Implementation and Refinement of a Comprehensive Model for Dense Granular Flows

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Princeton University

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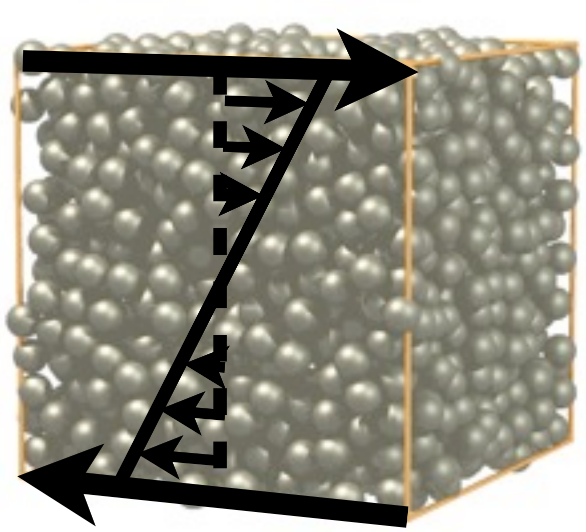

Shear flow of frictional particles in a periodic box

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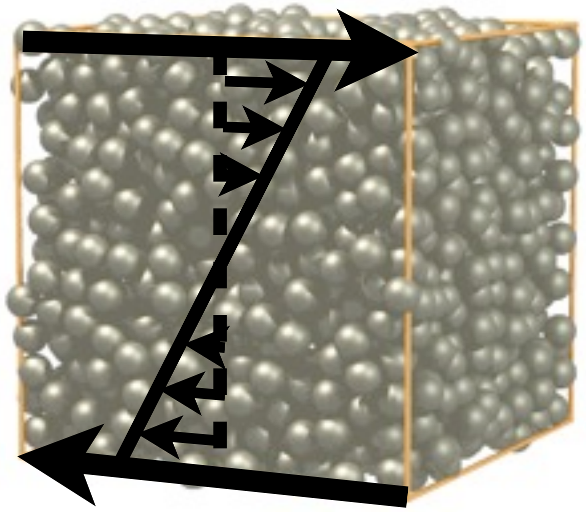

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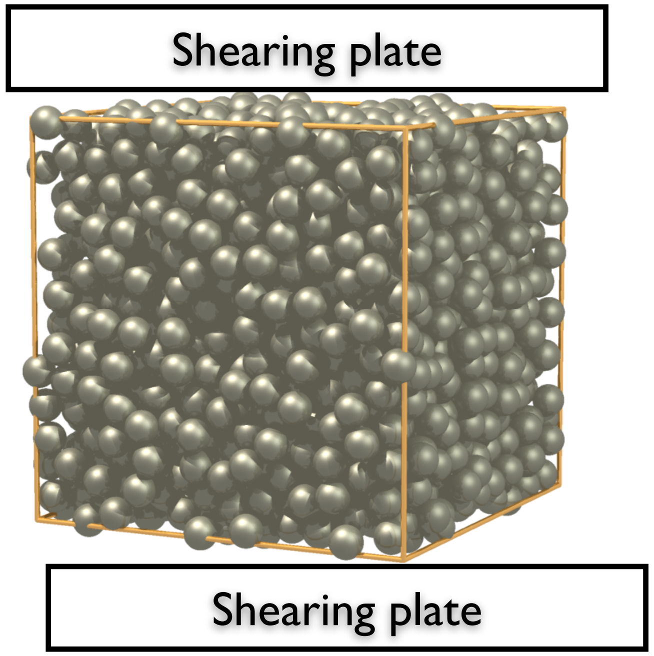

Shear flow of
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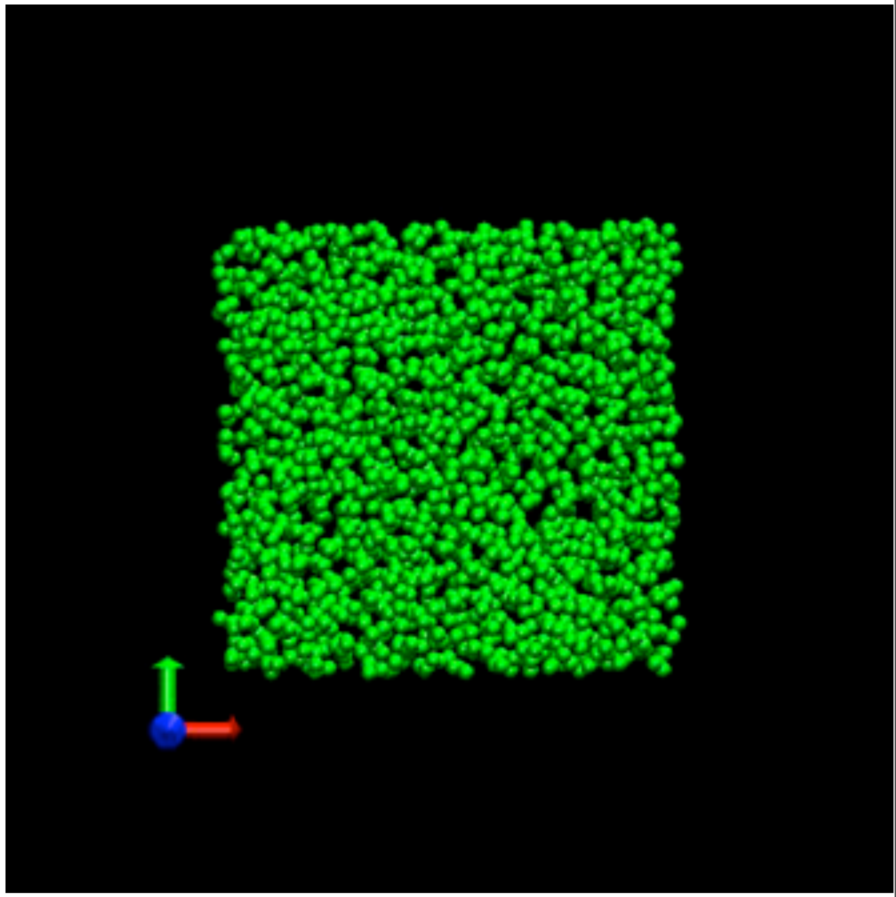
with bounding walls

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)

Dense phase rheology: Questions asked

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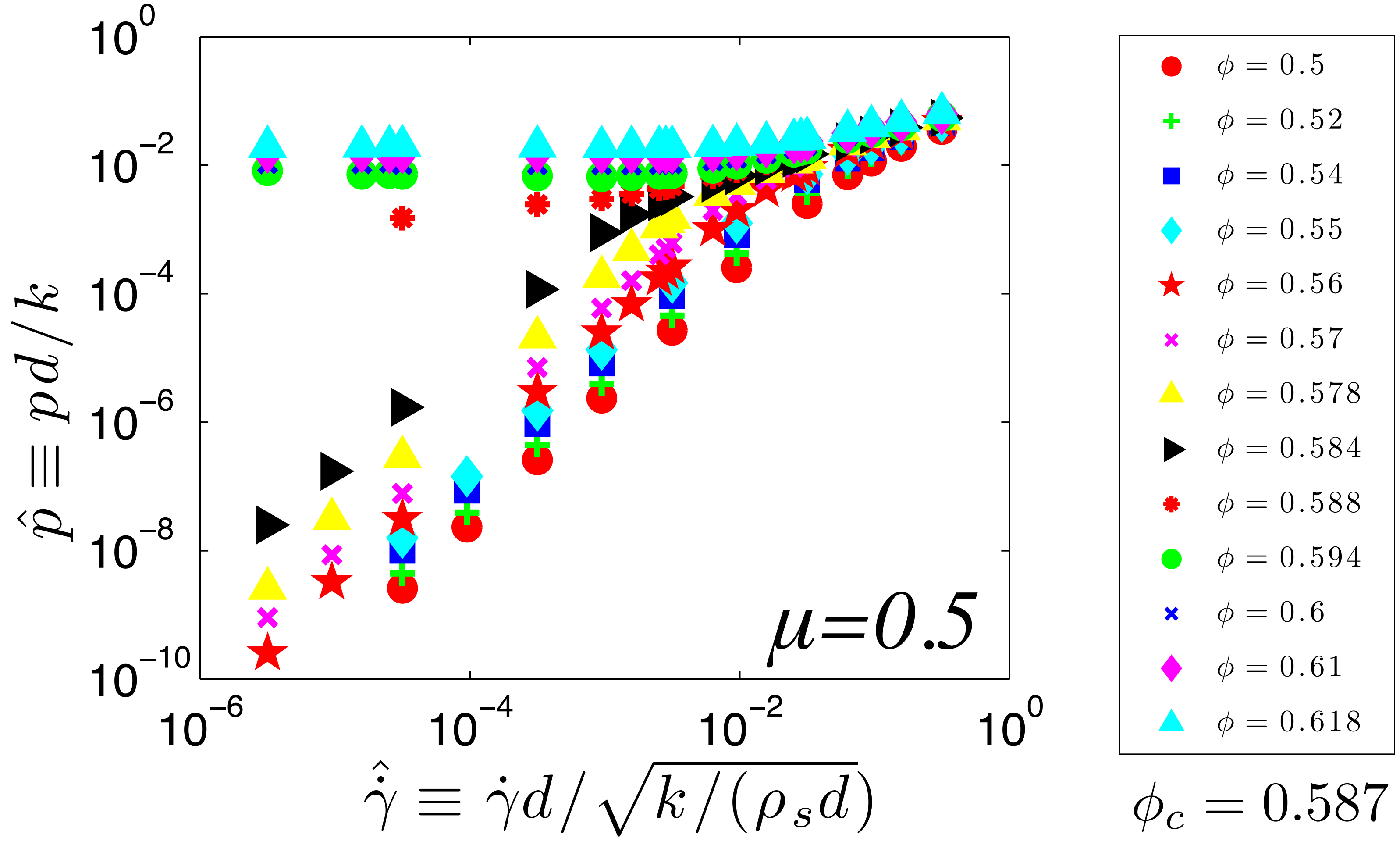
Flow map



$\phi_c = 0.587$

Previous studies

- Computational
  - C. S. Campbell, J. Fluid Mech. 465, 261 (2002).
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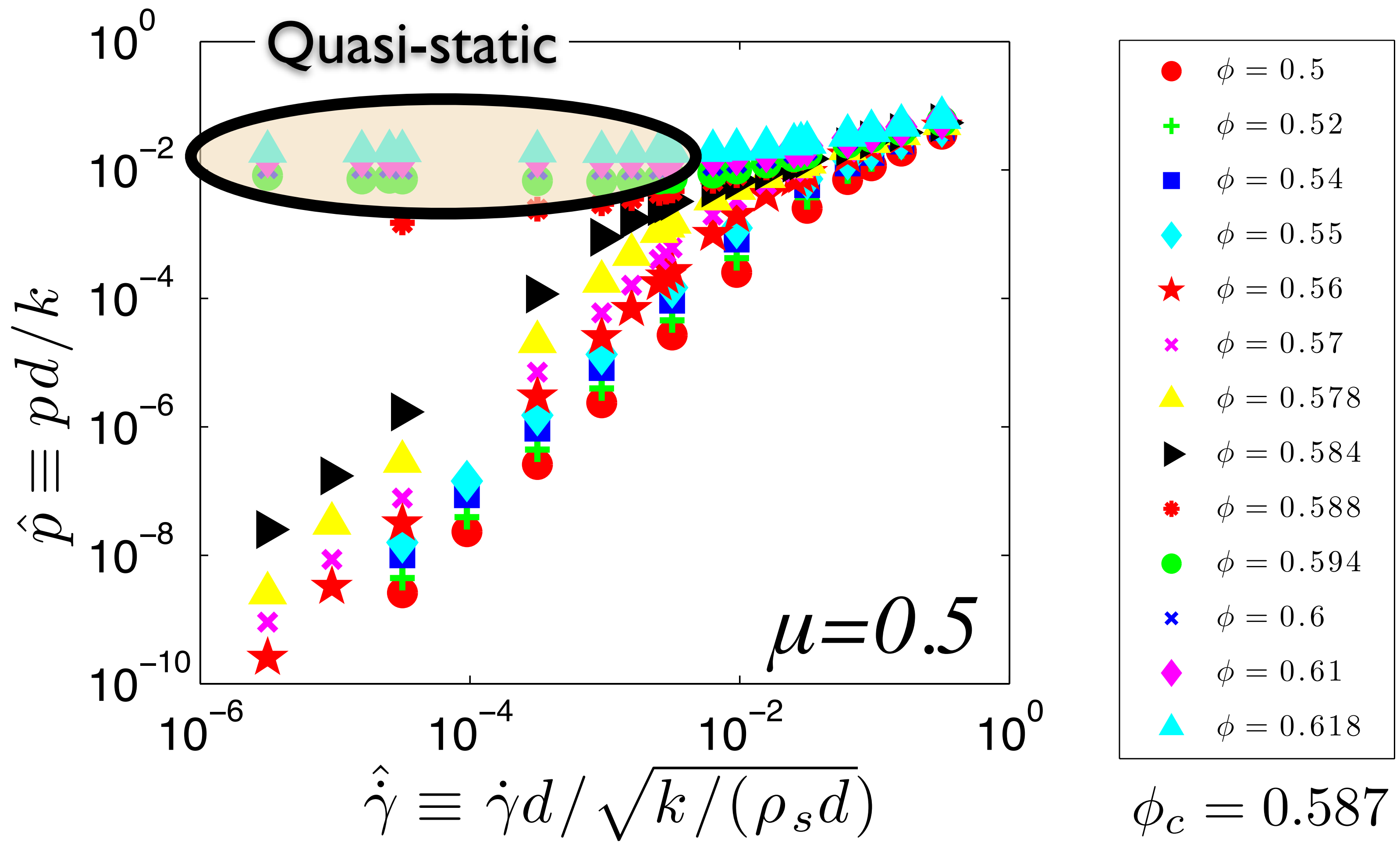

