Modified kinetic theory for flows of frictional granular materials

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Motivation

- Granular flows commonly modeled using kinetic theory
- Existing kinetic theories are valid for:
  - frictionless particles
  - low to moderate solids fractions
- However, granular materials are frictional and often densely packed
- Goal: To modify an existing kinetic theory[†] to handle dense frictional flows

[†]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

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

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

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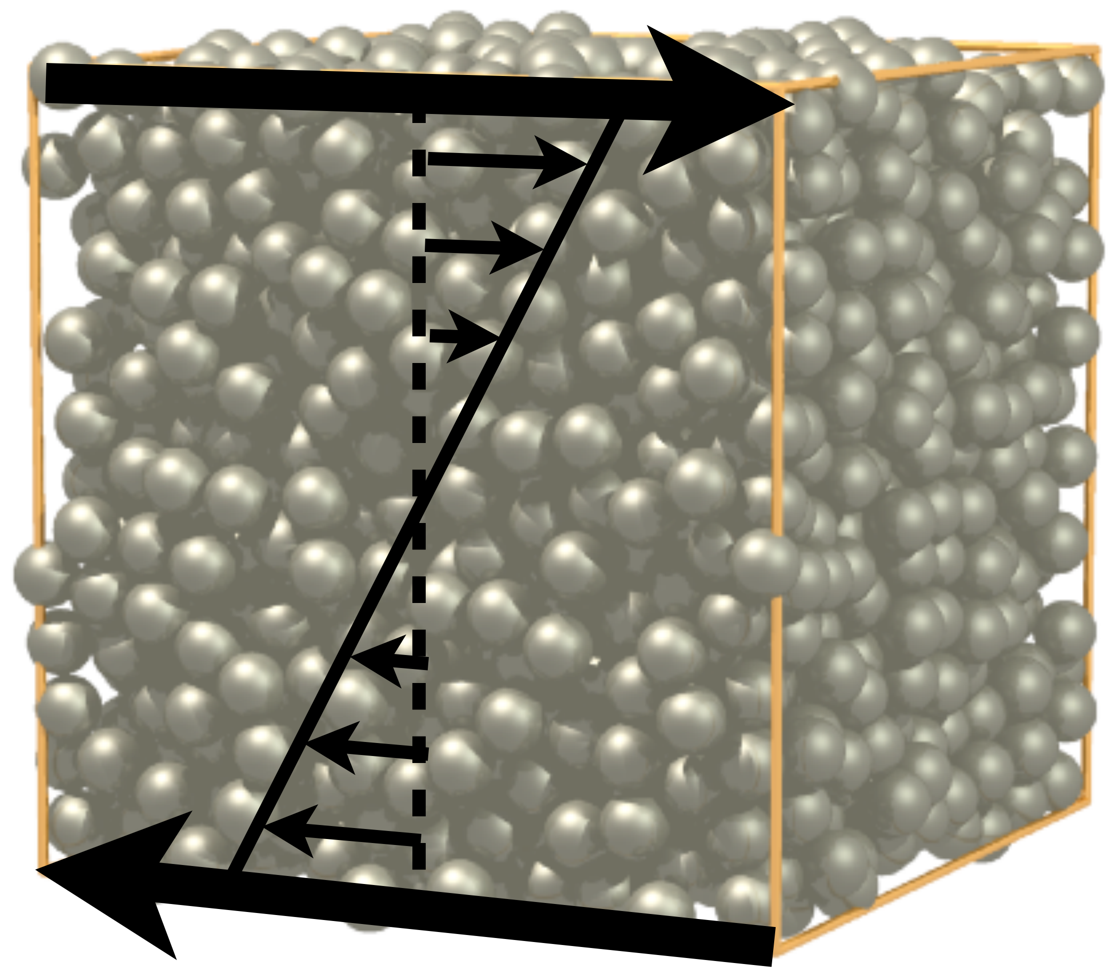
Important quantities:

- 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

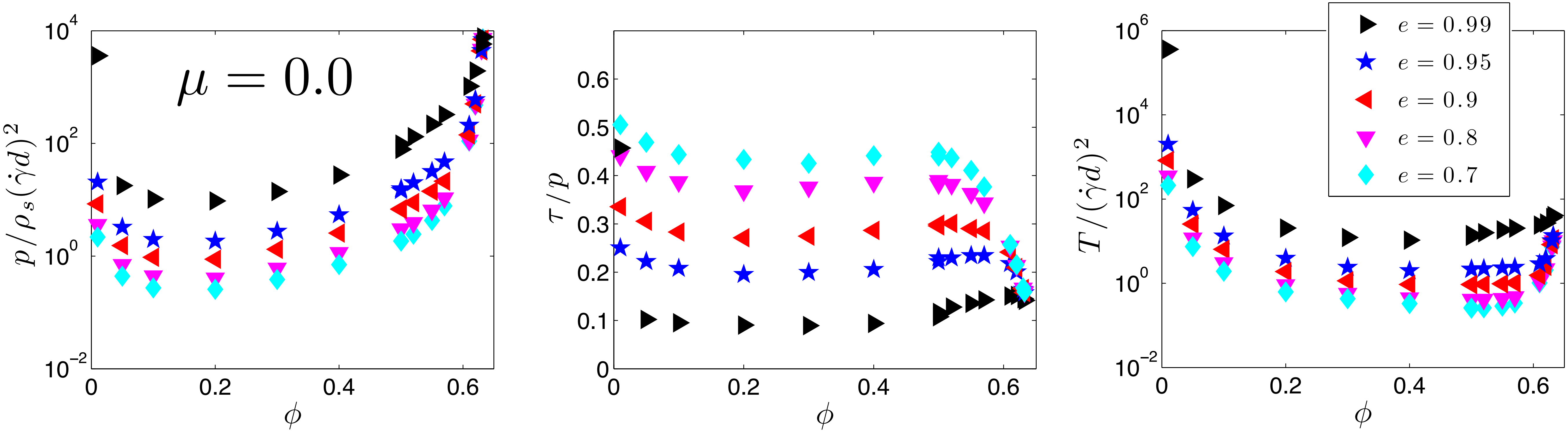
Computational methodology

- 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)

DEM results: without friction



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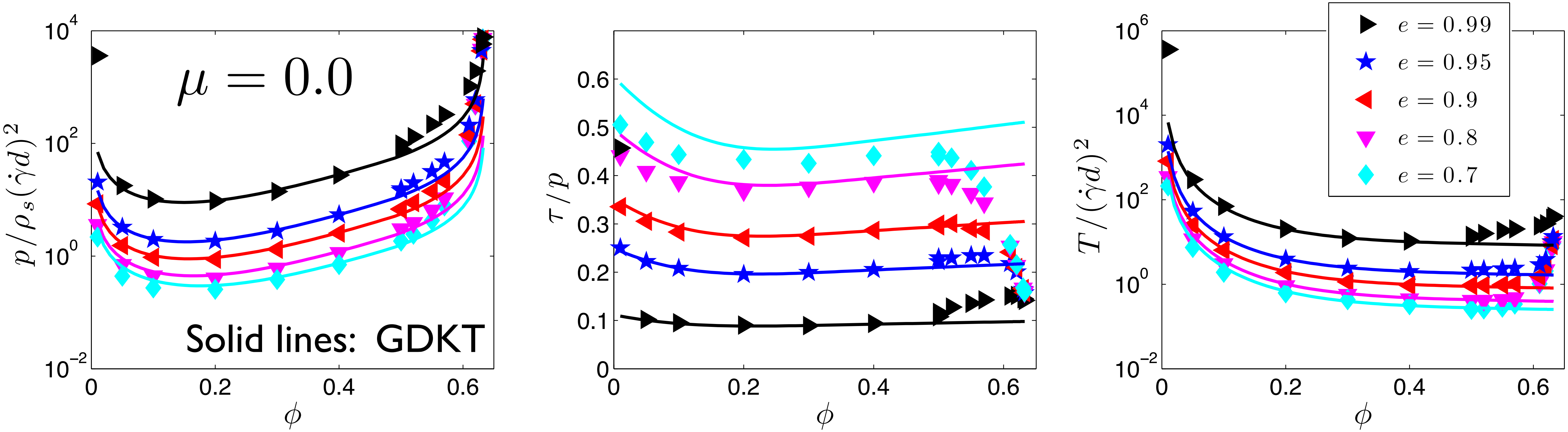

