Implementation and Refinement of a Comprehensive Model for Dense Granular Flows

Sebastian Chialvo and Sankaran Sundaresan
Princeton University

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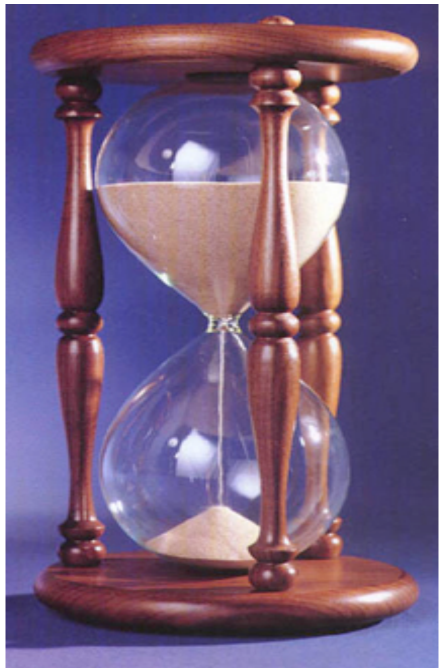
Motivation

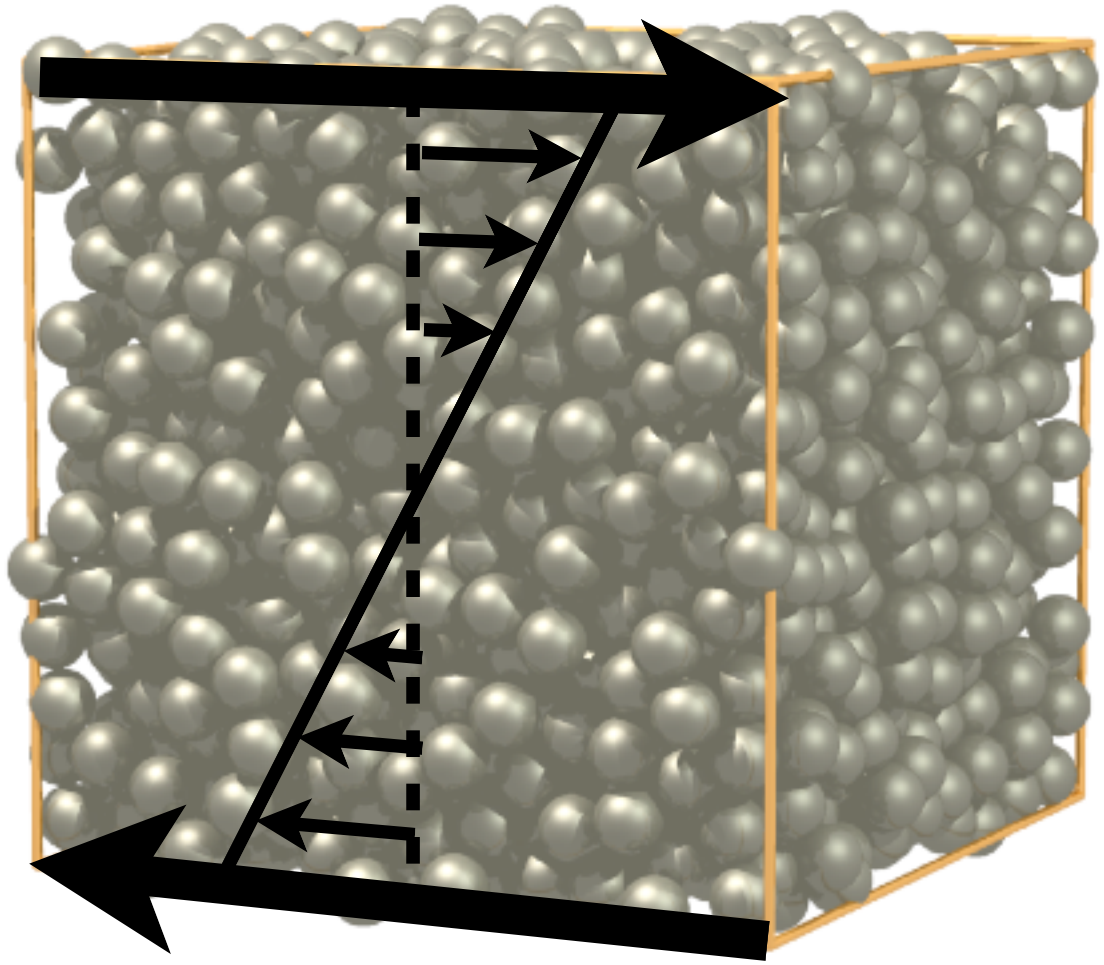
- Granular flows are ubiquitous in nature and in industry, e.g. avalanches and hopper discharge.
- Complex behavior: solid-, liquid-, or gas-like



- Goal: To probe flow behavior computationally and develop general rheological models.

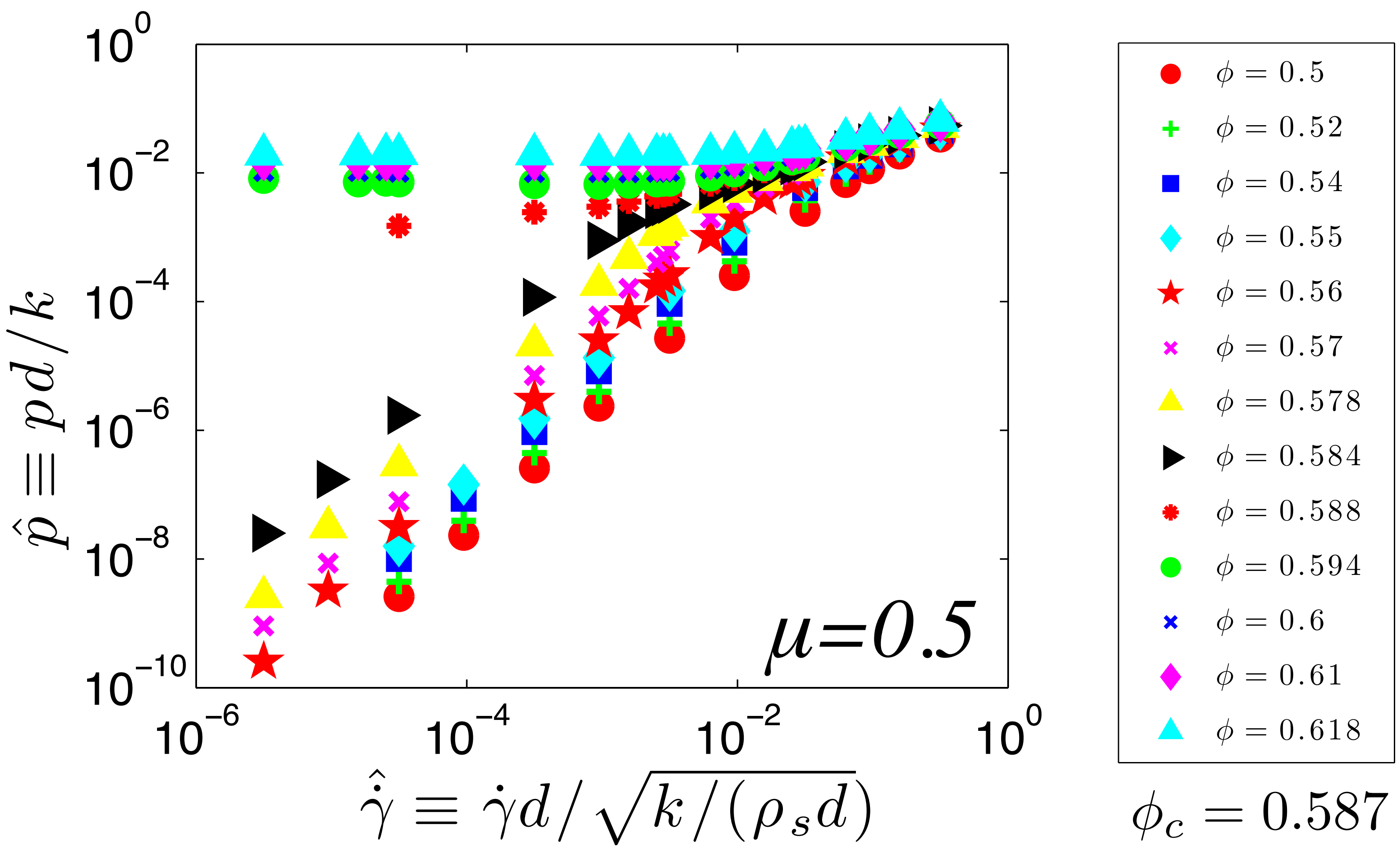
Computational methodology

- Simulate particle dynamics of homogeneous assemblies under simple shear using discrete element method (DEM).
  - Linear spring-dashpot with frictional slider.
  - 3D periodic domain without gravity
  - Lees-Edwards boundary conditions
- Extract stress and structural information by averaging.



LAMMPS code. http://lammps.sandia.gov S. J. Plimpton. J Comp Phys, 117, 1-19 (1995)

Flow map



$\phi_c = 0.587$

Previous studies

- Computational
  - C. S. Campbell, J. Fluid Mech. 465, 261 (2002).
  - T. Hatano, J. Phys. Soc. Japan 77, 123002 (2008).
- Experimental
  - K. N. Nordstrom *et al.* Phys. Rev. Lett. 105, 175701 (2010).