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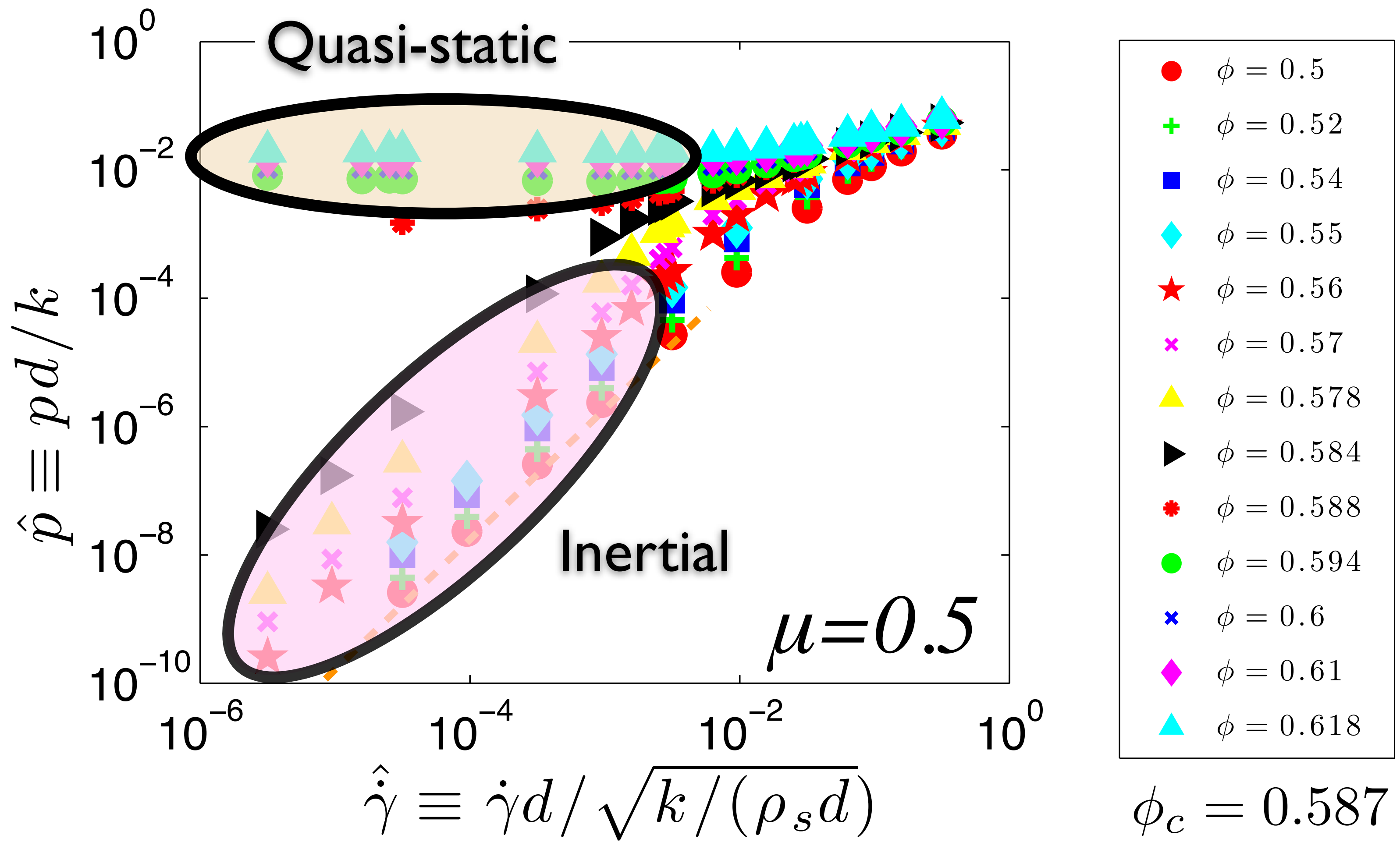

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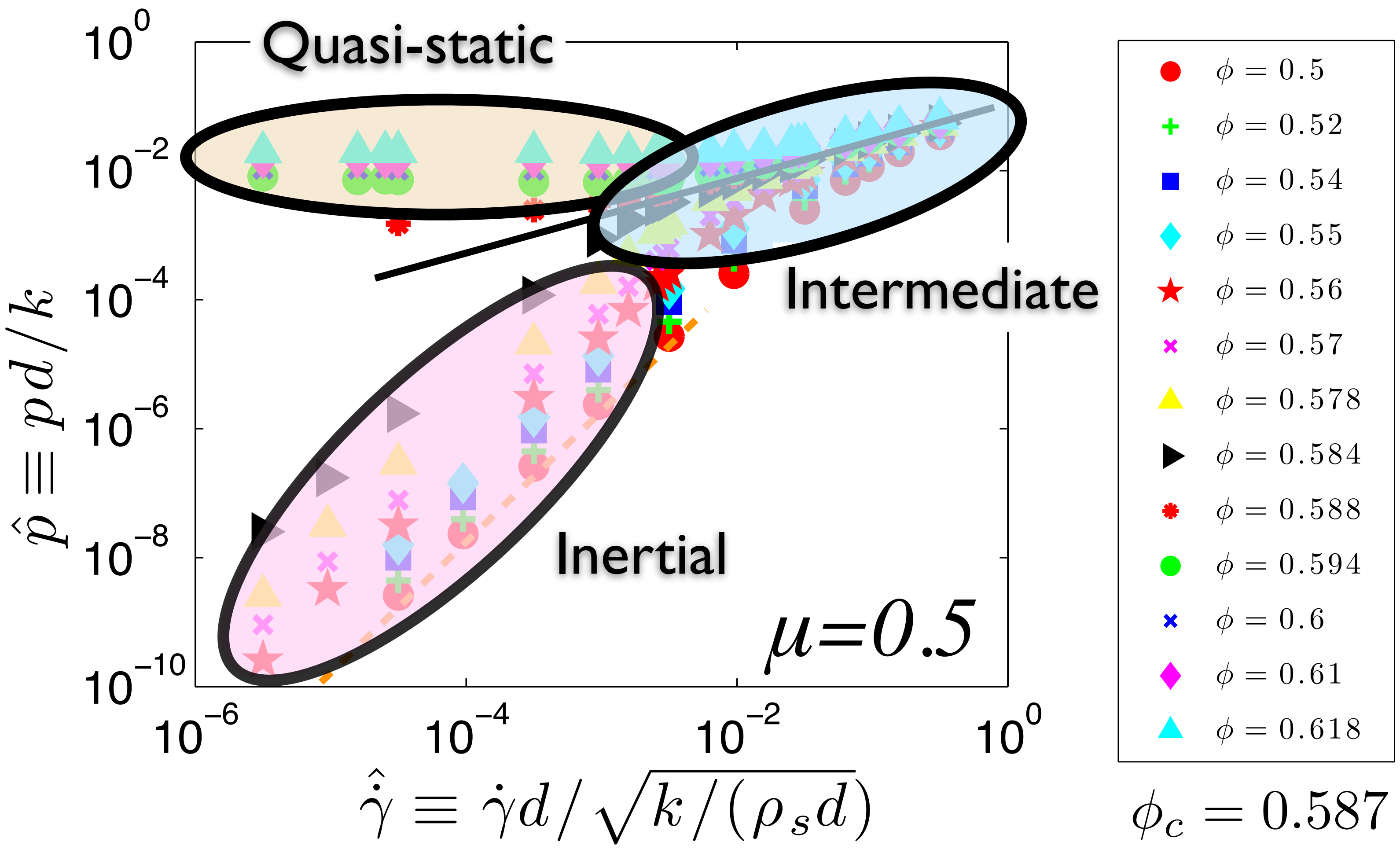

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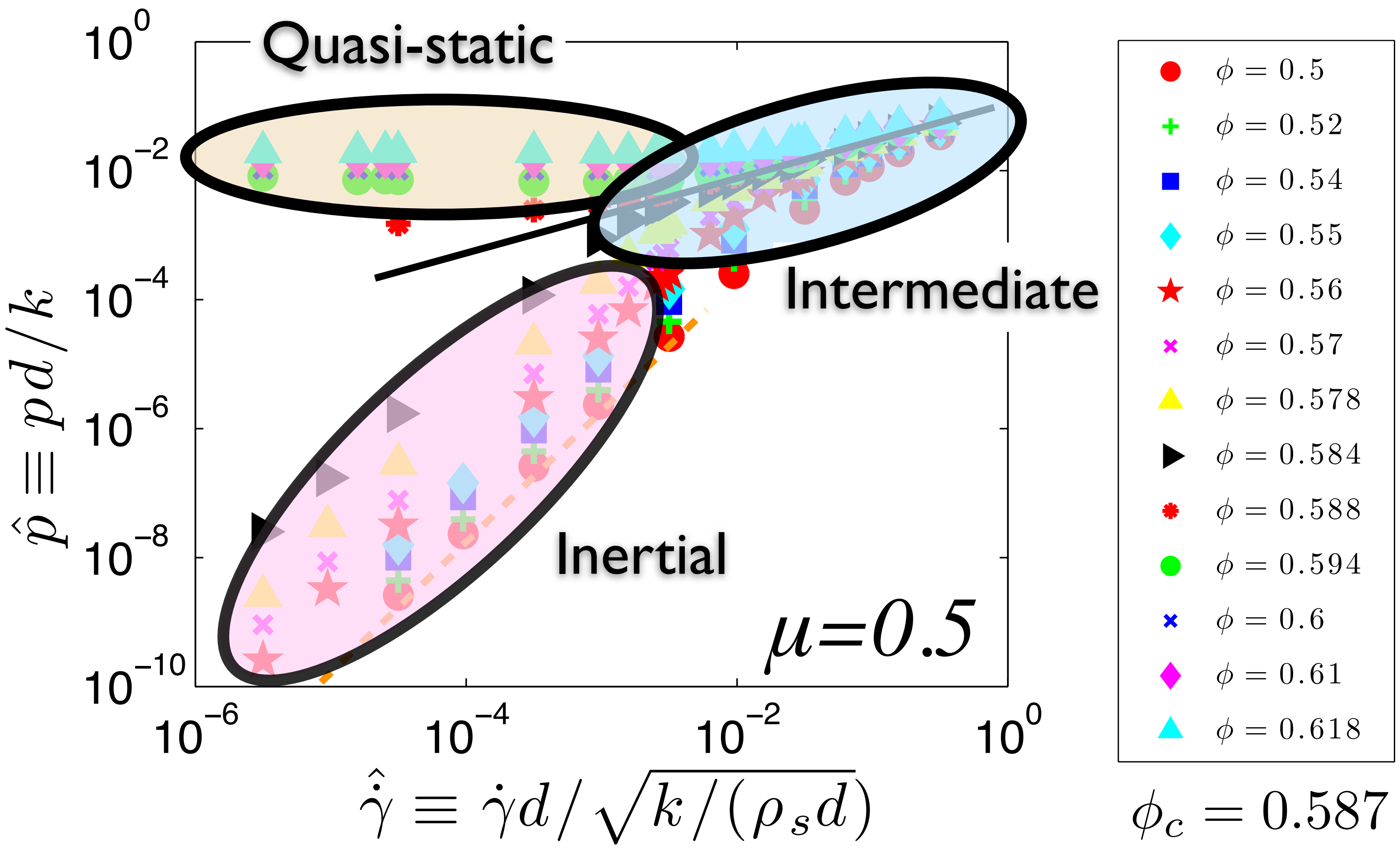

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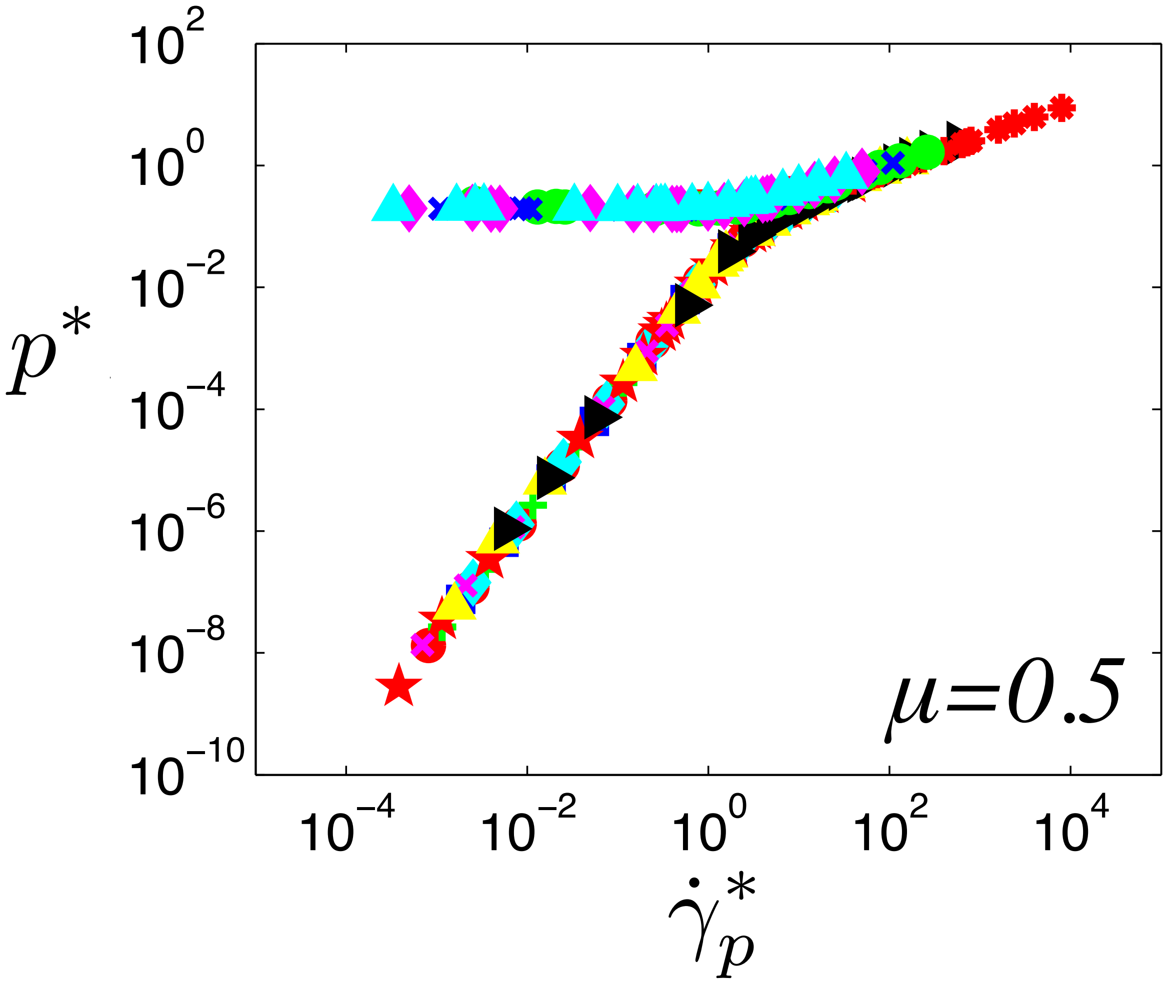
- Critical volume fraction ϕ_c and its flow curve $\hat{p} = \alpha \hat{\dot{\gamma}}^m$ distinguish the three flow regimes.
- Role of particle softness:
  - Large k $\Longrightarrow$ quasi-static or inertial regime
  - Small k $\Longrightarrow$ intermediate regime