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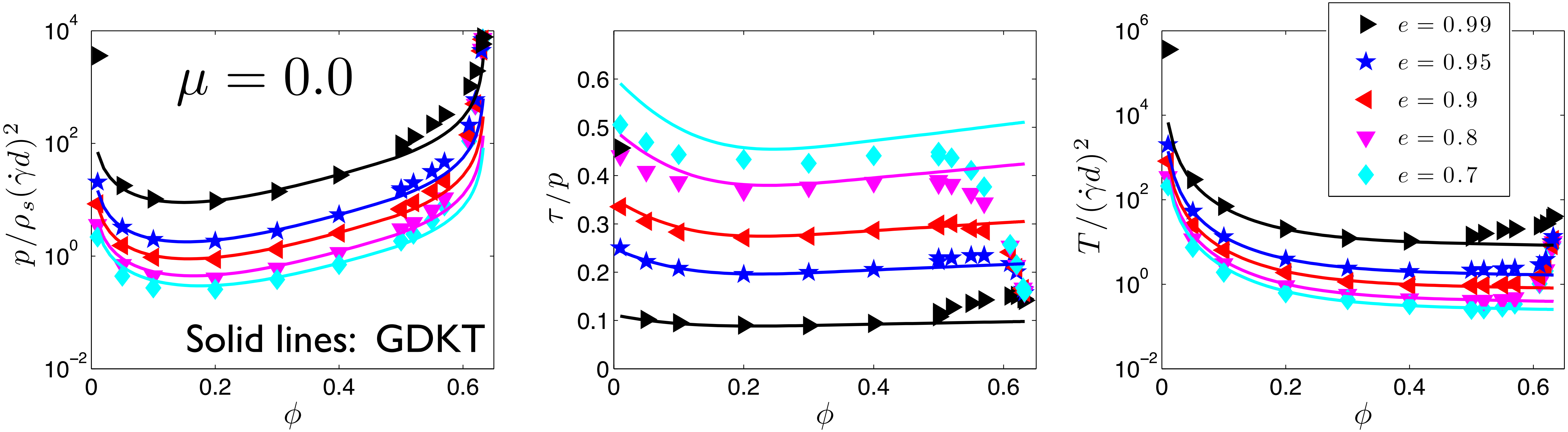
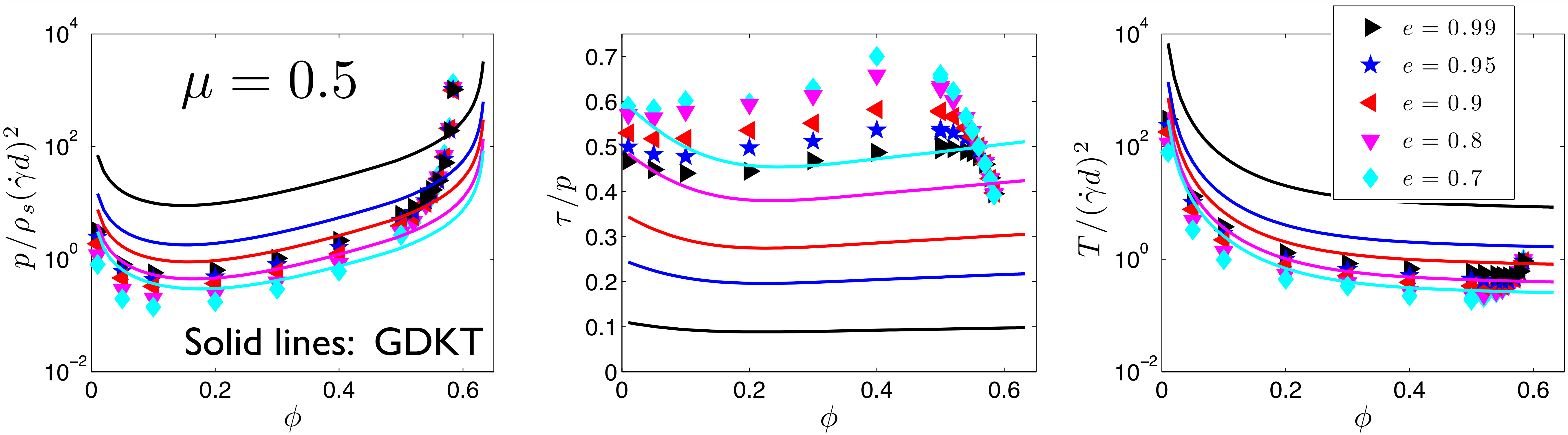


- GD theory agrees with DEM results for dilute systems
- GD theory fails for dense systems
  - Predicts incorrect scaling of pressure with volume fraction
  - Cannot predict yield stress in close-packed limit
  - Derived from false assumption of uncorrelated, isotropically-distributed collisions

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

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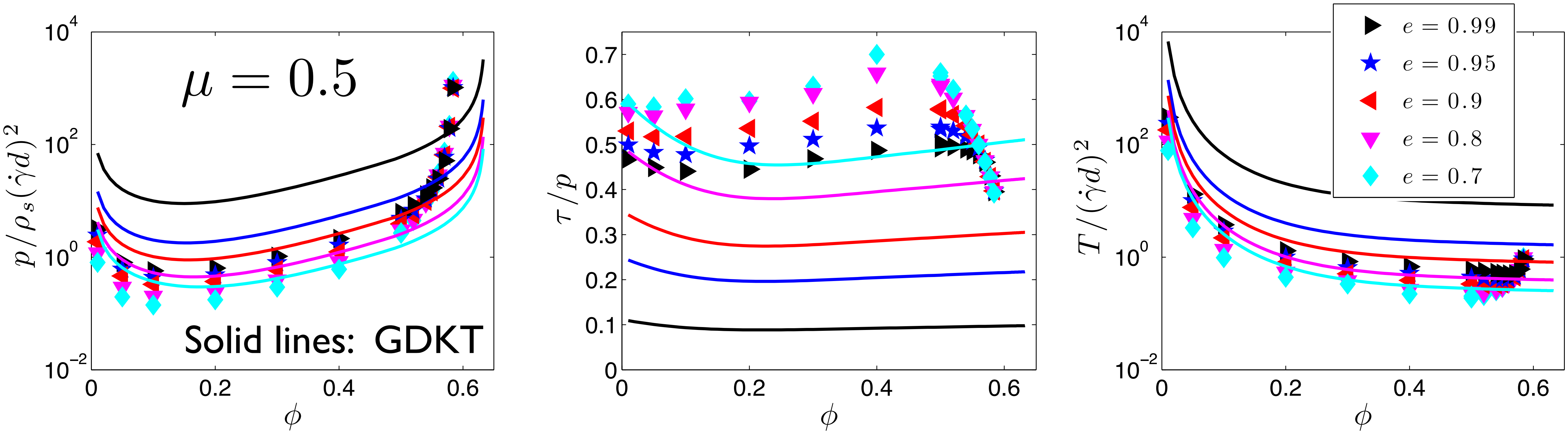

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  - Increased collisional stress in dense regime
  - Increased dissipation in dilute regime
- Possible modifications
  - Modified RDF at contact $g_0 = g_0(\phi, e, \mu) \longrightarrow p$
  - Effective restitution coefficient† $e_{\text{eff}} = e_{\text{eff}}(e, \mu) \longrightarrow T$
  - 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

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

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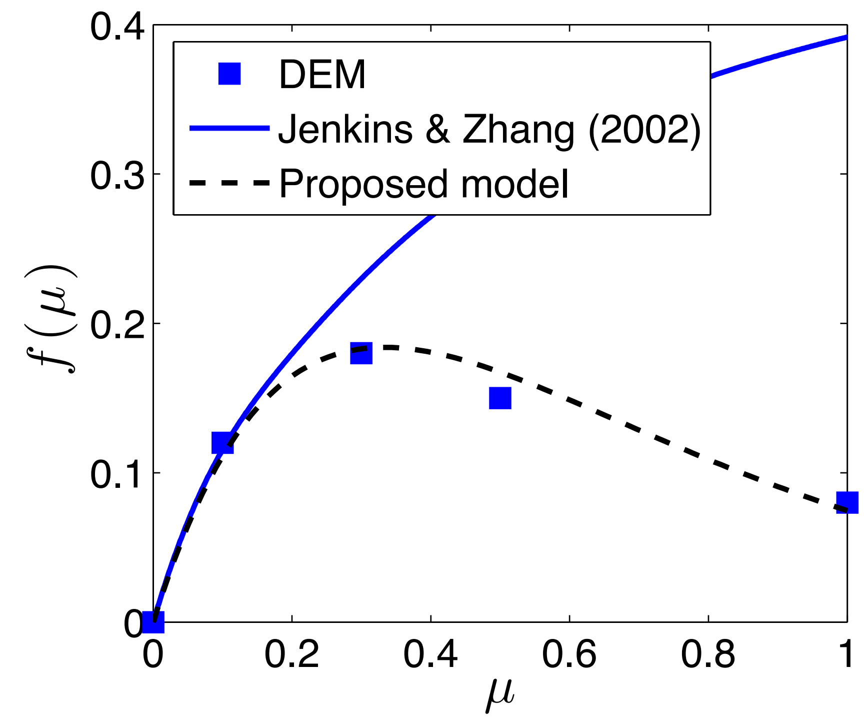
$$e_{\text{eff}} = e - f(\mu)$$

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



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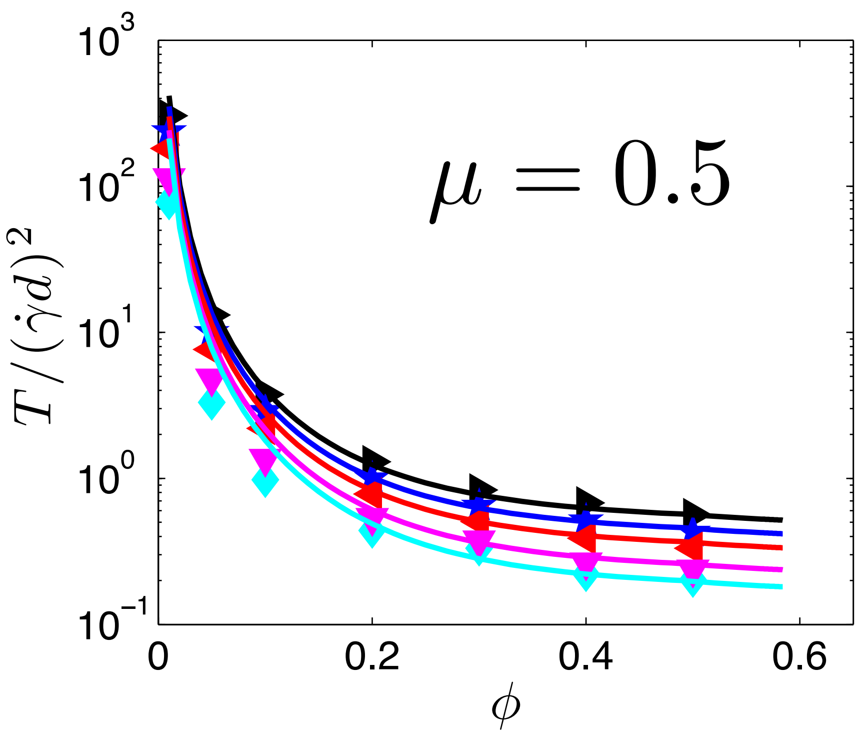
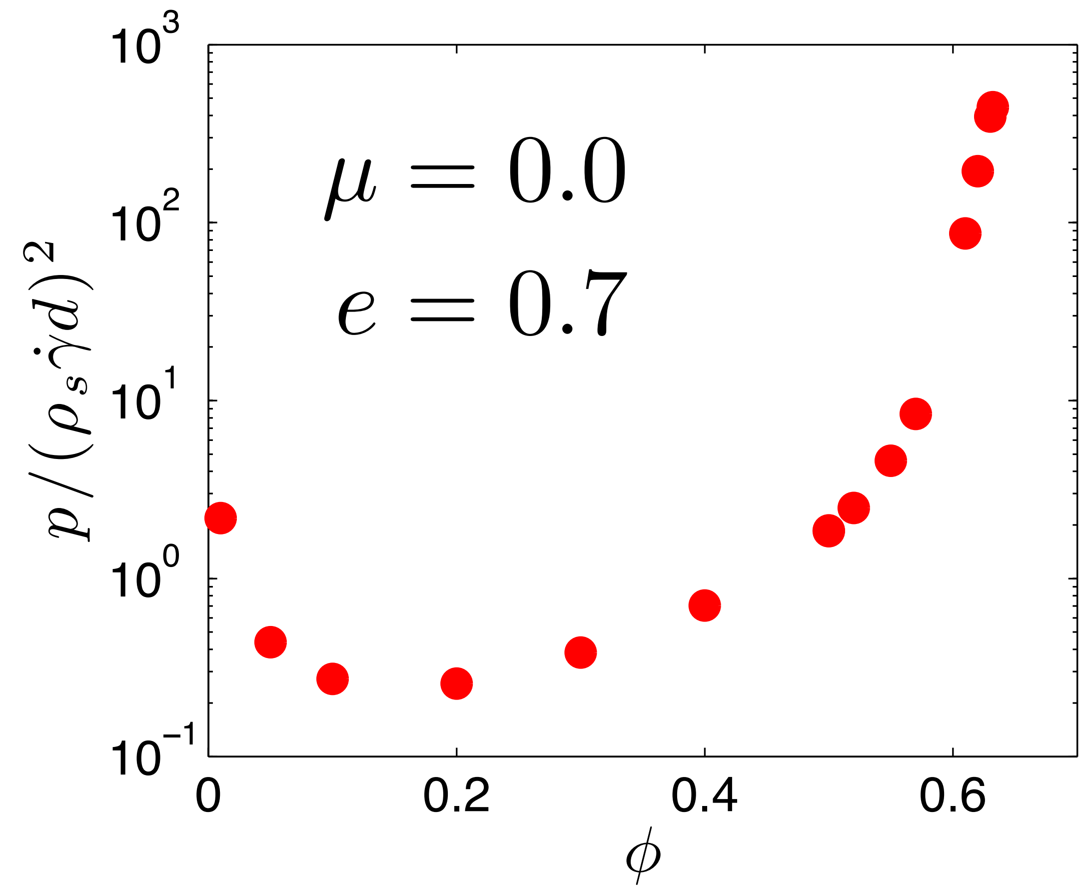


