Implementation and Refinement of a Comprehensive Model for Dense Granular Flows

Yile Gu, Ali Ozel, Sebastian Chialvo, and Sankaran Sundaresan
Princeton University

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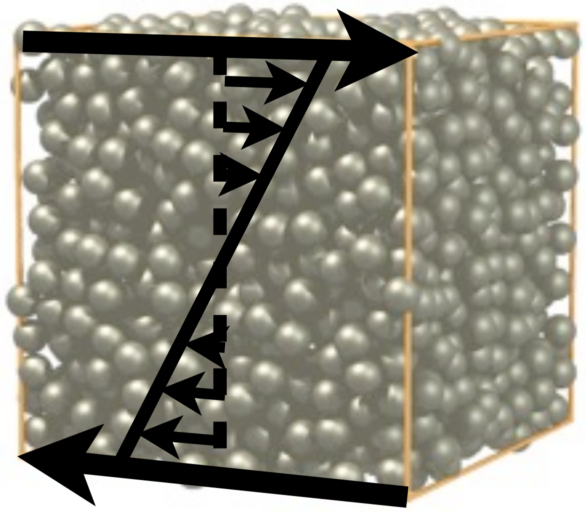

Shear flow of frictional particles in a periodic box

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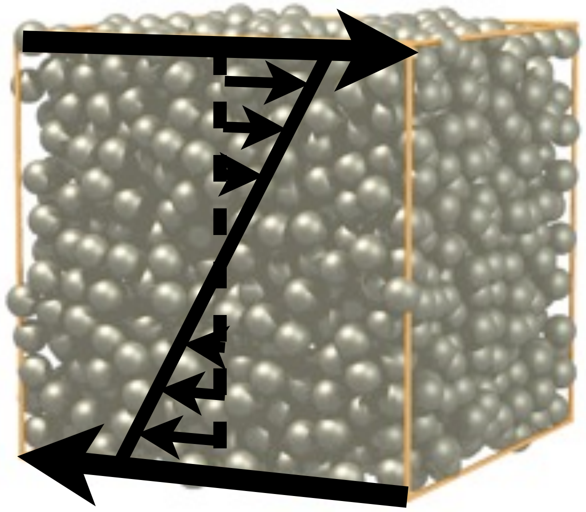

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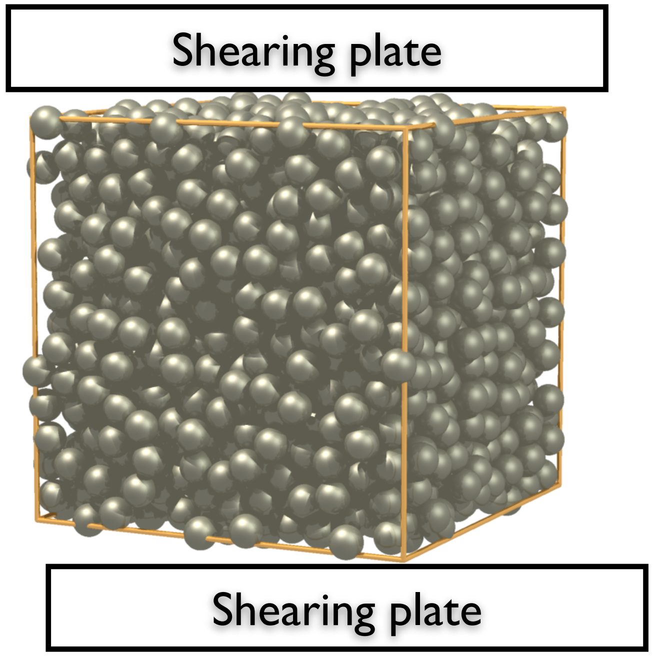
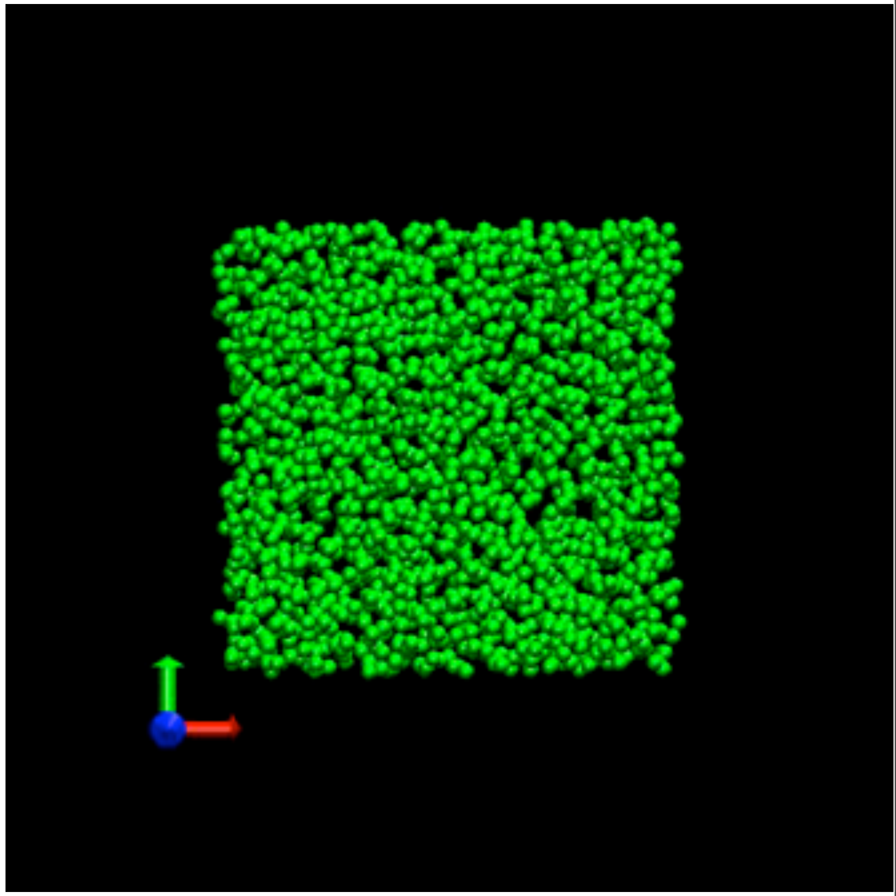


Shear flow of
frictional particles
with bounding walls

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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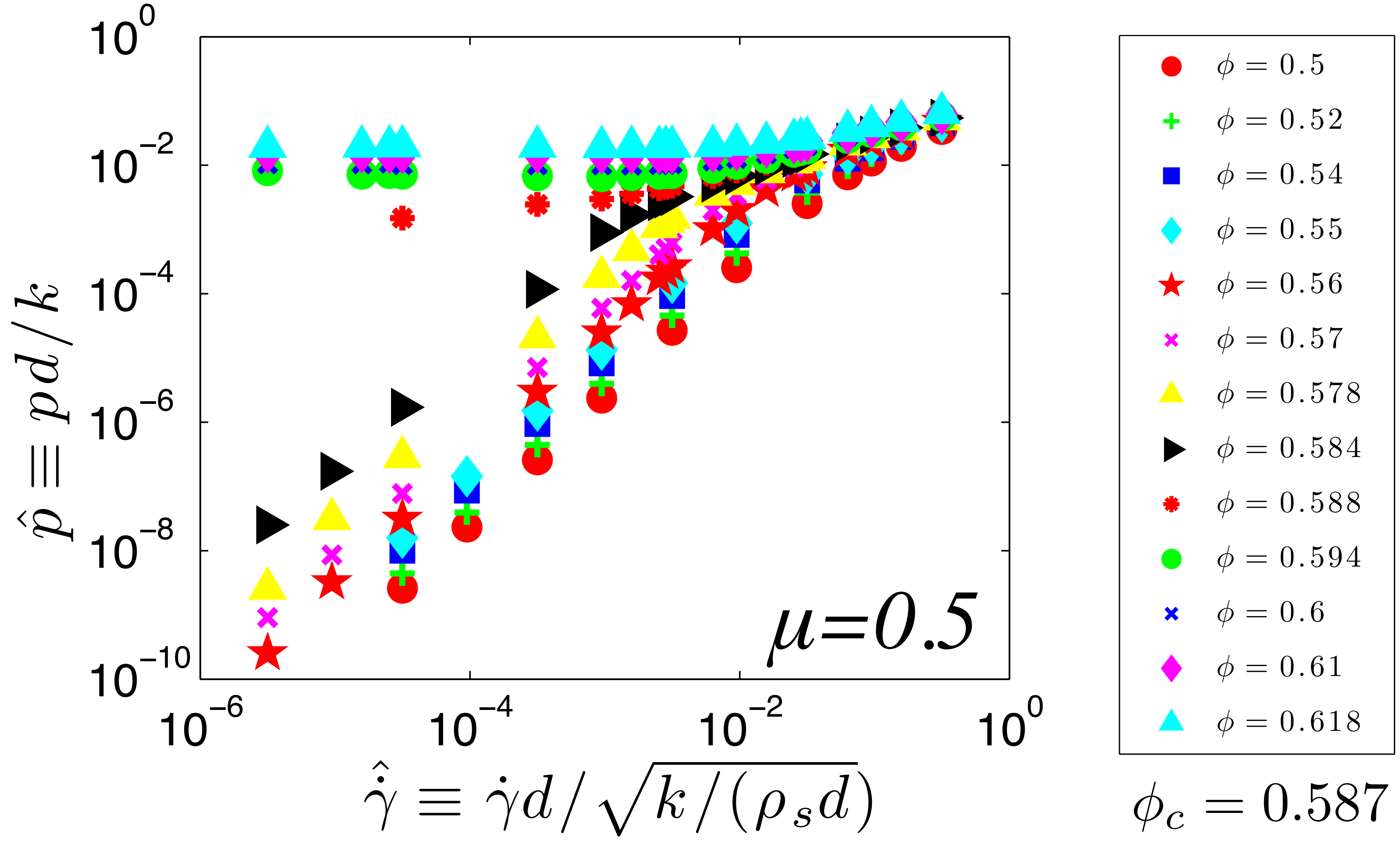
- Implementation of modified kinetic theory in MFIX/ openFOAM