Pressure scalings for frictional particles



Scaled pressure and shear rate†:

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

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

Choose exponents:

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

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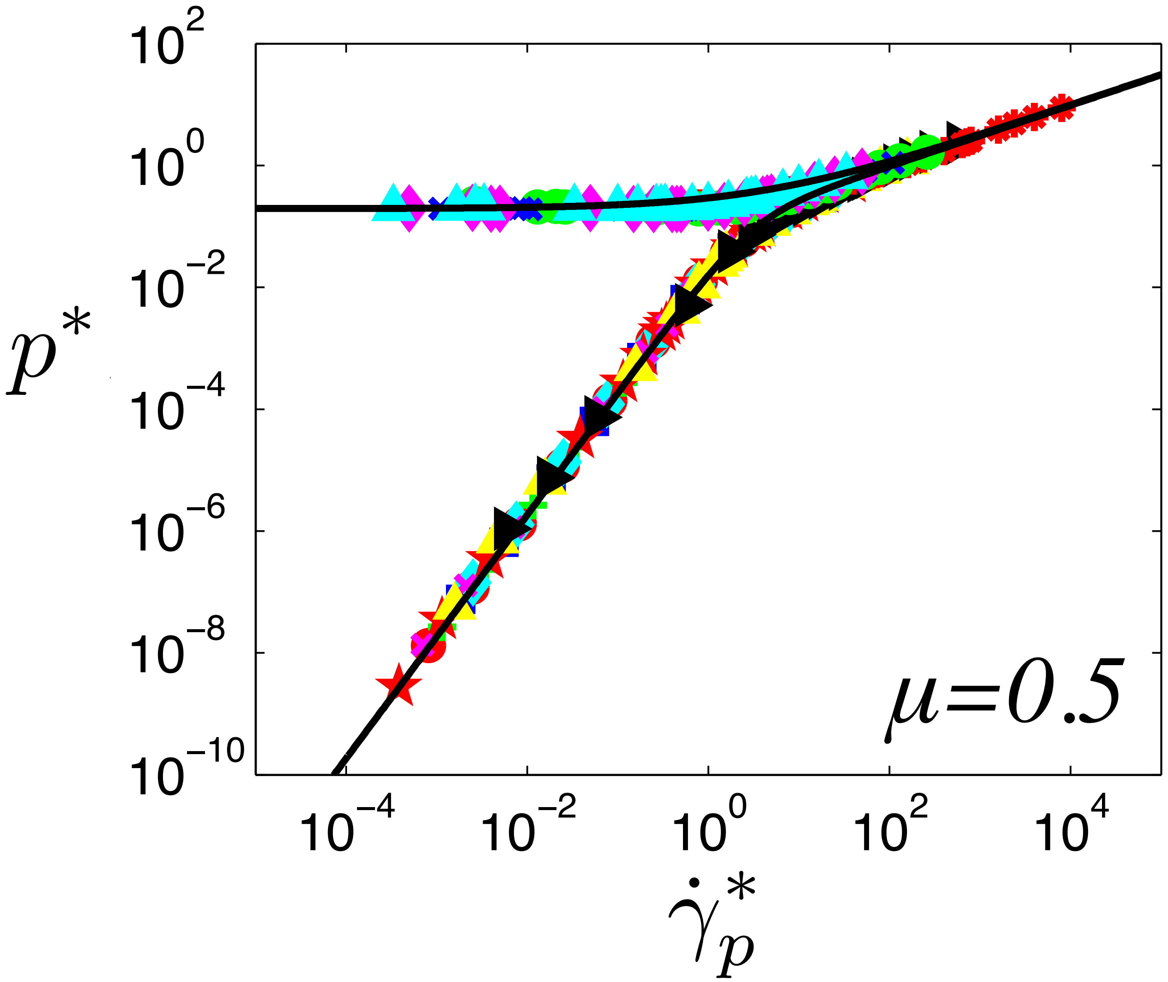

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- Three pressure asymptotes:

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

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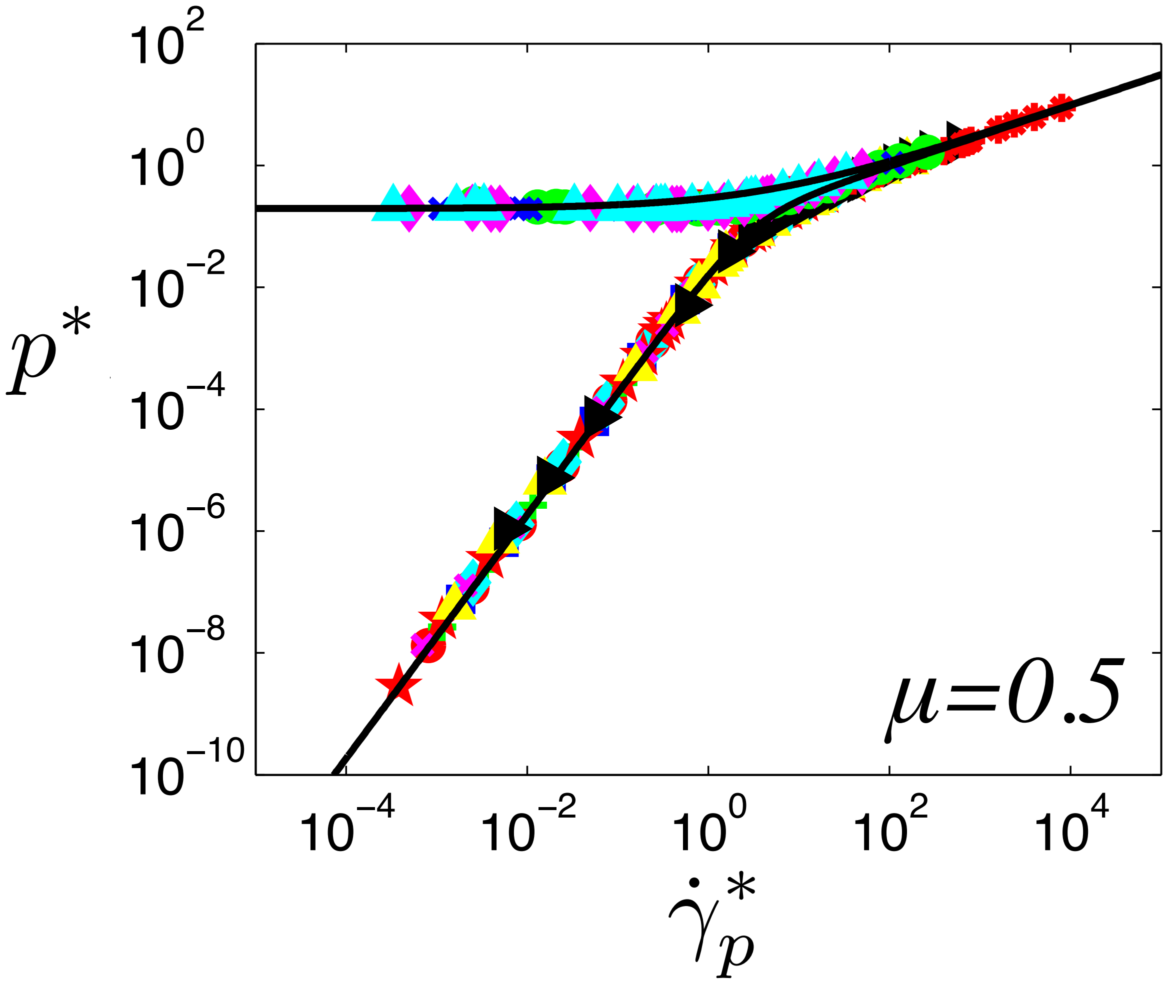

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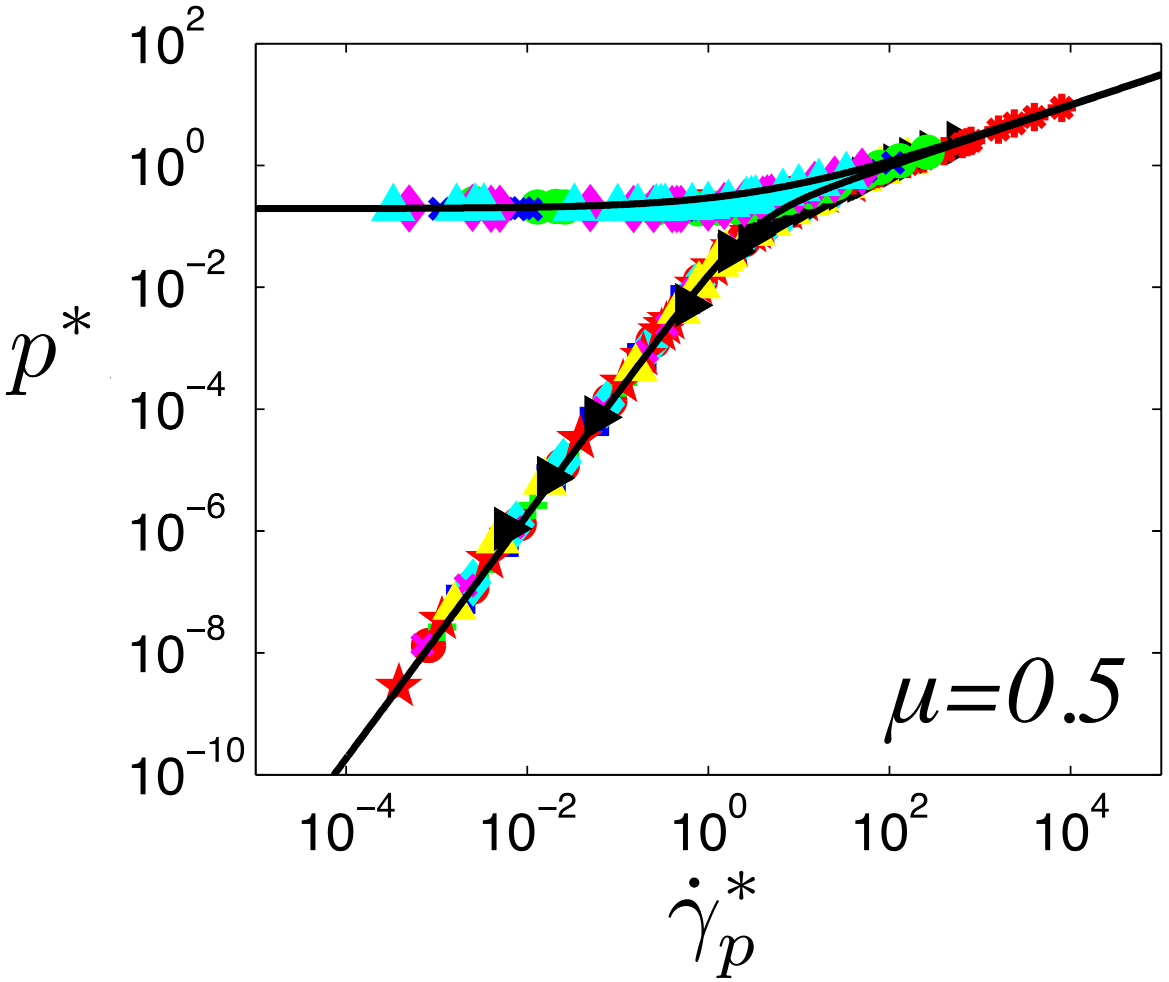

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S. Chialvo et al., PRE 85, 021305 (2012).

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- Flow regime map: What regimes of flow are observed in shear flow of soft, frictional, non-cohesive particles? (completed)
- Effect of cohesion: How does the addition of modest level of cohesion, such as in Geldart Group A particles change the flow regime map?
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  - Modified kinetic theory
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Kinetic-theory models

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- Most KT models designed for dilute flows of frictionless particles
- Can KT model be modified to capture dense-regime scalings?
- Seek modifications to KT model of Garzó-Dufty (1999)†

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

Kinetic theory equations

Garzó-Dufty kinetic theory for simple shear flow

Pressure

$$p = \rho_s H(\phi, g_0(\phi))T$$

Energy dissipation rate

$$\Gamma = \frac{\rho_s}{d} K(\phi, e) T^{3/2}$$

Shear stress

$$\tau = \rho_s d \dot{\gamma} J(\phi) \sqrt{T}$$

Steady-state energy balance

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

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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

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Modifications (in red)

$$p = \rho_s H(\phi, g_0(\phi, \phi_c(\mu)))T$$

$$\Gamma = \frac{\rho_s}{d} K(\phi, e_{\mathrm{eff}}(e, \mu)) T^{3/2} \delta_\Gamma$$

$$\tau = \tau_s + \rho_s d \dot{\gamma} J(\phi)\sqrt{T}\delta_\tau$$

$$\Gamma - (\tau - \tau_s)\dot{\gamma} = 0$$

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    S. Chialvo & S. Sundaresan, Phy. of Fluids, 25, 070603 (2013).
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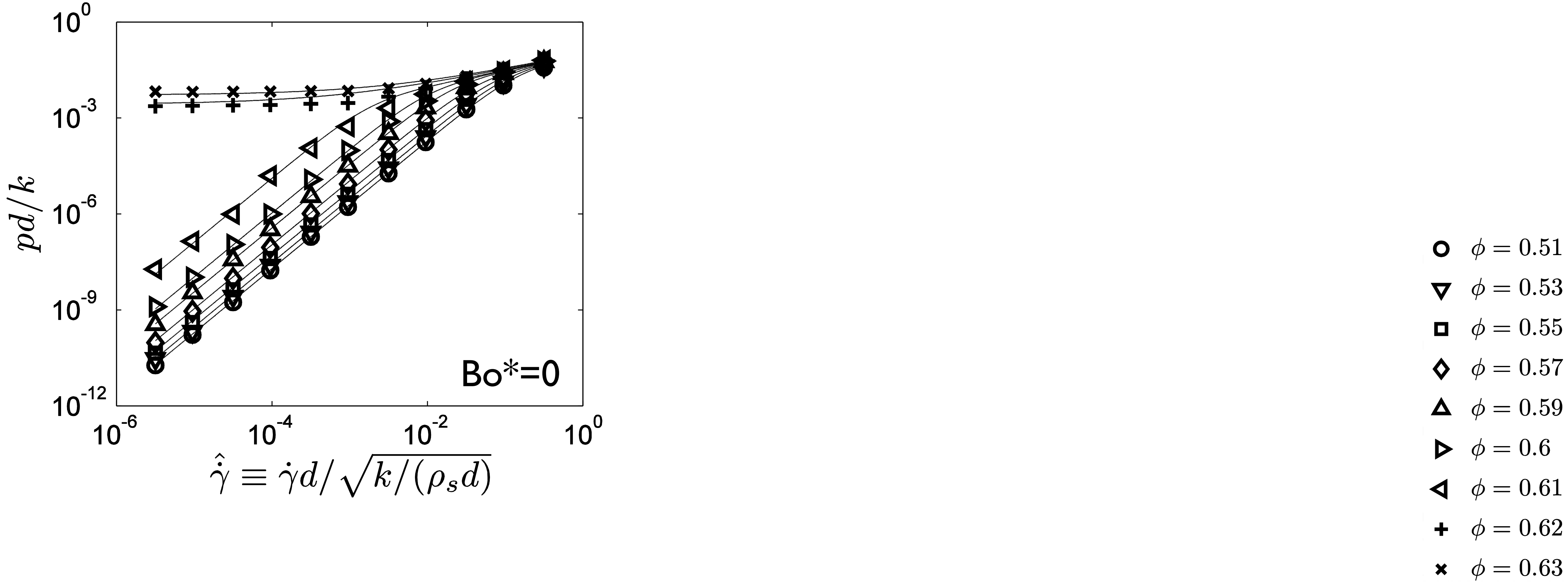
Cohesive particles



