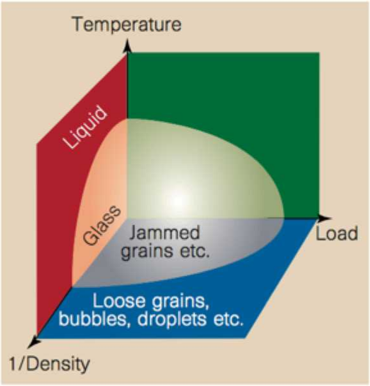




(Houssais et al., Nat. Comm., 6 2015)

# Flow Regimes in Frictional Granular Matter

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



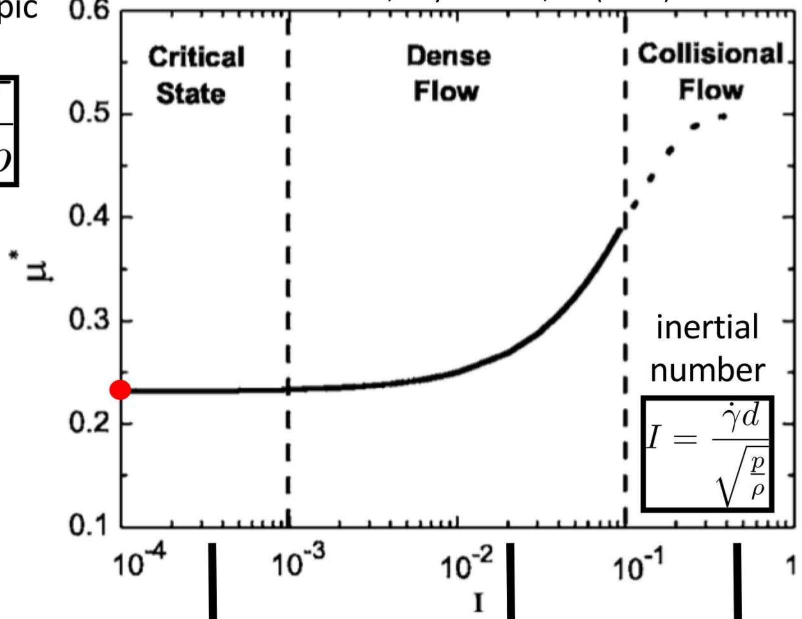




Liu and Nagel, Nature (1998)

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

macroscopic friction

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




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

rate-independent quasi-static; yield surface concept (Mohr-Coulomb, Critical State)

Bingham-type visco-plastic rheology

Bagnold regime; kinetic theories

# Key Unresolved Issues and Implications

**Issue #1**: Highly stochastic transient behavior near solid-fluid transition. What are its statistics?
**Implications**: Extend deterministic steady-state rheology to include stochastic and transient events.

**Issue #2**: Does granular matter flow beyond simple shear? What is the rheology?
**Implications**: Granular rheology beyond simple shear will enable its practical deployment to predict complex flow fields.

**Issue #3**: Granular matter creeps below yield stress. What are the microscopic mechanisms of creep?
**Implications:** Creep of amorphous matter is long-standing challenge in classical physics. We aim to improvise our understanding of this phenomenon.

**transient, stochastic characterization of granular flows beyond simple shear, above and below yield**

# Constant Pressure and Shear Simulations

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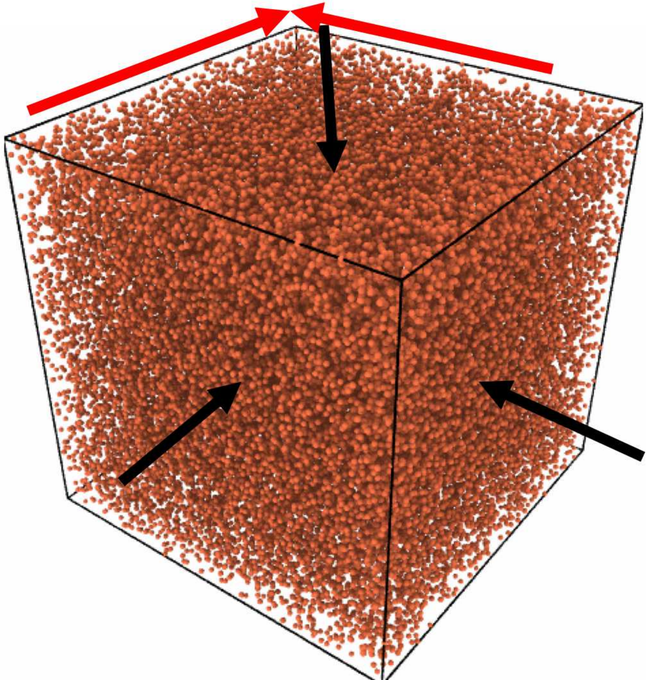
second Piola-Kirchhoff stress
(thermodynamic tension)

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



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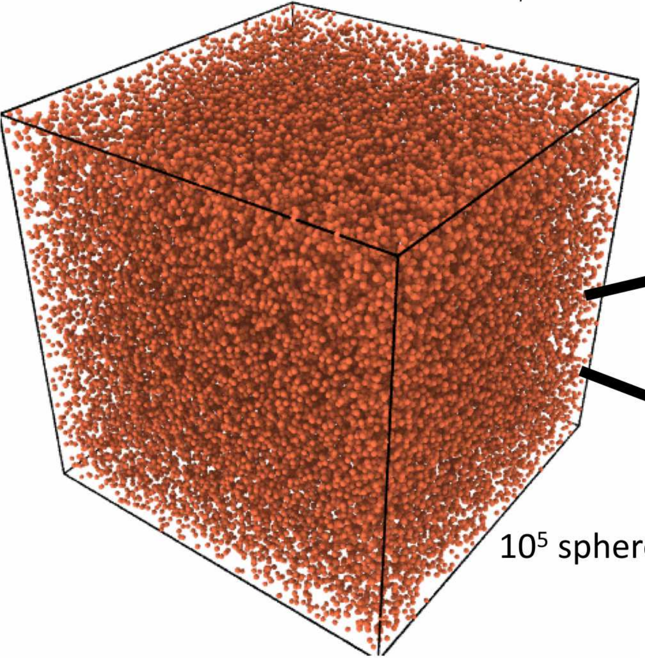
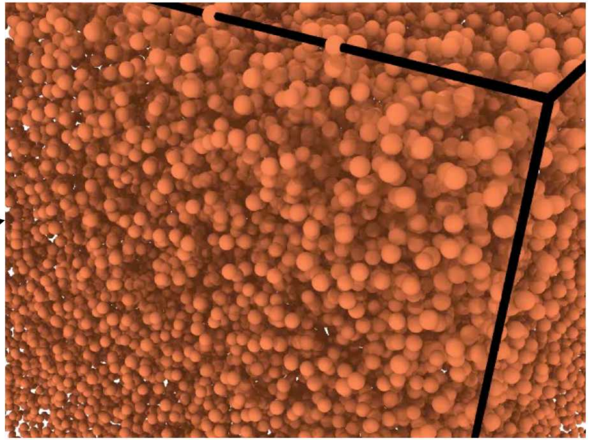
initial low-density assembly: $\phi = 0.05$