- Can capture temperature for frictional systems

Radial distribution function: no friction

- Pressure

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



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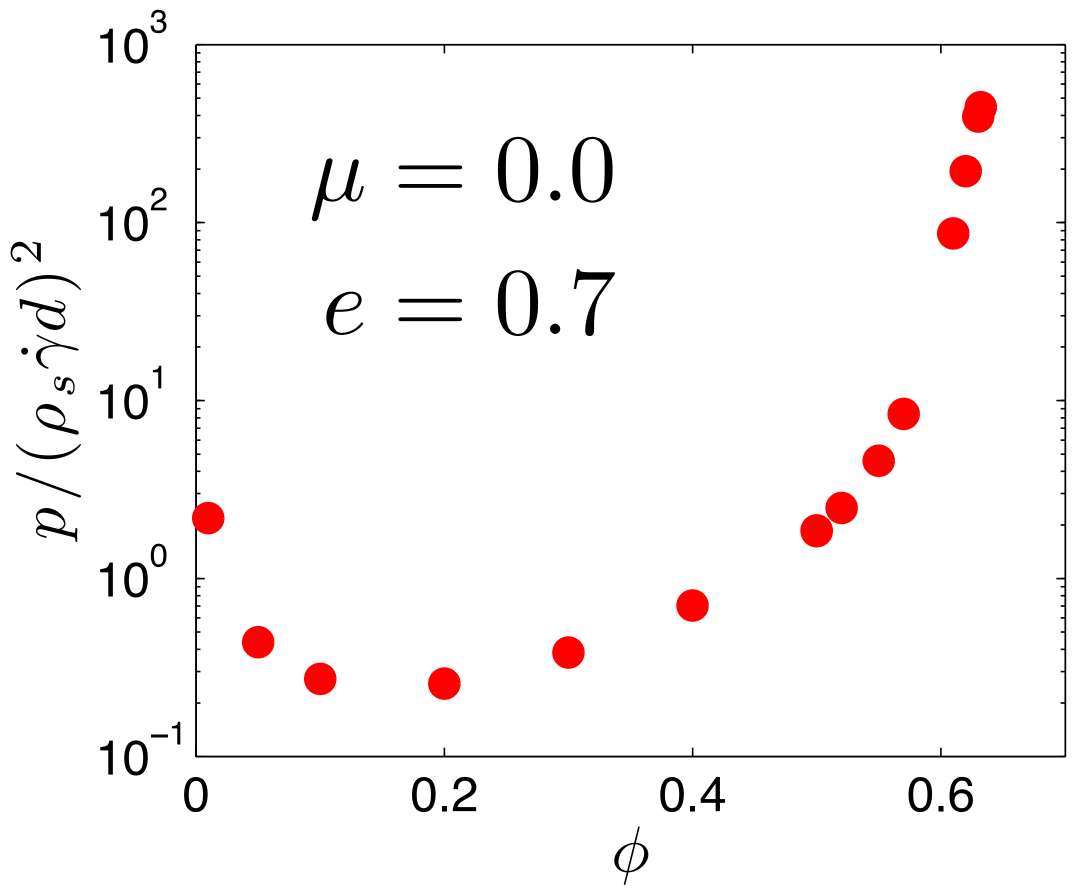
  - Carnahan-Starling[†]:

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



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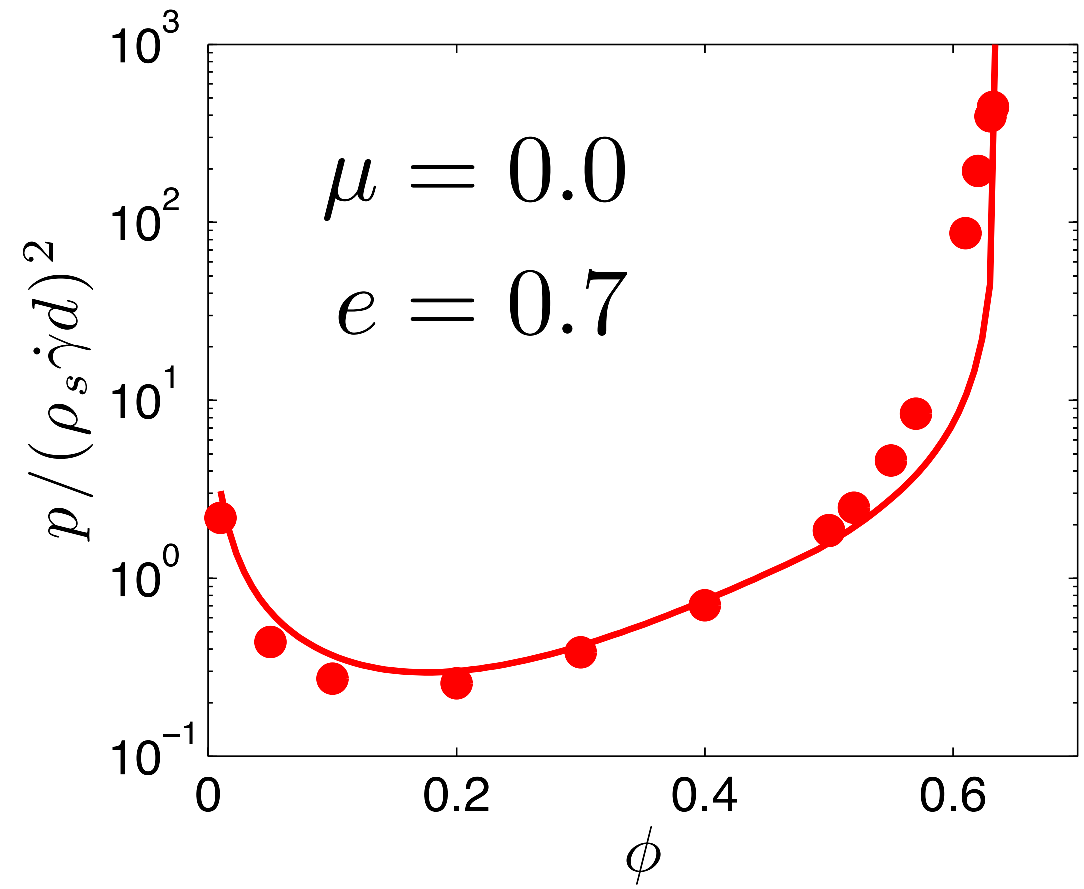
$$g_0 = \begin{cases} g_0^{CS}(\phi), & \phi \le \phi_f \\ g_0^{CS}(\phi_f)\frac{\phi_c - \phi_f}{\phi_c - \phi}, & \phi > \phi_f \end{cases}$$



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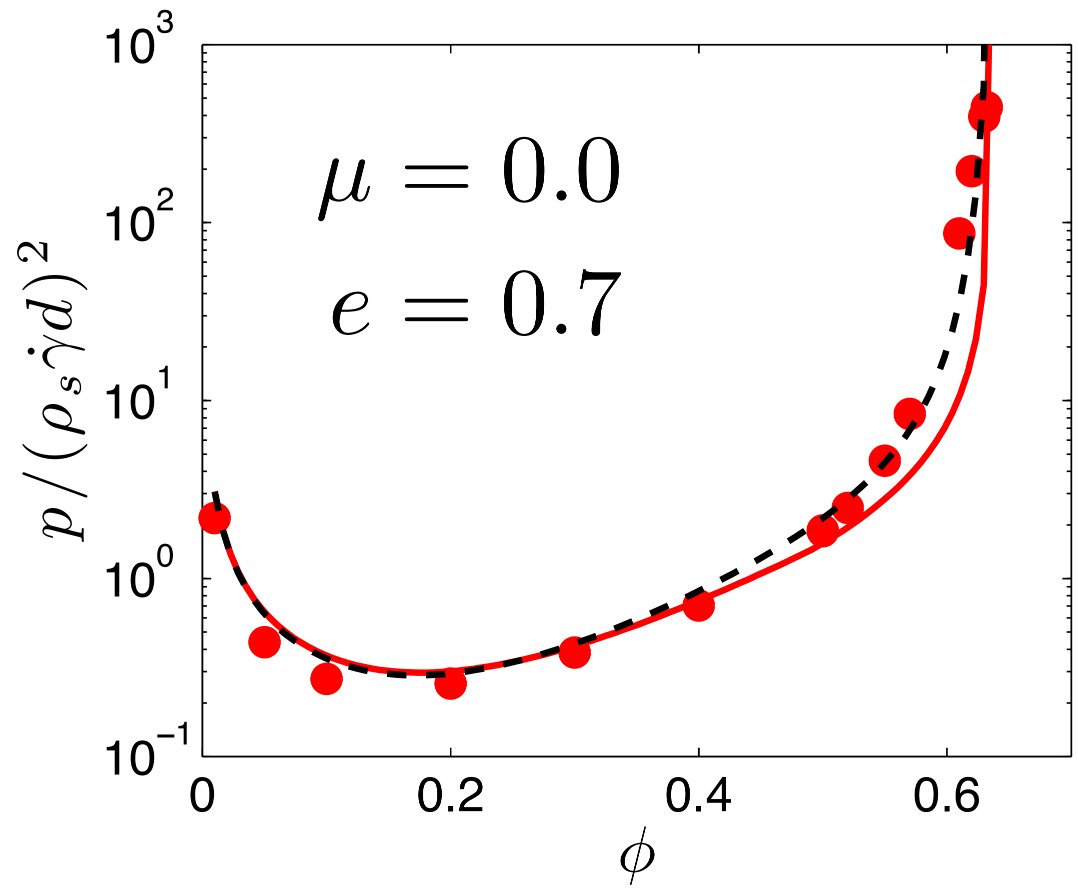