Flow map: Non-cohesive Particles



Previous studies

- Computational
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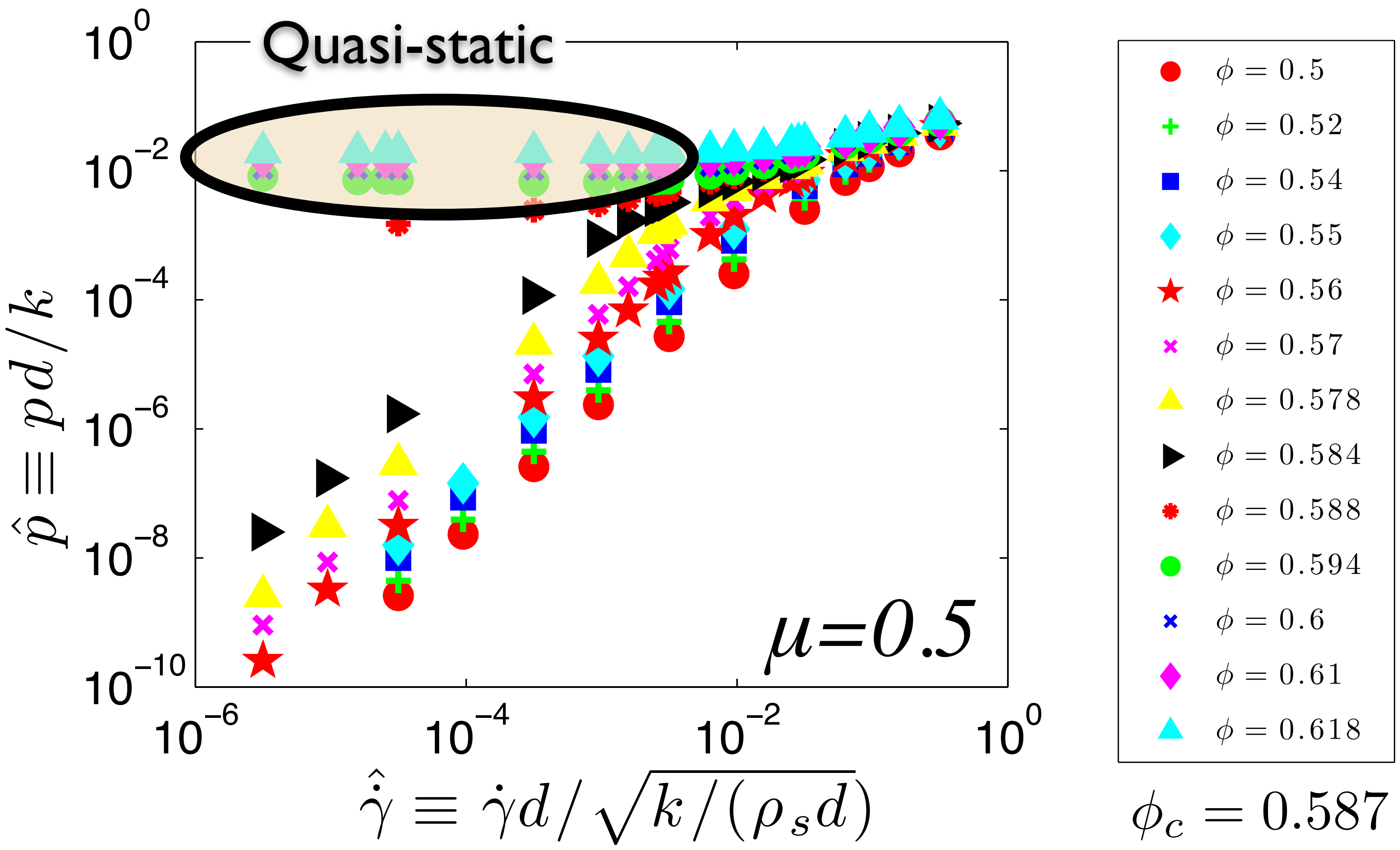

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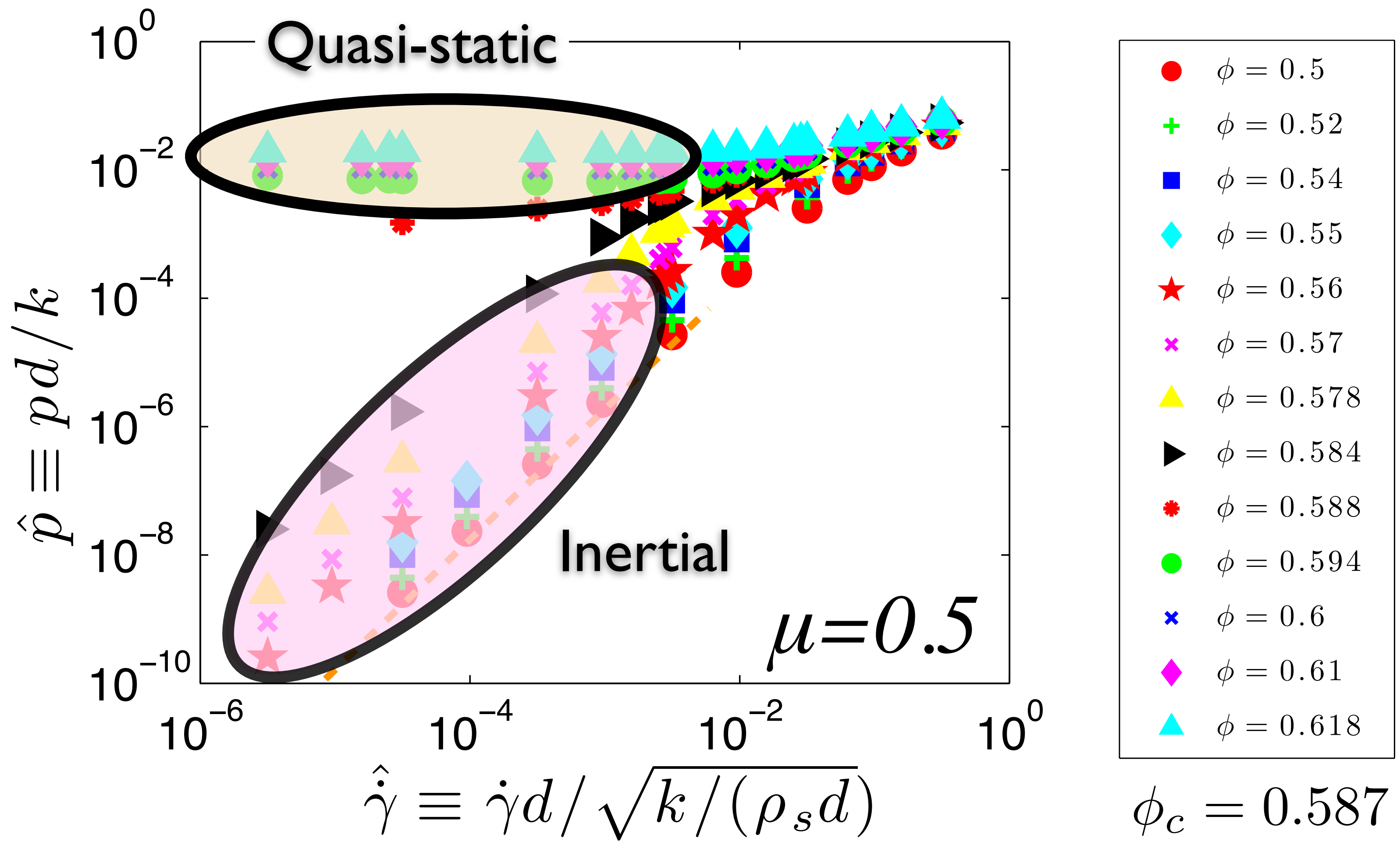

$\phi_c = 0.587$

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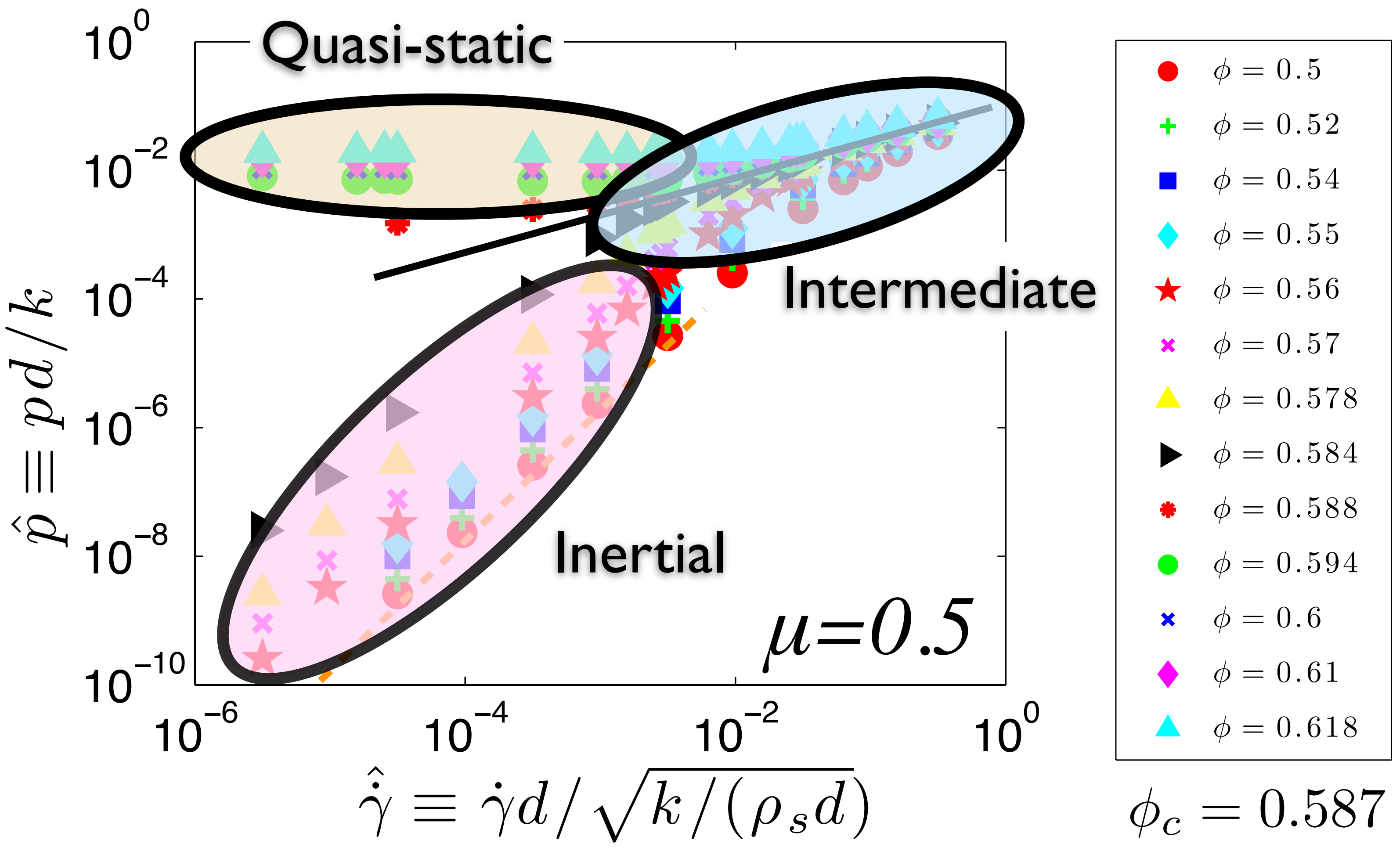