$10^5$ spheres

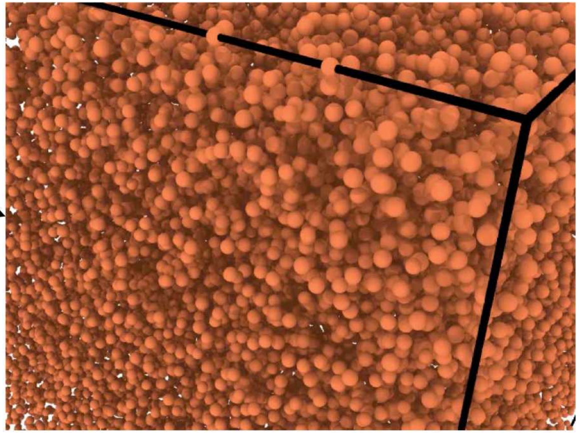
arrest



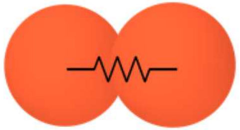
applied stress

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

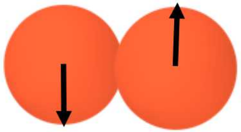
steady flow



harmonic contacts

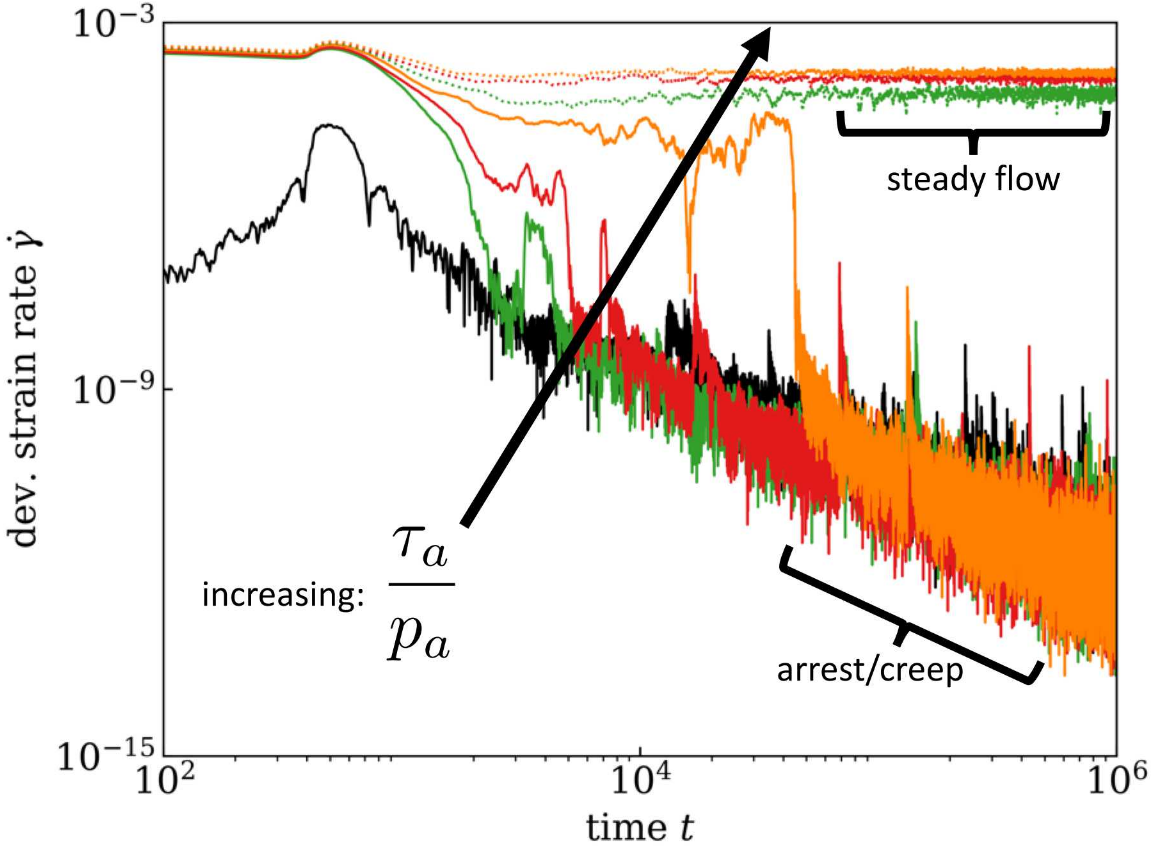


Coulomb microscopic friction



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

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




strain rate

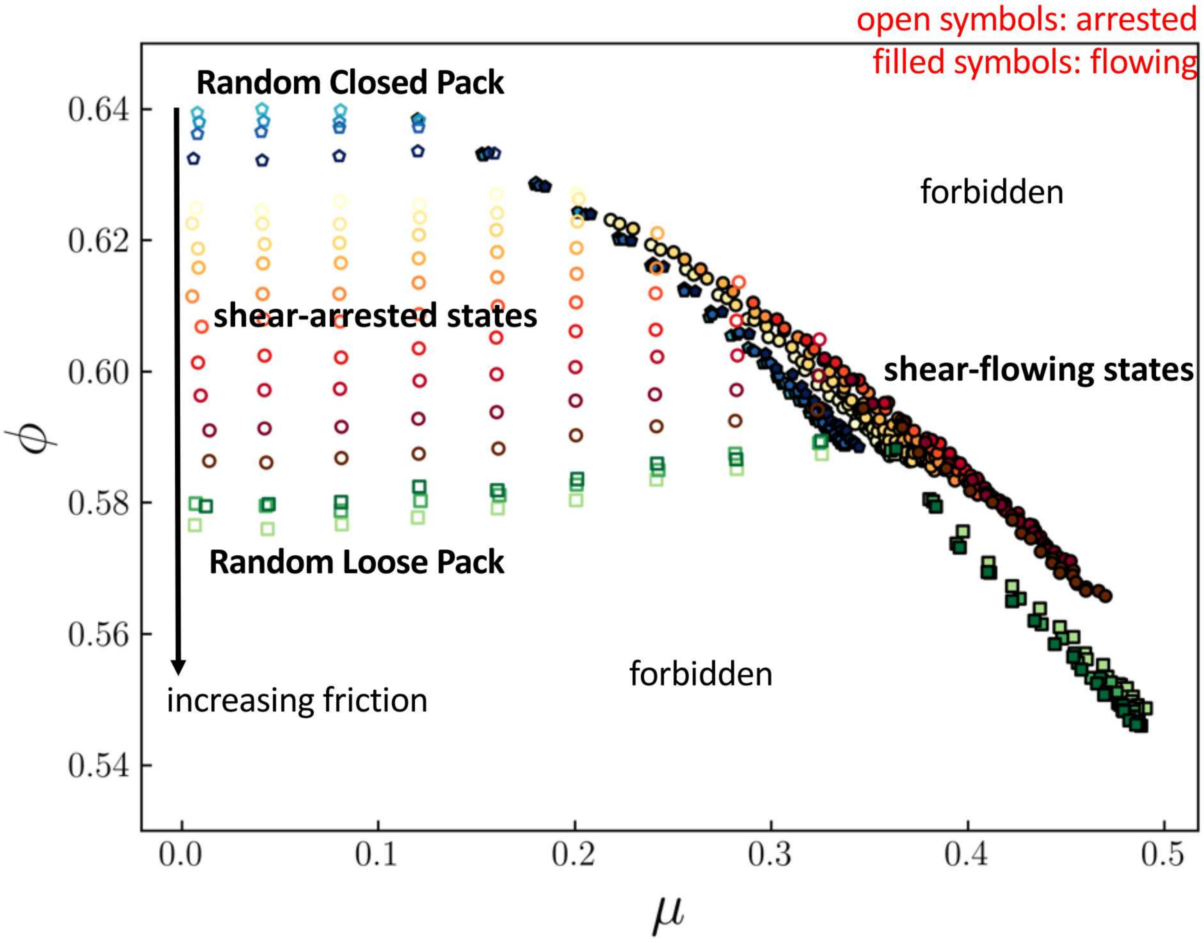
$$\dot{\gamma} = \sqrt{0.5\dot{\gamma}_{ij}\dot{\gamma}_{ij}}$$

**Steady Flow:**
shear-stress-dependent strain rate

**Arrest/Creep:**
massive drop in strain rate towards an arrested state

# Steady-State Flow-Arrest Phase Diagram






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

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

Drucker-Prager

**Steady Flow:**

- significant ***dilation*** to flow
- friction-dependent ***static yield stress***

**Arrest/Creep:**

mild compaction during shear arrest (shear jamming)

# Mechanics of Flow and Arrest

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

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

**Arrest (Jammed):**

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

equilibrium: balance of internal and external stress

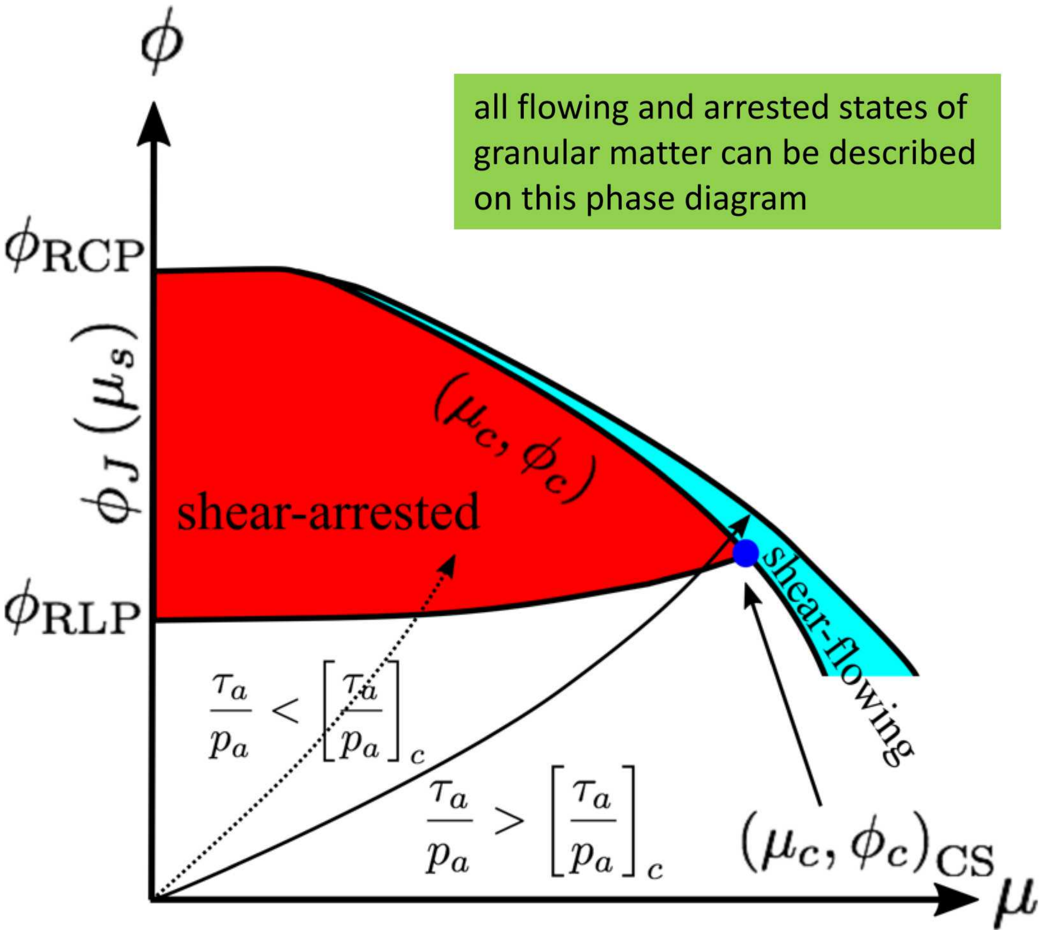
**Yielding:**

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

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

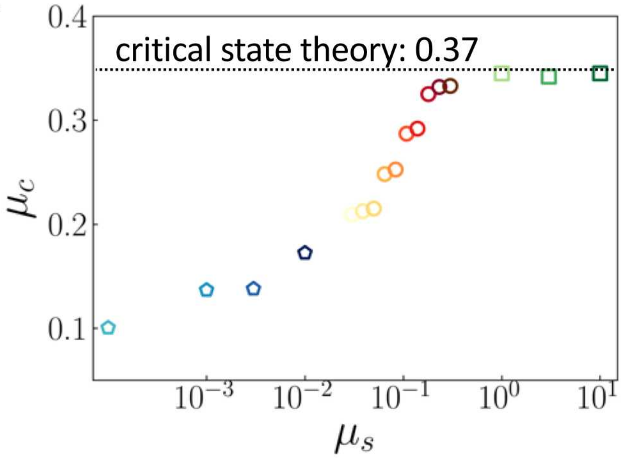
Nicot et al., IJP, 29 2012
Hill, J. Mech. Phys. Sol., 6, 1958

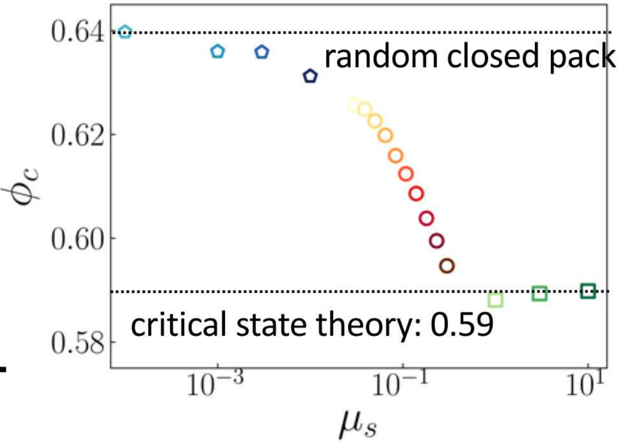
# Critical Flow-Arrest Phase Boundary




all flowing and arrested states of granular matter can be described on this phase diagram