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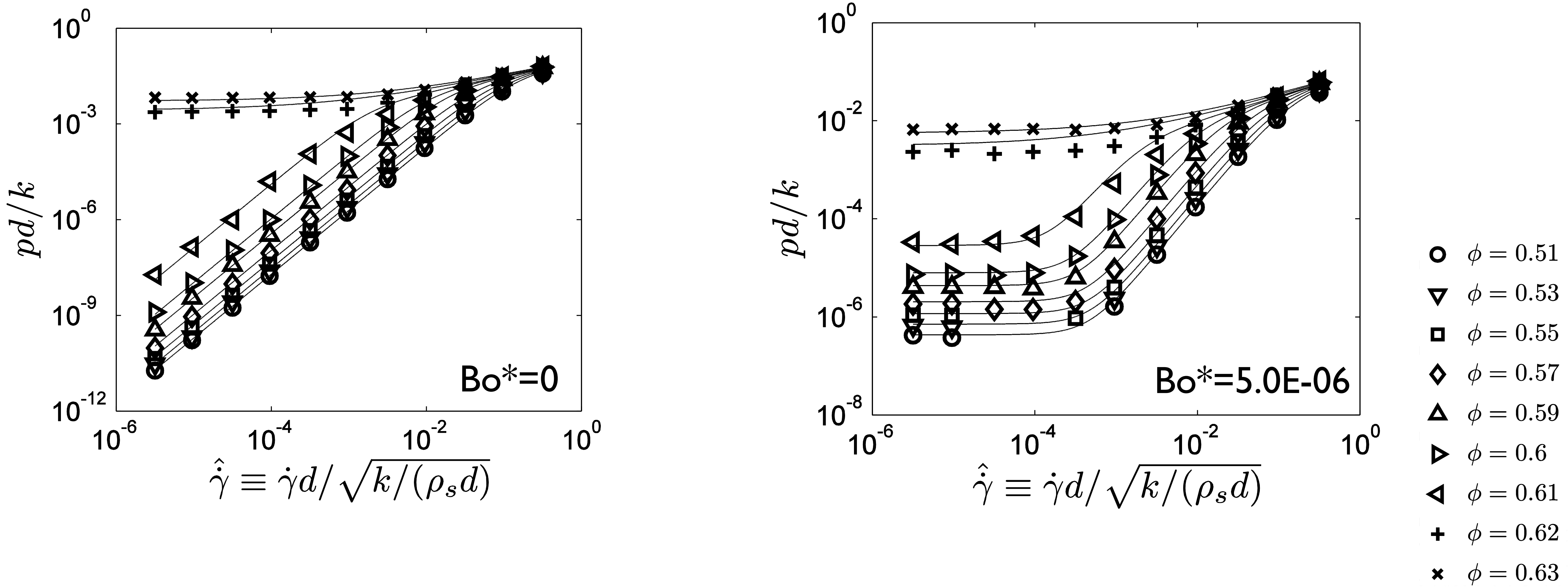

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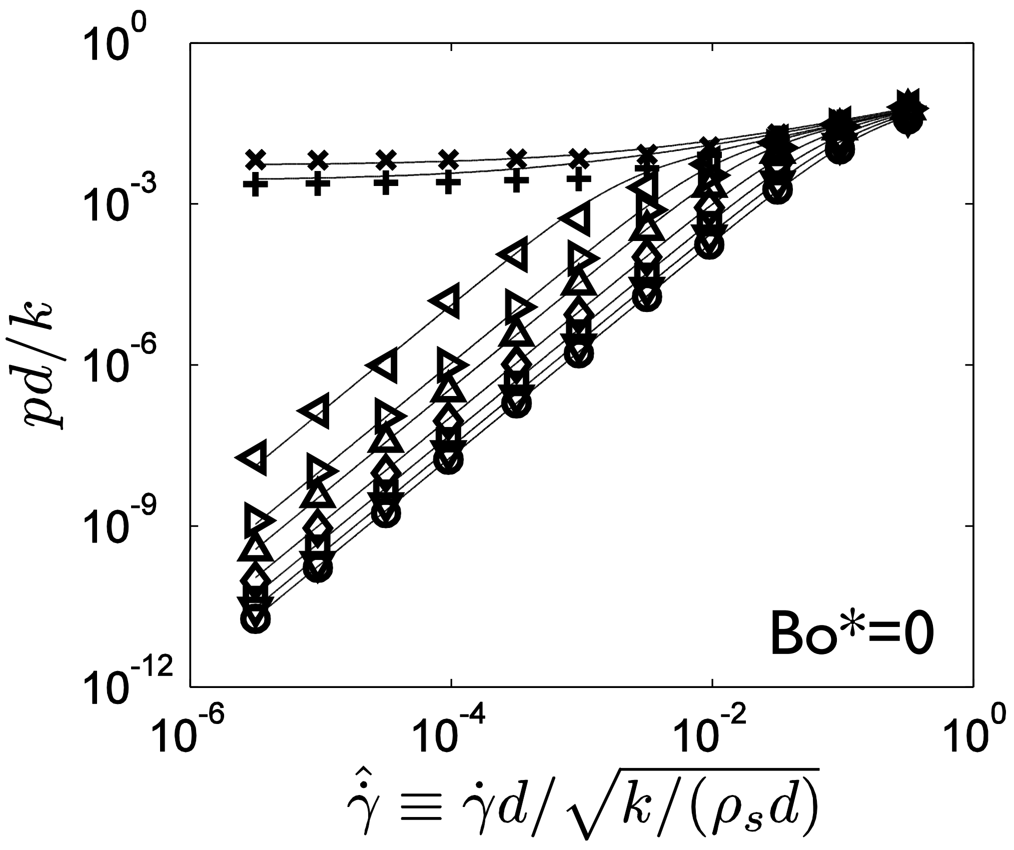

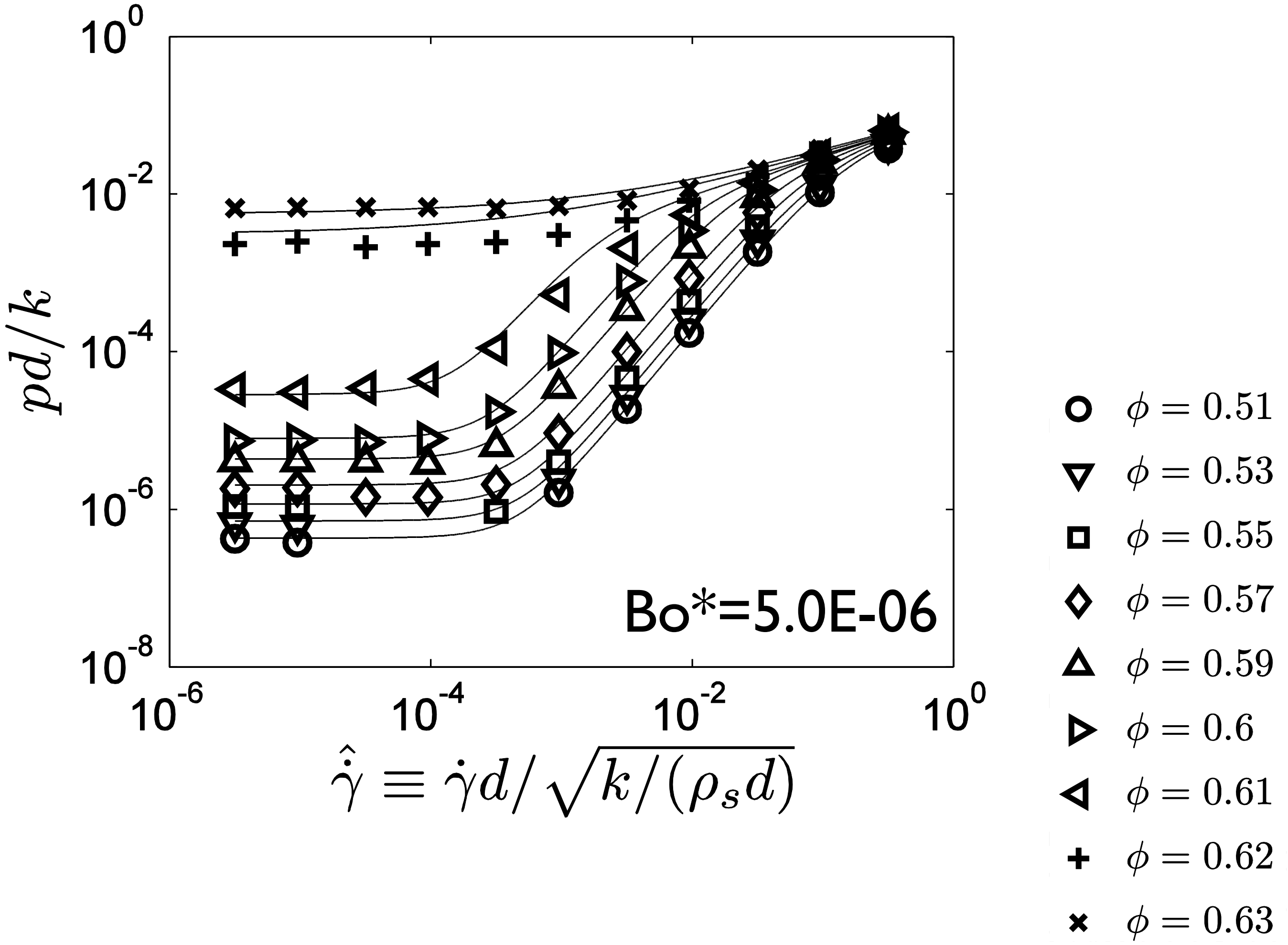

$$Bo^* \equiv F_{vdW}^{\max} / kd \approx A / 24ks_{\min}^2$$

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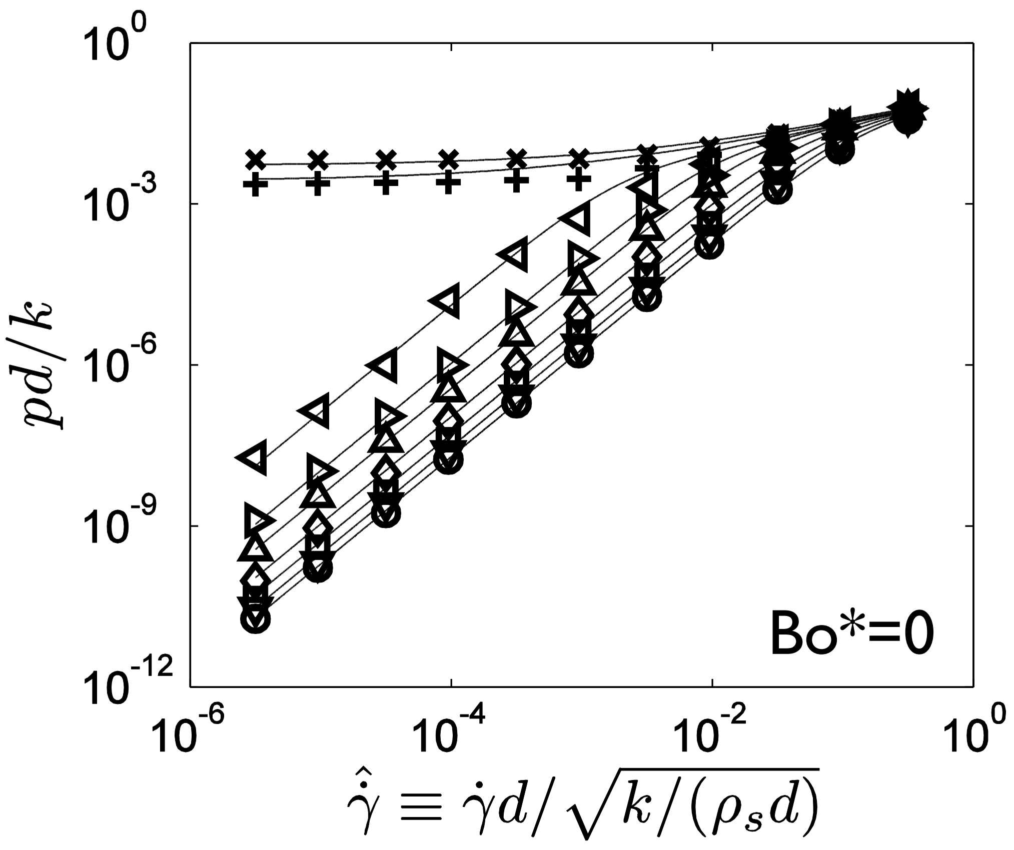