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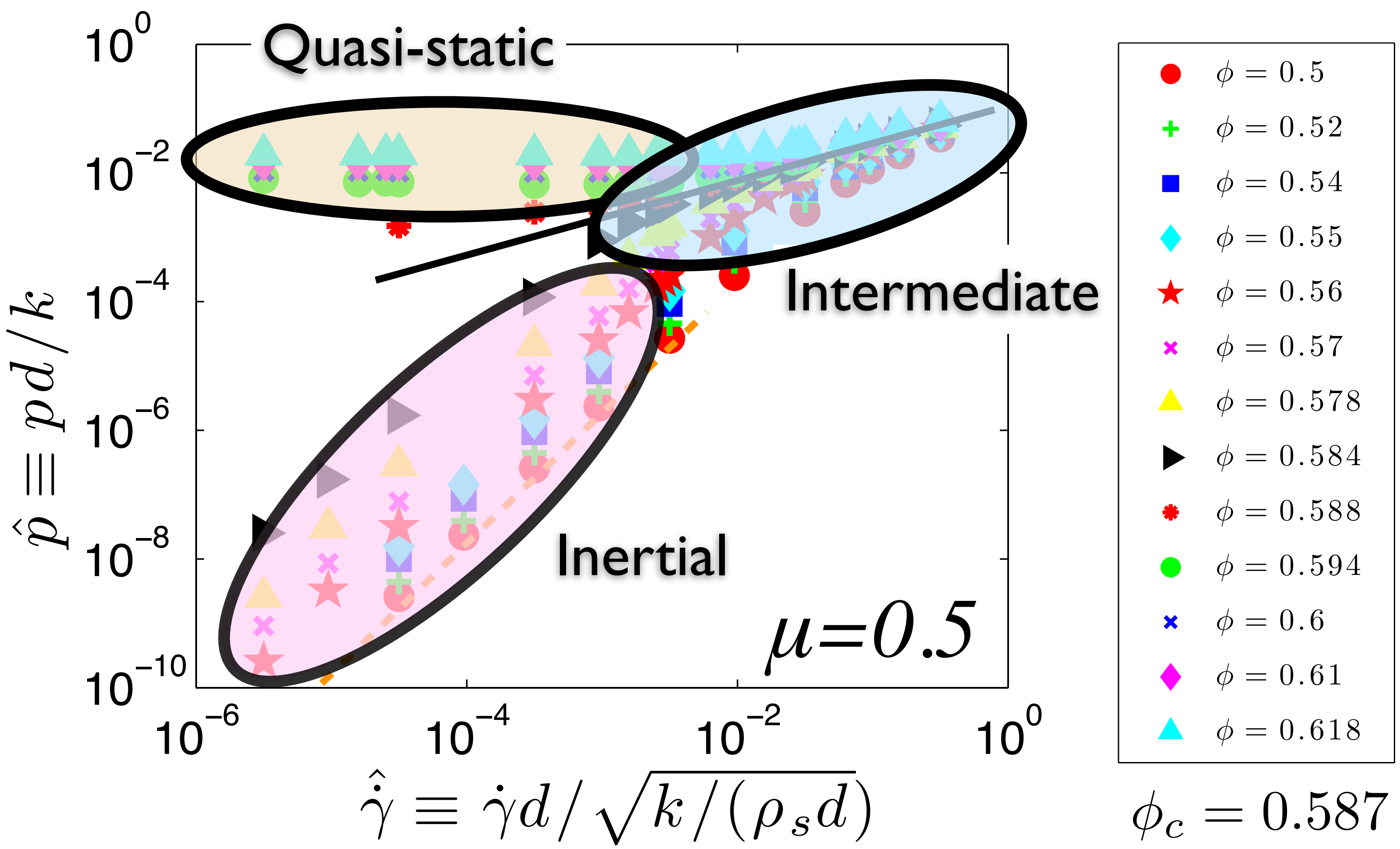

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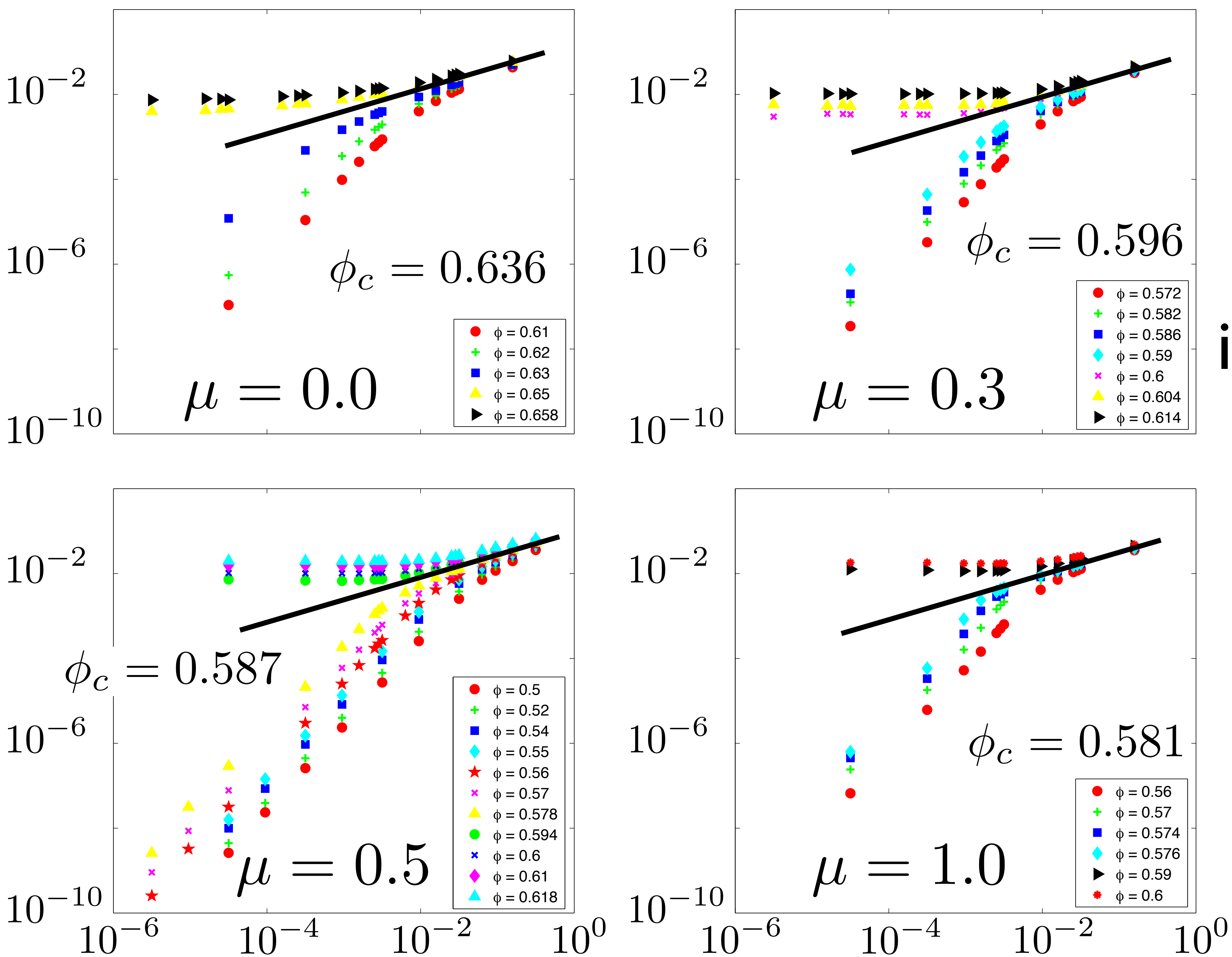
- Critical volume fraction ϕ_c and its flow curve $\hat{p} = \alpha \hat{\dot{\gamma}}^m$ distinguish the three flow regimes.
- Role of particle softness:
  - Large k $\Longrightarrow$ quasi-static or inertial regime
  - Small k $\Longrightarrow$ intermediate regime

Effect of μ on pressure

$\hat{p}$ vs. $\hat{\dot{\gamma}}$



Intermediate asymptote

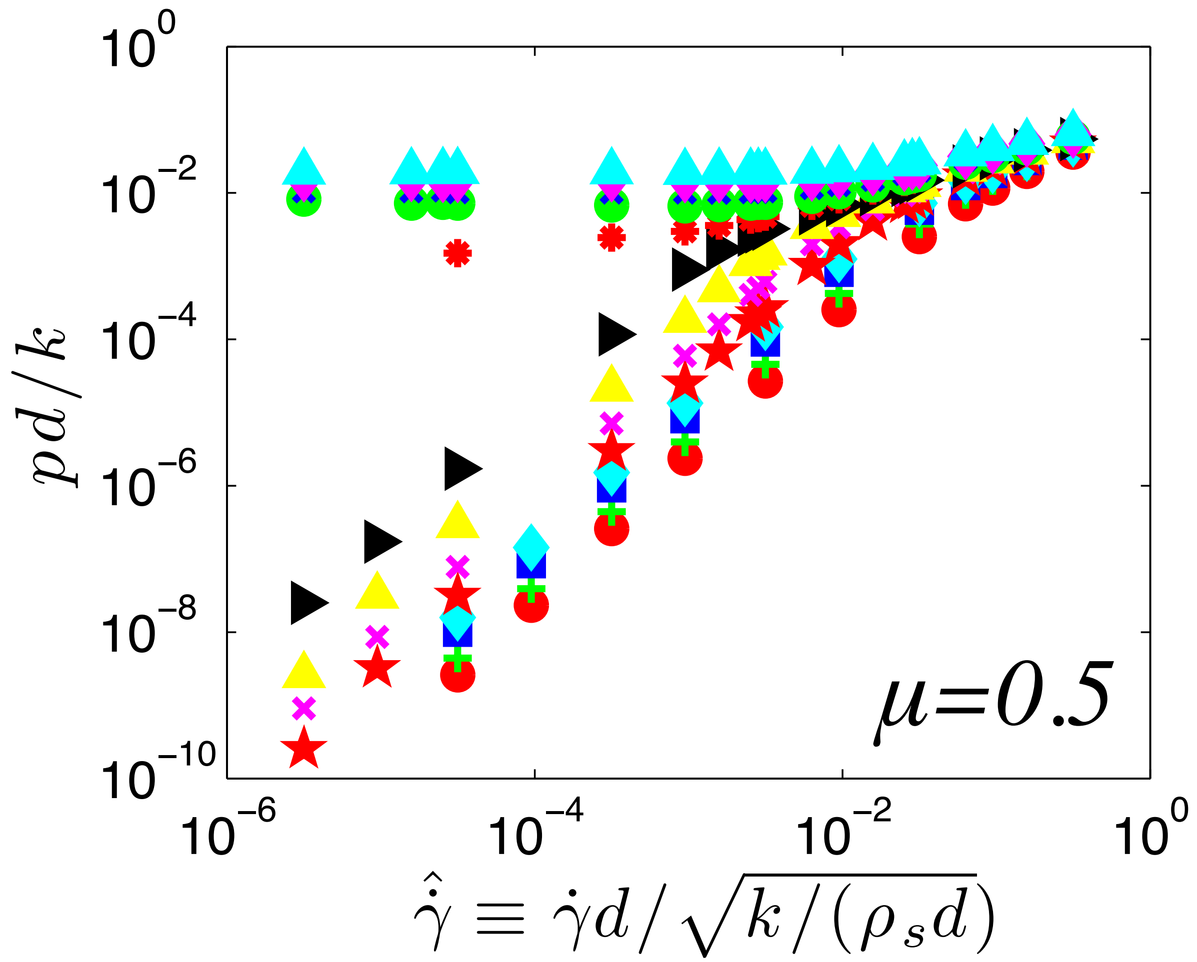
$$pd/k = \alpha \hat{\dot{\gamma}}^{1/2}$$

independent of μ

Critical volume fraction

$$\phi_c = \phi_c(\mu)$$

Pressure scalings for frictional particles



Scaled pressure and shear rate†:

$$p^* = \hat{p}/|\phi - \phi_c|^a$$

$$\dot{\gamma}^* = \hat{\dot{\gamma}}/|\phi - \phi_c|^b$$

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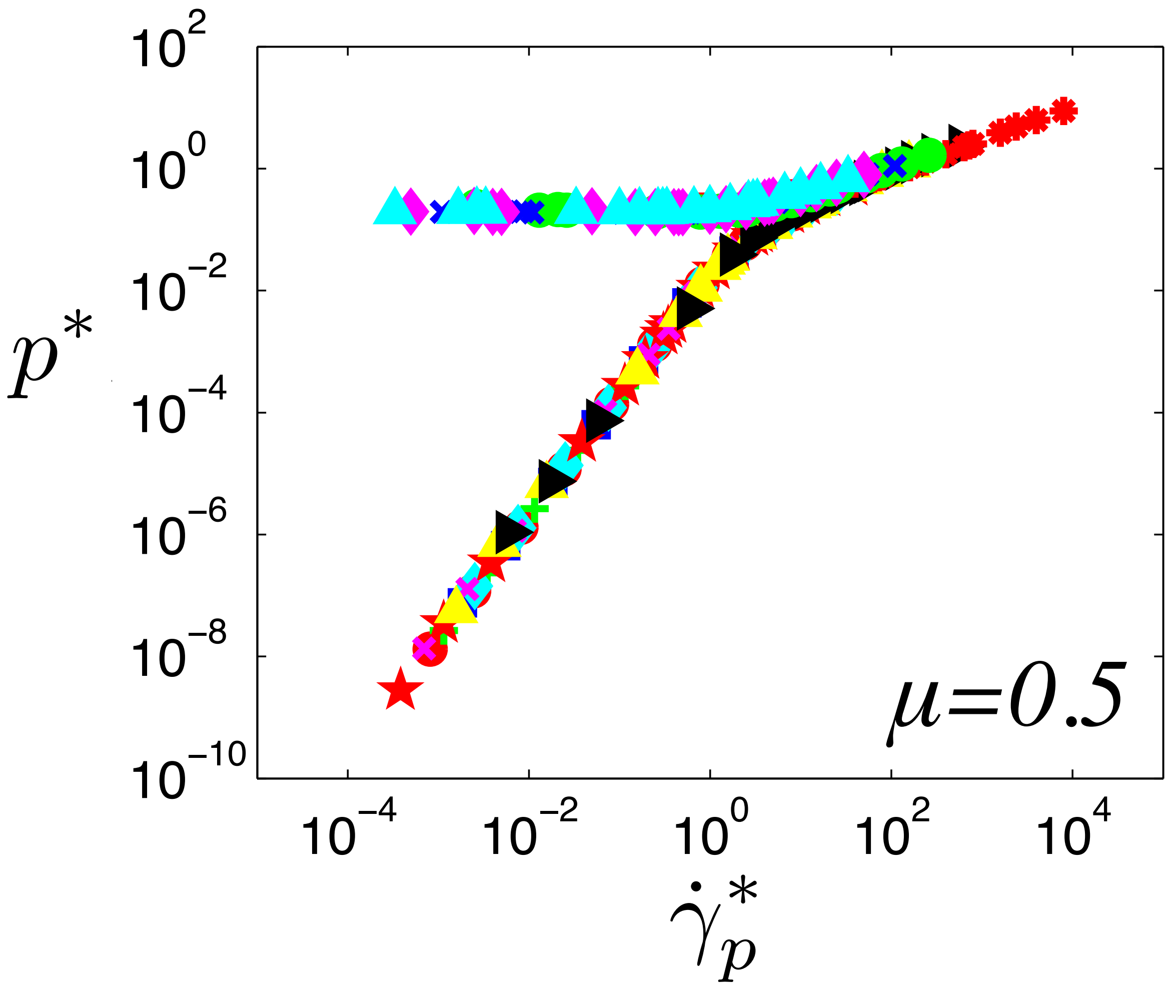

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$$\dot{\gamma}^* = \hat{\dot{\gamma}}/|\phi - \phi_c|^b$$

Choose exponents:

$$\left.\begin{aligned} a &= 2/3 \\ b &= 4/3 \end{aligned}\right\}$$ Independent of μ

- Three pressure asymptotes:

$$\frac{p_i}{|\phi - \phi_c|^{2/3}} = \alpha_i \left[\frac{\dot{\gamma}}{|\phi - \phi_c|^{4/3}} \right]^{m_i}$$

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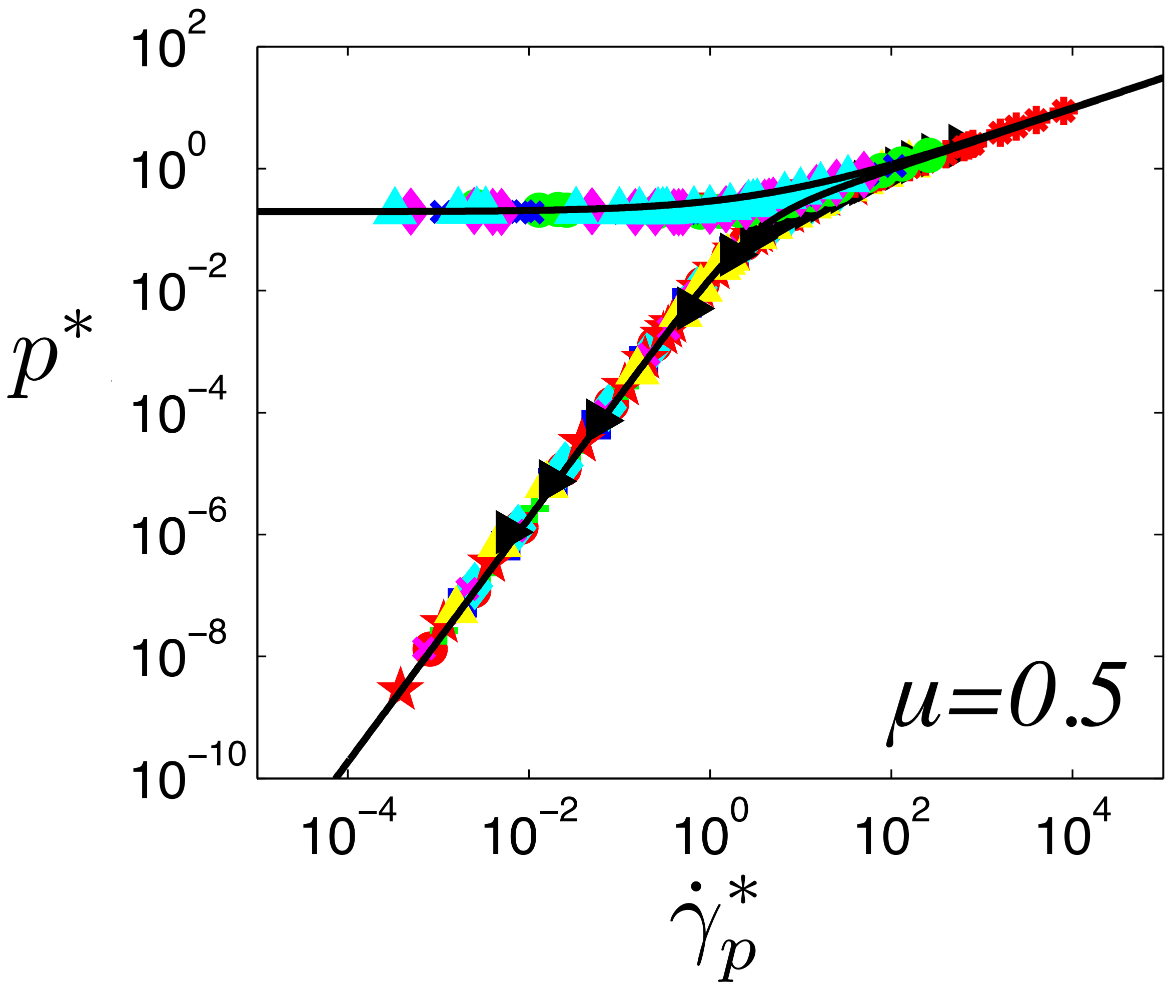

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- Three pressure asymptotes:

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- Transitions between regimes captured with a blending function:

$$B(y_1, y_2) = (y_1^w + y_2^w)^{1/w}$$

- $w = +1$ for top curve
- $w = -1$ for bottom curve

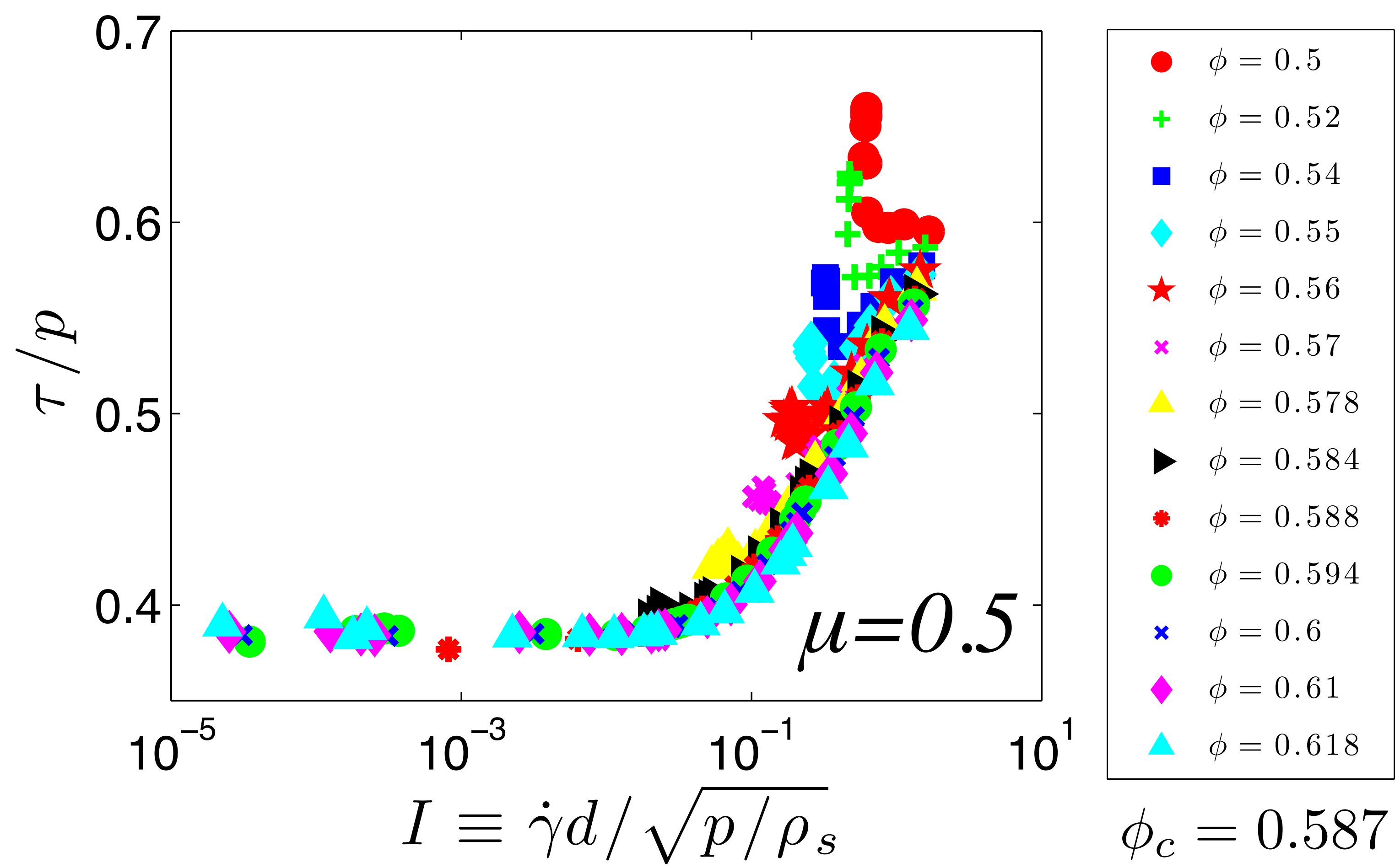
T. Hatano, J. Phys. Soc. Jpn. 77, 123002 (2008). K. N. Nordstrom et al., Phys. Rev. Lett. 105, 175701 (2010).