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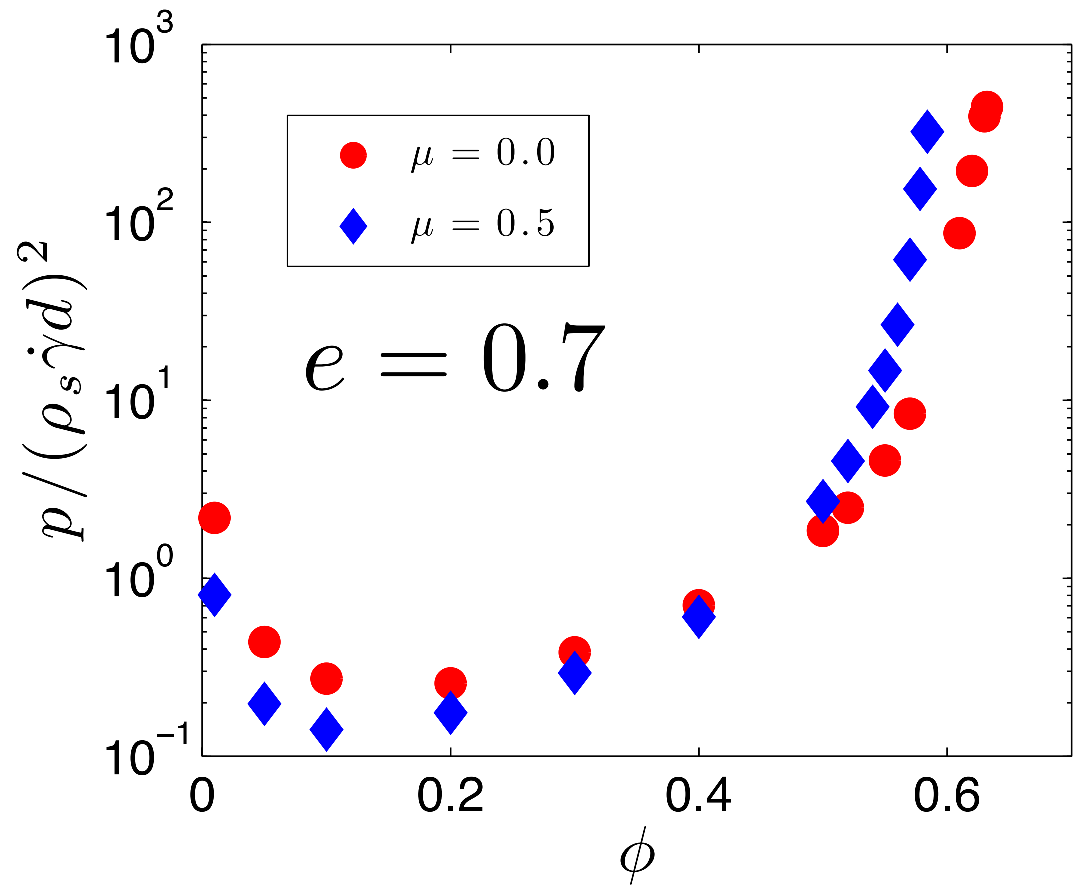

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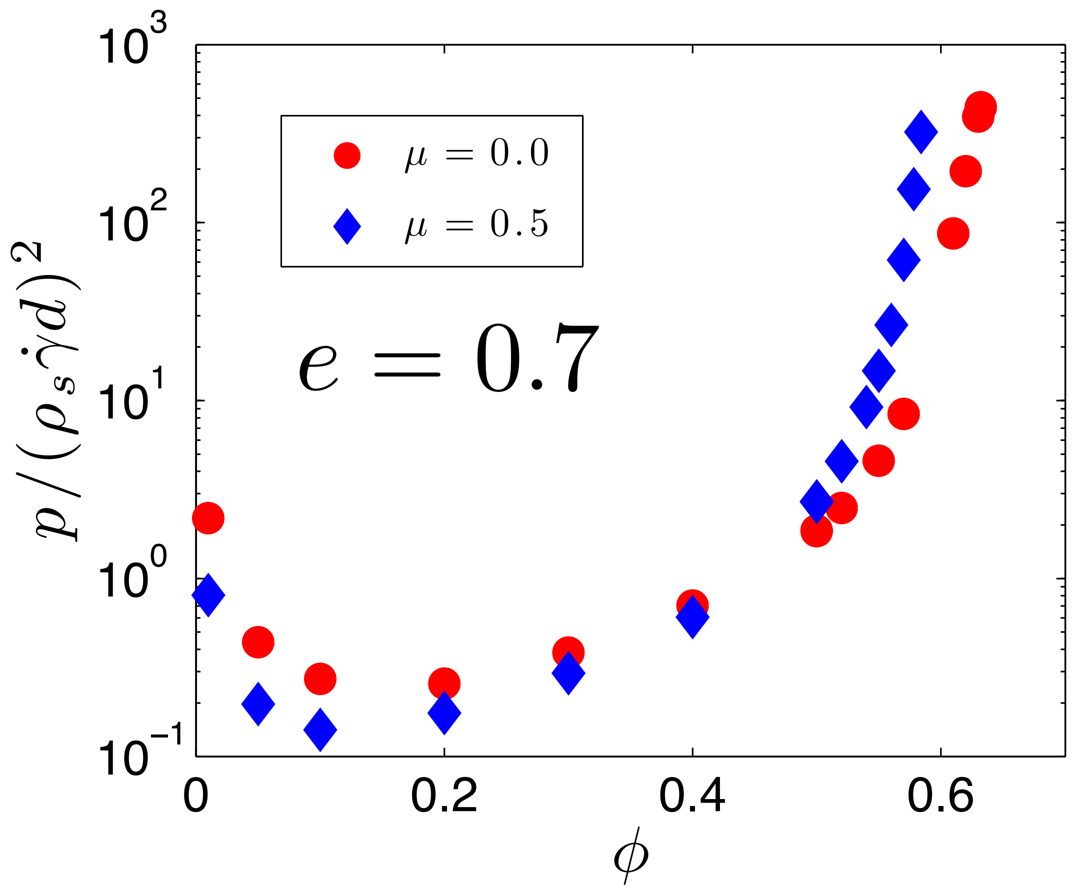

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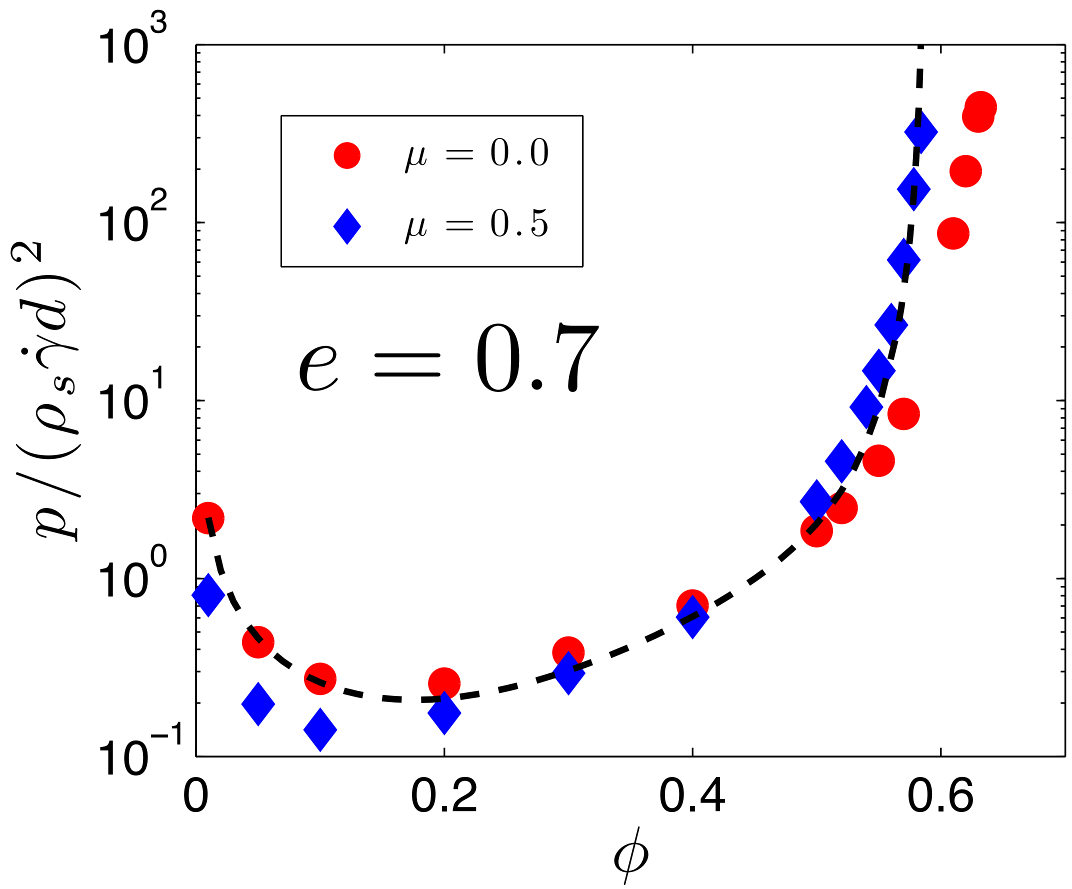