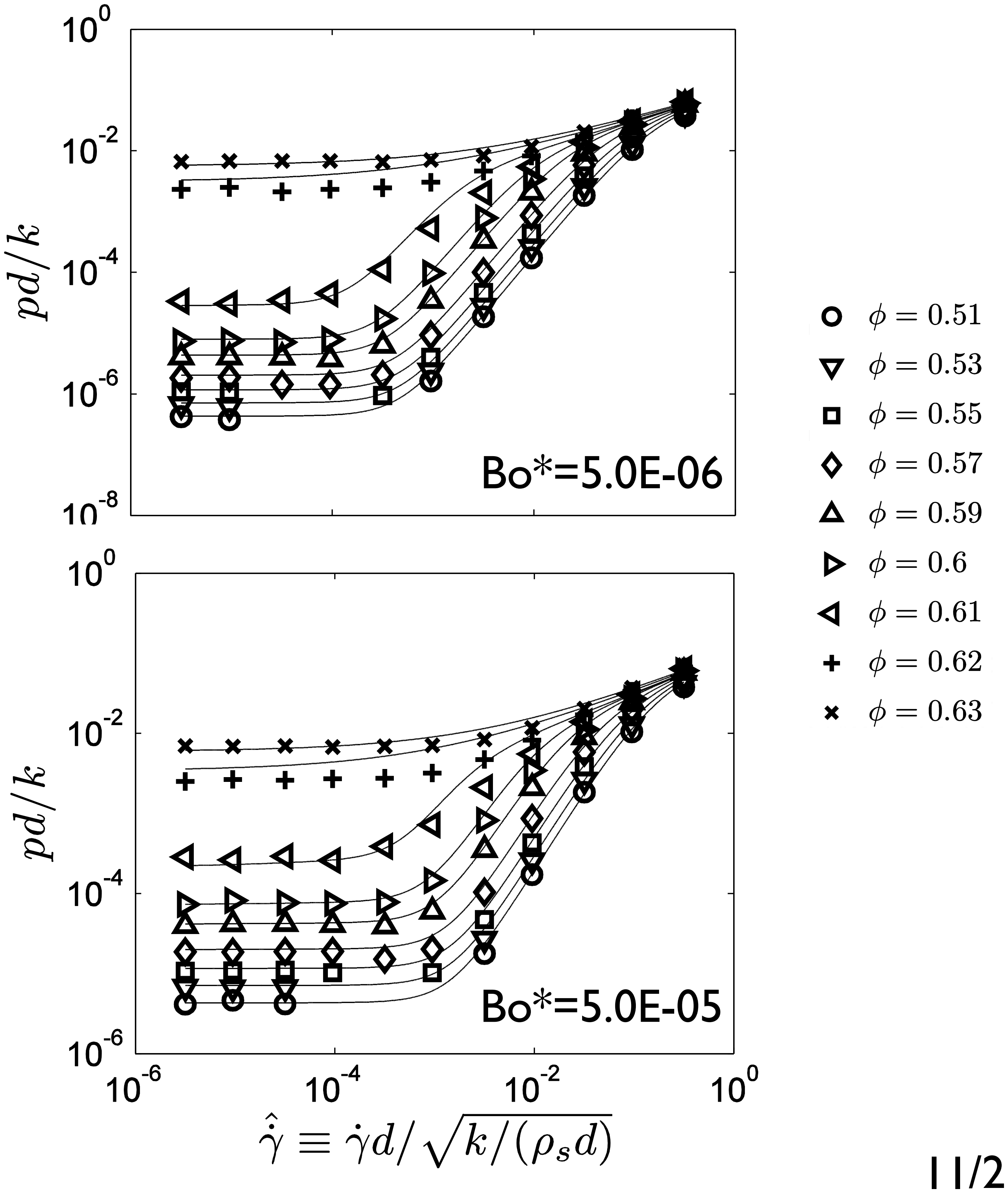

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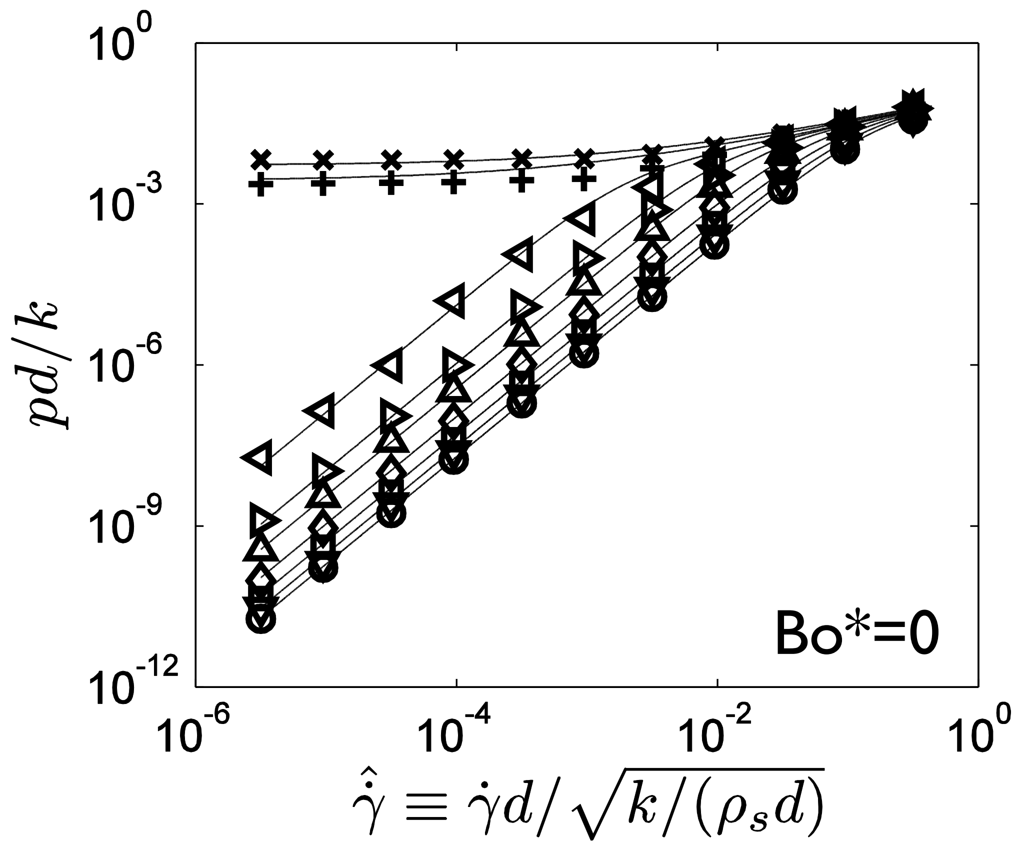

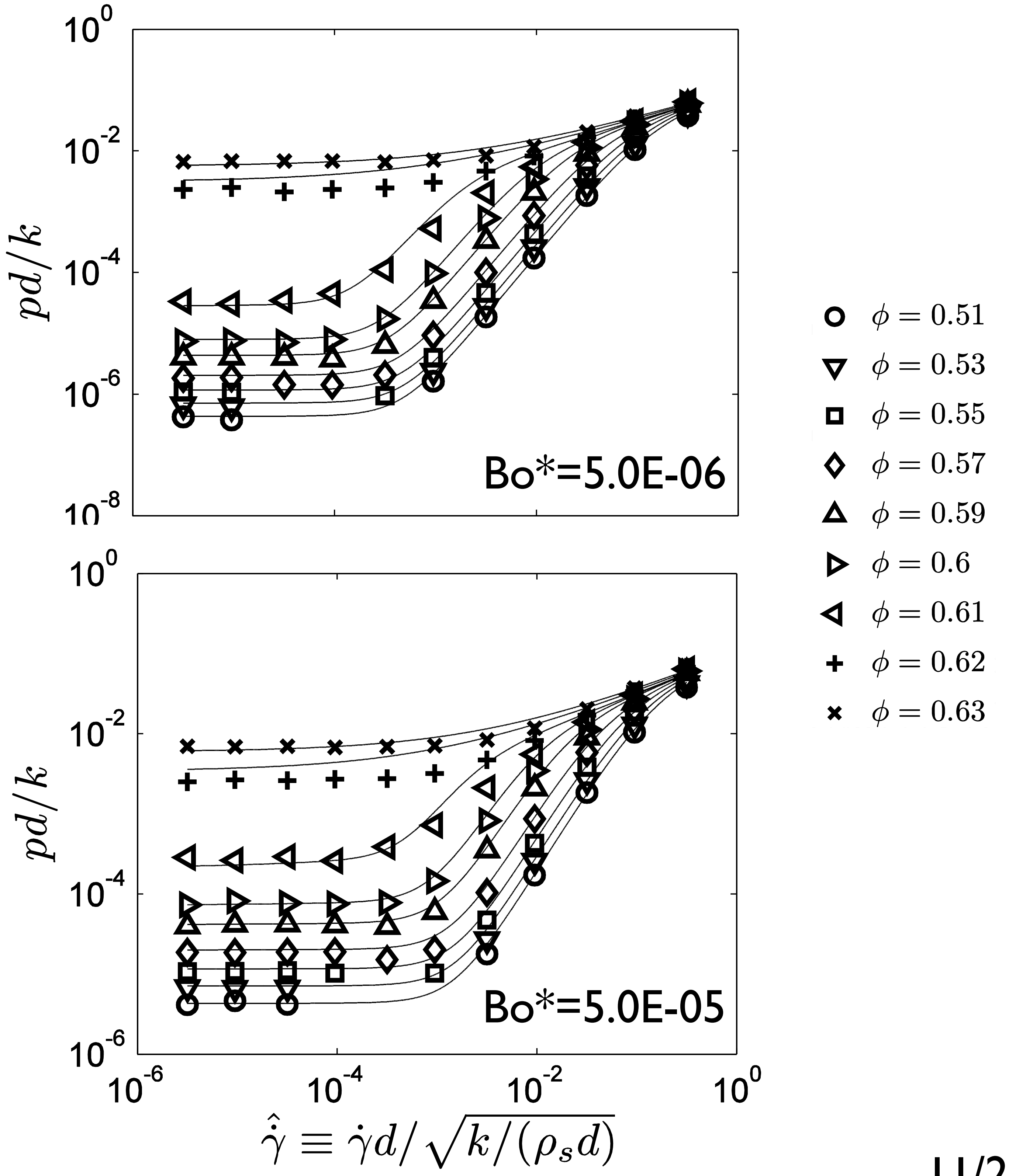

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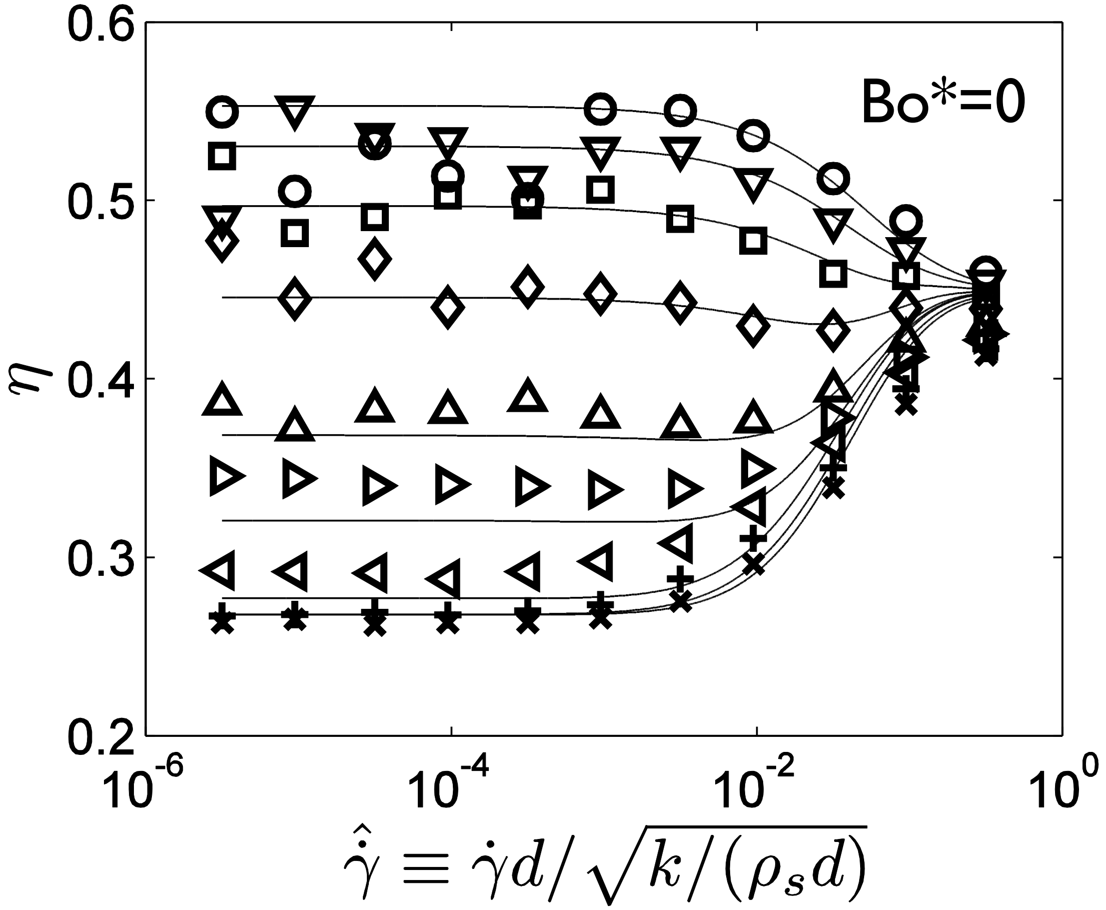
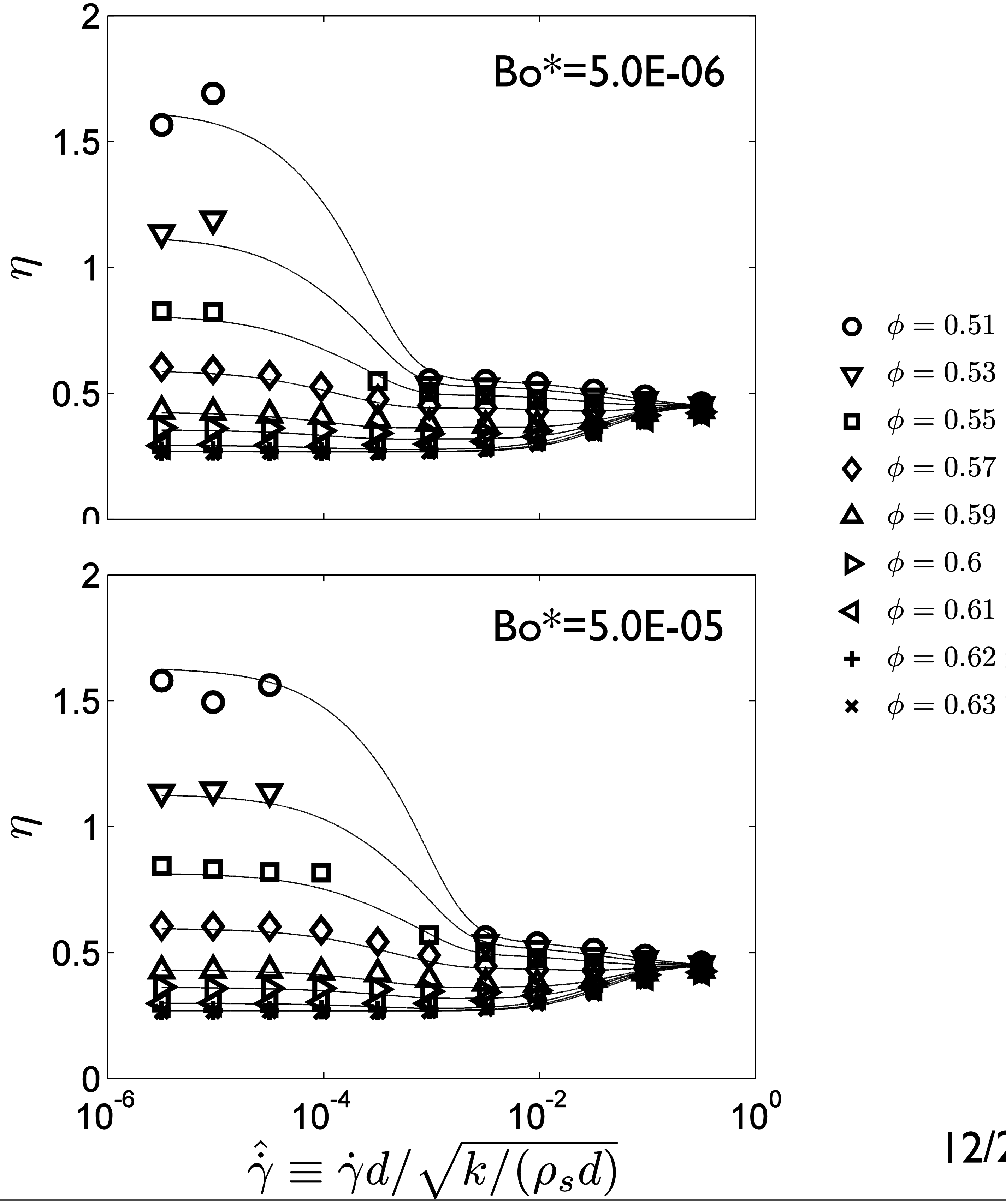
Quasi-static, inertial and intermediate regimes persist. A new cohesive regime emerges below the jamming conditions for equivalent non-cohesive particles.