Shear stress ratio

- Definition: $\eta \equiv \tau / p$
- Inertial number†: $I \equiv \dfrac{\dot{\gamma} d}{\sqrt{p/\rho_s}} = \dfrac{\left(\text{timescale of particle rearrangement}\right)}{\left(\text{timescale of macroscopic deformation}\right)}$
- Existing hard-sphere models:

$$\eta = \eta(I)$$

- Scatter at large I due to particle softness



$\phi_c = 0.587$

- G. D. R. Midi, Eur. Phys. J. E 14, 341 (2004).
- P. Jop, Y. Forterre, and O. Pouliquen, Nature 441, 727 (2006).
- F. da Cruz et al, Phys. Rev. E 72, 021309 (2005).

Contributions to shear stress ratio

- Propose a model of the form:

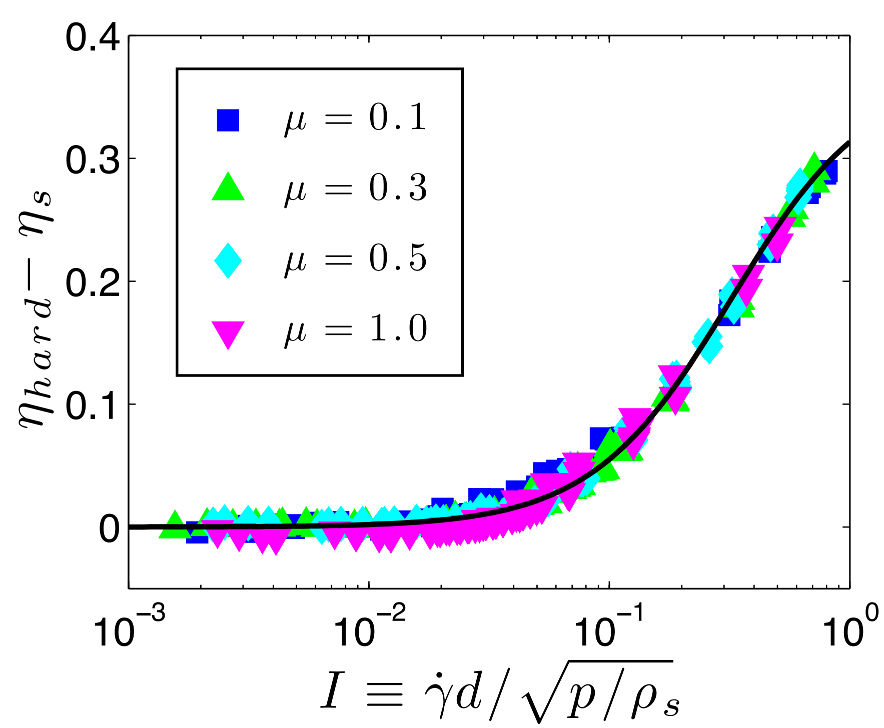
$$\eta(I,\hat{\dot{\gamma}}) = \eta_{hard}(I) + \eta_{soft}(\hat{\dot{\gamma}})$$

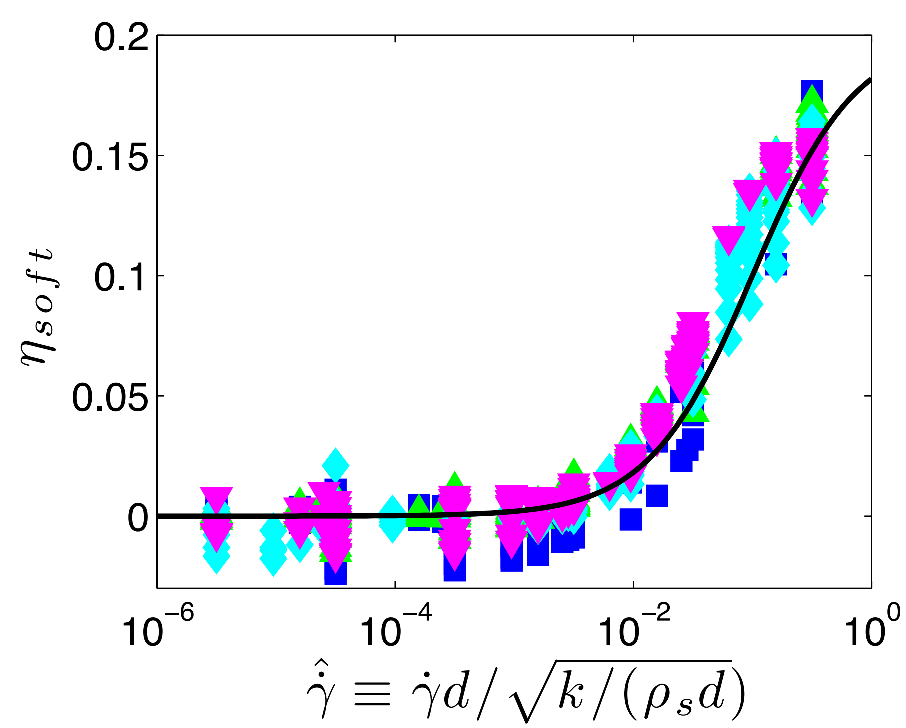
$$I \equiv \frac{\dot{\gamma} d}{\sqrt{p/\rho_s}}$$

$$\hat{\dot{\gamma}} \equiv \frac{\dot{\gamma} d}{\sqrt{k/(\rho_s d)}}$$

- Can fit each contribution to DEM data:

$$\eta_{\rm hard}(I) = \eta_s(\mu) + \frac{\alpha_1}{\left(\frac{I_0}{I}\right)^{\beta_1} + 1} \qquad \eta_{\rm soft}(\hat{\dot{\gamma}}) = \frac{\alpha_2}{\left(\frac{\hat{\dot{\gamma}}_0}{\hat{\dot{\gamma}}}\right)^{\beta_2} + 1}$$





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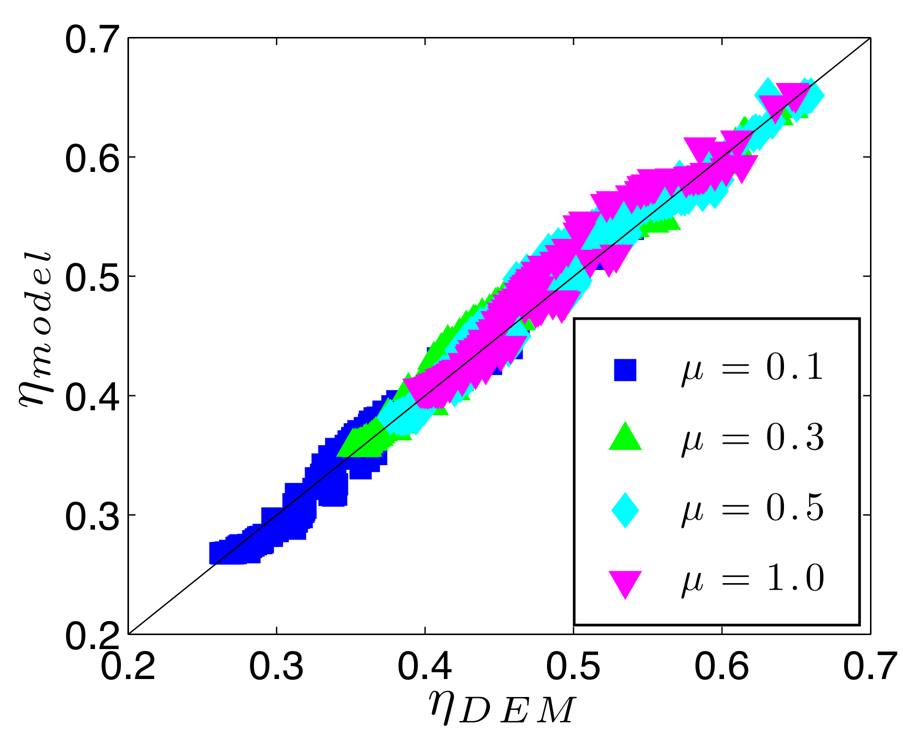
- Model works well for $\mu \geq 0.1$



Model summary

$$p = \begin{cases} p_{QS} + p_{Int} & \text{for } \phi \geq \phi_c \\ \left(p_{Inert}^{-1} + p_{Int}^{-1}\right)^{-1} & \text{for } \phi < \phi_c \end{cases}$$

$$\tau = \eta(I, \hat{\dot{\gamma}})\, p = \left[\eta_{hard}(I) + \eta_{soft}(\hat{\dot{\gamma}})\right] p$$

$$p_{QS} = \alpha_{QS} |\phi - \phi_c|^{2/3}$$

$$p_{Int} = \alpha_{Int} \hat{\dot{\gamma}}^{1/2}$$

$$p_{Inert} = \frac{\alpha_{Inert} \hat{\dot{\gamma}}^2}{|\phi - \phi_c|^2}$$

$$\eta_{hard}(I) = \eta_s + \frac{\alpha_1}{\left(\frac{I_0}{I}\right)^{\beta_1} + 1}$$

$$\eta_{soft}(\hat{\dot{\gamma}}) = \frac{\alpha_2}{\left(\frac{\hat{\dot{\gamma}}_0}{\hat{\dot{\gamma}}}\right)^{\beta_2} + 1}$$

- Model features:
  - Captures behavior in all three flow regimes.
  - Describes transitions between regimes.
  - Continuous in shear rate – no arbitrary cutoffs.
  - C^0 continuous in volume fraction

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$$\eta_{soft}(\dot{\hat{\gamma}}) = \frac{\alpha_2}{\left(\frac{\dot{\hat{\gamma}}_0}{\dot{\hat{\gamma}}}\right)^{\beta_2} + 1}$$

- Model features:
  - $\phi_c = \phi_c(\mu)$
  - Valid for $\mu \geq 0.1$ but can be extended to the frictionless case.