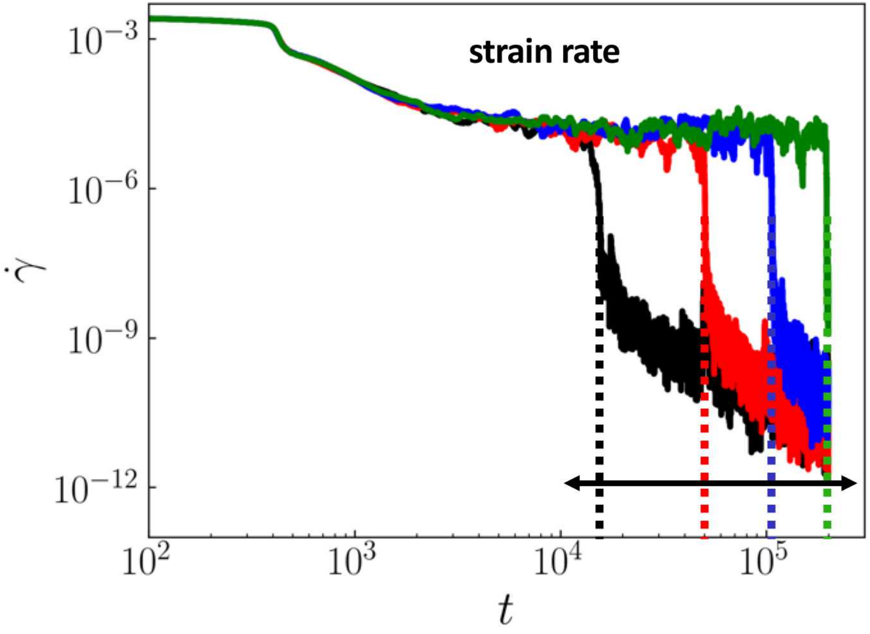
**phase boundary**

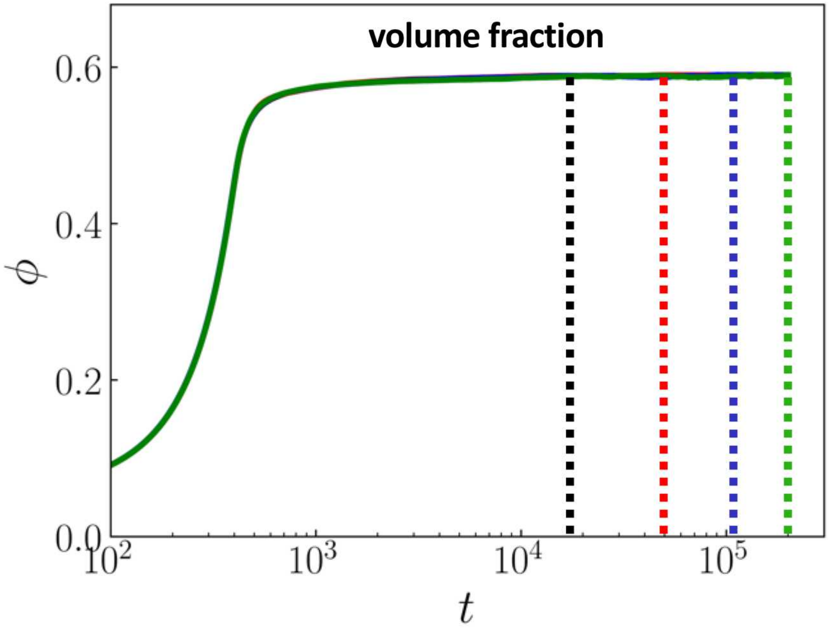


# Stochastic Granular Arrest: Below Yield

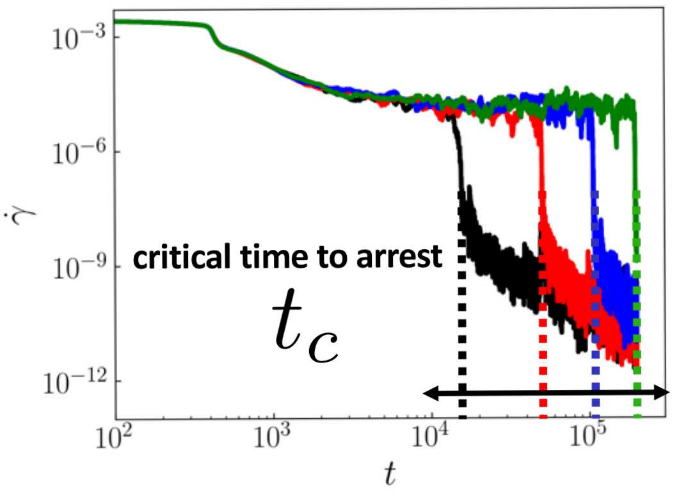
**same:** applied shear below yield, pressure, particle friction
**different:** initial positions of particles

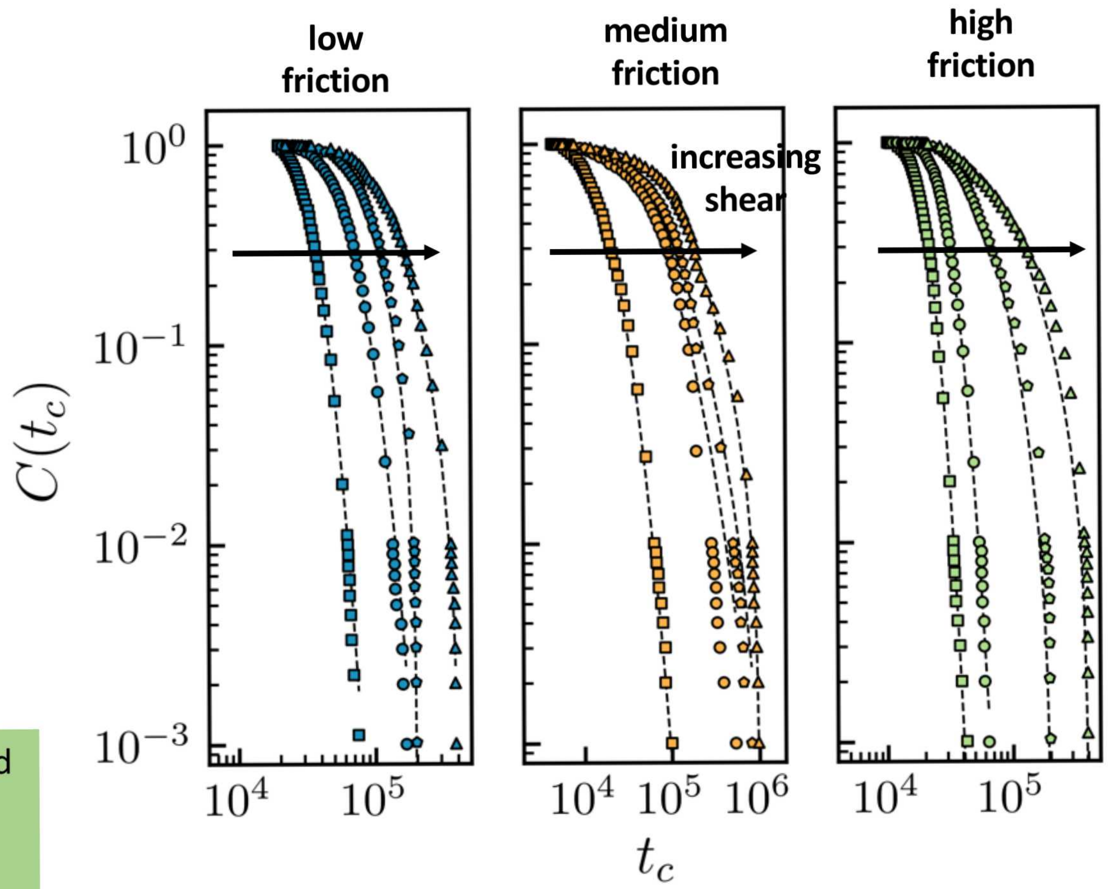



- wide variation of times taken to arrest for same applied shear
- volume fraction, however, is invariant: pressure sensitive only

# Stochastic Granular Arrest: Statistics




complementary cumulative distribution

- critical time to arrest is **log-normal** distributed for all frictions
- width of distribution increasing closer to critical yield

# Granular Arrest: Critical Phase Transition

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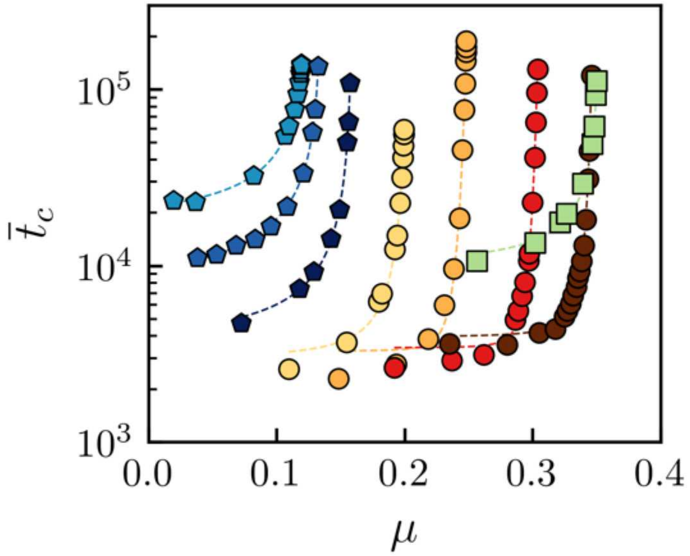
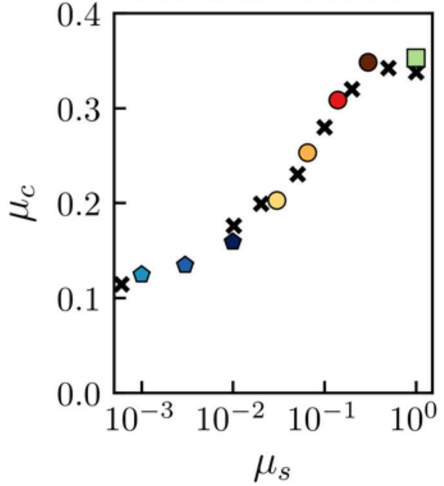
**mean critical time to arrest**
(statistics from $10^6$ simulations)



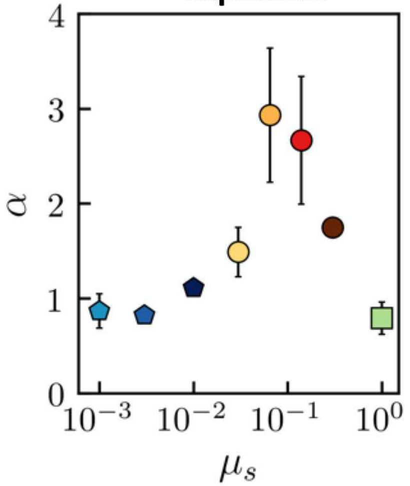

**power-law divergence of time to arrest at critical shear stress**

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

**friction-dependent critical shear stress**




**friction-dependent exponent**

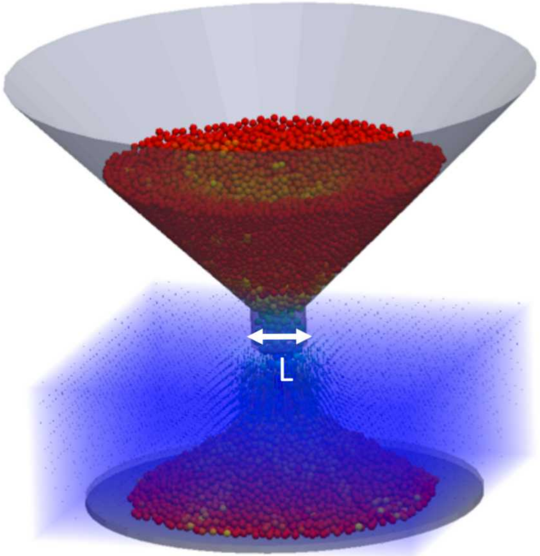



- mean times to arrest diverge at critical yield stress as a power law
- critical yield stress and power-law exponents are highly friction-dependent
- no universality of criticality?