Cohesive particles: Stress ratio





$$\boldsymbol{\sigma} = p\mathsf{I} - p\eta\hat{\mathsf{S}}$$

- cohesion increases effective stress ratio

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- Rheological models (non-cohesive particles)
  - Steady state models that bridge various regimes (completed)

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- Wall Boundary conditions

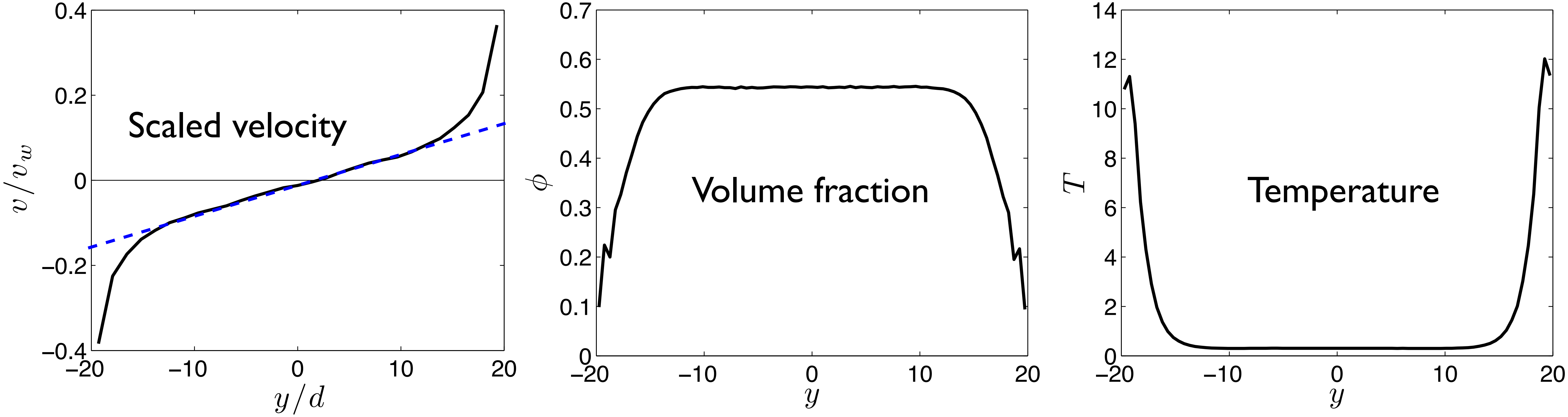
Boundary vs. core regions

Core region

- comprises the bulk of the flow
- exhibits uniform flow properties
- obeys local, inertial-number rheological models[*][†]

Boundary layer

- lies within ~10d of each wall
- exhibits large variations in field variables
- due to nonlocal conduction of pseudothermal energy



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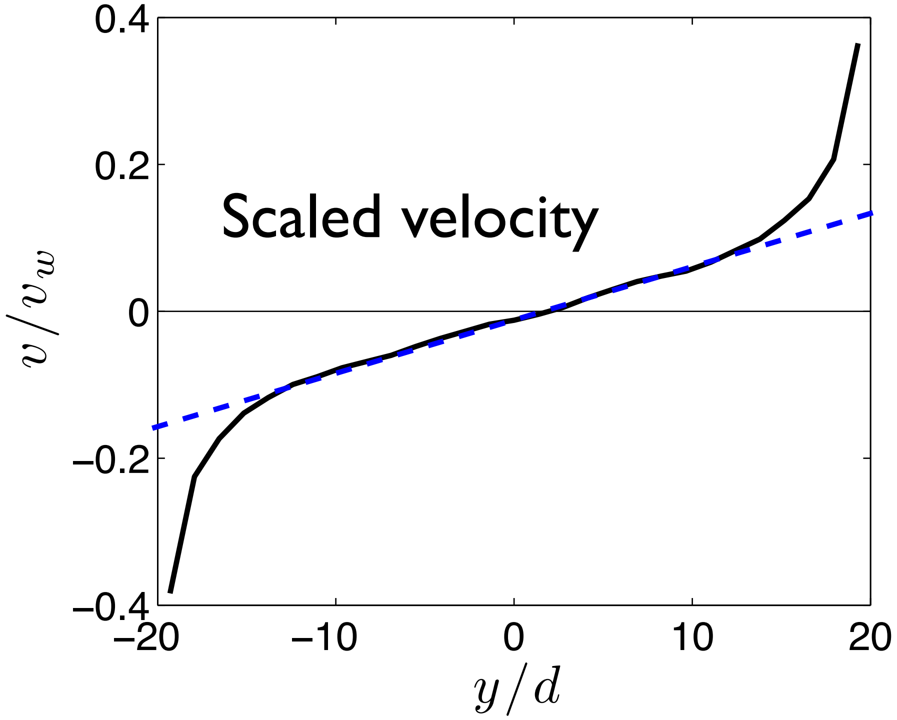
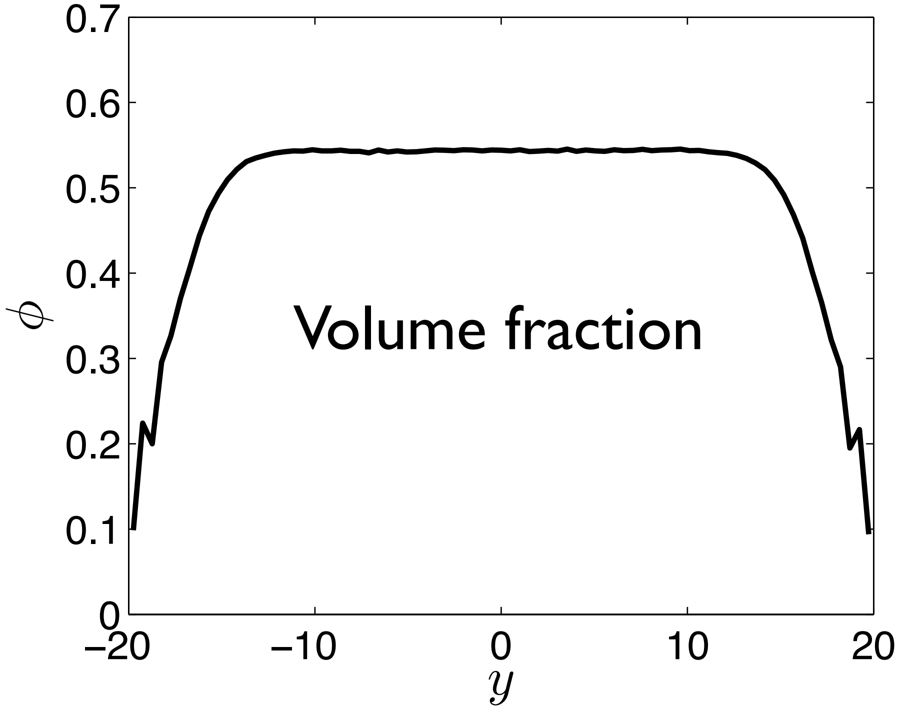
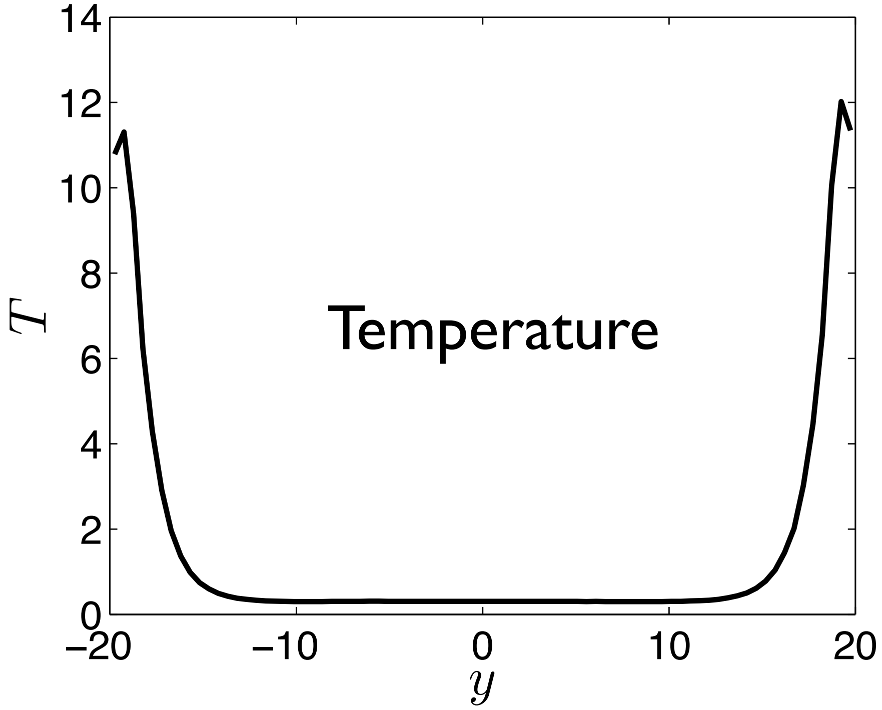
Questions:

- How to define the slip velocity to get simple scaling to work?
- What if we want to avoid the need to resolve the small boundary layer?







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Core rheology

Core region

- comprises the bulk of the flow
- exhibits uniform flow properties
- obeys local, inertial-number rheological models[*†]
  - interparticle friction coefficient μ affects yield stress ratio η_s
  - wall friction coefficient μ_w has no effect on rheological model

Inertial number:

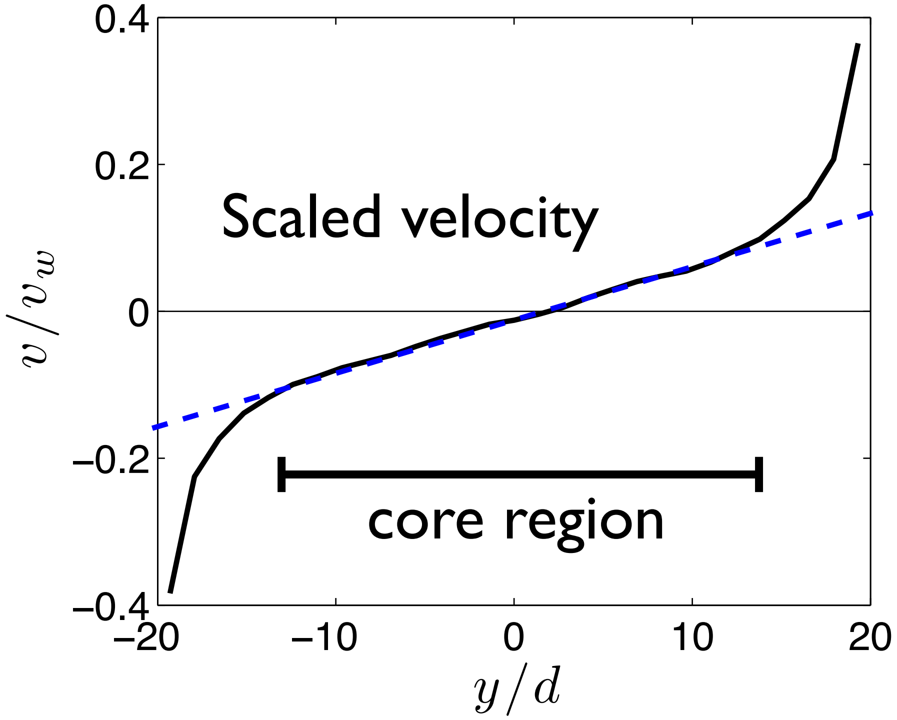
$$I_{\text{core}} \equiv \frac{\dot{\gamma}_{\text{core}} d}{\sqrt{p_{\text{core}}/\rho_s}}$$