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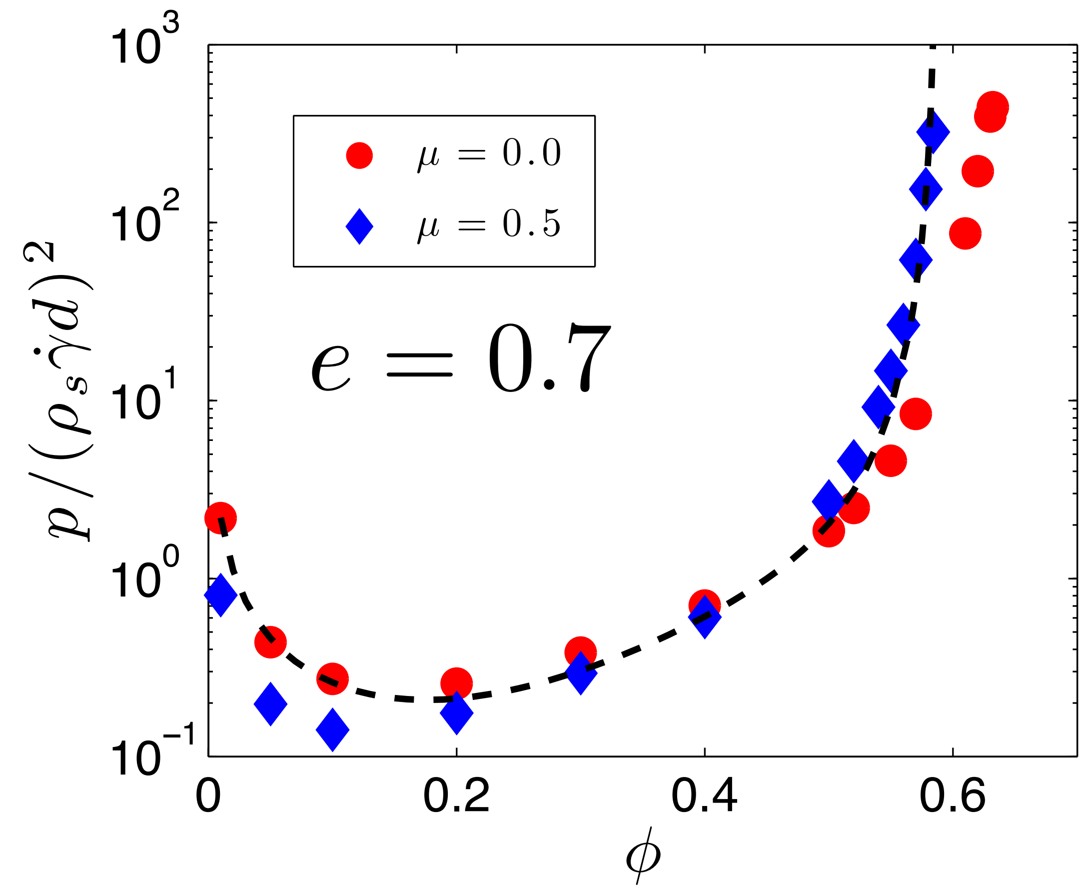

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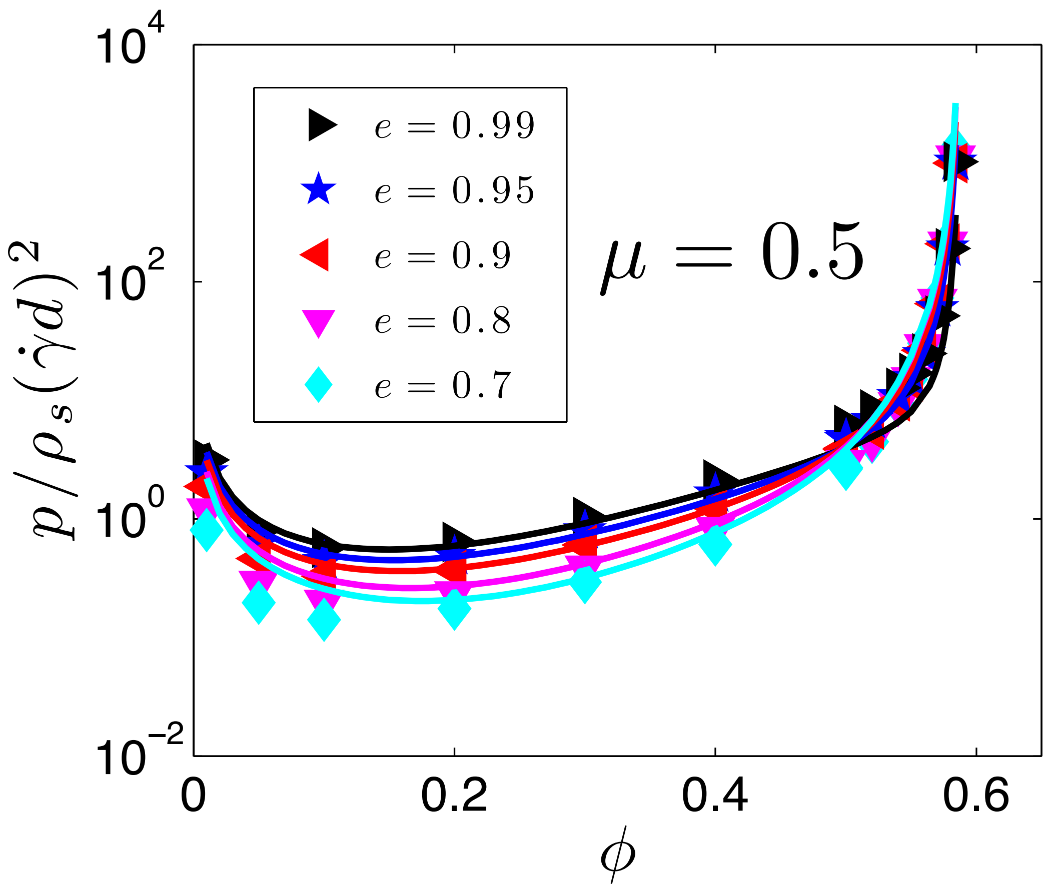

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S. Chialvo et al. Phys. Rev. E 85, 021305 (2012).

Shear stress ratio for dense regime

- Garzó-Dufty (1999)

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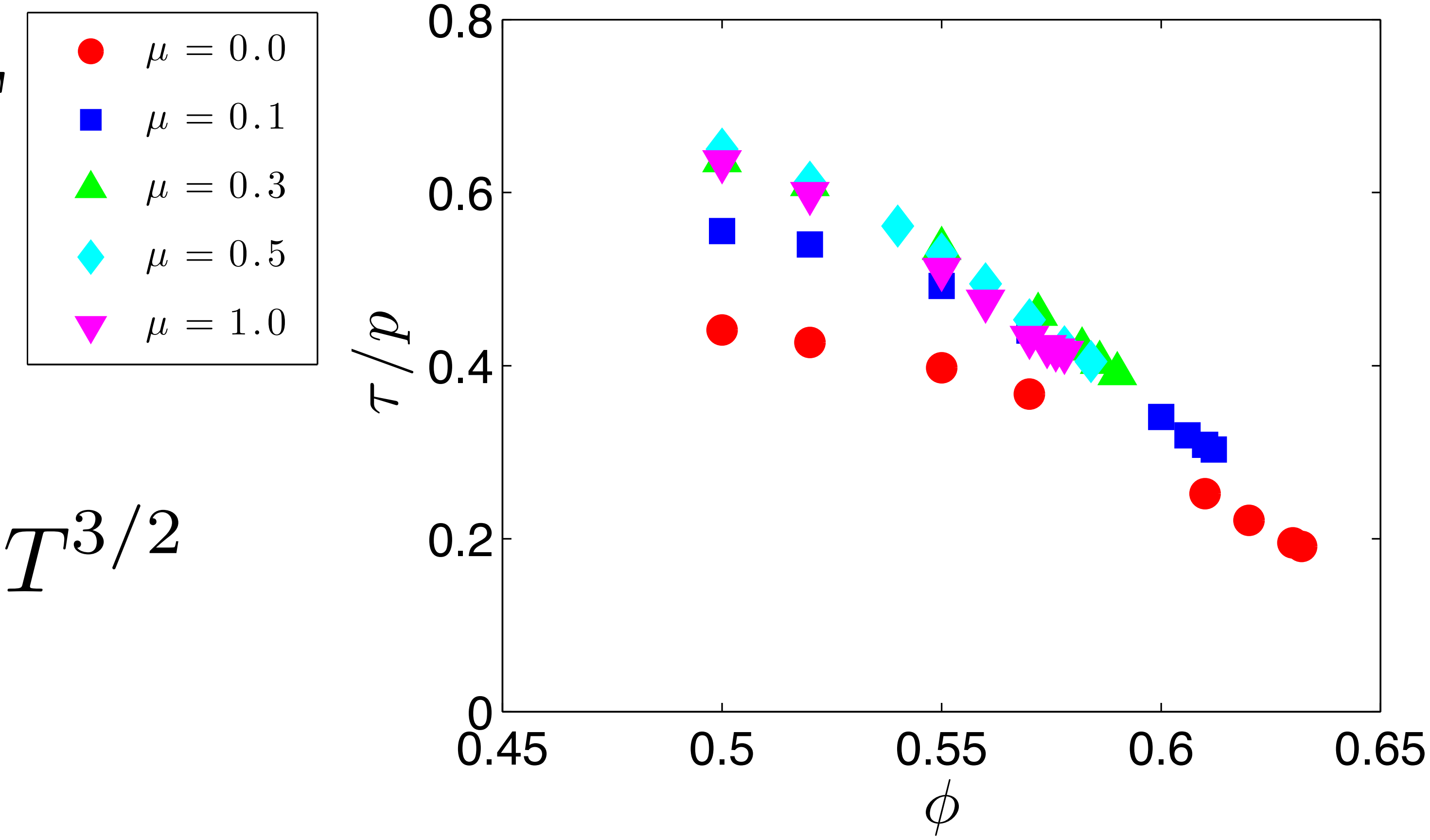