# Stochastic Arrest: Practical Implications

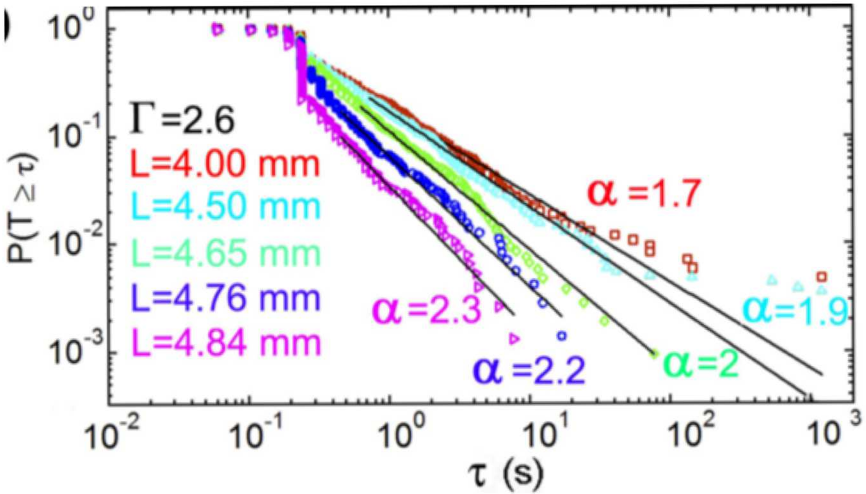


flow/clogging through a hopper

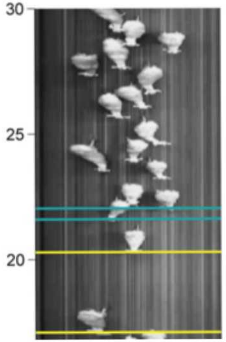



Zhao and Shan, Powder Tech., 239 (2013)

distribution of times between clogs



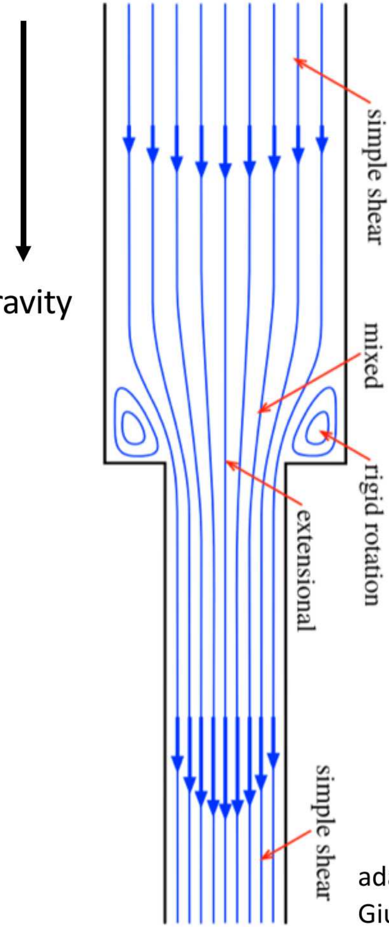

Zuriguel et al., Sci. Reports, 4 (2014)




- mean times to arrest is ***akin*** to intermittent clogging through hopper
- wide distributions: engineering design very challenging (lack of predictability)

# Complex Flows of Granular Matter

gravity

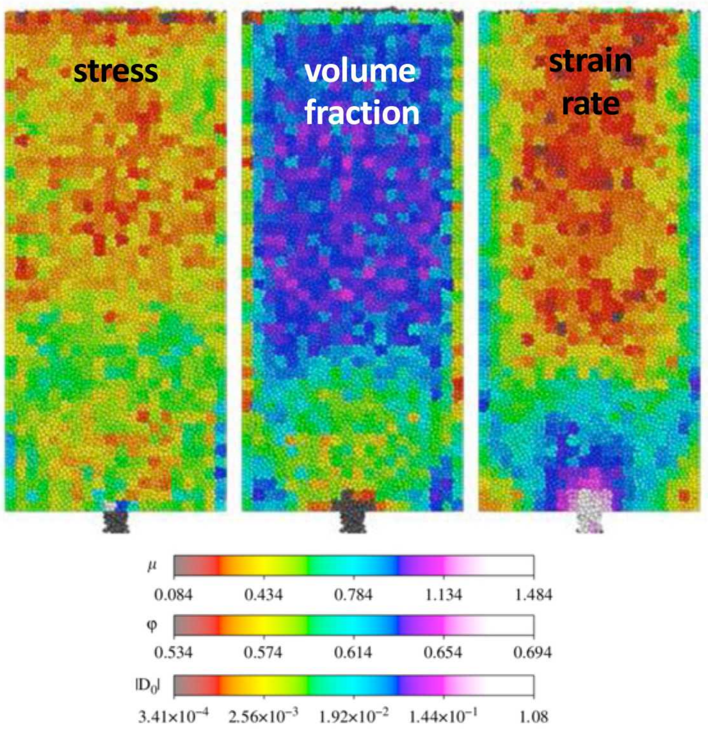



paradigmatic example of granular flow fields in practice

Can existing rheological constitutive laws predict such complex flows?

adapted from:
Giusteri and Seto, J. Rheology, 62 (2018)

complex flow field of granular discharge through orifice




Rycroft, Kamrin and Bazant, J. Mech. Phys. Sol., 57 (2009)

# Simple Shear Rheology of Granular Matter

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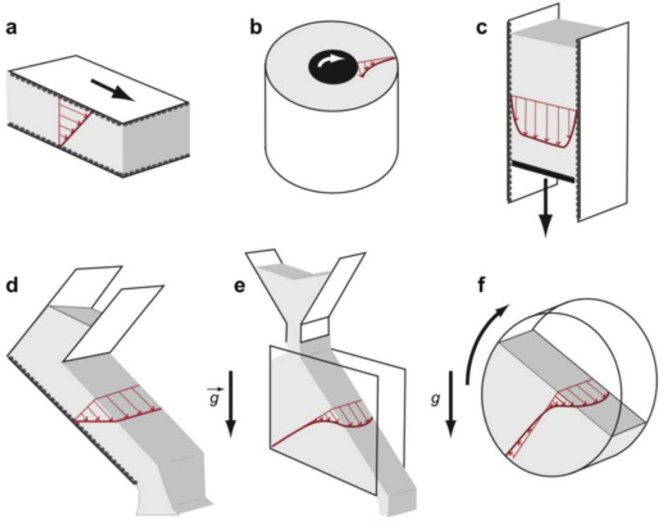
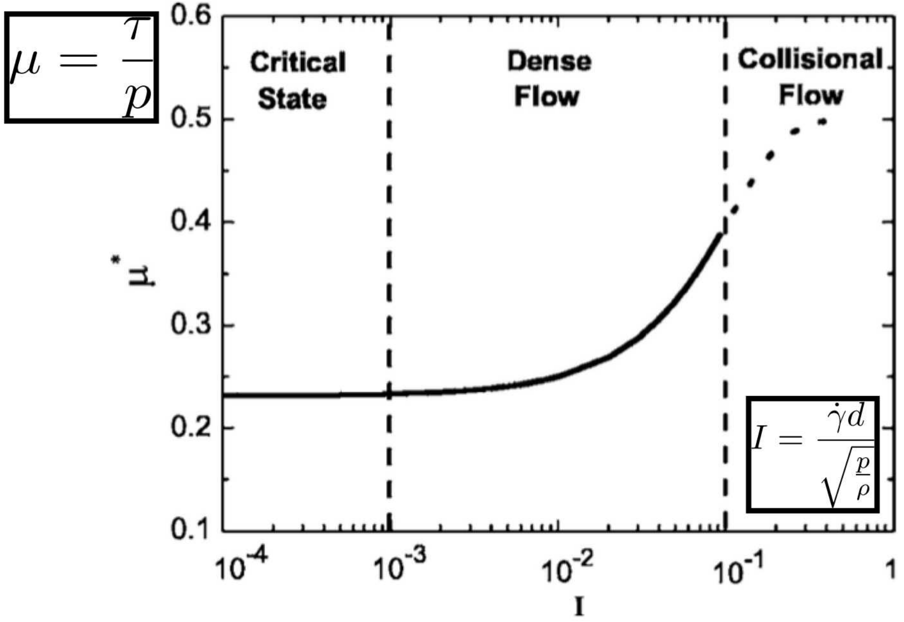
**simple shear flow scenarios**




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

$\mu(I)$ **rheology**




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

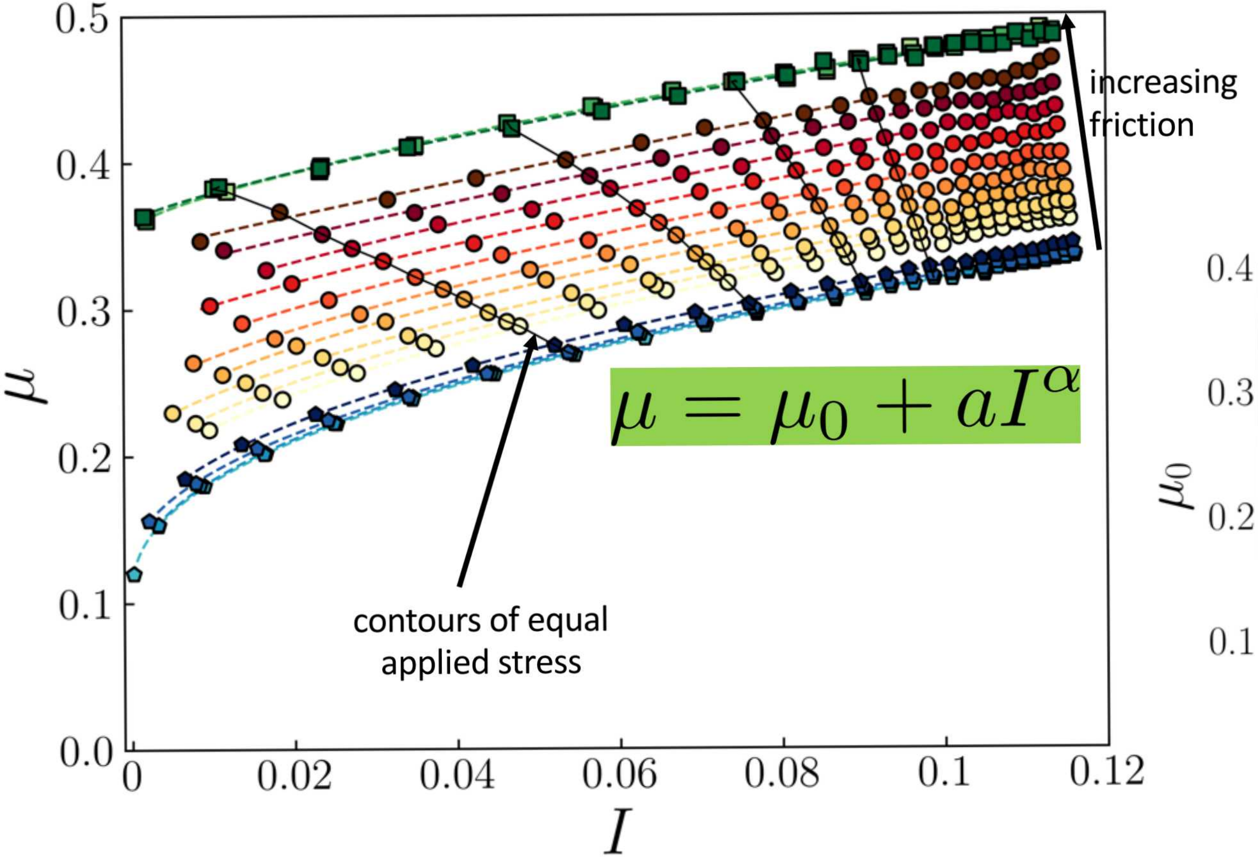
- dense granular rheology for simple shear is well-characterized by $\mu(I)$ rheology
- what about more complex flows?