Hard-particle limit

- As $k \to \infty$:
  - $\dot{\hat{\gamma}} \to 0 \implies$ No intermediate regime
  - $\phi \geq \phi_c$ is possible only in static packings
  - $\phi < \phi_c$ for sheared systems
  - Model can be simplified to:

$$p = p_{\mathrm{Inert}} \sim \dot{\gamma}^2$$
$$\tau = \eta_{\mathrm{hard}}(I)\, p \sim \dot{\gamma}^2$$

  - This form suggests a way to modify existing kinetic theories, e.g. Garzó-Dufty (1999)[†]

[†] **Garzó, V., Dufty, J.W. Phys. Rev. E 59, 5895 (1999).**

Kinetic theory equations

Garzó-Dufty kinetic theory for simple shear flow

Pressure

$$p = \rho_s \phi \left[1 + 2(1+e)\phi g_0\right] T$$

Shear stress

$$\tau = \left(\frac{2J}{5\sqrt{\pi}}\right) \frac{pd\dot{\gamma}}{F\sqrt{T}}$$

Energy dissipation rate

$$\Gamma = \frac{12}{\sqrt{\pi}} \frac{\rho \phi g_0}{d} (1-e^2) T^{3/2}$$

Steady-state energy balance

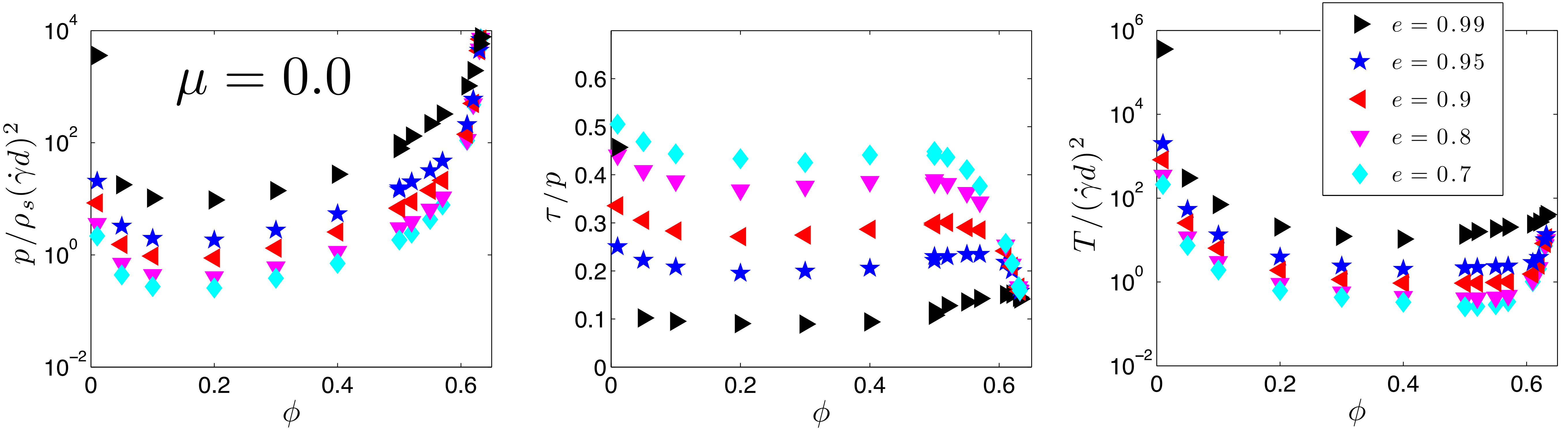
$$\Gamma - \dot{\gamma}\tau = 0$$

$$F = F(e, \phi)$$
$$J = J(e, \phi)$$

Important quantities:

- Radial distribution function at contact $g_0 = g_0(\phi)$
  - Measure of packing
  - Diverges at random close packing
- Restitution coefficient e
  - Measure of dissipation
  - Has strong effect on temperature

DEM results: without friction



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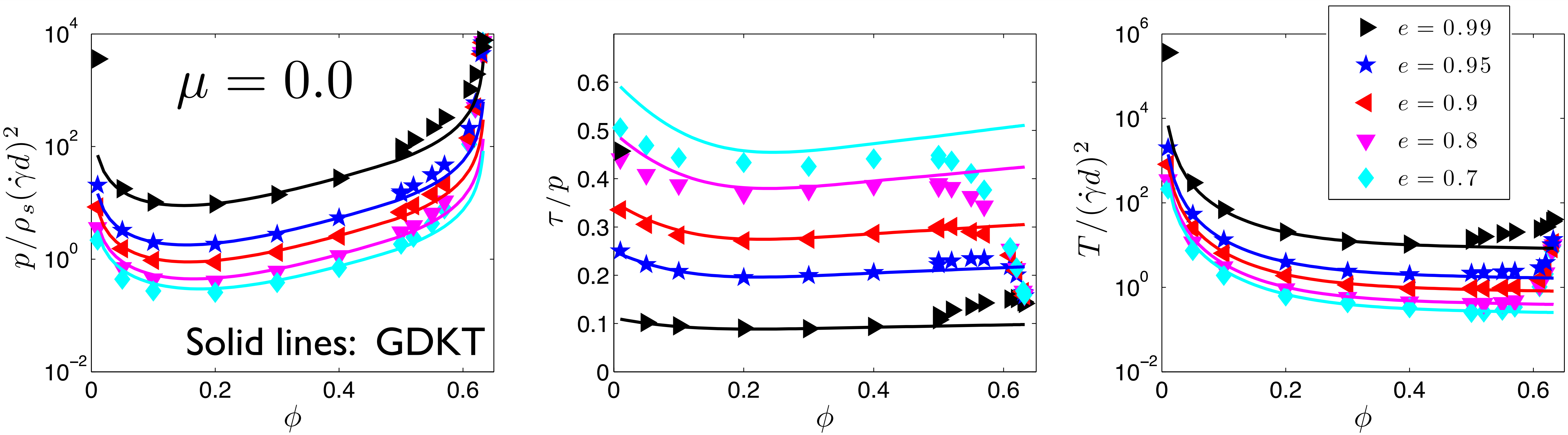
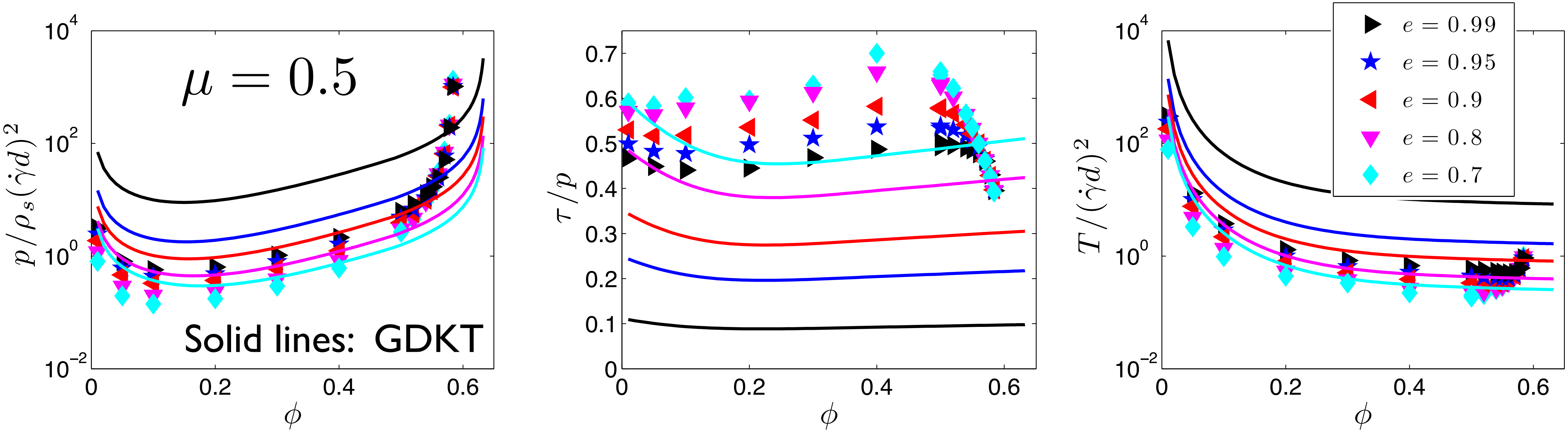


- GD theory agrees with DEM results for dilute systems
- GD theory fails for dense systems
  - Predicts incorrect scaling of pressure with volume fraction
  - Cannot predict yield stress in close-packed limit
  - Derived from false assumption of uncorrelated, isotropically-distributed collisions

DEM results: with friction



- GD theory fails to capture DEM results for frictional particles
  - Increased collisional stress in dense regime
  - Increased dissipation in dilute regime
- Possible modifications
  - Modified RDF at contact $g_0 = g_0(\phi, e, \mu) \longrightarrow p$
  - Effective restitution coefficient† $e_{\text{eff}} = e_{\text{eff}}(e, \mu) \longrightarrow T$
  - Correction factors* $\delta_i = \delta_i(\phi, e, \mu) \longrightarrow \tau/p$

† **Jenkins, J.T. and Zhang, C. Phys. Fluids 14, 1228 (2002).**
* **Jenkins, J.T. and Berzi, D. Granul. Matter 12, 151 (2010).**

Effective restitution coefficient

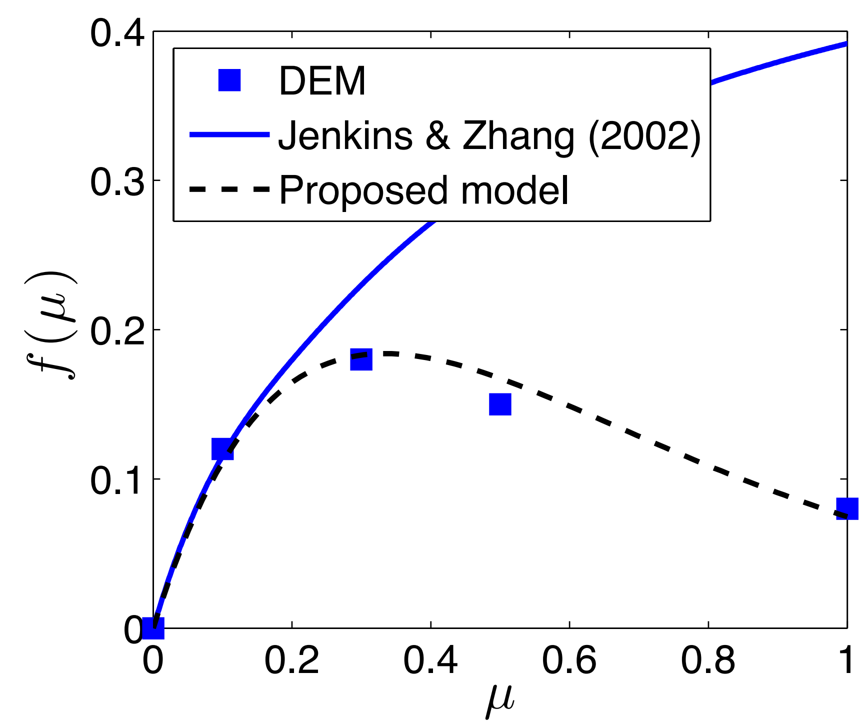
- Can use dilute regime temperature to calculate effective restitution coefficient

$$T = \frac{2J(\dot{\gamma}d)^2}{15(1-e^2)} \implies e_{\text{eff}} = \sqrt{1 - \frac{2J(\dot{\gamma}d)^2}{15T}}$$