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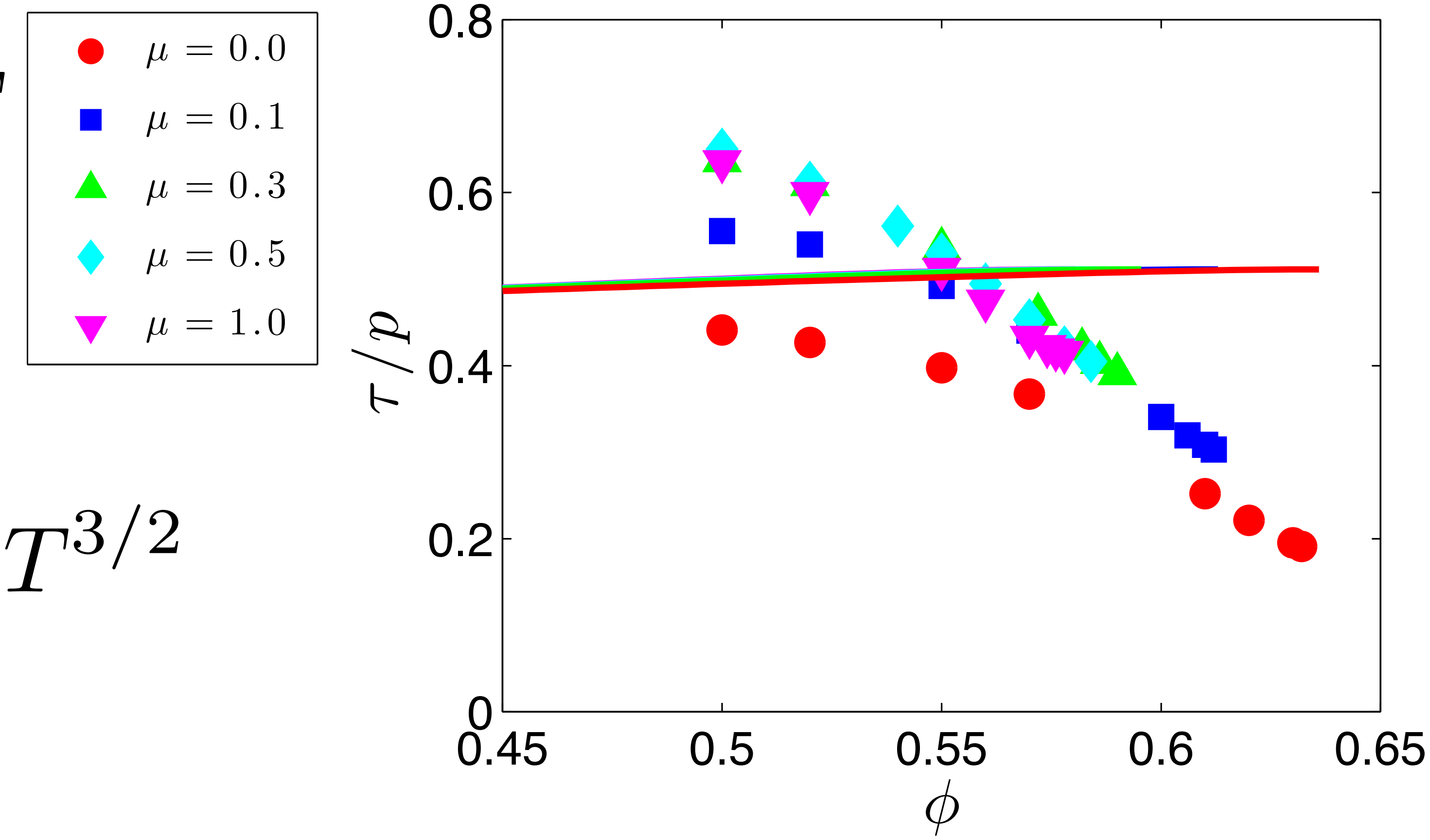

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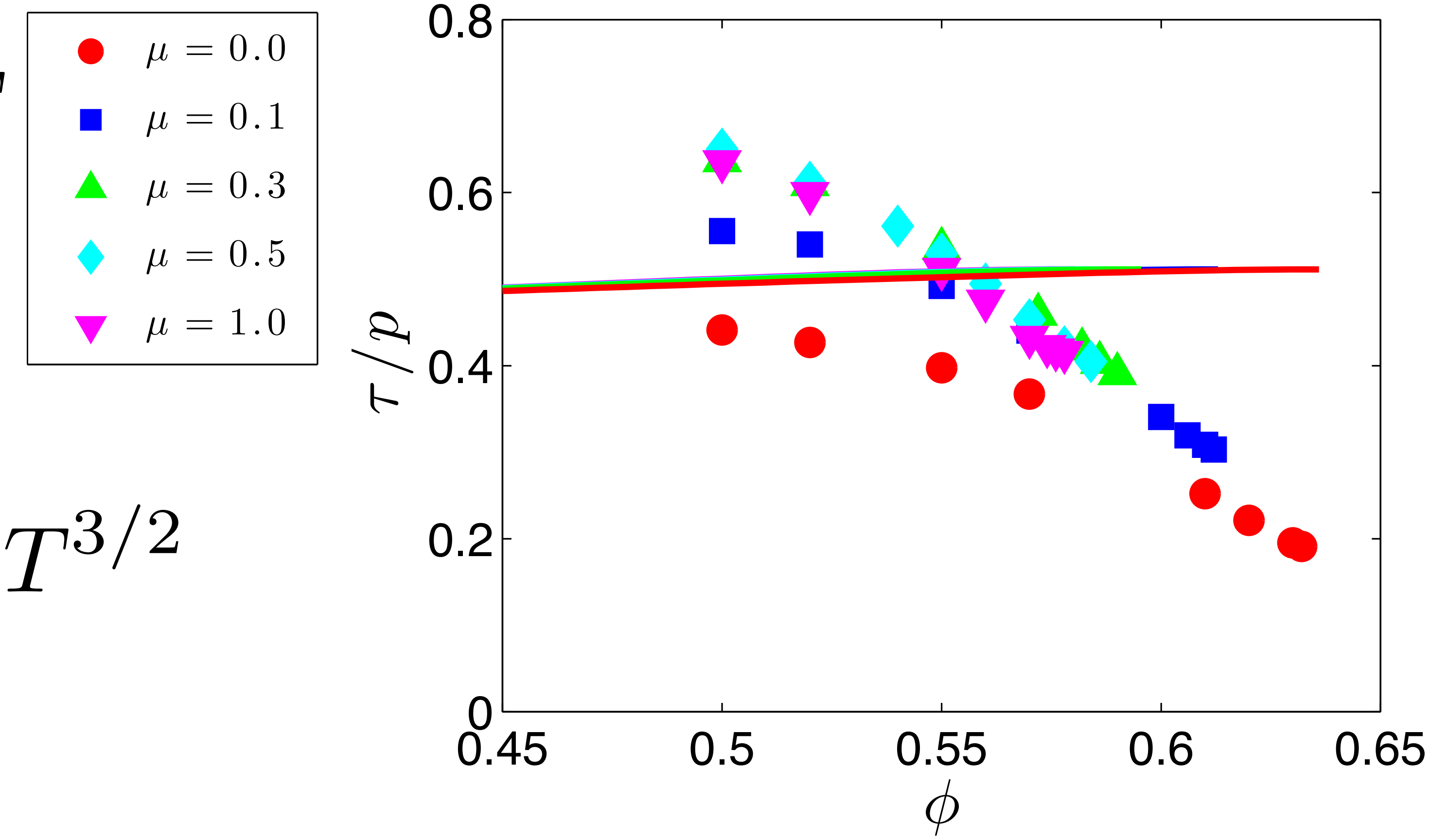

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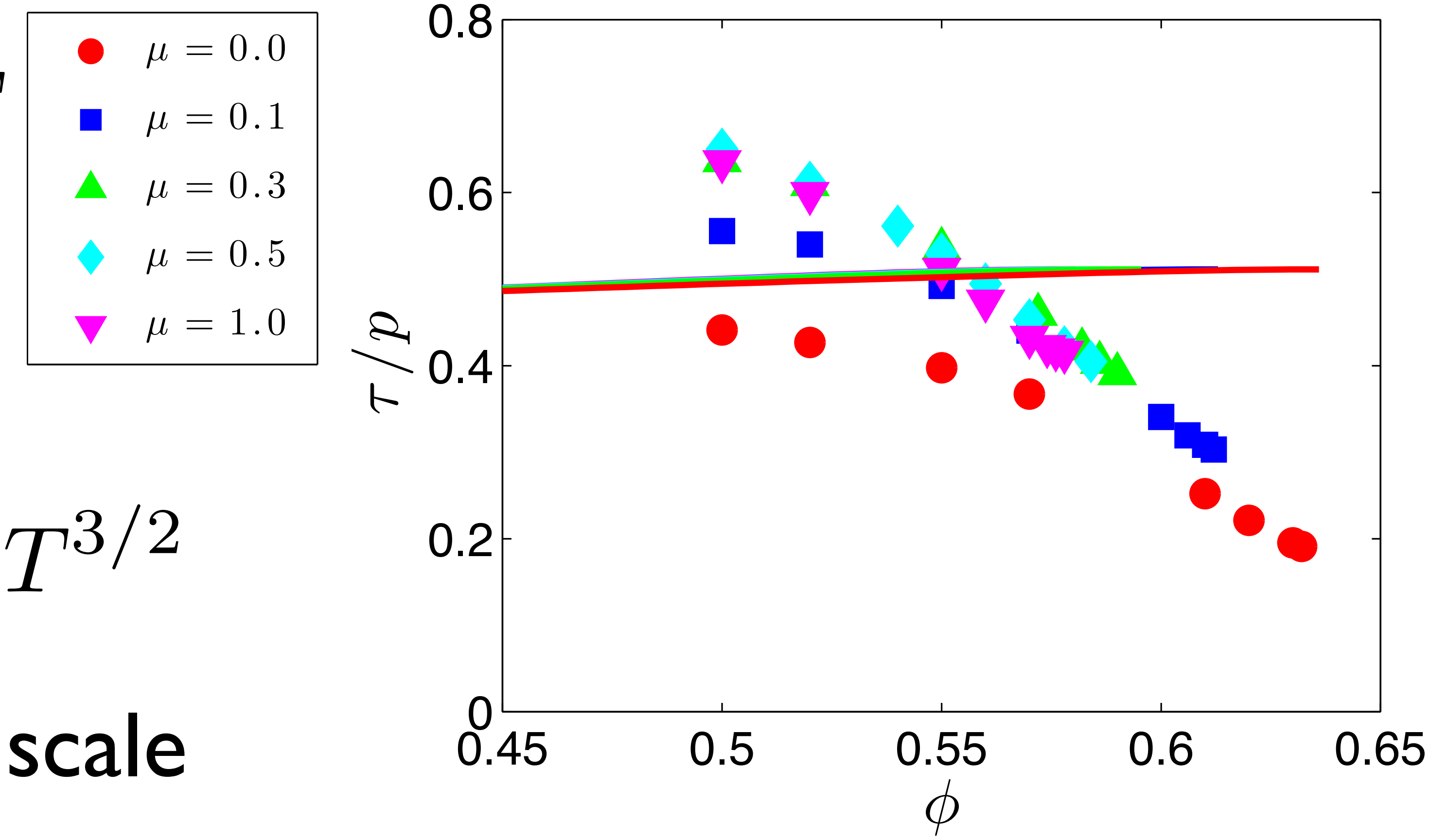