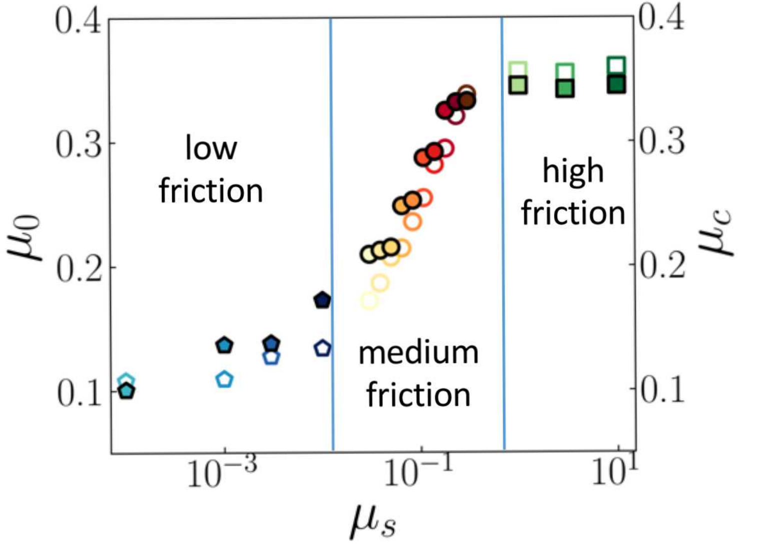
# Rheology beyond Simple Shear

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

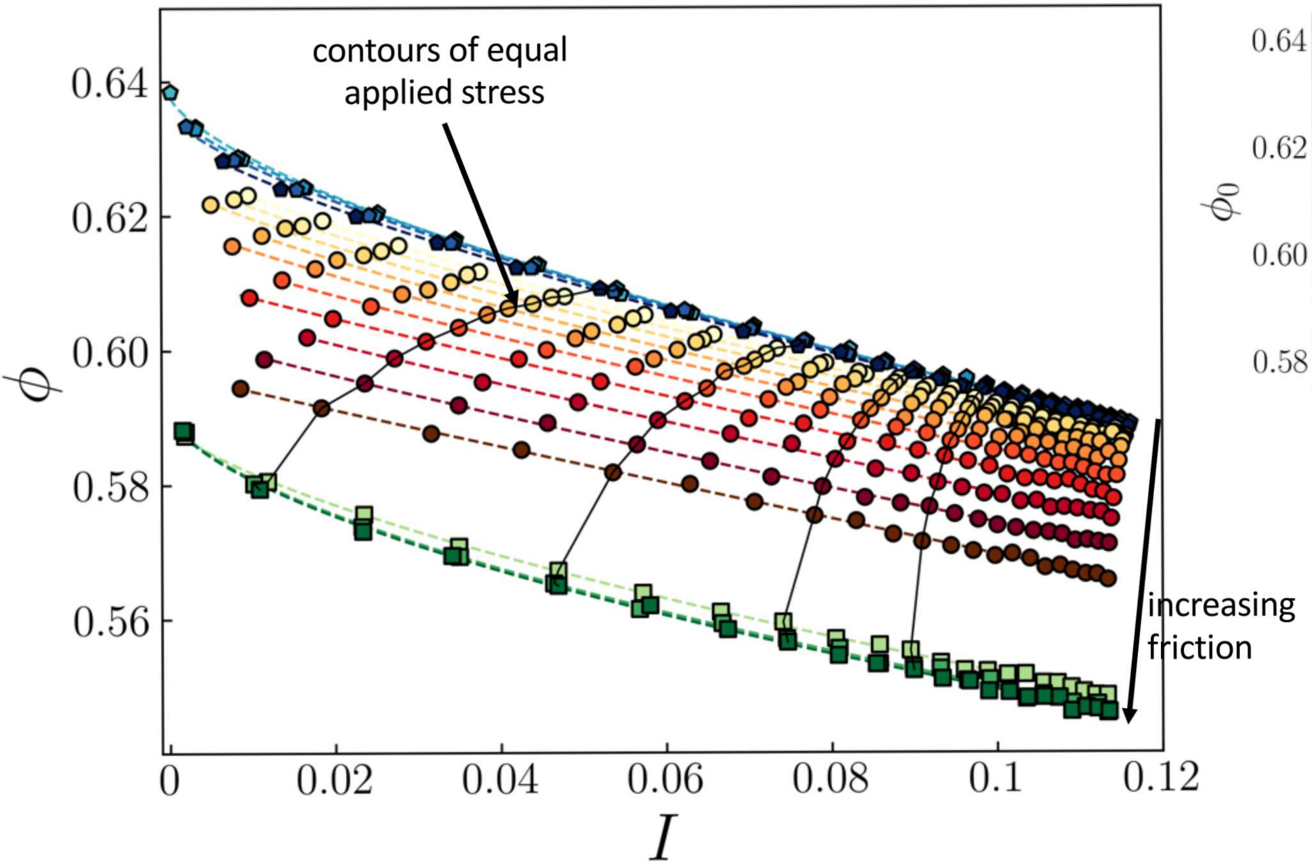
$$I = |\dot{\gamma}|d/\sqrt{p/\rho}$$

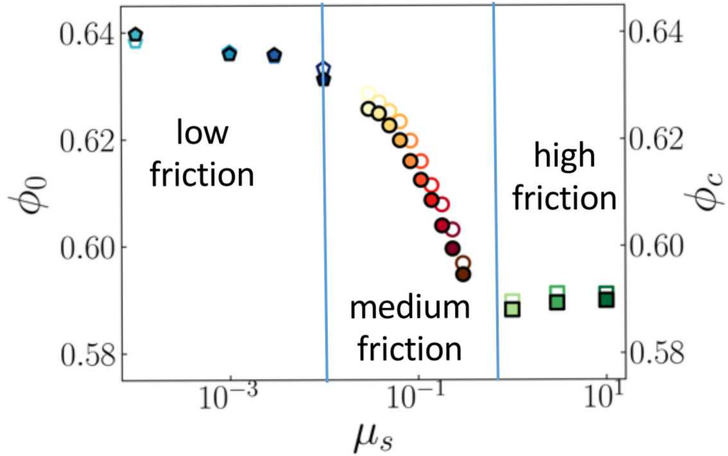
Jop et al., Nature, 441, 2008



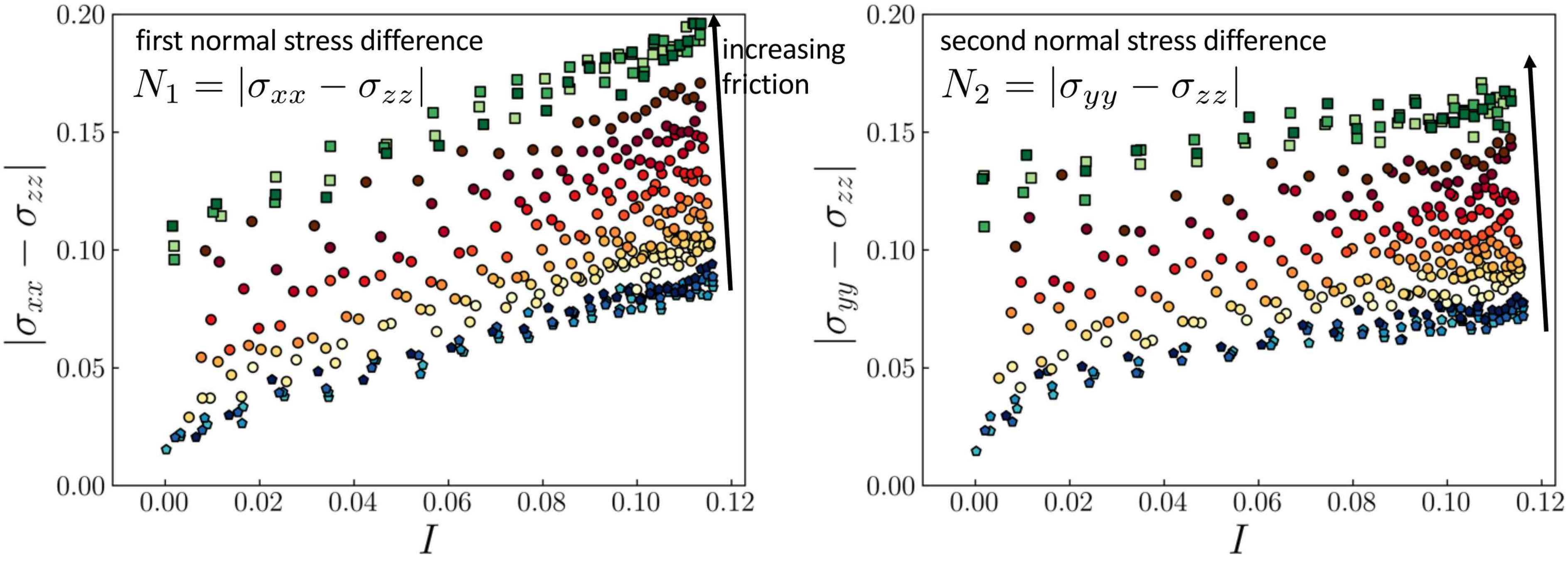
# Rheology beyond Simple Shear: Dilation




$$\phi = \phi_0 - bI^{\beta}$$

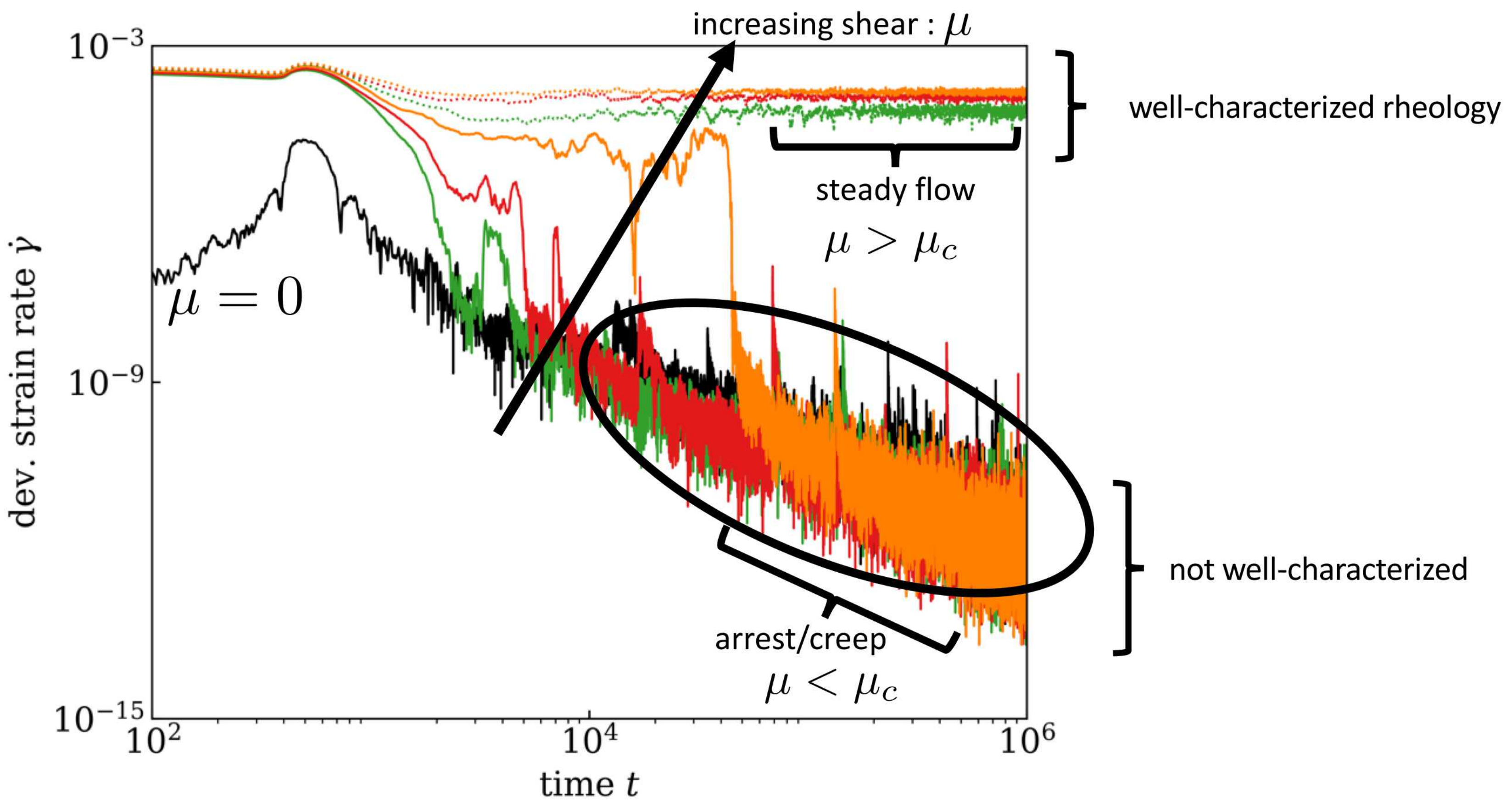
# Rheology beyond Simple Shear: Normal Stress Differences




simple shear viscosity — normal stress differences

proposed rheology beyond $\mu(I)$: $$\sigma_{ij} = f\left[p, \eta(p, |\dot{\gamma}|), N_1(p, |\dot{\gamma}|), N_2(p, |\dot{\gamma}|)\right]$$