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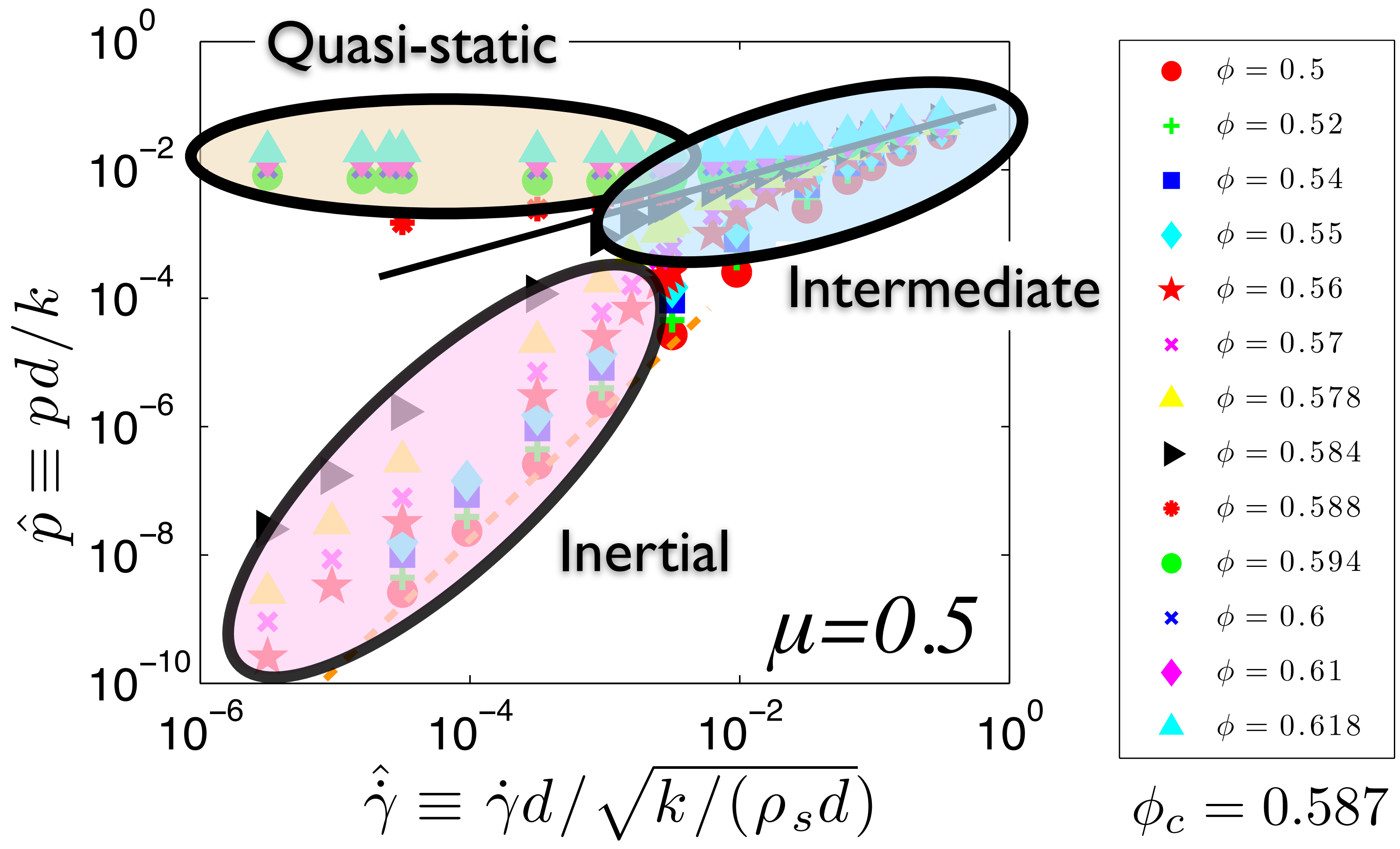

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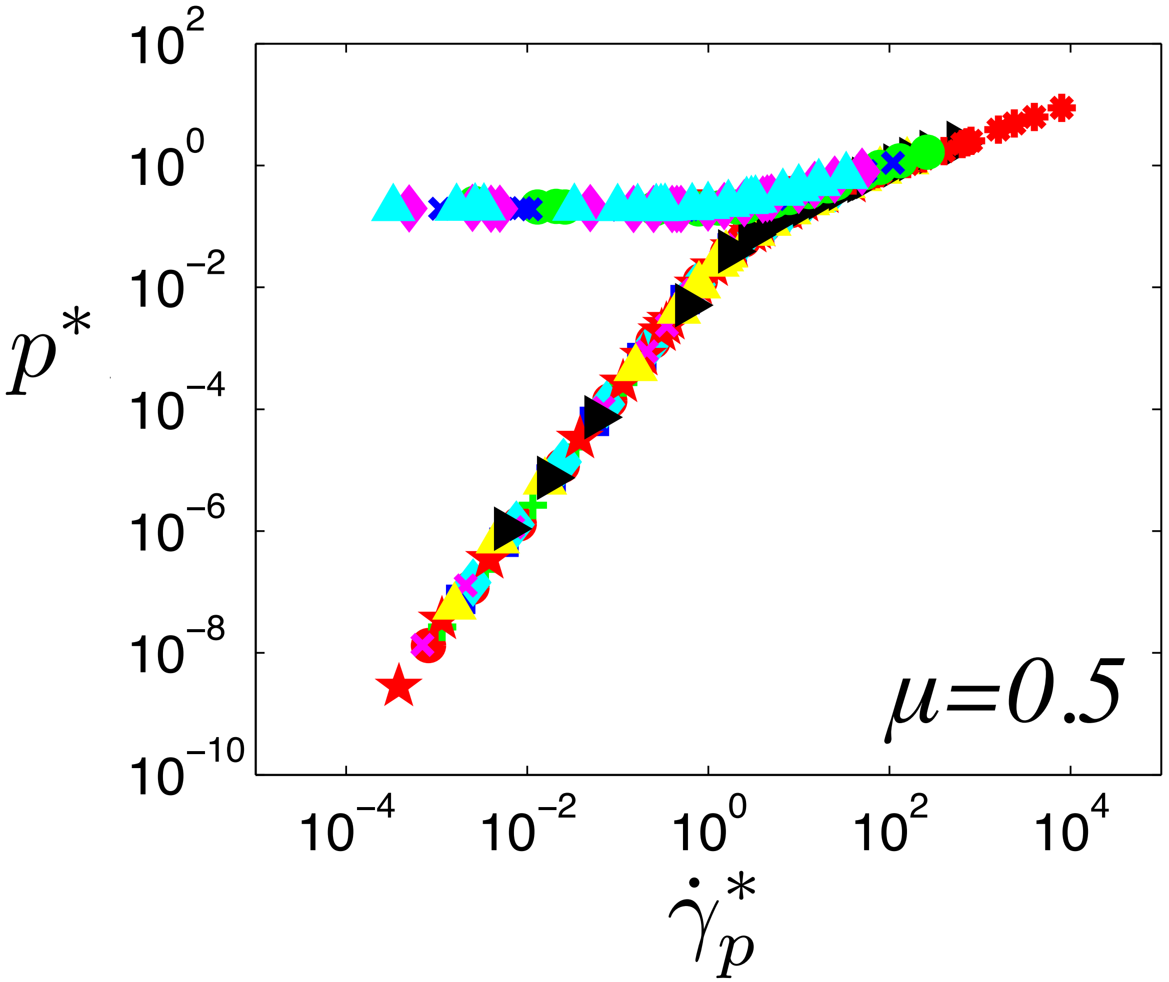
- Critical volume fraction ϕ_c and its flow curve $\hat{p} = \alpha \hat{\dot{\gamma}}^m$ distinguish the three flow regimes.
- Role of particle softness:
  - Large k $\Longrightarrow$ quasi-static or inertial regime
  - Small k $\Longrightarrow$ intermediate regime

Pressure scalings for frictional, non-cohesive particles



Scaled pressure and shear rate[†]:

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

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

Choose exponents:

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

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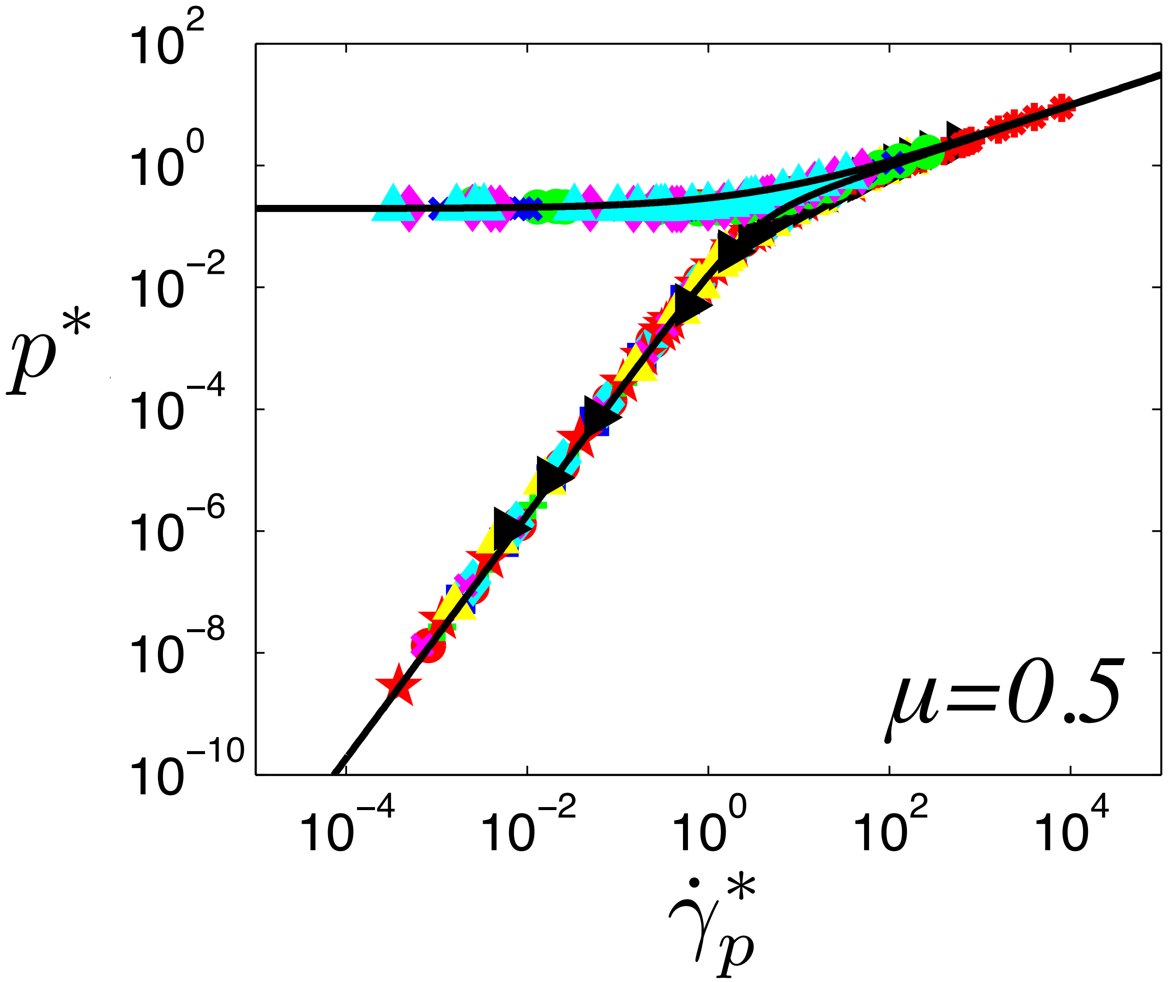

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- Three pressure asymptotes:

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

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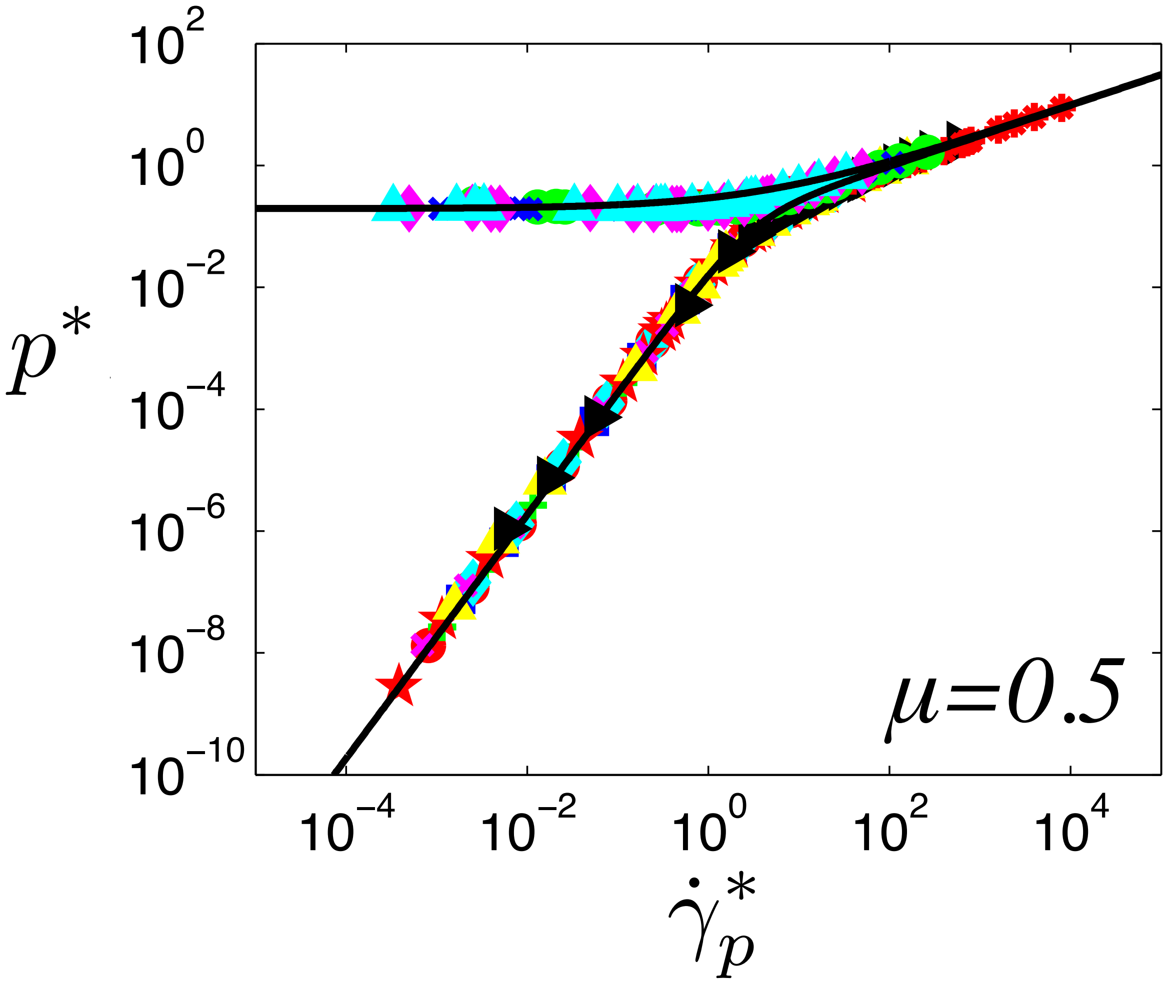

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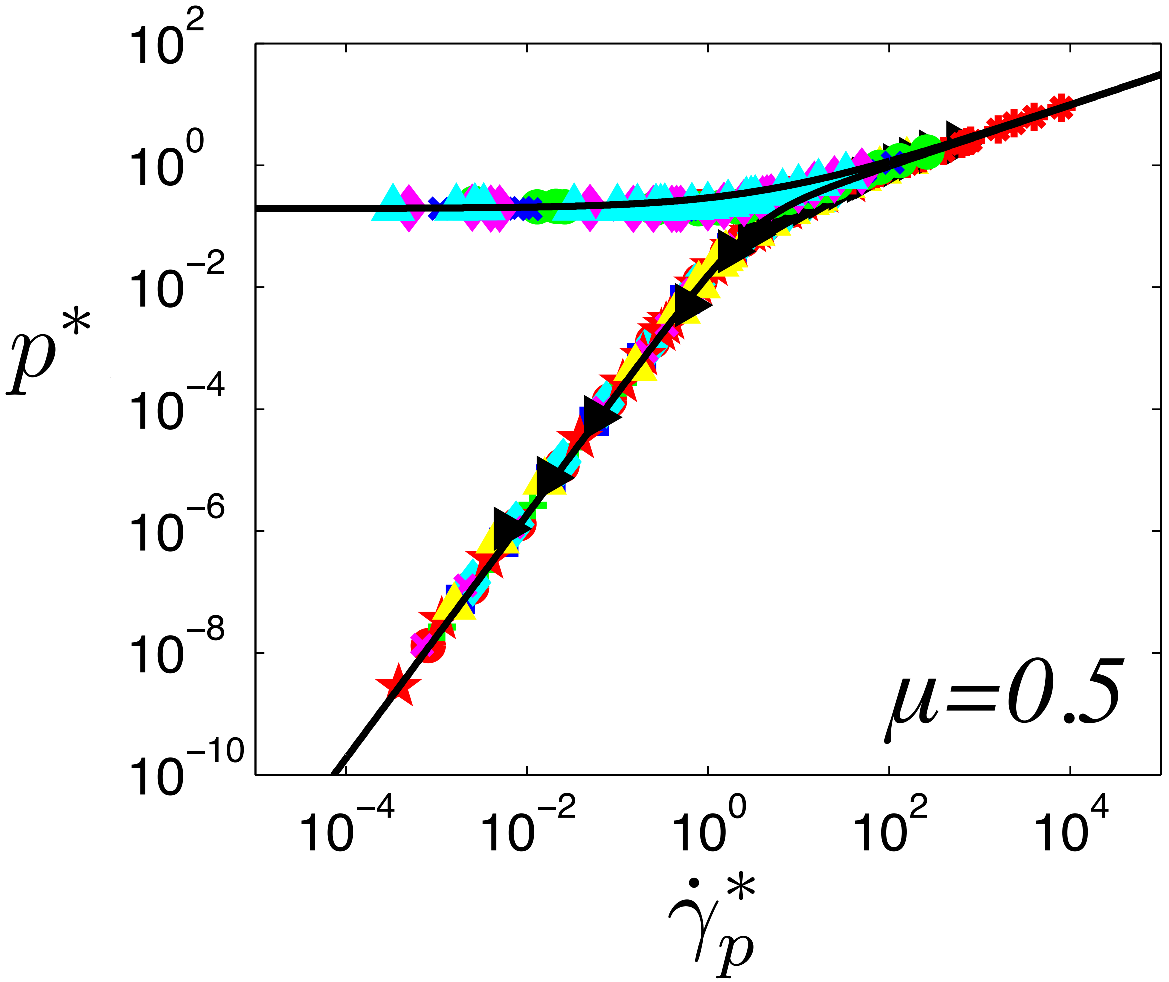

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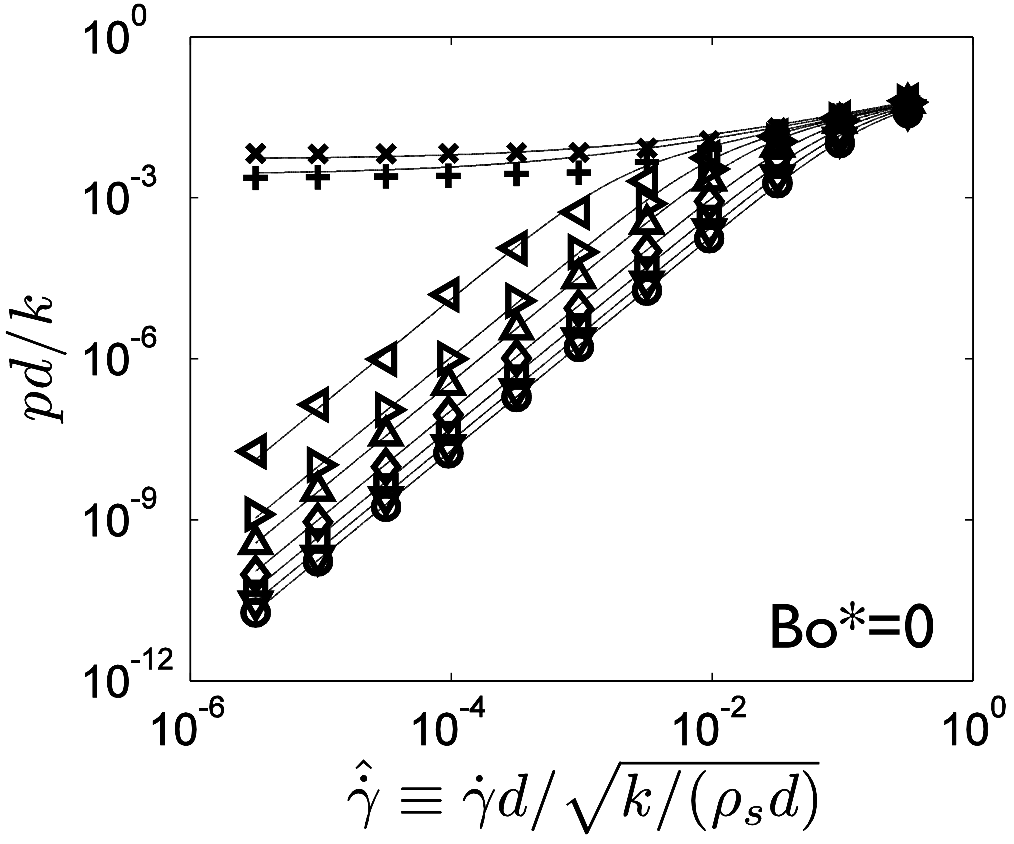
Pressure in frictional, cohesive particles



○ $\phi = 0.51$
▽ $\phi = 0.53$
□ $\phi = 0.55$
◇ $\phi = 0.57$
△ $\phi = 0.59$
▷ $\phi = 0.6$
◁ $\phi = 0.61$
+ $\phi = 0.62$
× $\phi = 0.63$