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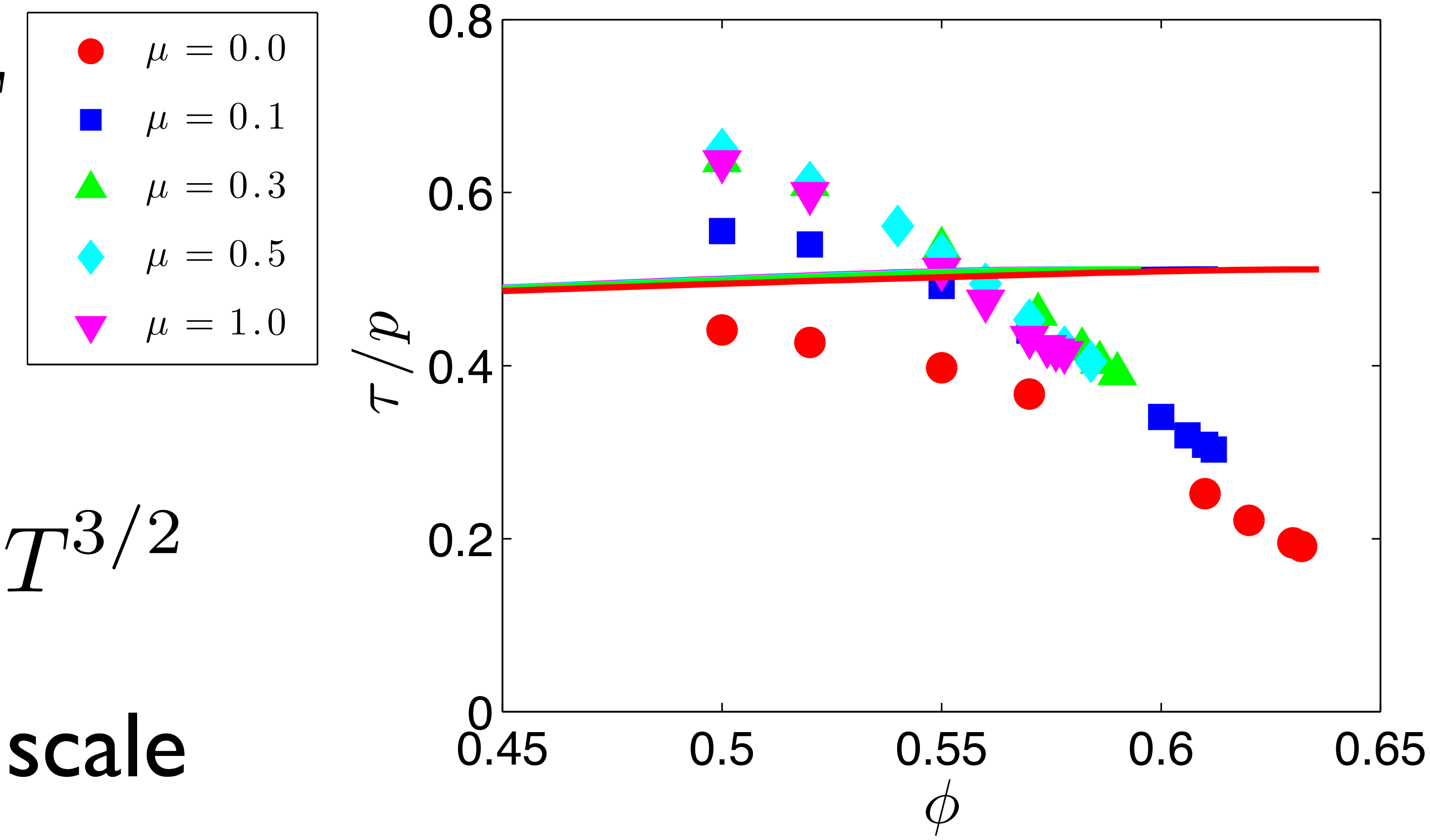

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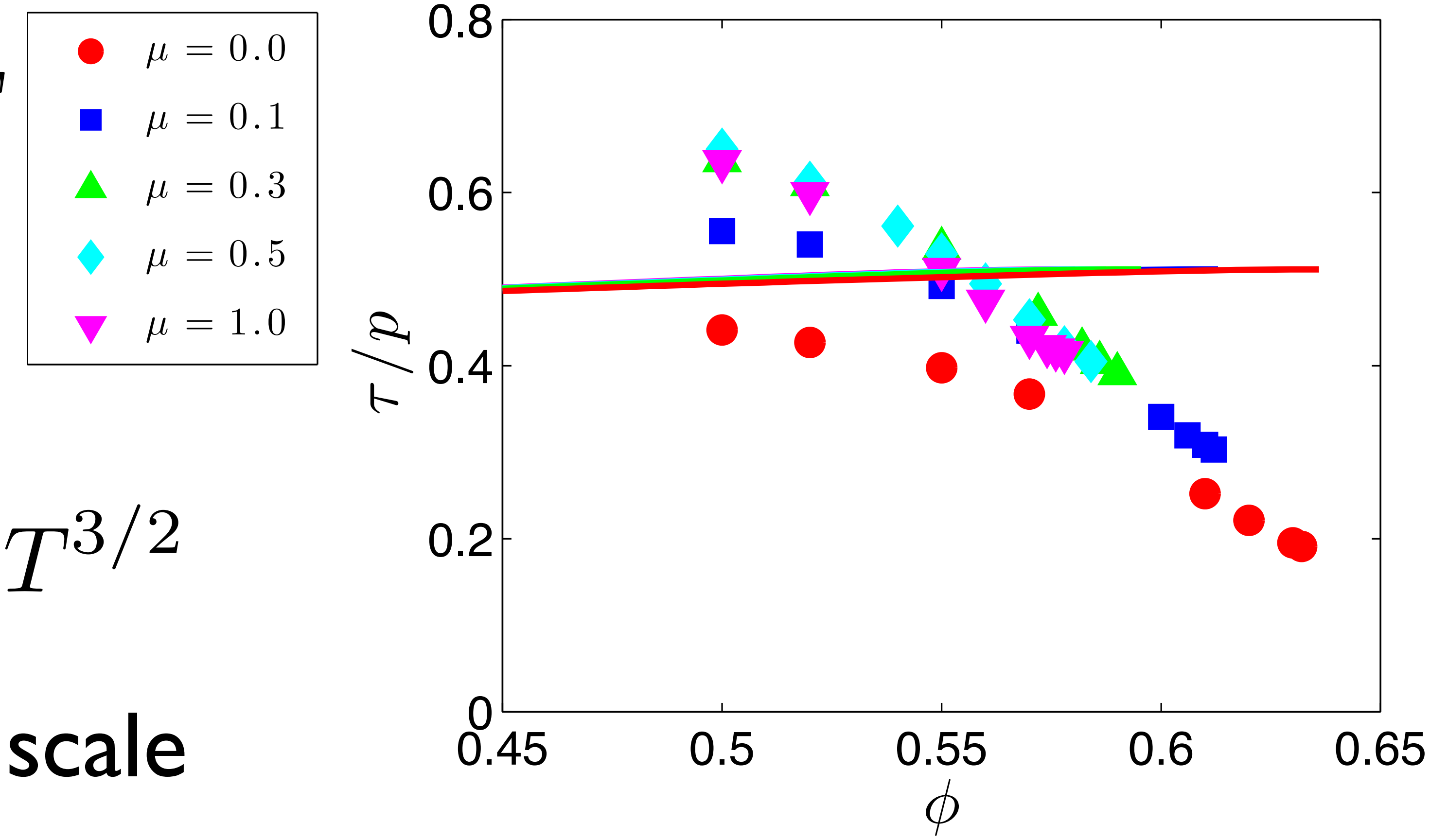