- Proposed form:

$$e_{\text{eff}} = e - f(\mu)$$

$$f(\mu) = 1.5\mu e^{-3\mu}$$



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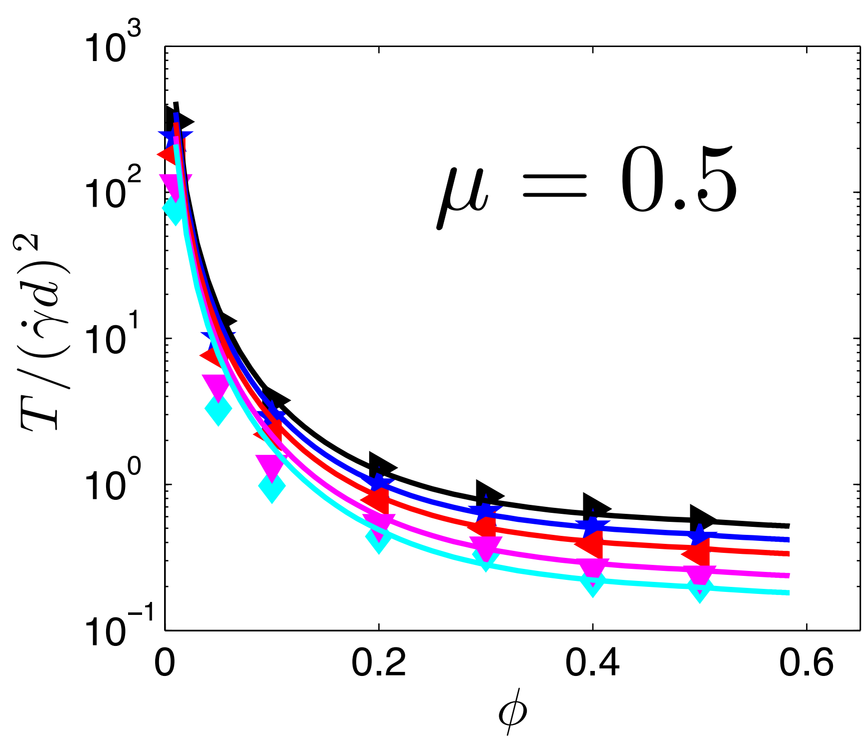


- Can capture temperature for frictional systems

Radial distribution function: no friction

- Pressure

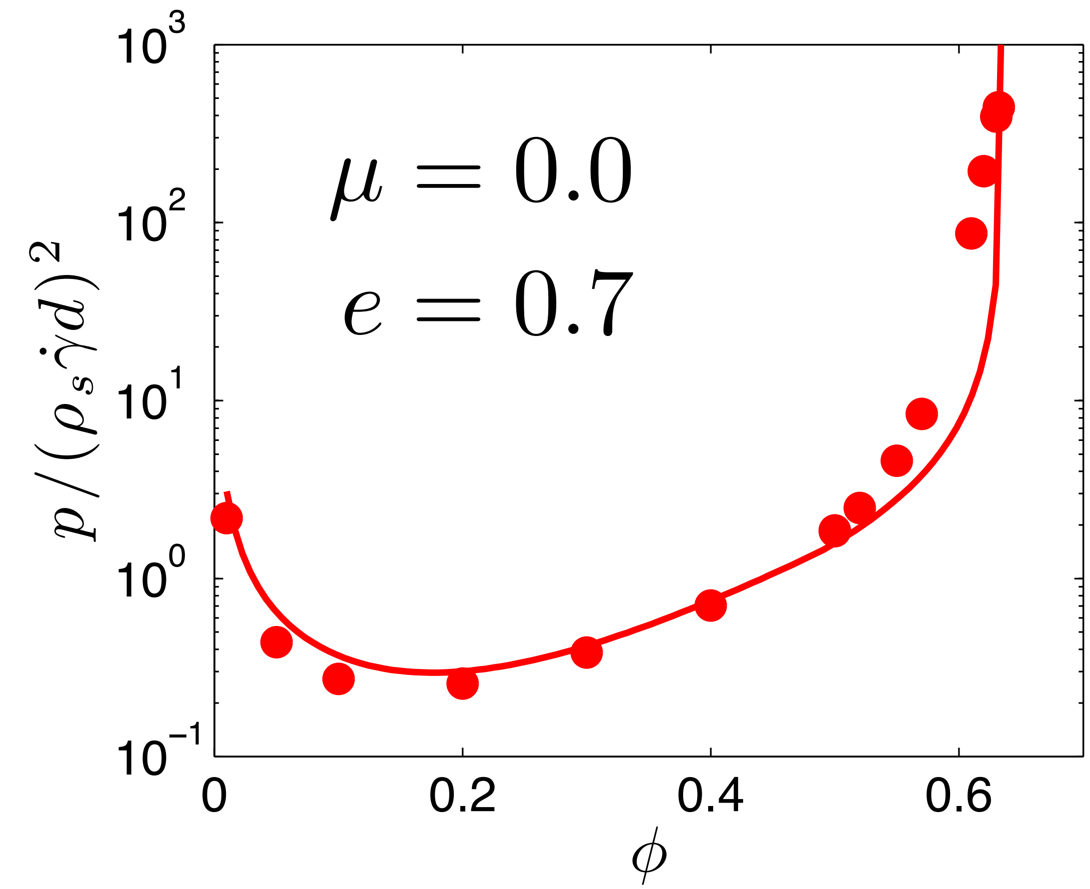
$$p = \rho_s \phi \left[1 + 2(1+e)\phi g_0\right] T$$

- Radial distribution function
  - Carnahan-Starling[†]:

$$g_0^{CS} = \frac{1 - \phi/2}{(1-\phi)^3}$$

  - Torquato (1995)*:

$$g_0 = \begin{cases} g_0^{CS}(\phi), & \phi \le \phi_f \\ g_0^{CS}(\phi_f)\frac{\phi_c - \phi_f}{\phi_c - \phi}, & \phi > \phi_f \end{cases}$$



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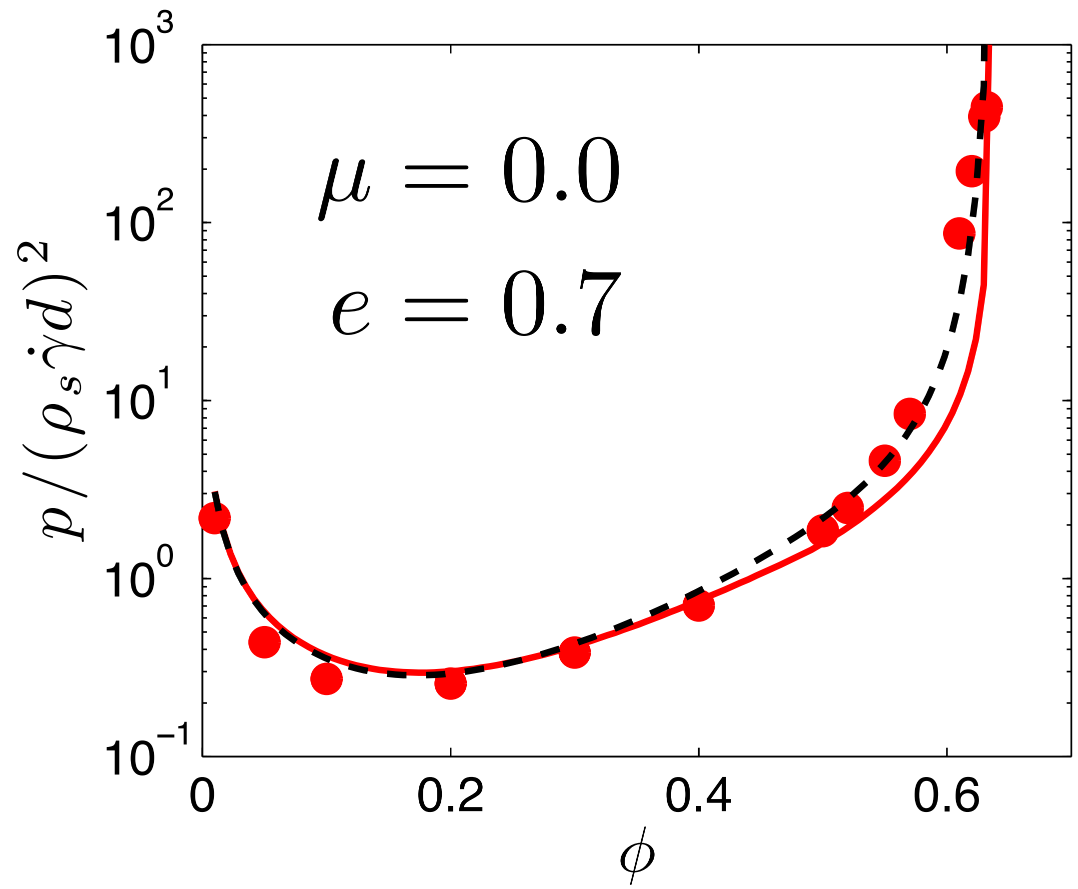
  - Proposed form:

$$\boxed{g_0 = g_o^{CS} + \frac{\alpha(e,\mu)\phi^2}{(\phi_c-\phi)^2}}$$



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Radial distribution function: friction

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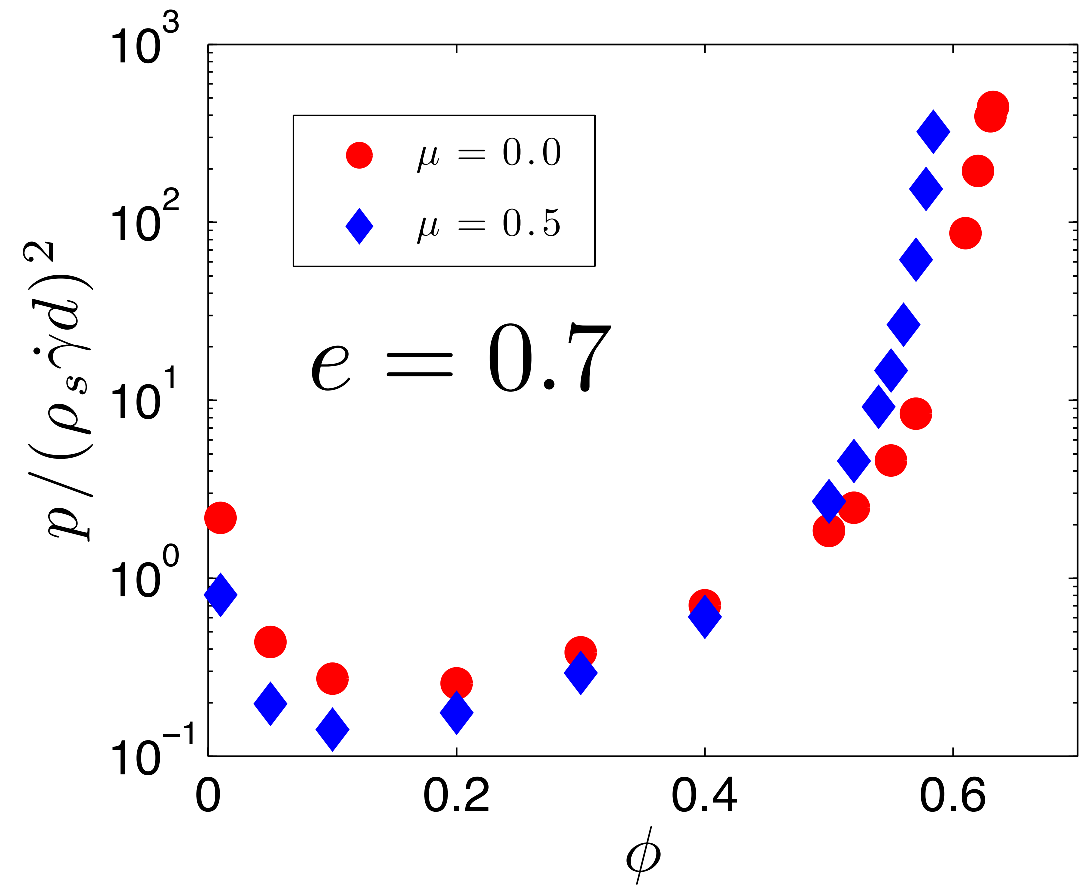
$$p = \rho_s \phi \left[1 + 4\eta\phi g_0\right] T$$