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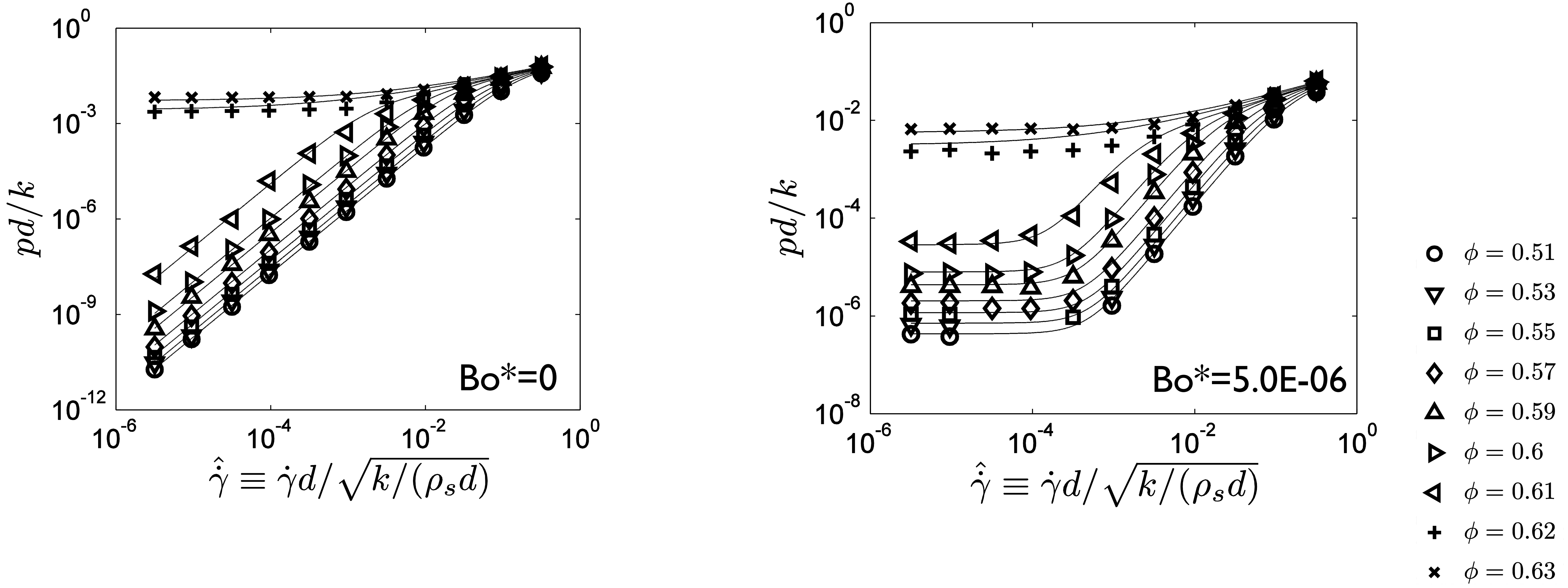

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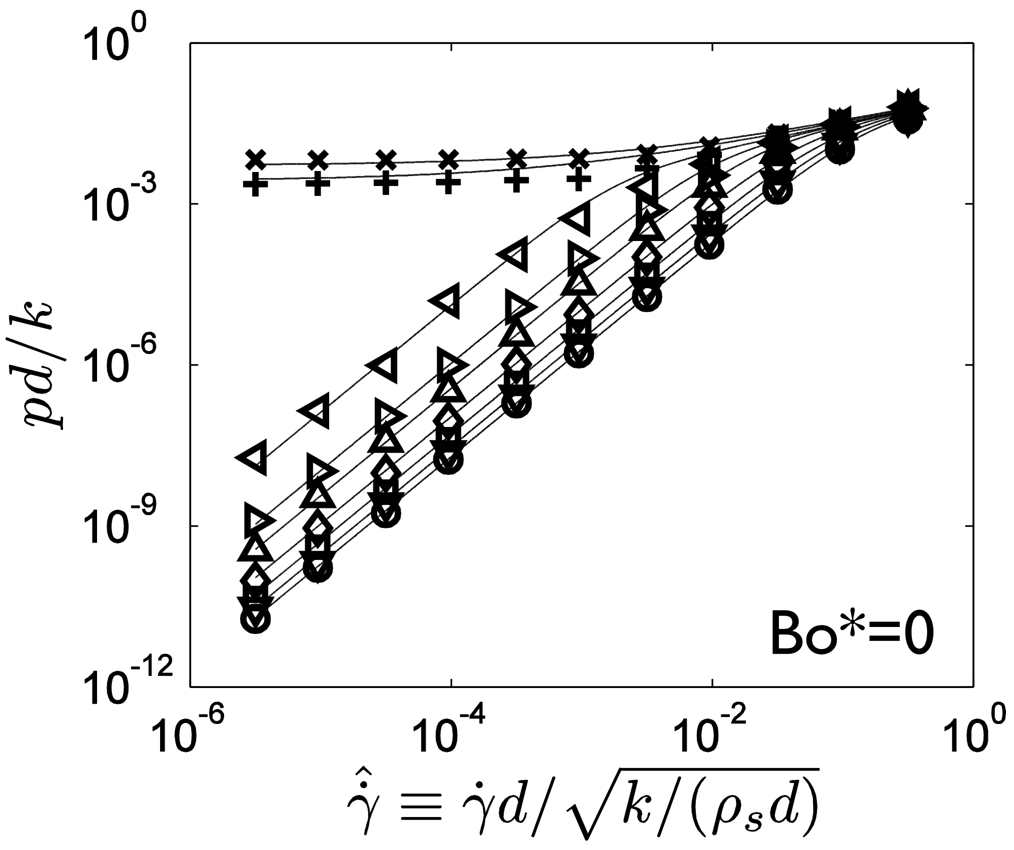

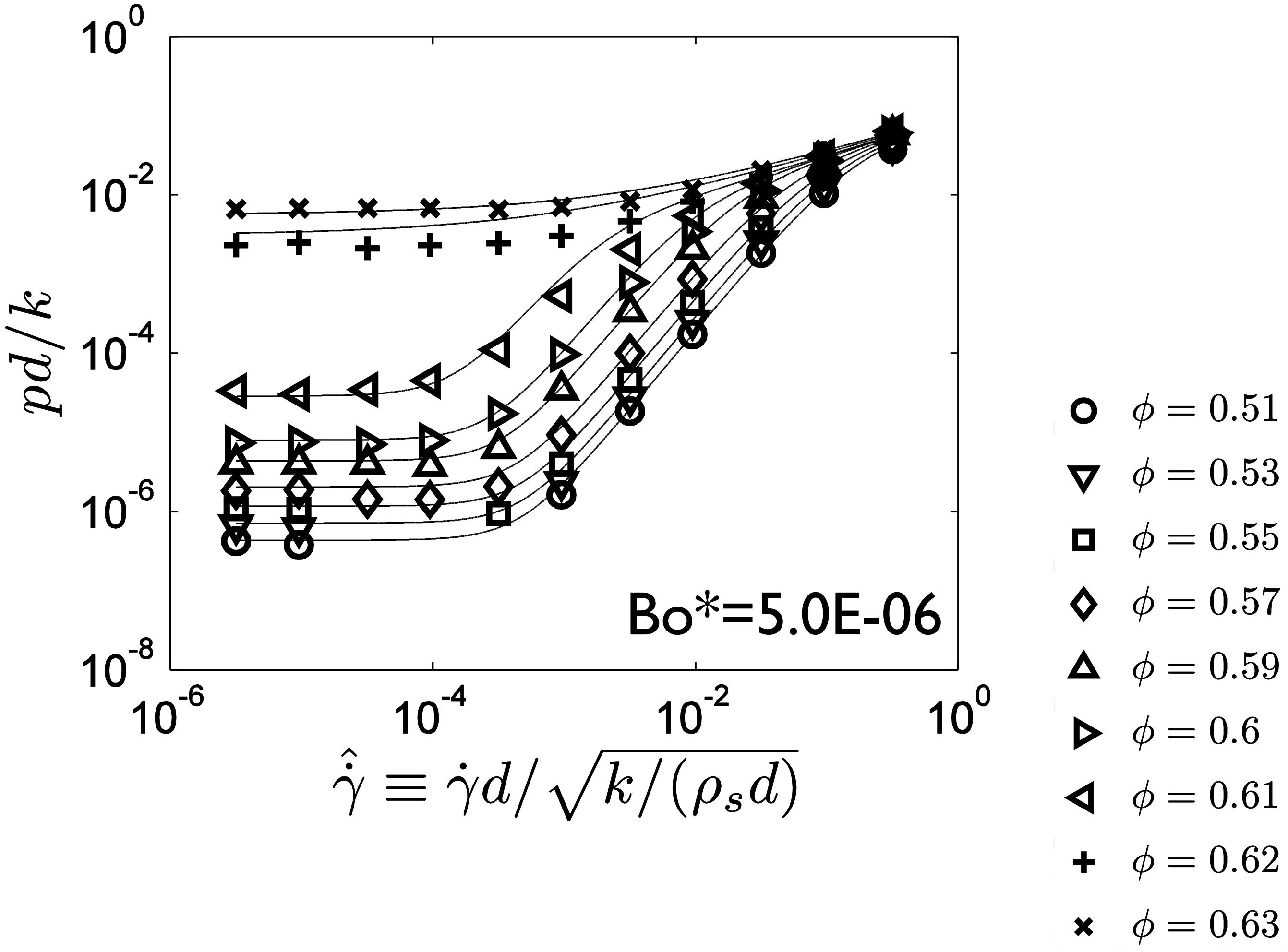

$$Bo^* \equiv F_{vdW}^{\max} / kd \approx A / 24ks_{\min}^2$$

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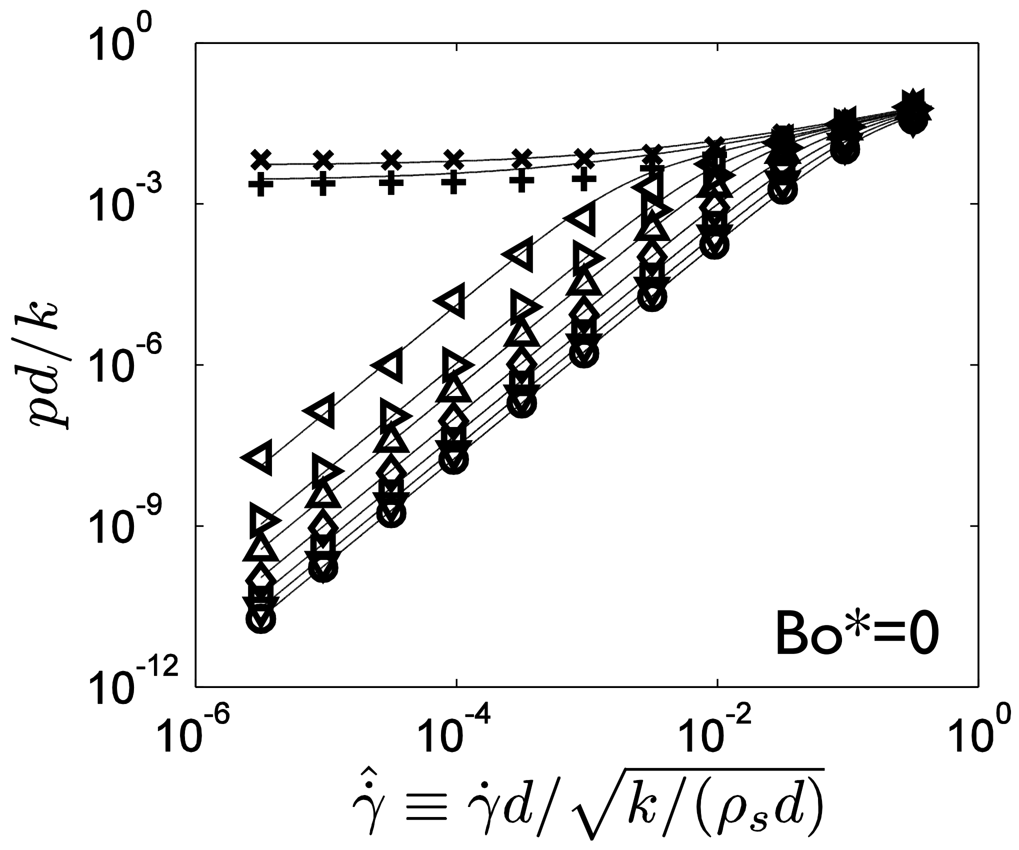