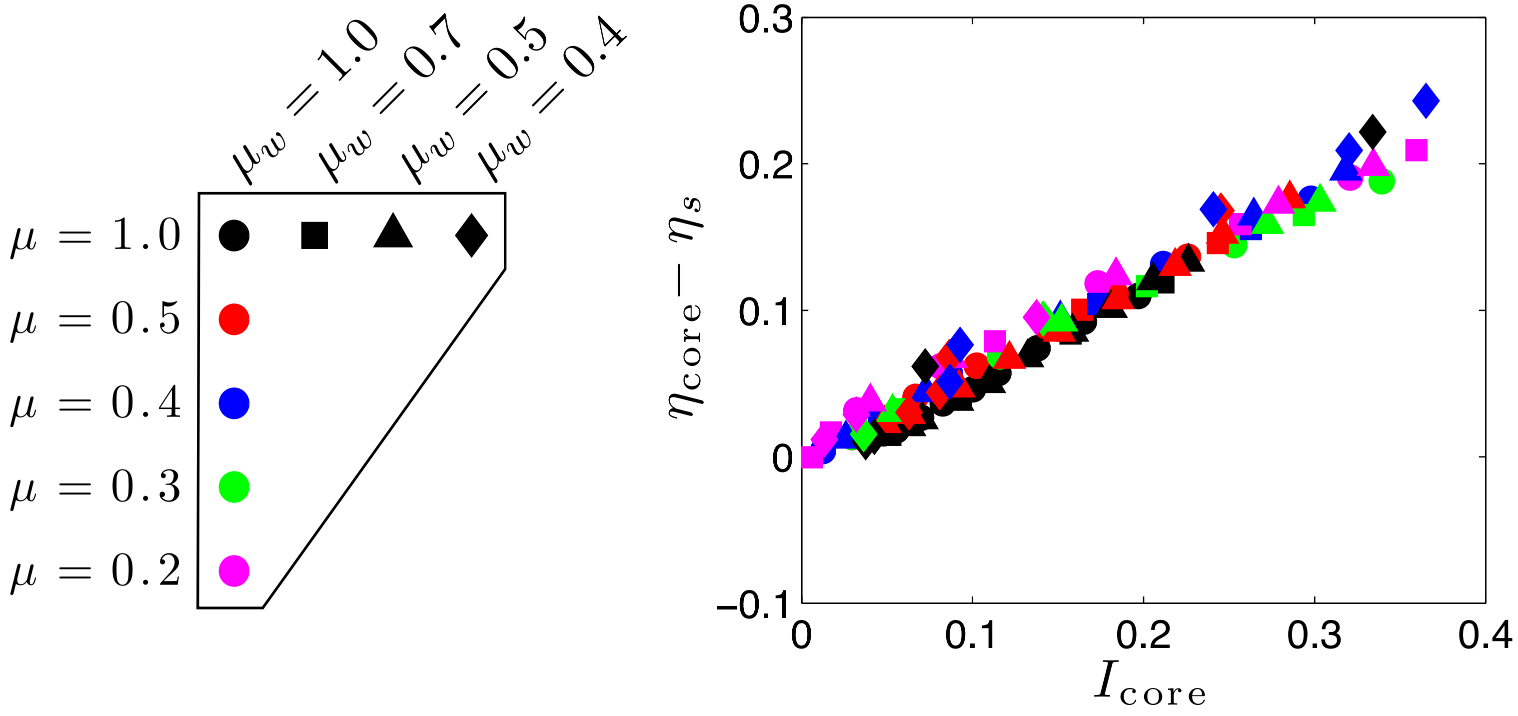
$$I_{\text{core}} \approx f(\phi) \text{ for } \phi < \phi_c(\mu)$$

Shear stress ratio:

$$\eta_{\text{core}} \equiv \frac{\tau_{\text{core}}}{p_{\text{core}}}$$

$$\eta_{\text{core}} = \eta_s(\mu) + \alpha I_{\text{core}}$$





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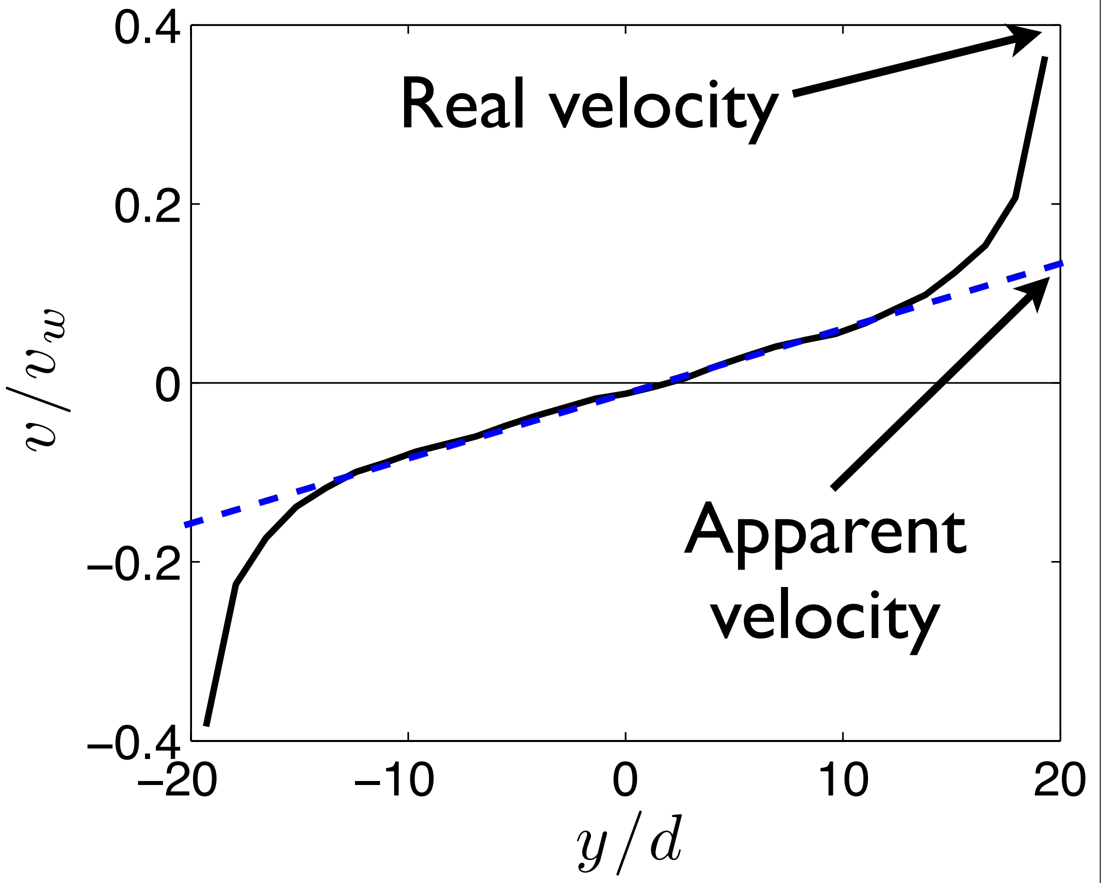
Definitions of slip velocity

- Slip velocity: $v^{(\cdot)}_{\text{slip}} = v^{(\cdot)} - v_w$

Some solids velocity at the wall

Velocity of wall



- Options for velocity $v^{(\cdot)}$:

a) 'Standard' slip velocity: based on translational velocity of particles at wall

$$v^{\text{tr}}_{\text{slip}} = v^{\text{tr}} - v_w$$

b) 'Apparent' slip velocity: based on extrapolated velocity from core region to wall

$$v^{\text{app}}_{\text{slip}} = v^{\text{app}} - v_w$$

$$v^{\text{app}} \equiv \dot{\gamma}_{\text{core}} H/2$$

$$= v^{\text{tr}} - v'$$

Definitions of slip velocity

- Slip velocity: $v_{\text{slip}}^{(\cdot)} = v^{(\cdot)} - v_w$

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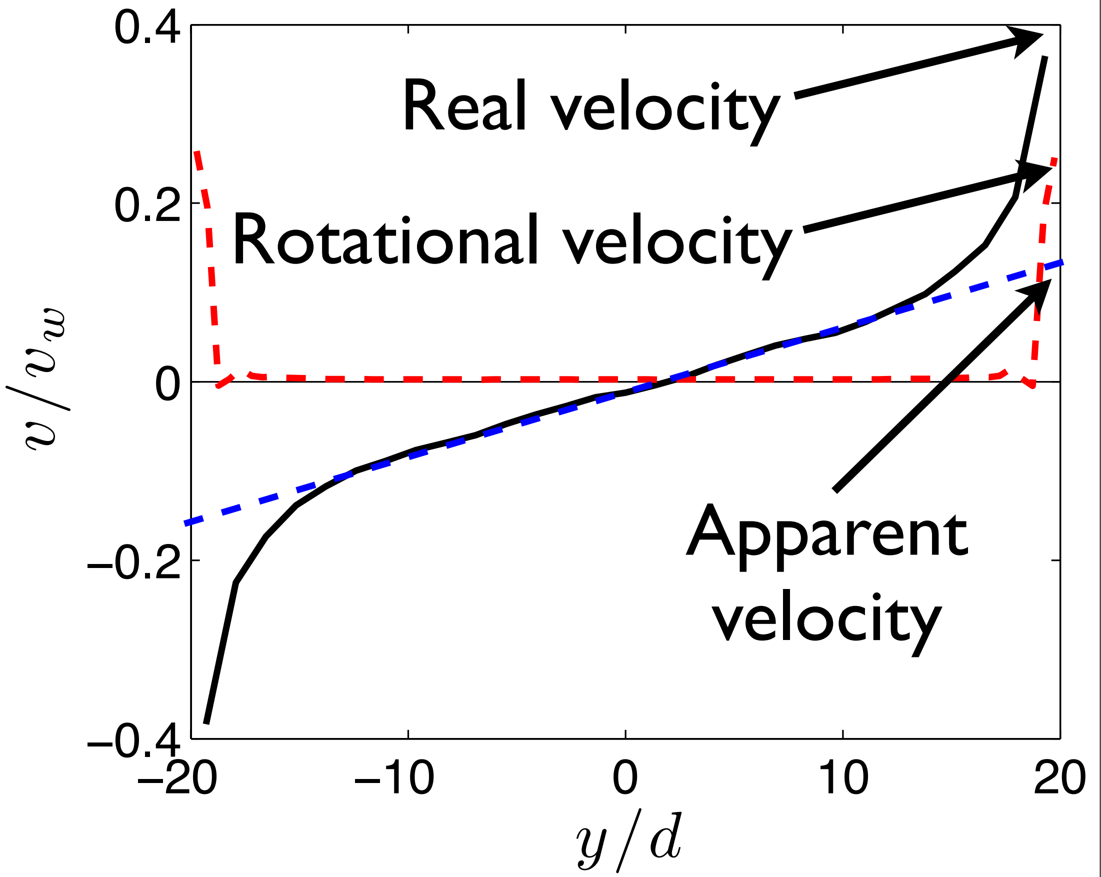
Velocity of wall

- Options for velocity $v^{(\cdot)}$:

  c) 'Surface' slip velocity: based on relative velocity of particle surface at wall

$$v_{\text{slip}}^{\text{surf}} = v^{\text{surf}} - v_w$$

$$v^{\text{surf}} = v^{\text{tr}} \pm \omega d/2$$



Definitions of slip velocity

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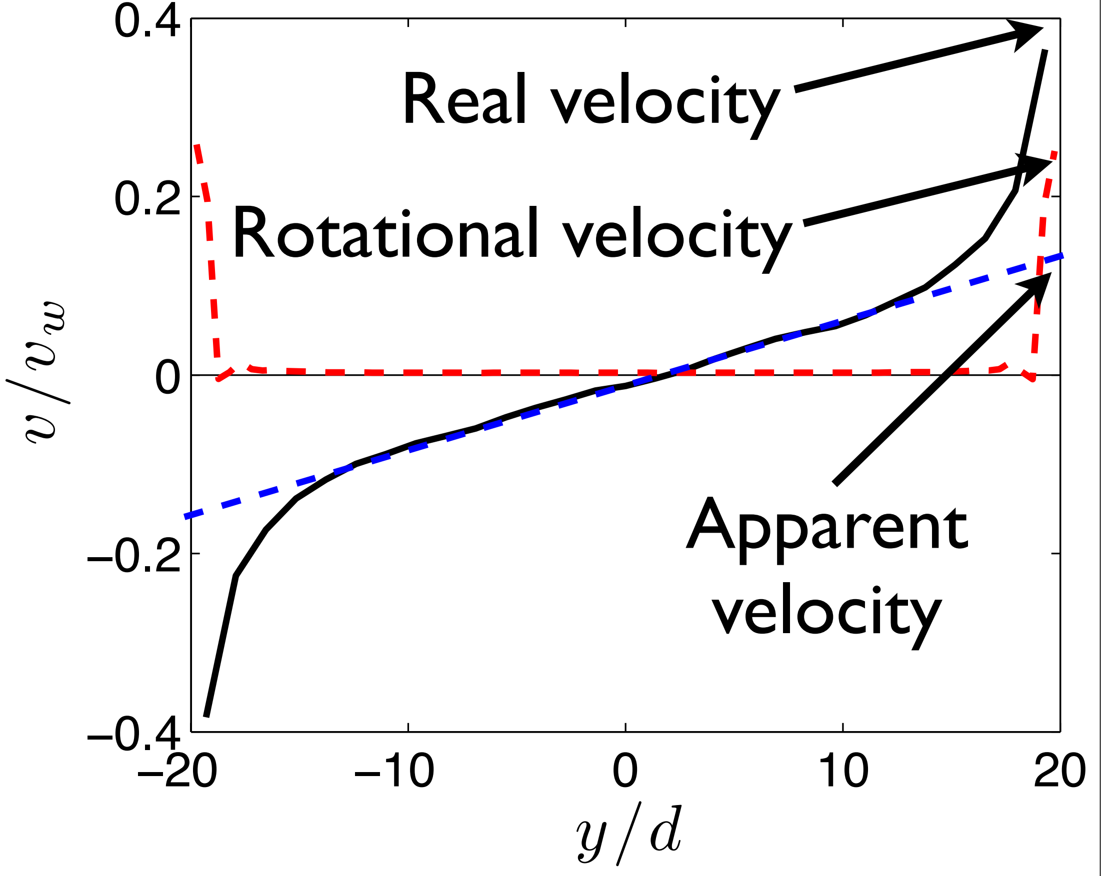
$$v_{\text{slip}}^{(\cdot)} = \underset{\substack{\uparrow \\ \text{Some solids velocity} \\ \text{at the wall}}}{v^{(\cdot)}} - \underset{\substack{\nwarrow \\ \text{Velocity} \\ \text{of wall}}}{v_w}$$



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$$v_{\text{slip}}^{\text{surf}} = v^{\text{surf}} - v_w$$

$$v^{\text{surf}} = v^{\text{tr}} \pm \omega d/2$$

Question:

- Is one (or more) of these slip velocities amenable to a scaling collapse?