- Radial distribution function
  - Proposed form:

$$\boxed{g_0 = g_o^{CS} + \frac{\alpha(e,\mu)\phi^2}{(\phi_c - \phi)^2}}$$

$$\uparrow$$

$$\boxed{\phi_c = \phi_c(\mu)}$$



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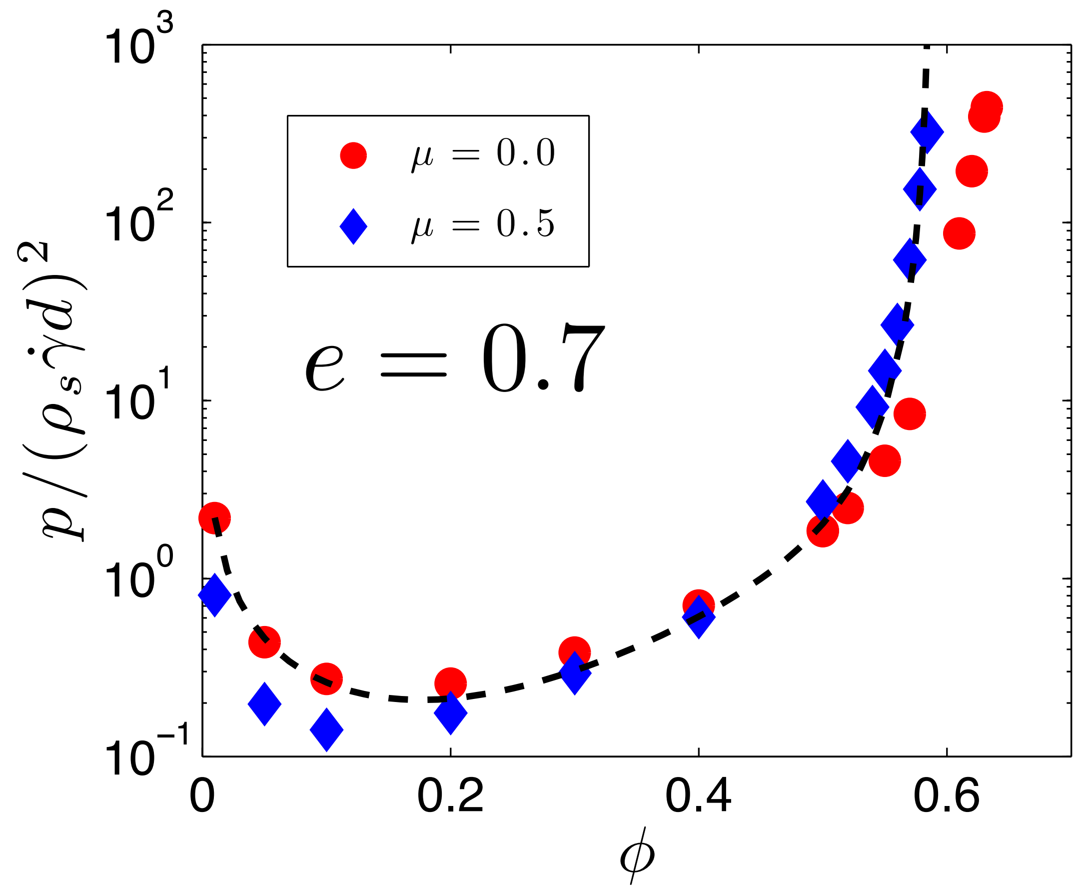

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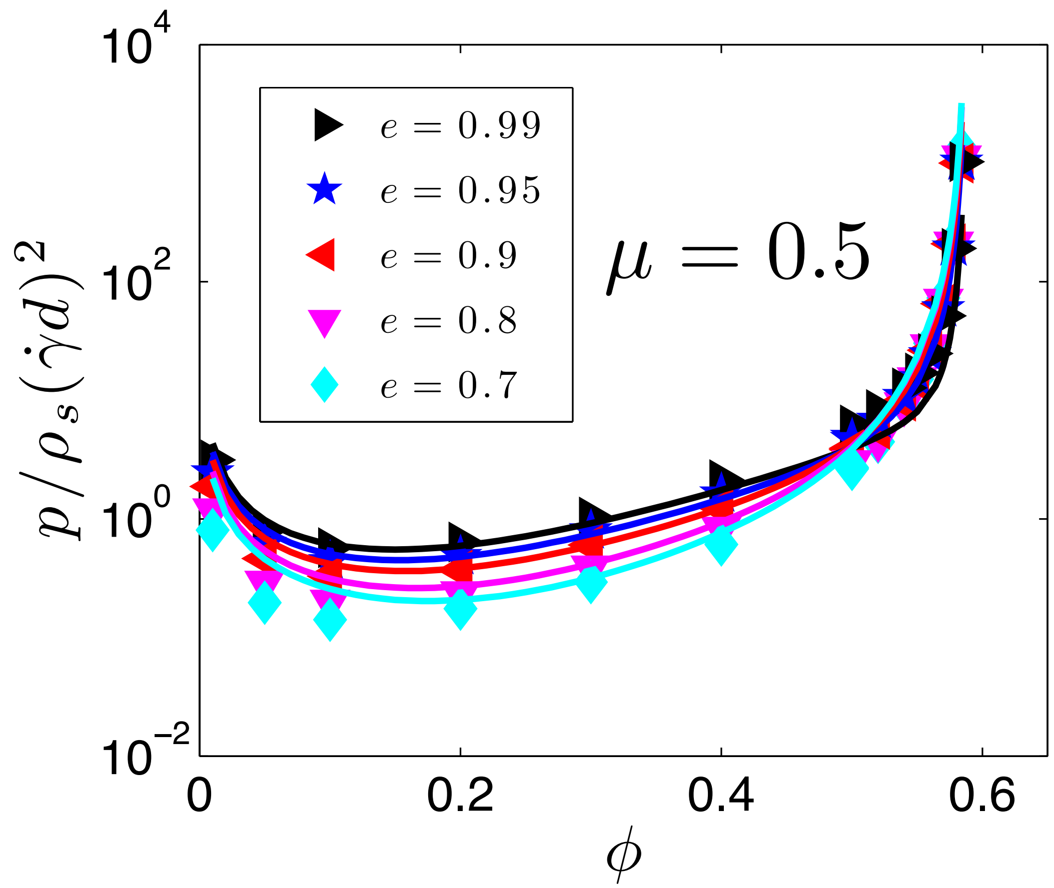


$$\alpha(e,\mu) = \left(\frac{1}{3} + \frac{3}{2}\mu\right)(1-e)$$

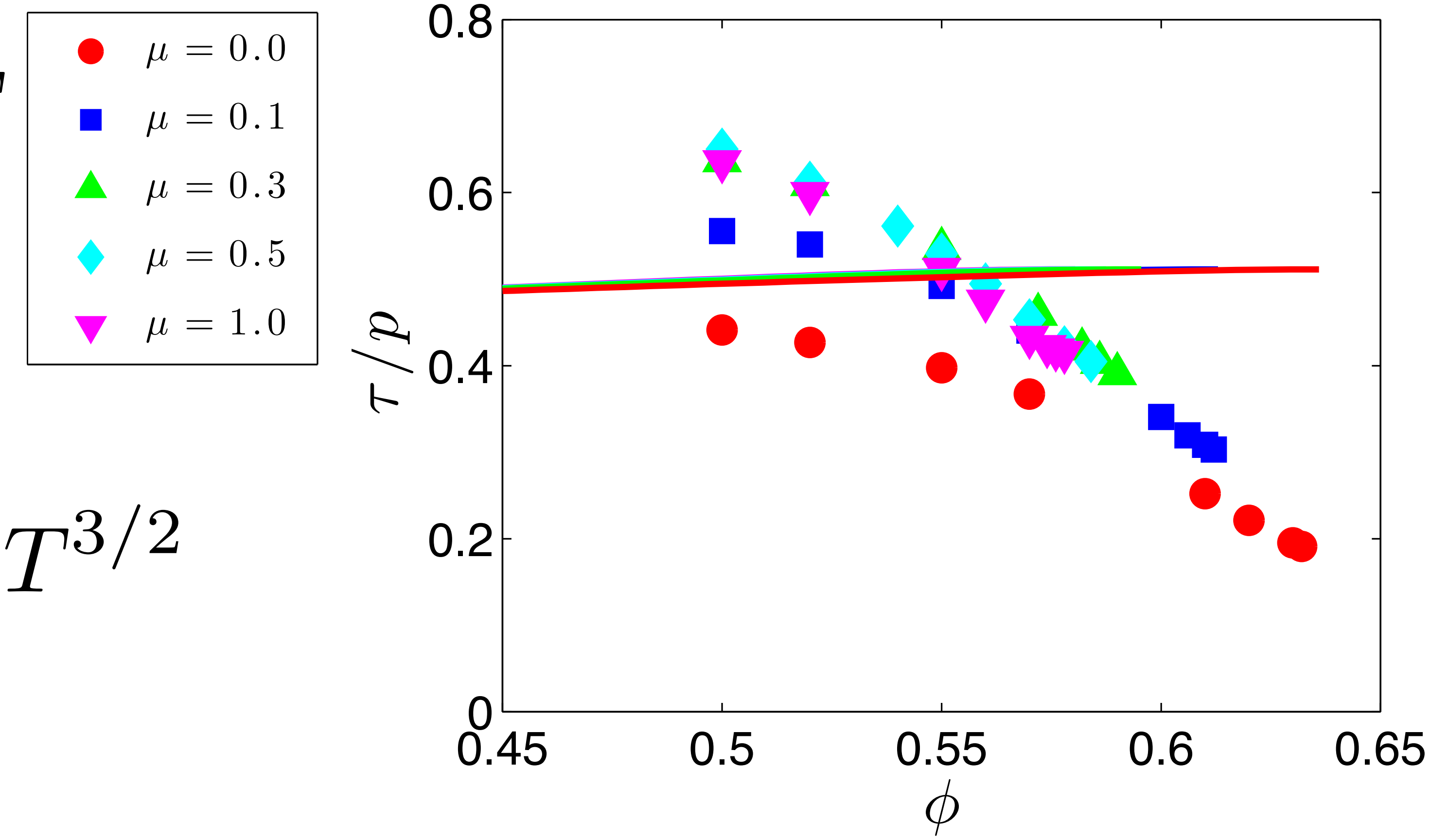
Shear stress ratio for dense regime

- Garzó-Dufty (1999)

$$p = \rho_s \phi \left[1 + 4\eta\phi g_0\right] T$$

$$\tau = \left(\frac{2J}{5\sqrt{\pi}}\right) \frac{pd\dot{\gamma}}{F\sqrt{T}}$$

$$\Gamma = \frac{12}{\sqrt{\pi}} \frac{\rho\phi g_0}{d}(1 - e^2)T^{3/2}$$



Shear stress ratio for dense regime

- Jenkins-Berzi (2010)