# Sub-Yield Creep in Granular Matter



# What is Creep?

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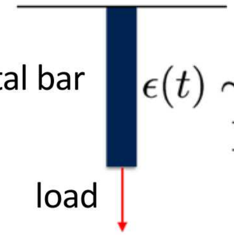
creep: slow irreversible deformation of a solid under stress

metal bar

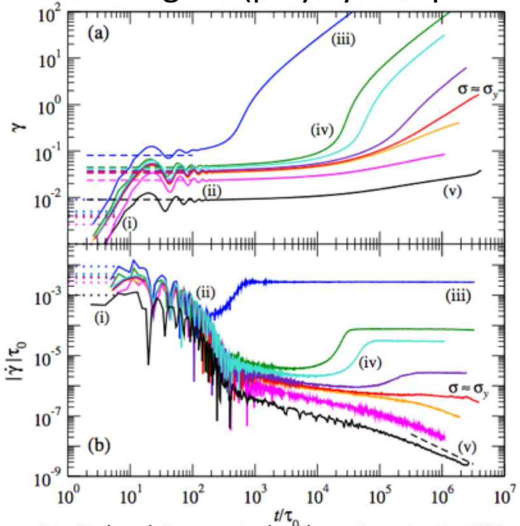


load

$$\epsilon(t) \sim \begin{cases} t^{1/3} & \text{Andrade creep} \\ \log(t) & \text{Logarithmic creep} \end{cases}$$

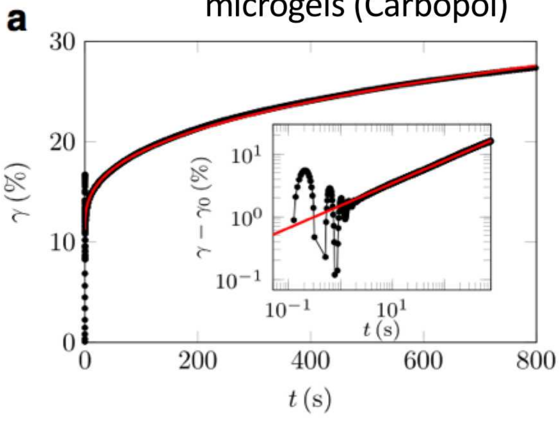
"… strain-hardening, *rather than turbulence*, is most difficult remaining problem in classical physics."- Alan Cottrell, Dislocations in Solids. Vol. 11. Elsevier, 2002.

colloidal glass (polystyrene particles)



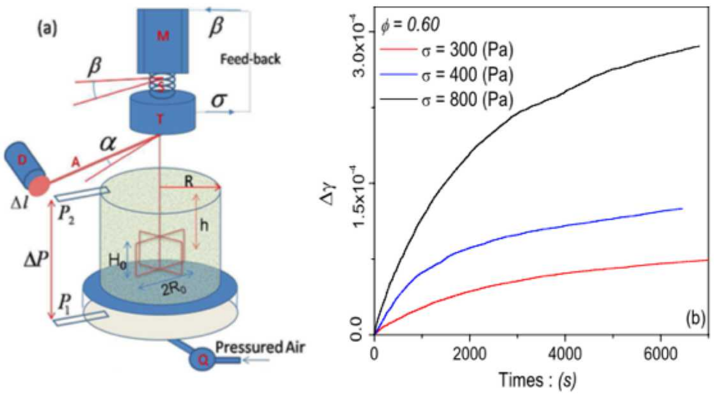

M. Siebenbürger et al., Phys. Rev. Lett. 108, 1 (2012)

microgels (Carbopol)




P. Lidon et al., Rheol. Acta 1 (2016)

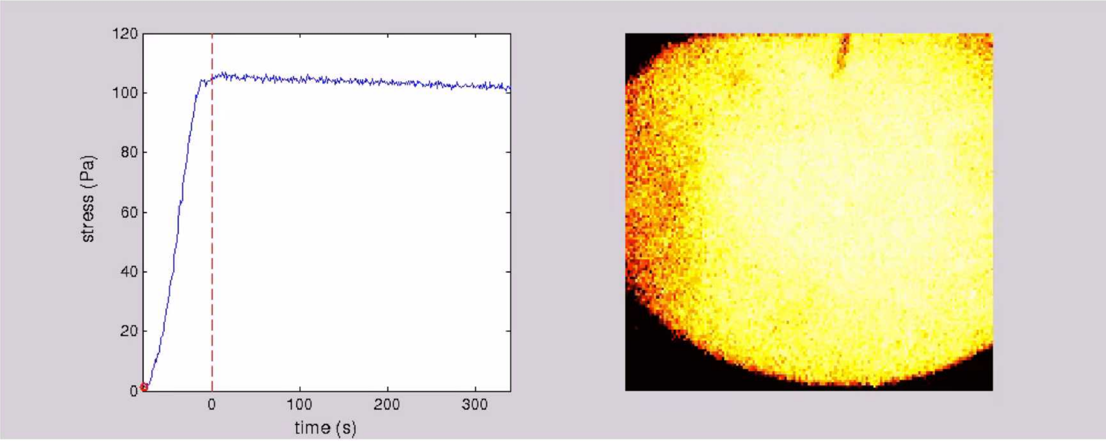
granular matter (glass beads)



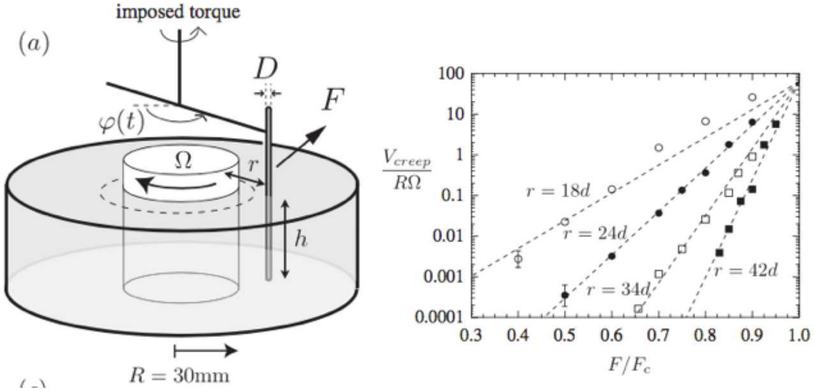

V. B. Nguyen et al., Phys. Rev. Lett. 107, 1 (2011)

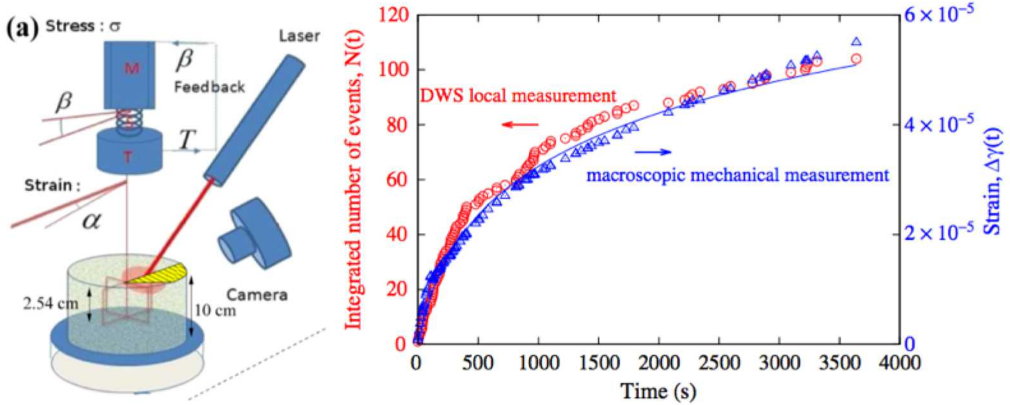
# Creep in Granular Matter: Novel Phenomena

Reddy et al., Phys. Rev. Lett. 106, (2011)

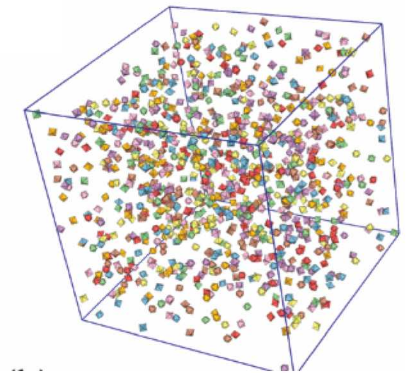



Amon et al., Phys. Rev. Lett. 108, (2012)

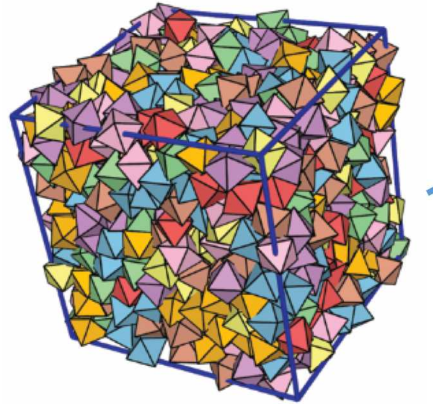


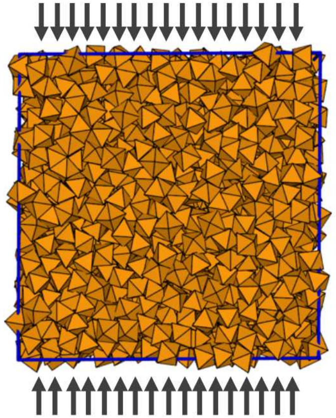
# Creep Simulations in Granular Matter



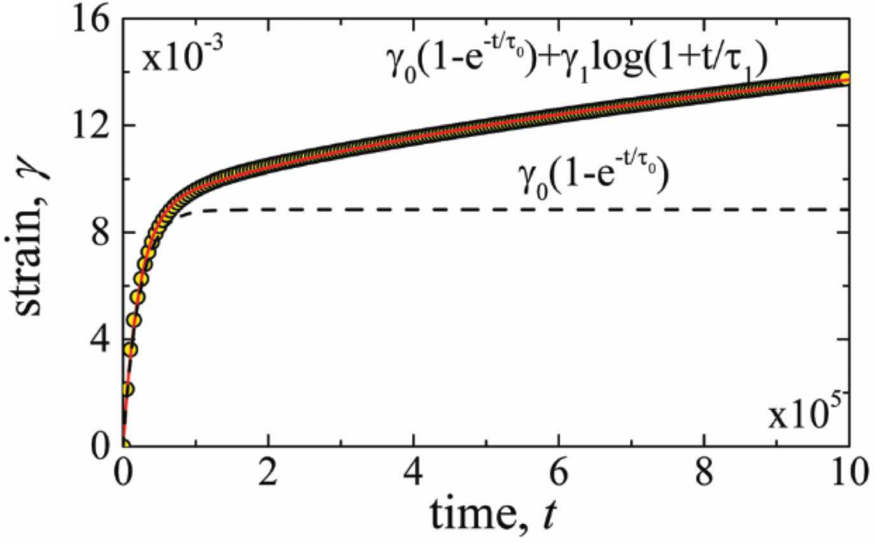
jam



$$\sigma^a = pI + \begin{bmatrix} \tau & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$



constant
pressure + uniaxial stress




$$\gamma(t) = \gamma_0\left(1 - e^{-t/\tau_0}\right) + \gamma_1 \log\left(1 + \frac{t}{\tau_1}\right)$$

early-time
Kelvin viscoelastic

long-time
logarithmic creep

# Constitutive Law: Creep and Fluidity

Complex Fluids Rheology


$$\partial_t \sigma = -\frac{G}{\eta}\sigma + G\dot{\gamma}$$

$$\partial_t \sigma = -f\sigma + G\dot{\gamma}$$

$$\partial_t f = -af^2 + r\dot{\gamma}^2$$

ageing rejuvenation

**Soft Glassy Rheology**

Derec et. al., Phys. Rev. Lett. 103, (2009)