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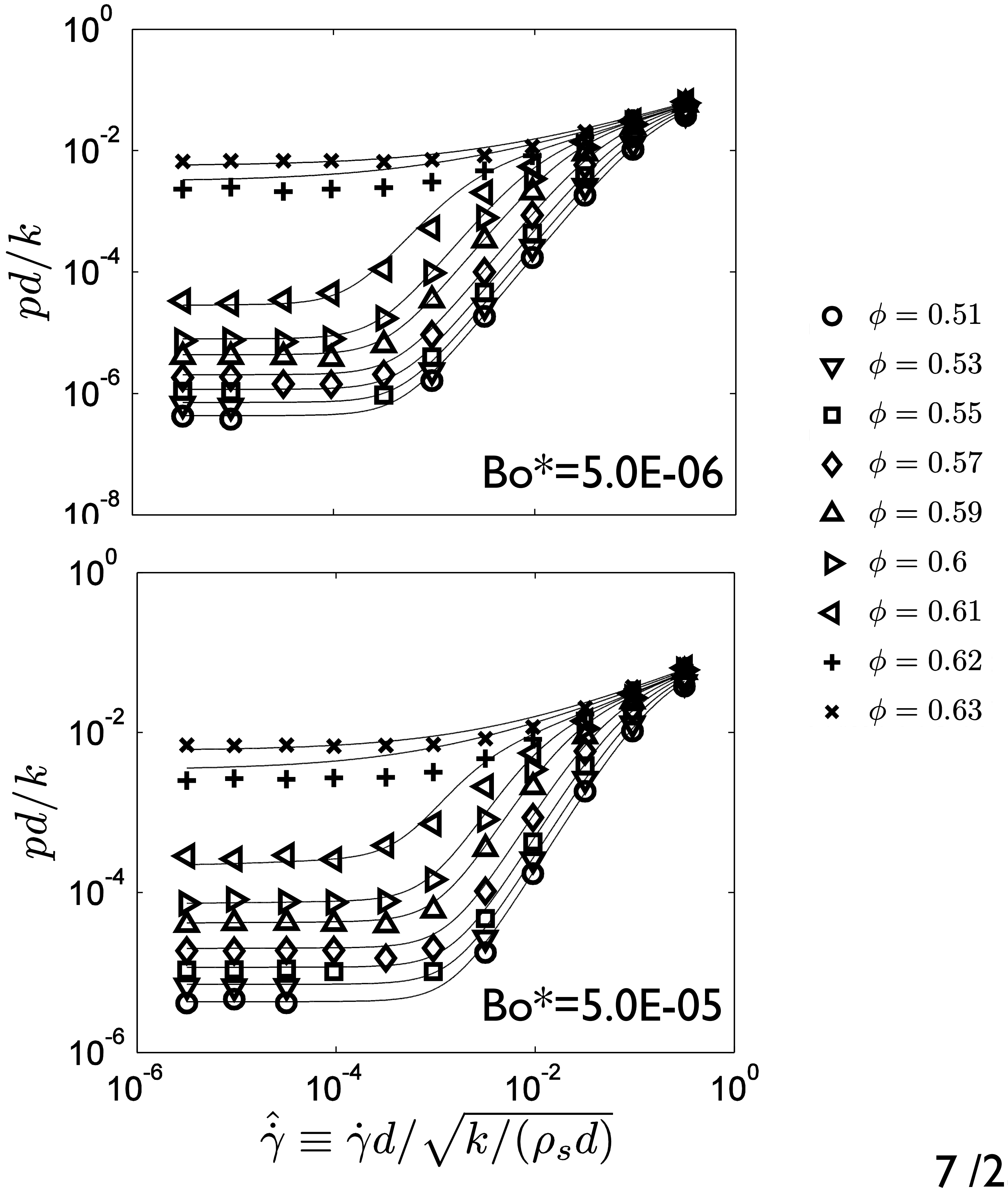

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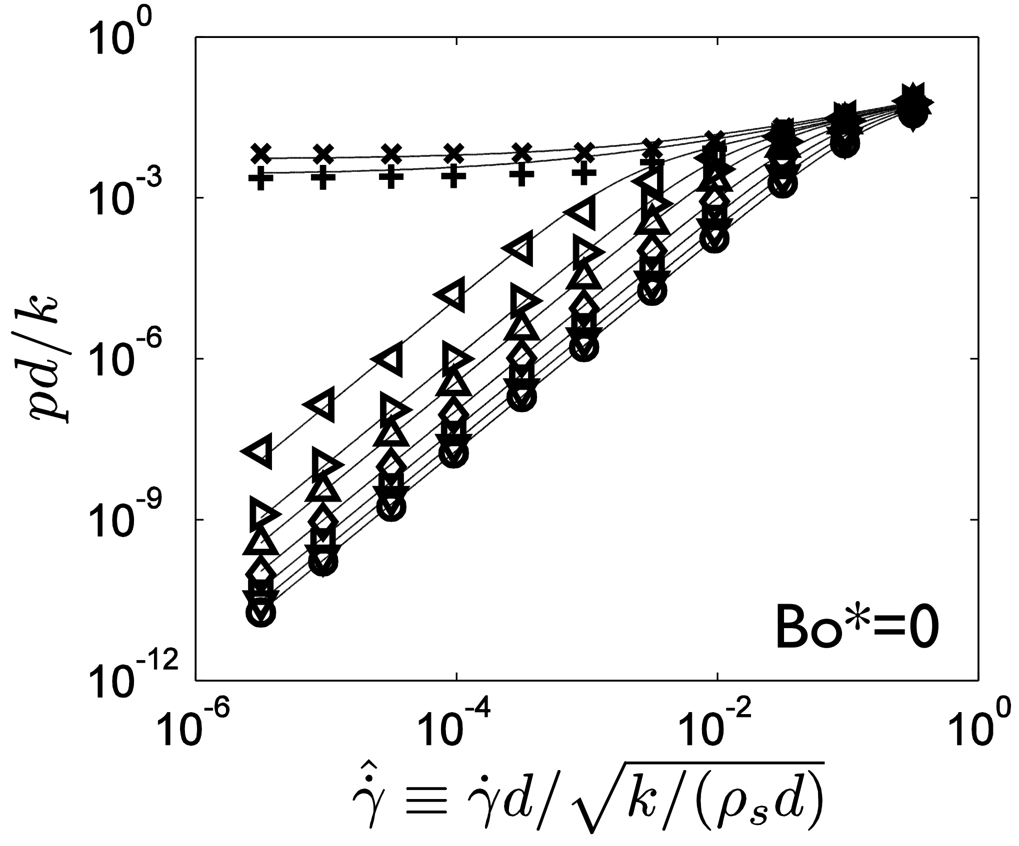