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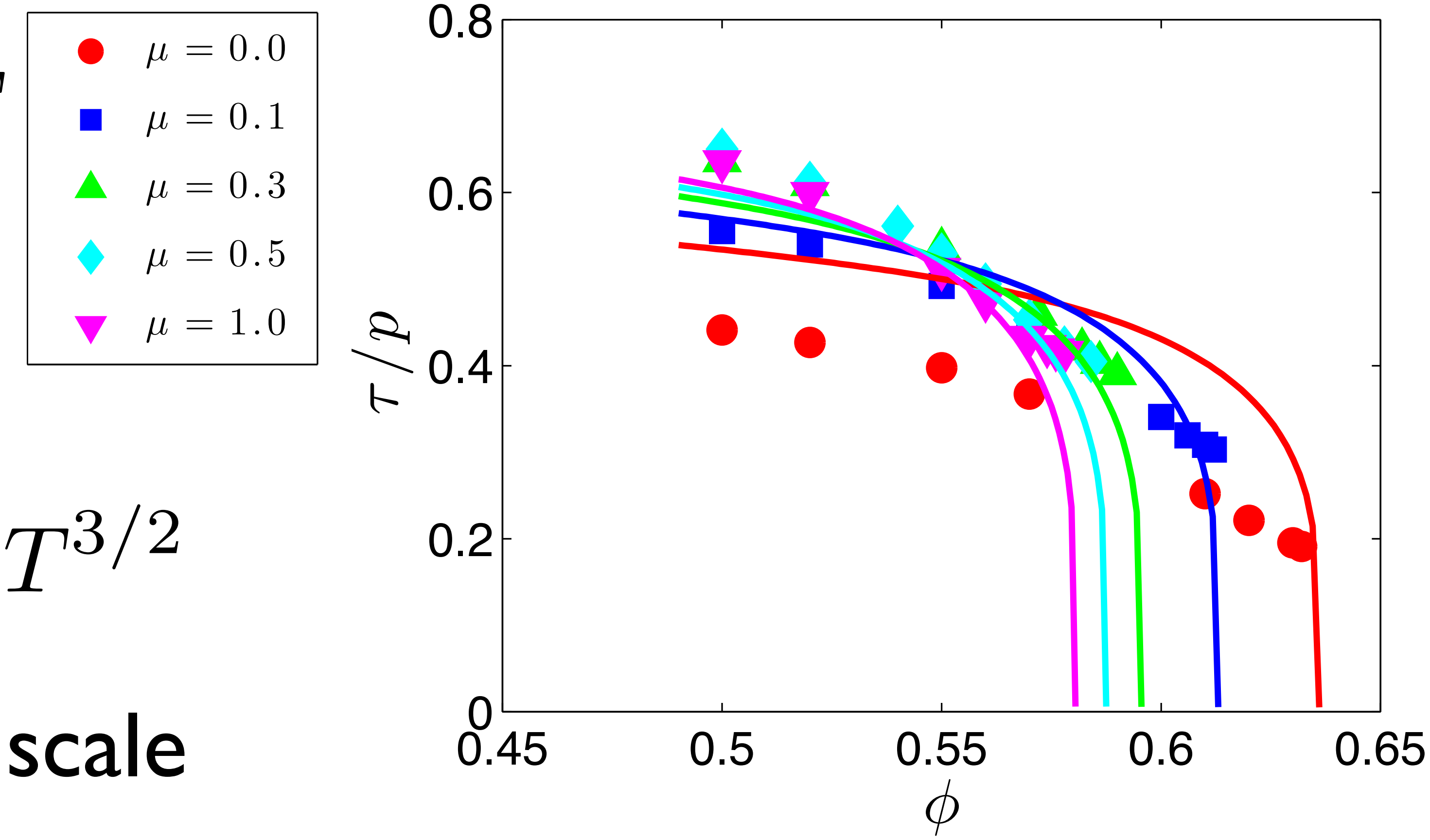
$$\Gamma = \frac{12}{\sqrt{\pi}} \frac{\rho\phi g_0}{\color{red}{L}} (1 - e^2) T^{3/2}$$

Length scale

$$\frac{L}{d} = \frac{1}{2} \hat{c} G^{1/3} \frac{\dot{\gamma} d}{\sqrt{T}}$$



- Undesirable features:
  - Does not predict a yield stress ratio η_s
  - Temperature diverges at ϕ_c

†Jenkins, J.T. and Berzi, D. Granul. Matter 12, 151 (2010).

Modifications for dense regime

- Our proposed model:

$$p = \rho_s \phi \left[1 + 4\eta\phi g_0\right] T$$

$$\tau = \left(\frac{2J}{5\sqrt{\pi}}\right) \frac{pd\dot{\gamma}}{F\sqrt{T}}\delta_1 \longrightarrow$$ to match DEM stress ratio

$$\Gamma = \frac{12}{\sqrt{\pi}} \frac{\rho\phi g_0}{d}(1-e^2)T^{3/2}\delta_2 \longrightarrow$$ to retain temperature expression, i.e. leave T unaffected

Steady-state:

$$\Gamma - \dot{\gamma}\tau = 0 \implies T = T\frac{\delta_1}{\delta_2} \implies \delta_1 = \delta_2 \equiv \delta$$

$$\eta = \eta(I) = \eta_s + \frac{\alpha_2}{(\frac{I_0}{I})^{1.5} + 1} \implies \delta = \frac{\eta(I)}{\eta_{\mathrm{KT,SS}}}$$

$$I \equiv \frac{\dot{\gamma} d}{\sqrt{p/\rho_s}}$$

S. Chialvo et al. Phys. Rev. E 85, 021305 (2012).

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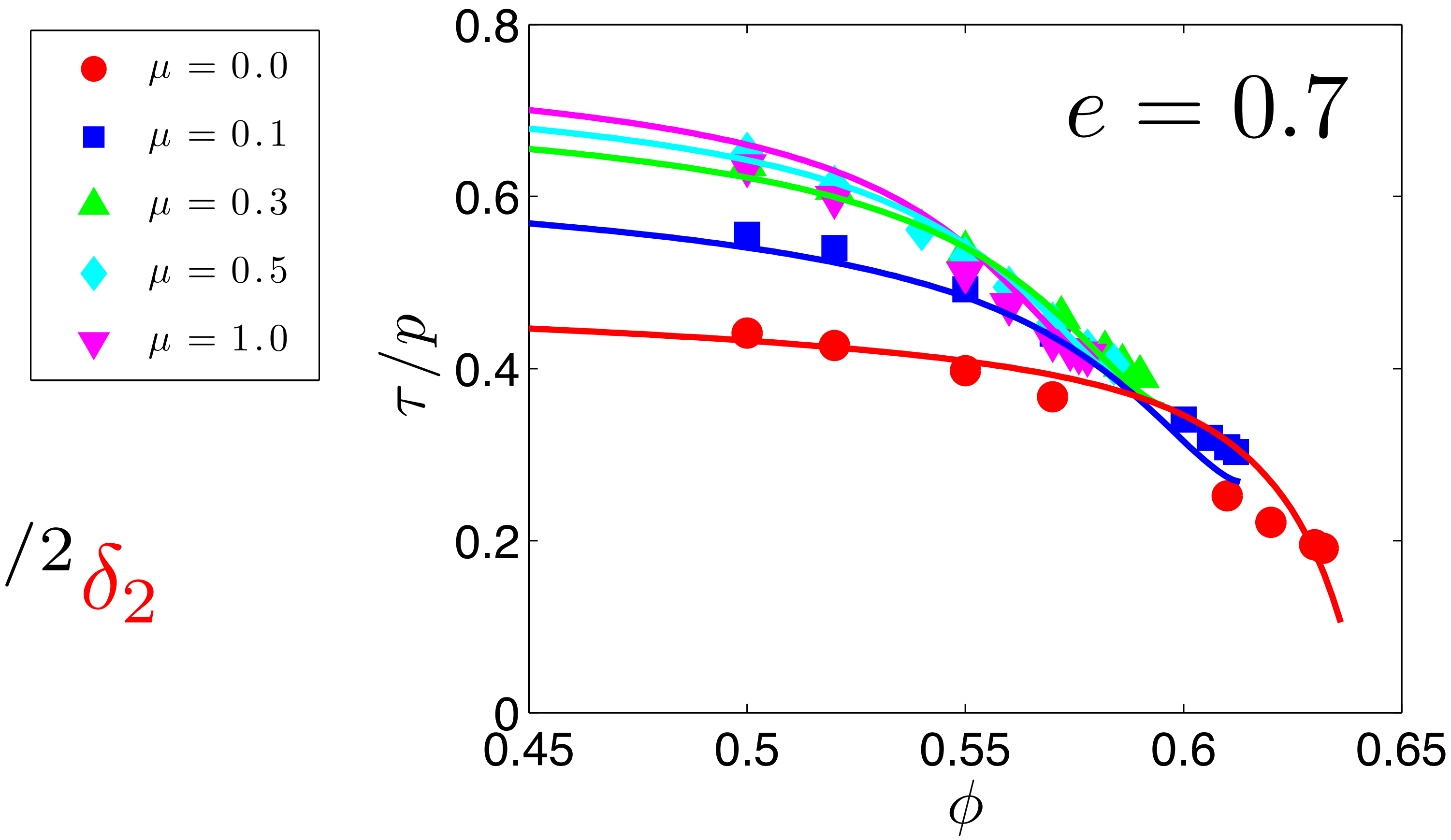

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Summary and future work

- Developed rheological model spanning three regimes of *dense* granular flow
- Proposed modified kinetic theory to capture rheological behavior for *dense and dilute* systems
- Will soon implement KT model into MFIX continuum solver for testing on process-scale flow problems