Pressure-dependent Granular Flows

$$P\partial_t \mu = Gg\mu + G\dot{\gamma}$$

$$g = \frac{\dot{\gamma}}{\mu}$$

granular fluidity at constant stress
inverse of viscosity
units: time inverse

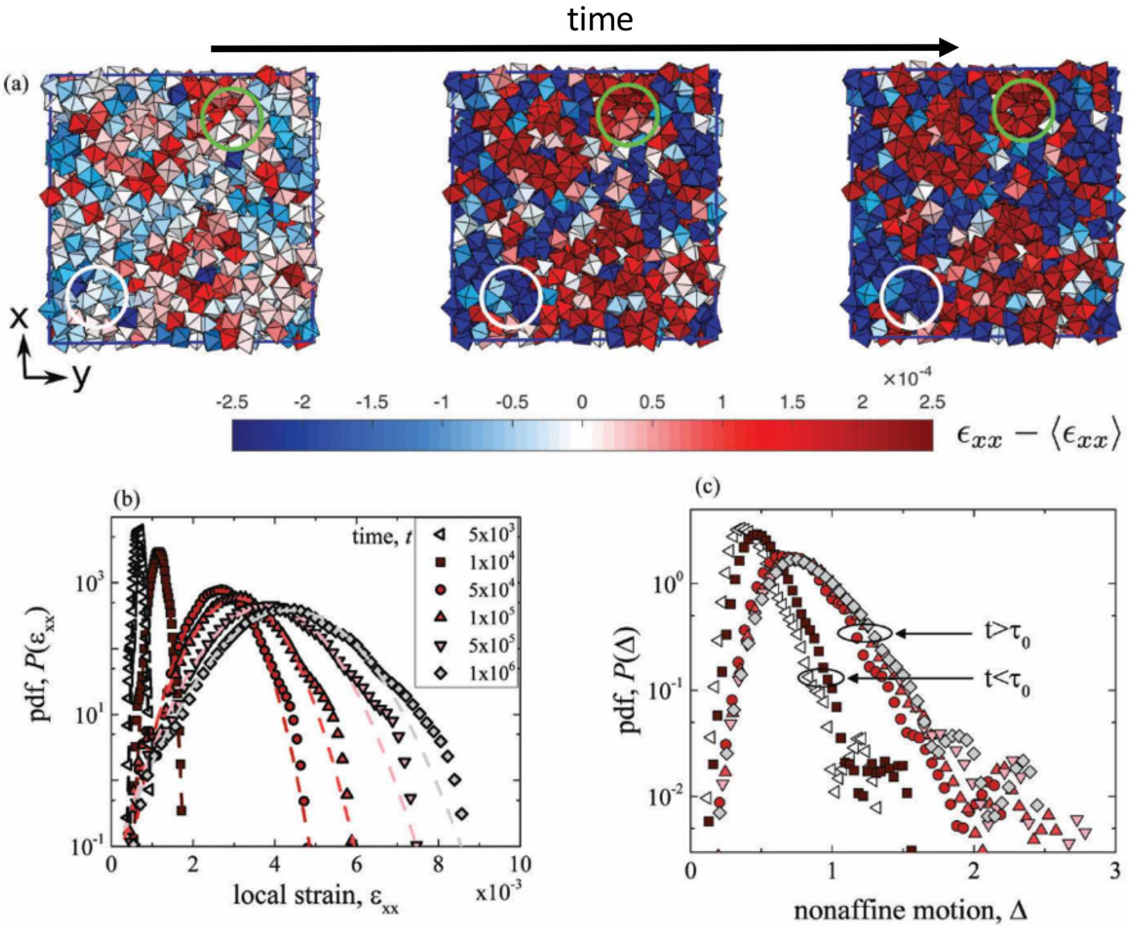
Ginzburg-Landau + Plasticity Theory:

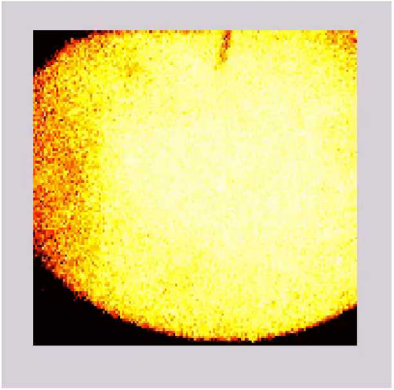
$$t_0\dot{g} = A^2 d^2 \nabla^2 g - \Delta\mu\left(\frac{\mu_s - \mu}{\mu_2 - \mu}\right)g - b\sqrt{\frac{\rho_s d^2}{P}}\mu g^2$$

[1]Kamrin and Koval, Phys. Rev. Lett., 108, 178301, 2012
[2]Henann and Kamrin, PNAS, 110, 17, 6730-6735, 2013
[3] Aranson and Tsimring, Rev. Mod. Phys.,78, 641-692, 2006

- what is fluidity in terms of microscopic mechanisms?

# Microscopic Mechanisms during Granular Creep



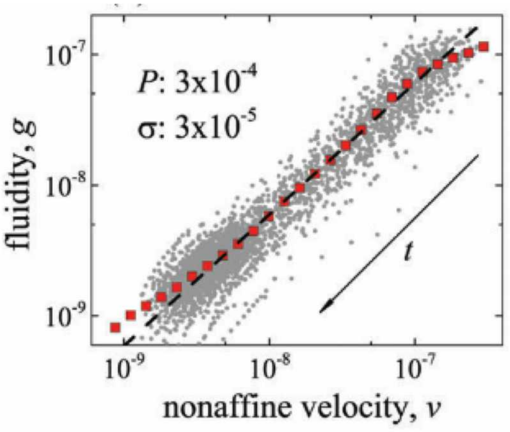



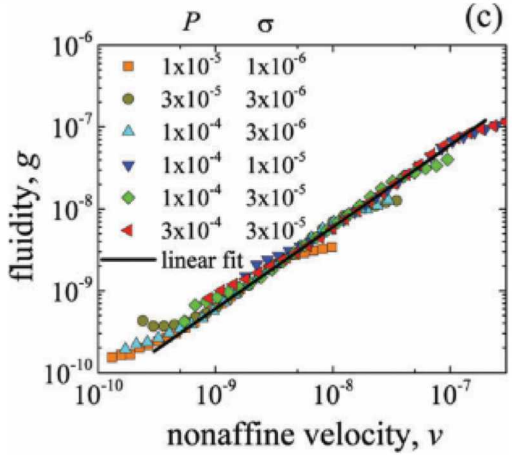
Amon et al., Phys. Rev. Lett. 108, (2012)

- regions of large strain and non-affine motion nucleate randomly with time
- regions of large strain and non-affine motion grow in time
- local response is random and heterogeneous

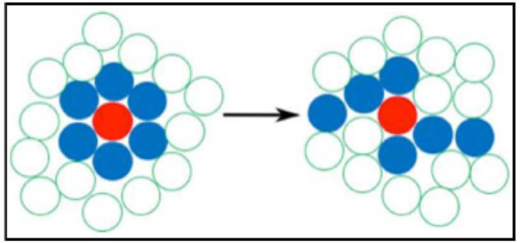
Srivastava and Fisher, Soft Matter, 13, (2017)

# Microscopic Definition of Granular Fluidity




non-affine velocity



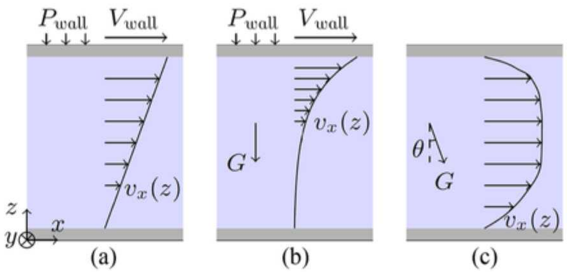
$$\min\left[D_i^2 = \sum_{j=1}^{n}\left[\mathbf{r}_{ij} - \mathbf{F}_i\mathbf{r}_{ij}\right]^2\right]$$

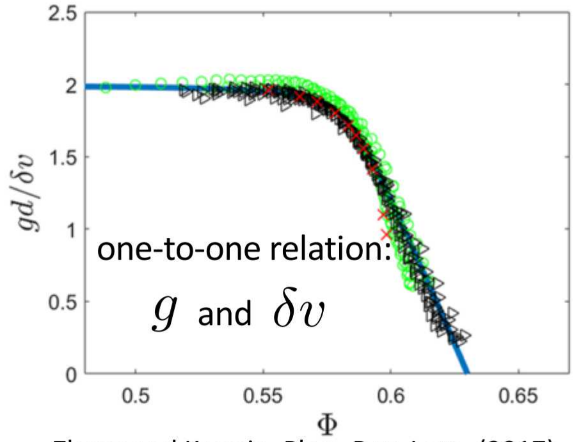
$$\boldsymbol{\epsilon}_i = \frac{1}{2}\left(\mathbf{F}_i^T\mathbf{F}_i - \mathbf{I}\right)$$

$$\dot{v}_i = \frac{\mathrm{d}}{\mathrm{d}t}D_i$$

Falk and Langer, Phys. Rev. E, (1998)

a measure of inelastic motion of a grain




Zhong and Kamrin, Phys. Rev. Lett., (2017)

**Fluidity is a kinematic variable governed by velocity fluctuations**

# Conclusions

**Key Phenomena Identified:**

- stressed granular matter exhibits a bifurcative behavior: (i) ***steady flow***, and (ii) ***creep arrest***
- transitions between these states is ***highly stochastic*** and friction dependent with ***power-law divergence***
- full 3D stress-controlled simulations reveal rheological signatures ***beyond simple shear***
- granular creep is often logarithmic, characterized by growing regions of high ***fluidity***
- ***fluidity*** acts a potential state variable characterizing local velocity fluctuations

# Publications:


K. C. Smith, **I. Srivastava**, T. S. Fisher, M. Alam, Phys. Rev. E 89 (4), 042203, 2014

**I. Srivastava**, T. S. Fisher, Soft Matter 13 (18), 3411-3421, 2017

**I. Srivastava**, L. E. Silbert, G. S. Grest, J. B. Lechman, "Flow-arrest transitions in frictional granular matter," arXiv:1810:00043