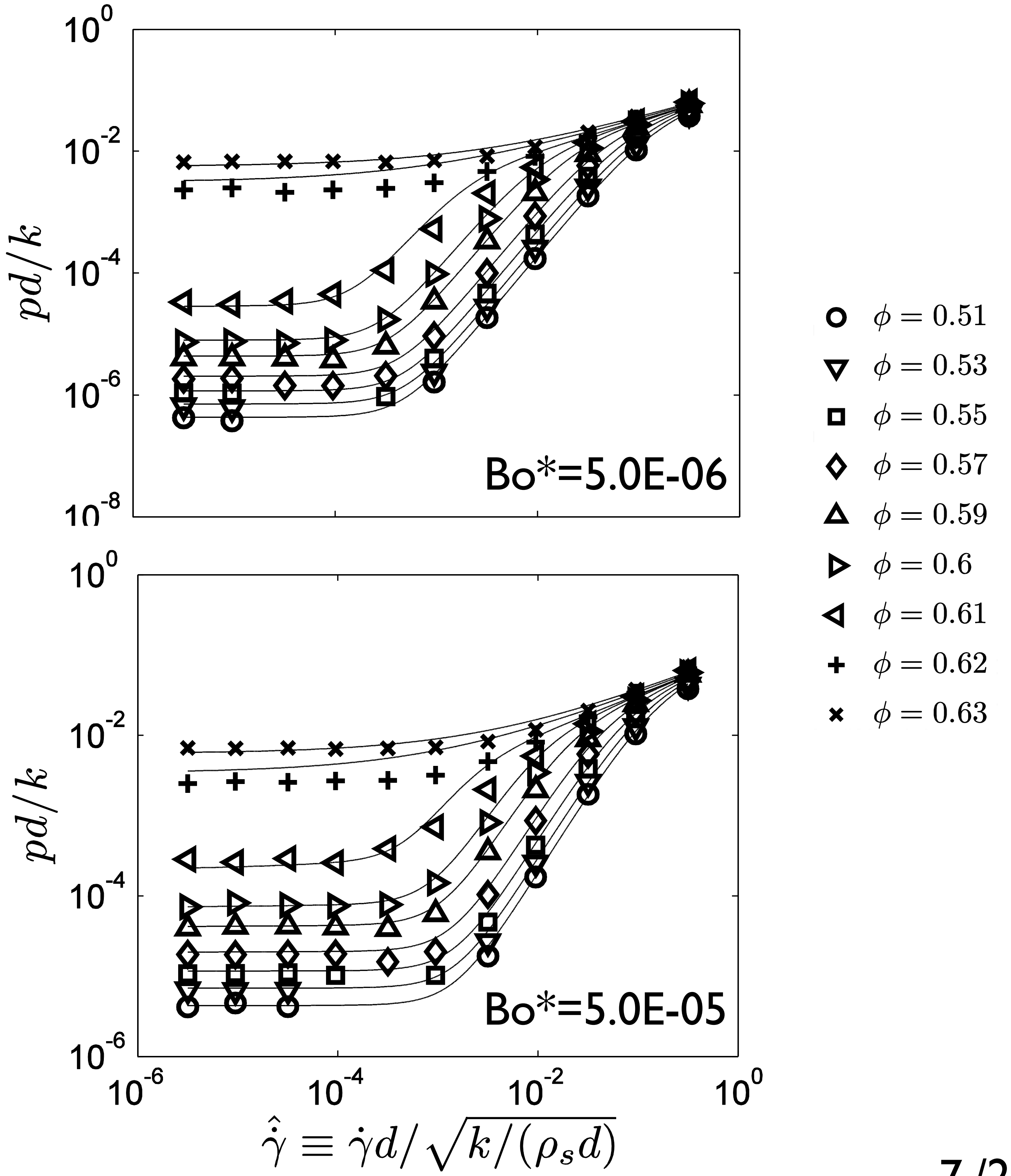

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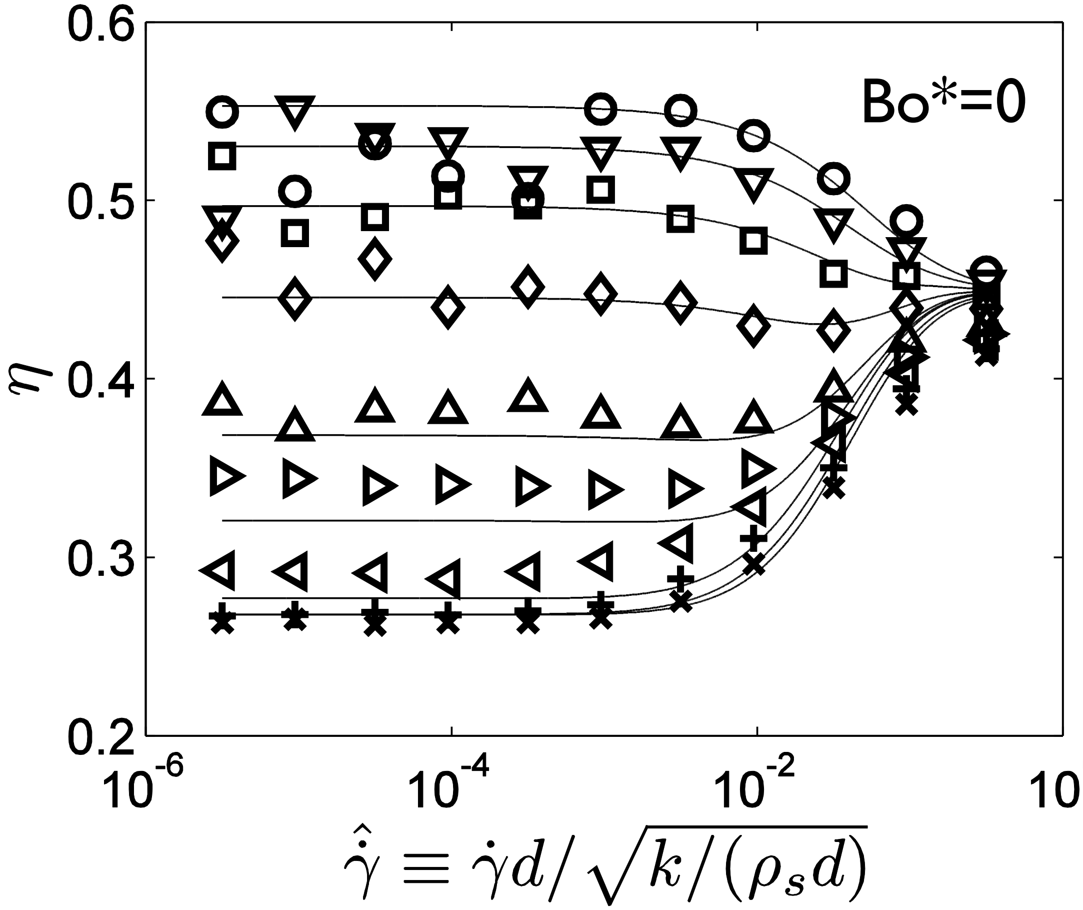
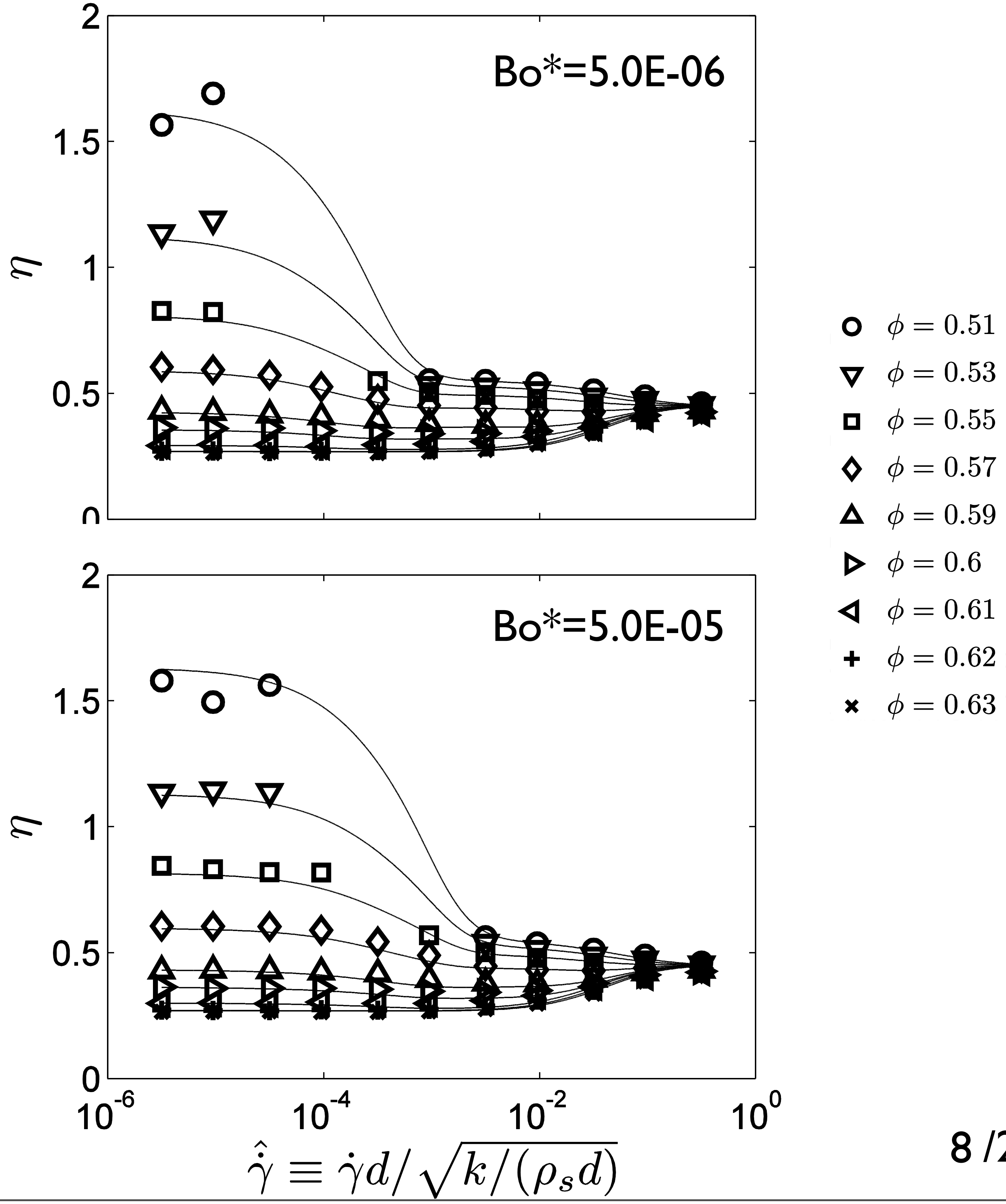
Quasi-static, inertial and intermediate regimes persist. A new cohesive regime emerges below the jamming conditions for equivalent non-cohesive particles.

Cohesive particles: Stress ratio





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

- cohesion increases effective stress ratio

Dense phase rheology: Summary

- Flow regime map: (completed)
- Rheological models
  - Steady state models that bridge various regimes (completed)
  - Modified kinetic theory
- Wall Boundary conditions
- Implementation

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

Y. Gu et al., PRE 90, 032206 (2014).

Kinetic-theory models

- Traditionally use kinetic-theory (KT) models for modeling inertial regime
- Most KT models designed for <u>dilute flows</u> of <u>frictionless particles</u>

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- Can KT model be modified to capture dense-regime scalings?

- Seek modifications to KT model of 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

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

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)

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

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

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

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

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

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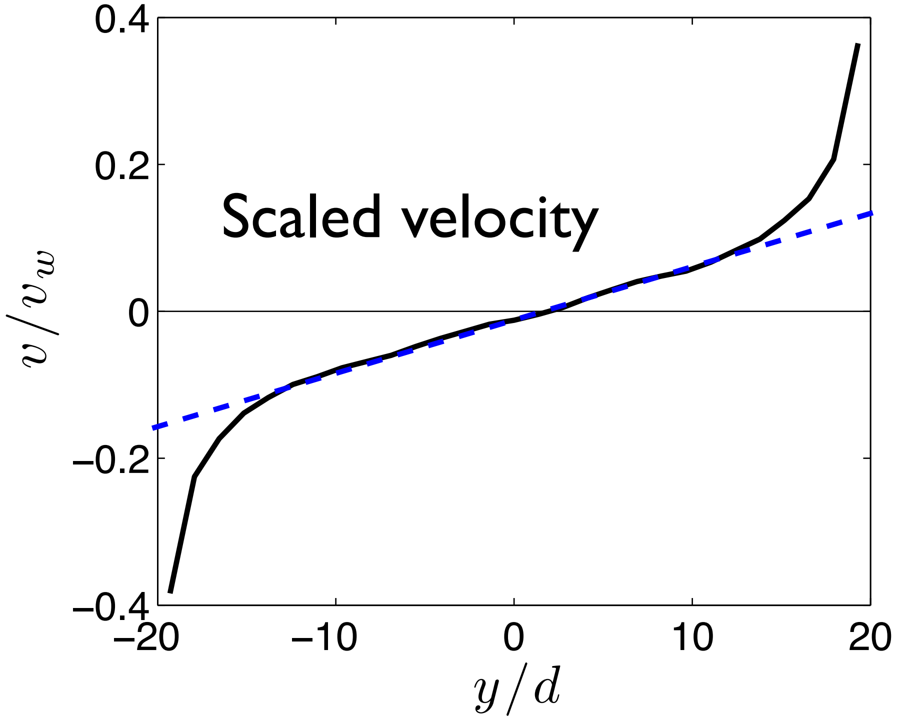
Boundary vs. core regions