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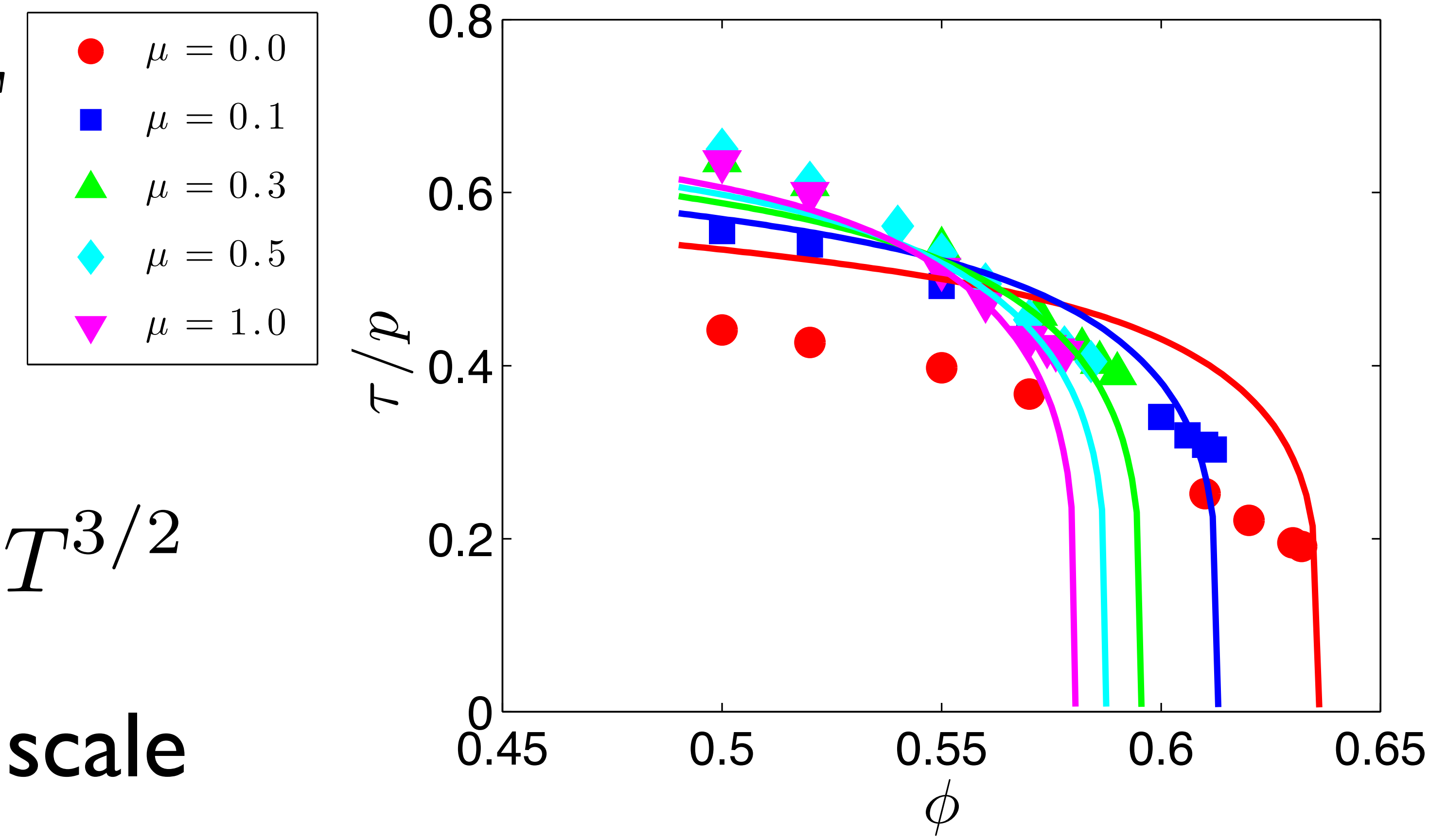

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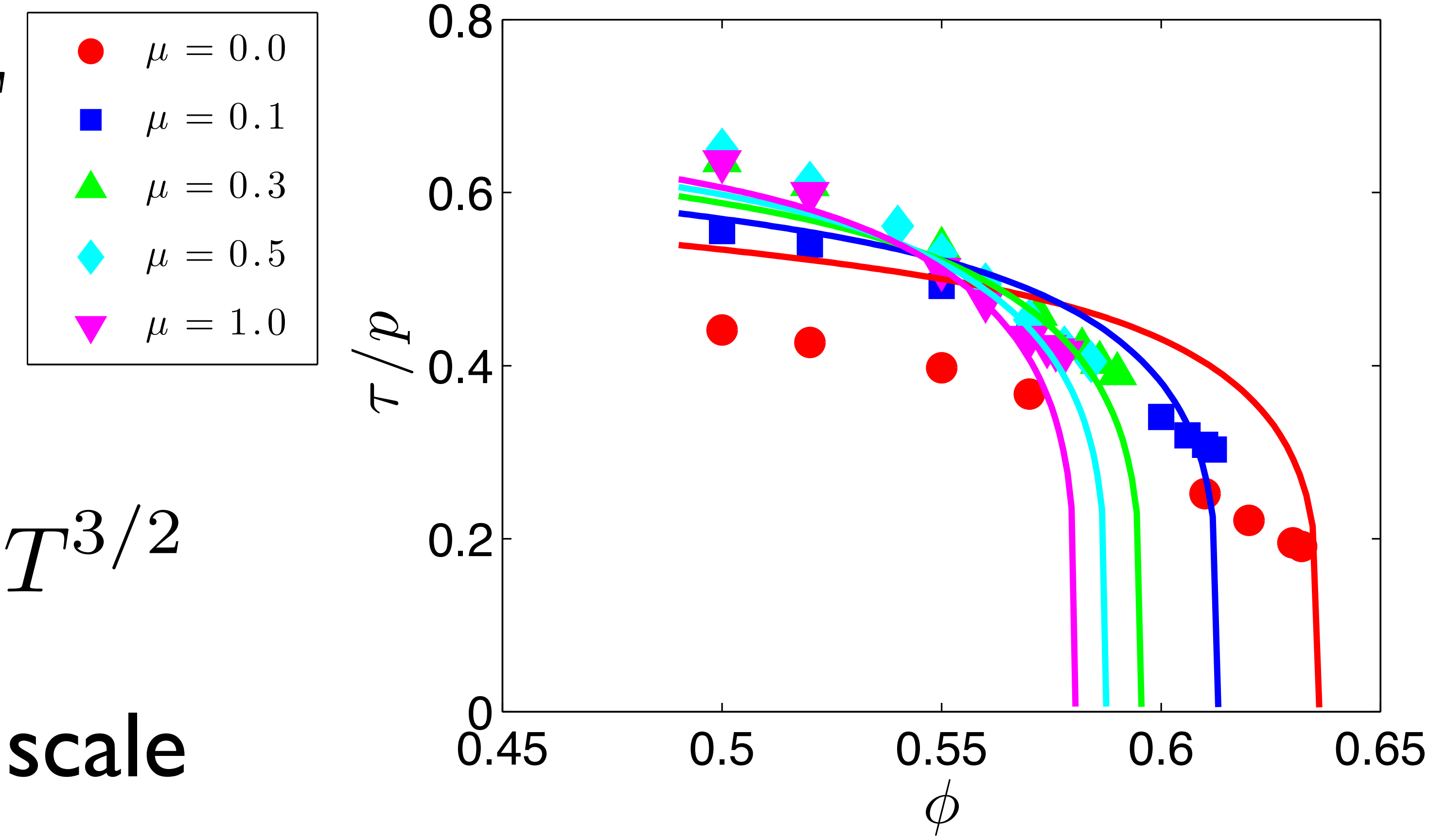

- Undesirable features:
  - Does not predict a yield stress ratio η_s
  - Temperature diverges at ϕ_c

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

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

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

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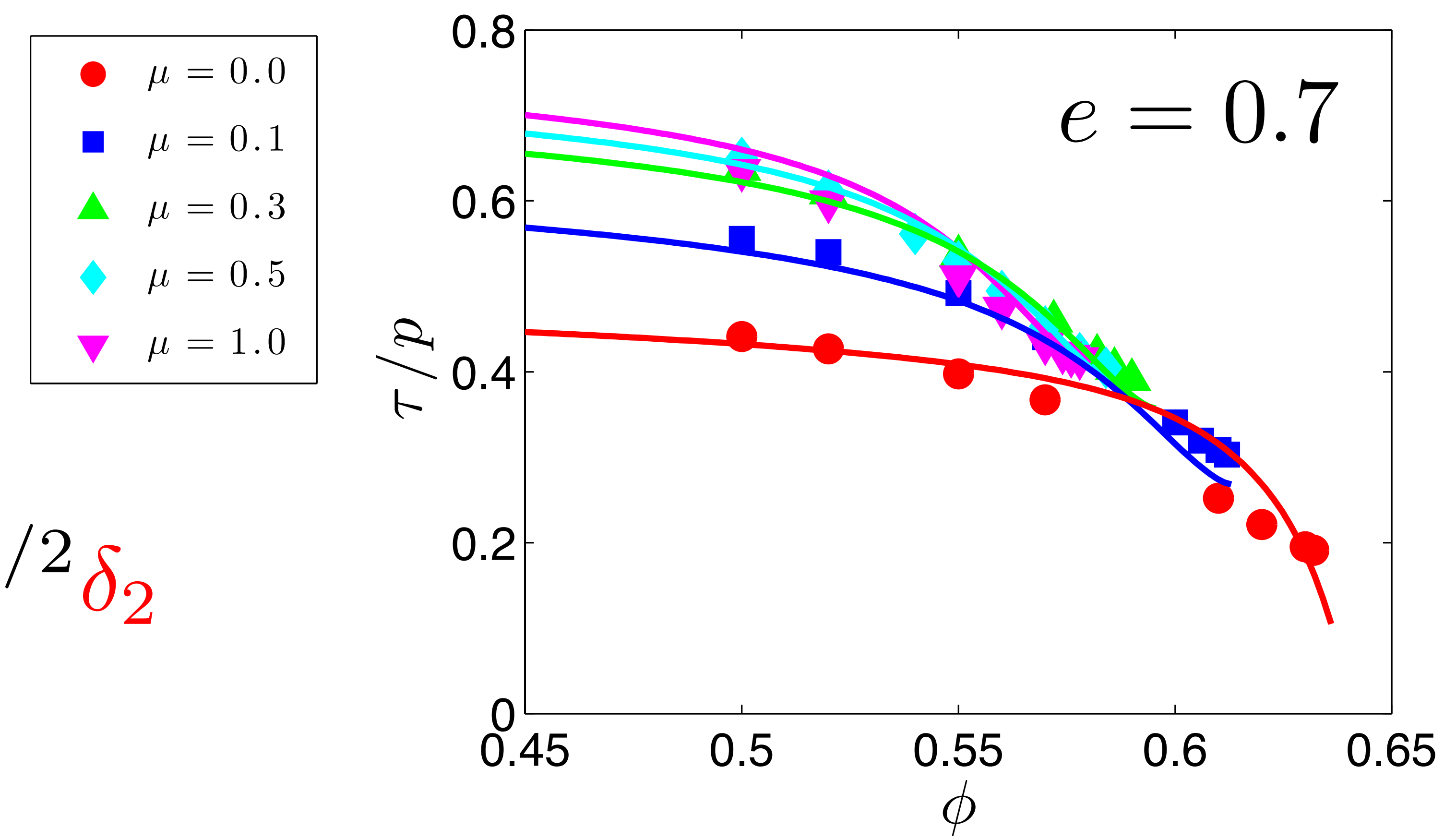

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$$\Gamma - \dot{\gamma}\tau = 0 \implies T = T\frac{\delta_1}{\delta_2} \implies \delta_1 = \delta_2 \equiv \delta$$

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

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

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

Summary and future work

- Proposed modified KT expressions that improves temperature, pressure, and shear stress predictions for frictional particles and dense flows
- Will soon implement model into MFIX continuum solver for testing on process-scale flow problems
  - Inclined chutes with/without sidewalls
  - Hoppers and bins
  - Fluidized beds