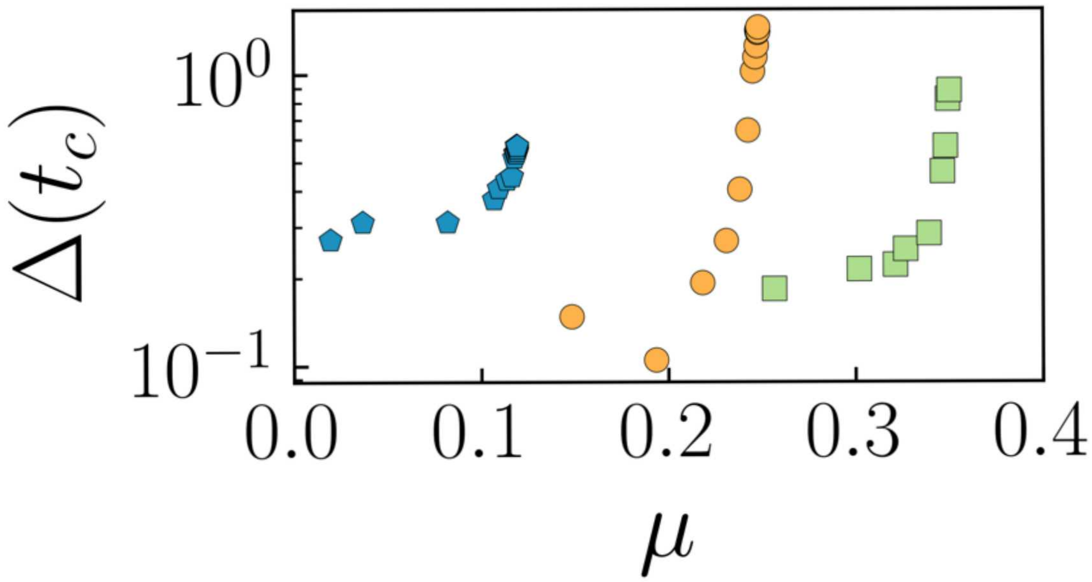
**I. Srivastava**, L. E. Silbert, G. S. Grest, J. B. Lechman, "Normal stress differences in granular shear flows," *in preparation*

**I. Srivastava**, L. E. Silbert, G. S. Grest, J. B. Lechman, "Hysteresis in granular shear arrest and flow initiation," *in preparation*



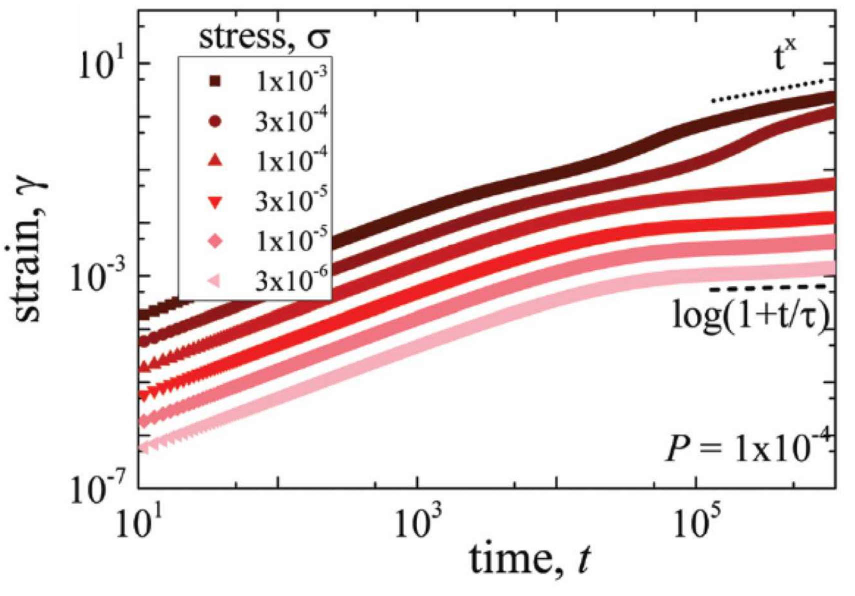
email: isriva@sandia.gov

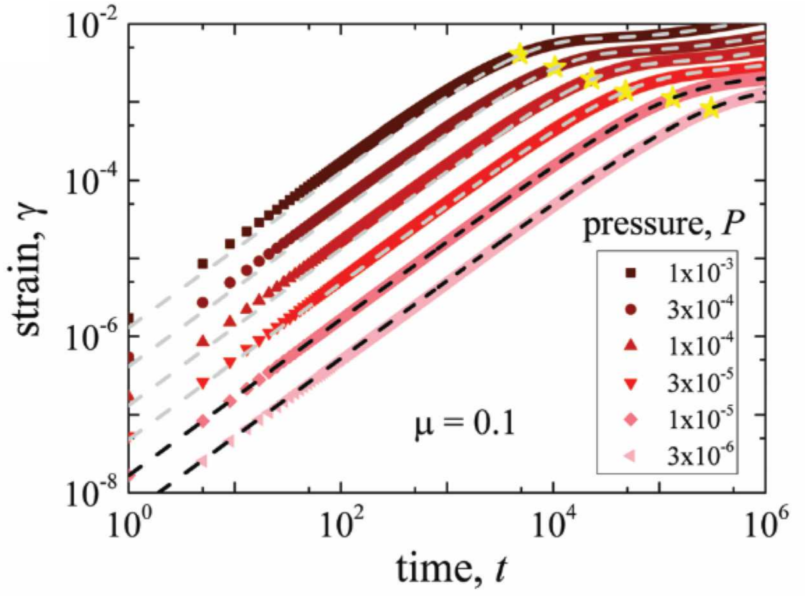
# Second Moment of Distribution




**Ratio of standard deviation to mean**

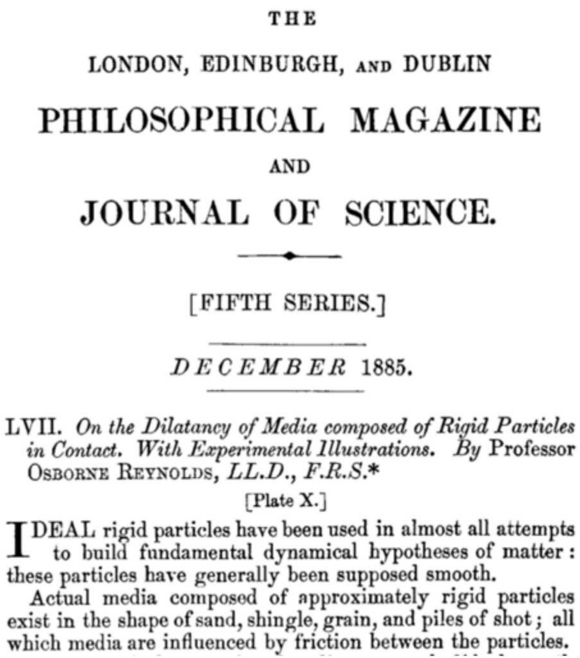
# Creep Simulations in Granular Matter




$$\gamma(t) = \gamma_0\left(1 - e^{-t/\tau_0}\right) + \gamma_1 \log\left(1 + \frac{t}{\tau_1}\right)$$

# Granular Matter: Illustrious History



THE

LONDON, EDINBURGH, AND DUBLIN

PHILOSOPHICAL MAGAZINE

AND

JOURNAL OF SCIENCE.

[FIFTH SERIES.]

*DECEMBER* 1885.

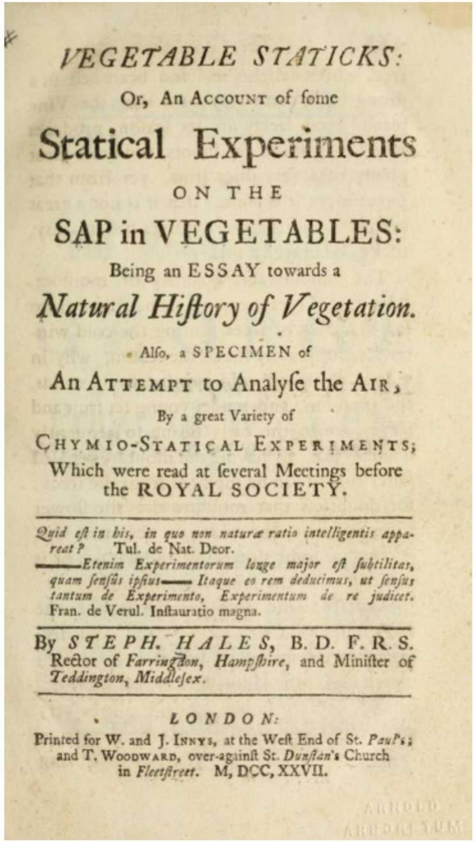
LVII. *On the Dilatancy of Media composed of Rigid Particles in Contact. With Experimental Illustrations.* By Professor OSBORNE REYNOLDS, *LL.D., F.R.S.**

[Plate X.]

IDEAL rigid particles have been used in almost all attempts to build fundamental dynamical hypotheses of matter: these particles have generally been supposed smooth.

Actual media composed of approximately rigid particles exist in the shape of sand, shingle, grain, and piles of shot; all which media are influenced by friction between the particles.

Reynolds Dilatancy
(1881)



*VEGETABLE STATICKS:*

Or, An ACCOUNT of fome

Statical Experiments

ON THE

SAP in VEGETABLES:

Being an ESSAY towards a

*Natural Hiftory of Vegetation.*

Alfo, a SPECIMEN of

An ATTEMPT to Analyfe the AIR,

By a great Variety of

CHYMIO-STATICAL EXPERIMENTS;

Which were read at feveral Meetings before the ROYAL SOCIETY.

*Quid eft in his, in quo non naturæ ratio intelligentis appareat?* Tul. de Nat. Deor.

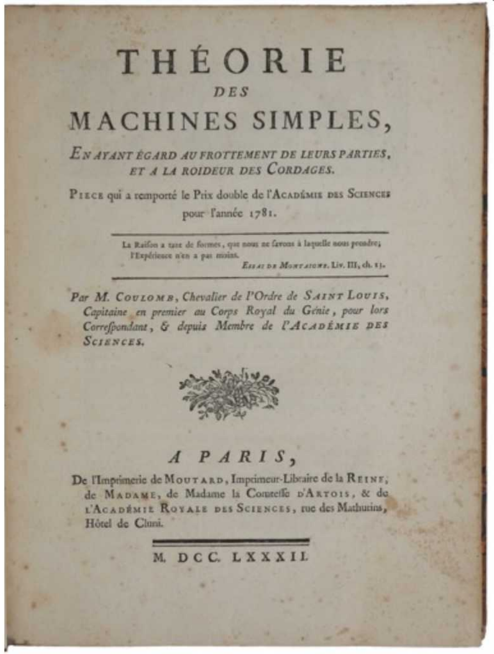
——*Etenim Experimentorum longe major eft fubtilitas, quam fenfûs ipfius*—— *Itaque eo rem deducimus, ut fenfus tantum de Experimento, Experimentum de re judicet.* Fran. de Verul. Inftauratio magna.

By *STEPH. HALES*, B. D. F. R. S. Rector of *Farringdon, Hampfhire*, and Minifter of *Teddington, Middlefex.*

*LONDON:*

Printed for W. and J. INNYS, at the Weft End of St. *Paul's*; and T. WOODWARD, over-againft St. *Dunftan's* Church in *Fleetftreet*. M, DCC, XXVII.

Sphere Packing Problem
(1727)



THÉORIE

*DES*

MACHINES SIMPLES,

*EN AYANT ÉGARD AU FROTTEMENT DE LEURS PARTIES, ET A LA ROIDEUR DES CORDAGES.*

PIECE qui a remporté le Prix double de l'ACADÉMIE DES SCIENCES pour l'année 1781.

La Raifon a tant de formes, que nous ne favons à laquelle nous prendre; l'Expérience n'en a pas moins.

*ESSAI DE MONTAIGNE*, Liv. III, ch. 13.

*Par M. COULOMB, Chevalier de l'Ordre de SAINT LOUIS, Capitaine en premier au Corps Royal du Génie, pour lors Correfpondant, & depuis Membre de l'ACADÉMIE DES SCIENCES.*

*A PARIS,*

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M. DCC. LXXXII.

Mohr-Coulomb Yield Theory
(1772)

*"Who could ever calculate the path of a molecule? How do we know that the creation of worlds are not determined by falling grains of sand?"*

**Victor Hugo, Les Misreables (1862)**