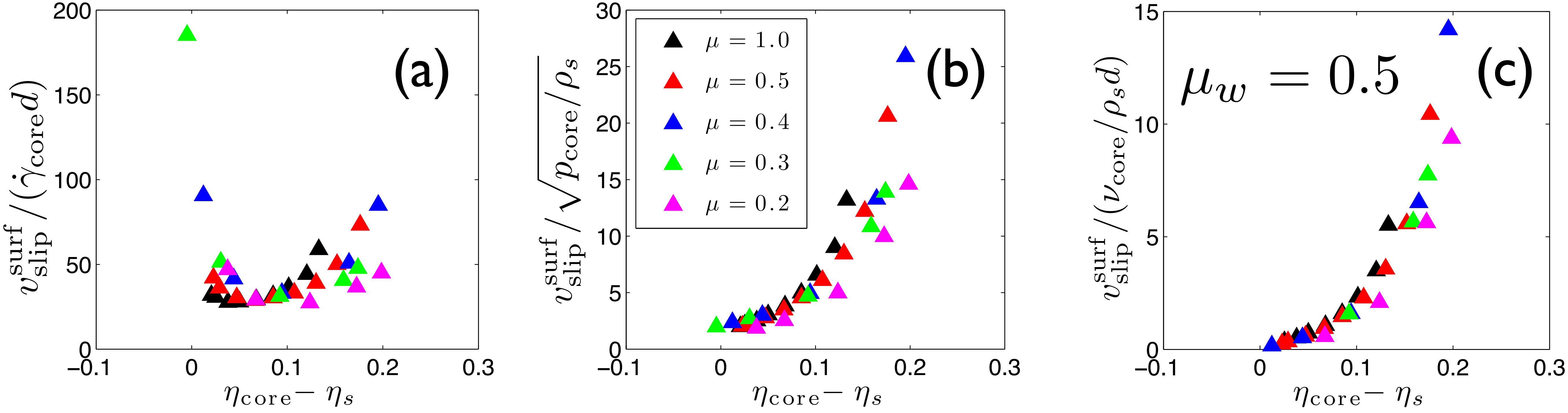
Velocity scales

- Dimensionless slip velocity: $I_{\mathrm{slip}}^{(\cdot)} = \dfrac{v_{\mathrm{slip}}^{(\cdot)}}{v_{\mathrm{char}}}$ ← Some slip velocity ← Some characteristic velocity in the core
- Options for v_{char}:

a) shear-rate-based†: $v_{\mathrm{char}} = \dot{\gamma} d$

b) stress-based*: $v_{\mathrm{char}} = \sqrt{p/\rho_s}$ or $\sqrt{\tau/\rho_s}$

c) viscosity-based: $v_{\mathrm{char}} = \nu/\rho_s d = \tau/\rho_s \dot{\gamma} d$



†**Artoni et al. PRL 108, 238002 (2012).**

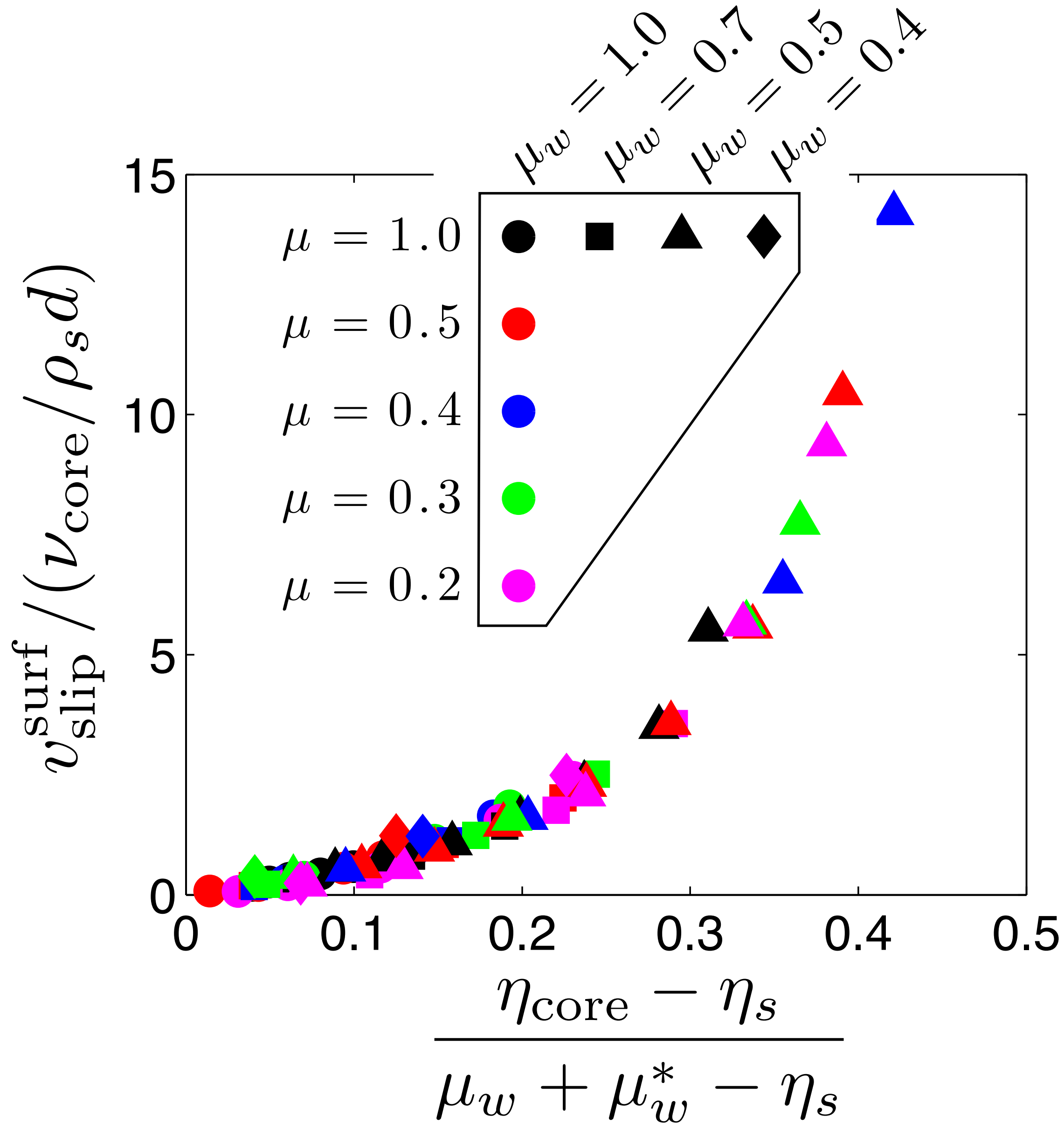
***Artoni et al. PRE 79, 031304 (2009).**

DEM results: dimensionless slip velocity

- Full collapse achieved by scaling of $\eta_{\text{core}} - \eta_s$:
    - $\eta_{\text{wall}} = \mu_w + \mu_w^*$
    - Critical wall friction coefficient $\mu_w^* \approx 0.33$ separates partial- and full-slip regimes[†]
- Possible model form:

$$y = \frac{1.5x^{2/3}}{(1-x)^5}$$

- This form still requires solving for rotational velocity and boundary layer



$$\begin{cases} v_{\text{slip}}^{\text{surf}} = v^{\text{surf}} - v_w \\ v^{\text{surf}} = v^{\text{tr}} \pm \omega d/2 \end{cases}$$

[†] Z. Shojaaee et al. PRE 86, 011302 (2012).

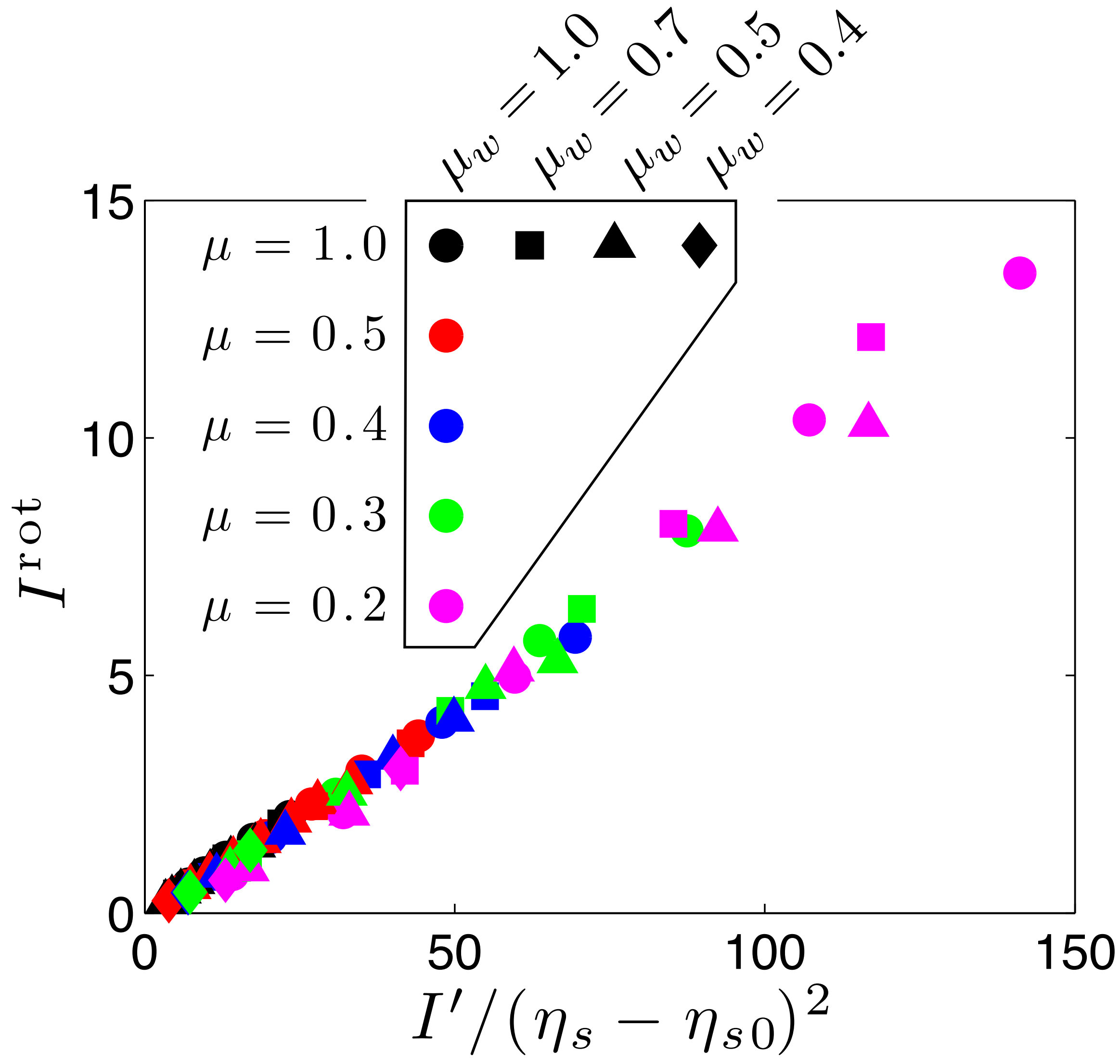
DEM results: dimensionless slip velocity

- Extend $v_{\text{slip}}^{\text{surf}}$ model to coarsely-resolved, translation-only problems

$$I_{\text{slip}}^{\text{app}} = \underbrace{I_{\text{slip}}^{\text{surf}}}_{\text{from last slide}} + \underbrace{I^{\text{rot}} + I'}_{\text{fitted below}}$$

$$I^{\text{rot}} = \frac{mI'}{(\eta_s - \eta_{s0})^2}$$ (see figure)

$$I' = \alpha(\eta - \eta_s)^\beta$$



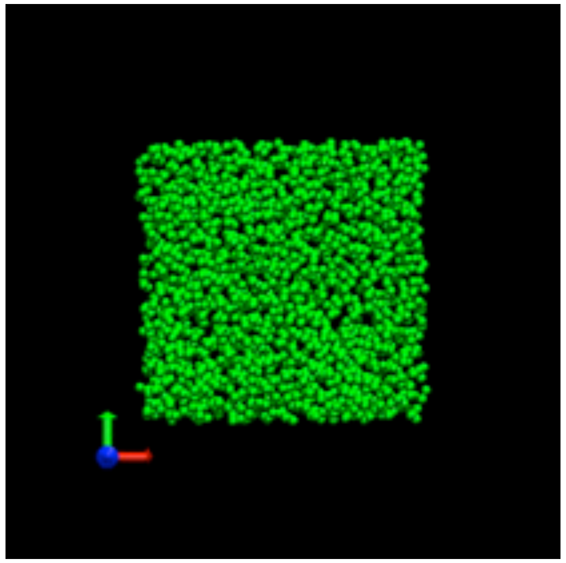
$$\eta_{s0} = \eta_s(\mu = 0) = 0.105$$

- Model can be coupled with simple rheological models (e.g. inertial-number models)

Dense phase rheology: Summary

- Flow regime map: What regimes of flow are observed in shear flow of soft, frictional, non-cohesive particles? (completed)
- Effect of cohesion: How does the addition of modest level of cohesion, such as in Geldart Group A particles change the flow regime map? (work nearly complete, manuscript under revision)
- Rheological models (non-cohesive particles)
  - Steady state models that bridge various regimes (completed)
    S. Chialvo et al. PRE 85, 021305 (2012).
  - Modified kinetic theory (completed)
    S. Chialvo & S. Sundaresan, Phy. of Fluids, 25, 070603 (2013).
- Wall Boundary conditions (work nearly complete, manuscript under preparation)

Research questions: Looking ahead



- Complete wall boundary condition manuscript (Sebastian Chialvo)
- Implementation of the modified kinetic theory and the wall BCs in a CFD code (such as MFIX) and testing. Will be collaborating with NETL researchers
- Implementation of the steady-shear rheology model in MFIX and testing - already completed

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
- Developed boundary-condition model for dense flows
- Will soon implement MKT and wall BCs into MFIX continuum solver and test