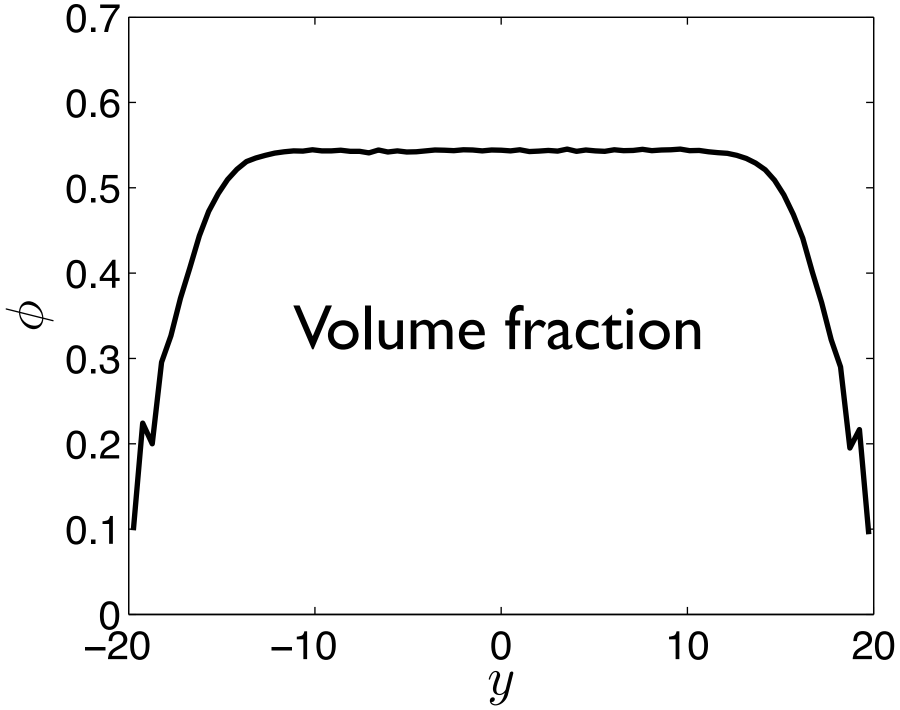
Core region

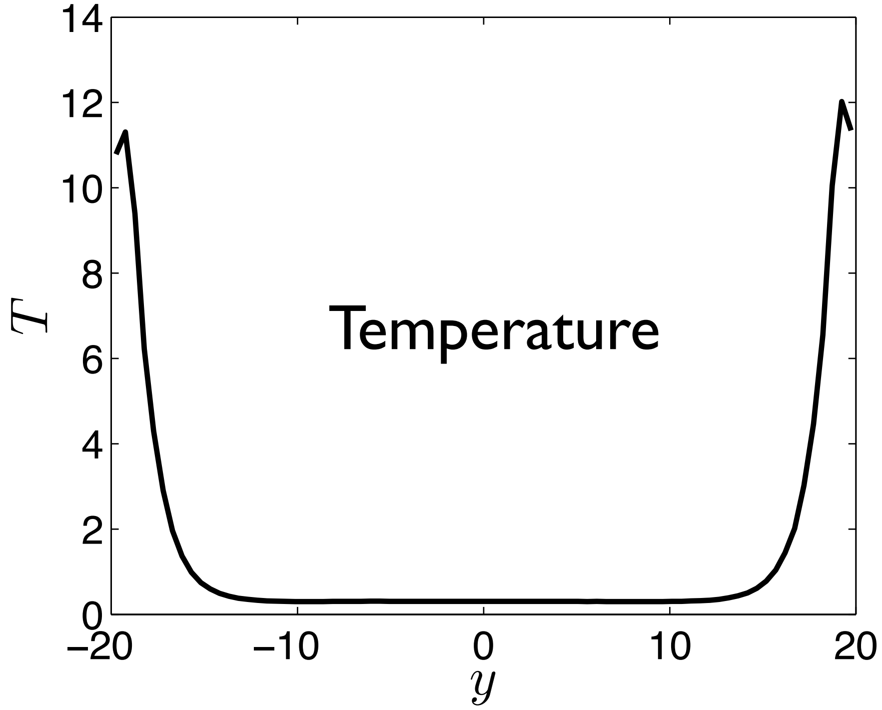
- comprises the bulk of the flow
- exhibits uniform flow properties
- obeys local, inertial-number rheological models[*†]

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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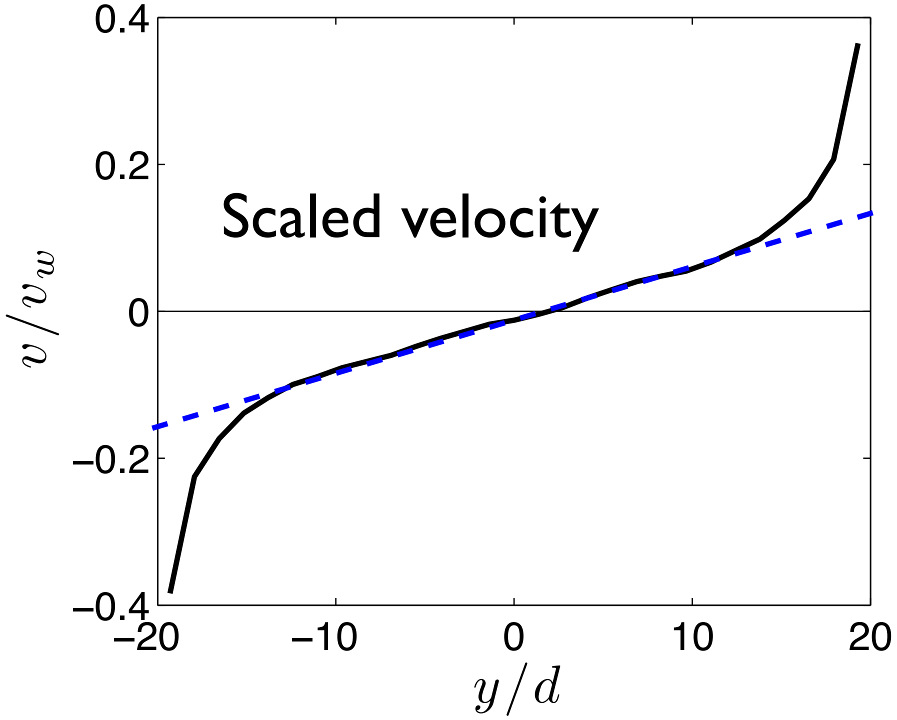
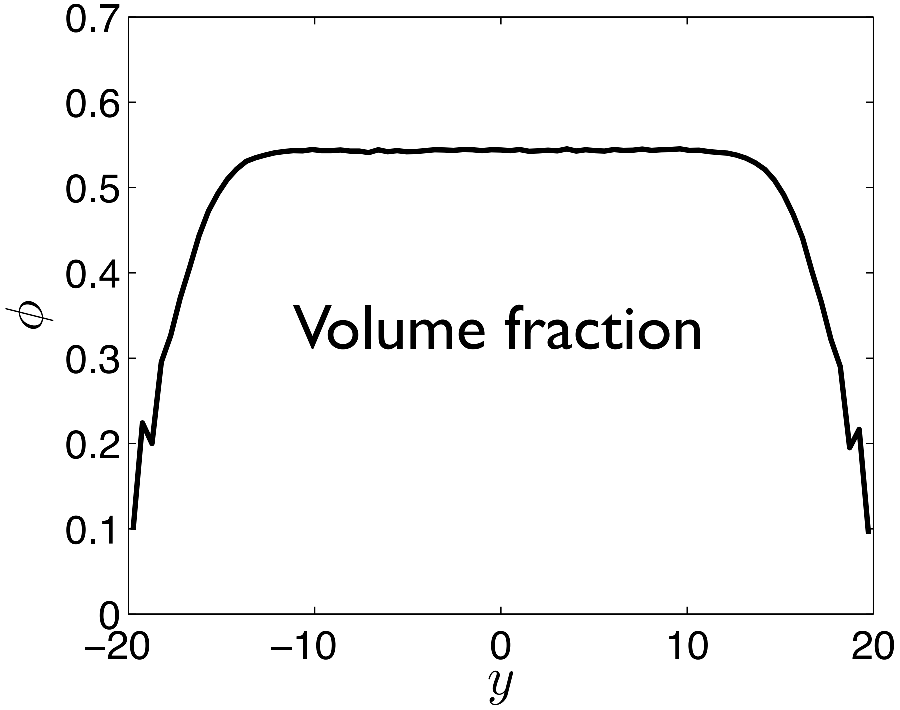
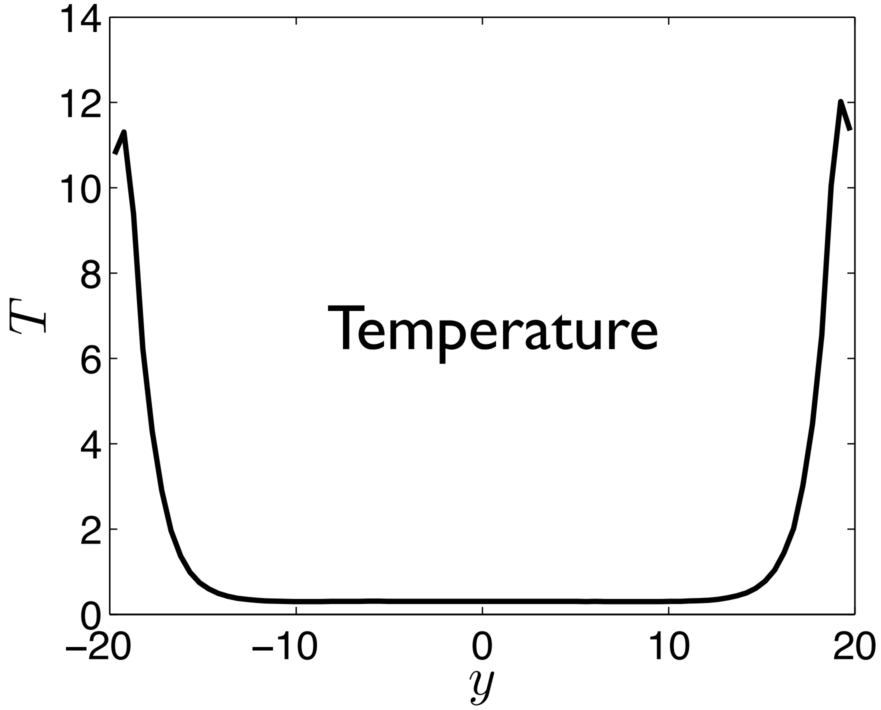
Questions:

- 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:

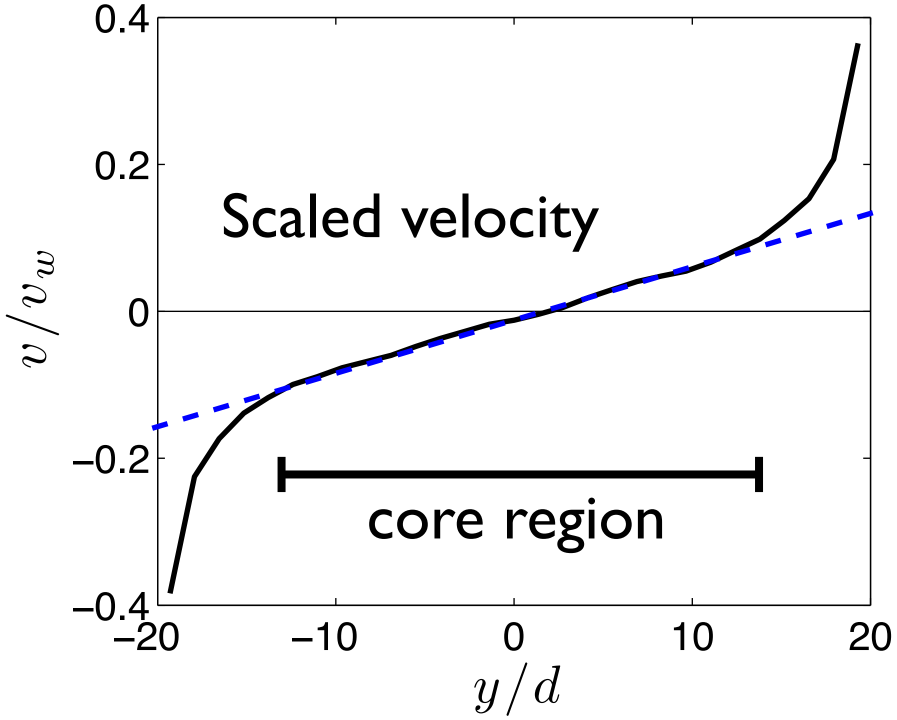
$$I_{\text{core}} \equiv \frac{\dot{\gamma}_{\text{core}} d}{\sqrt{p_{\text{core}}/\rho_s}}$$

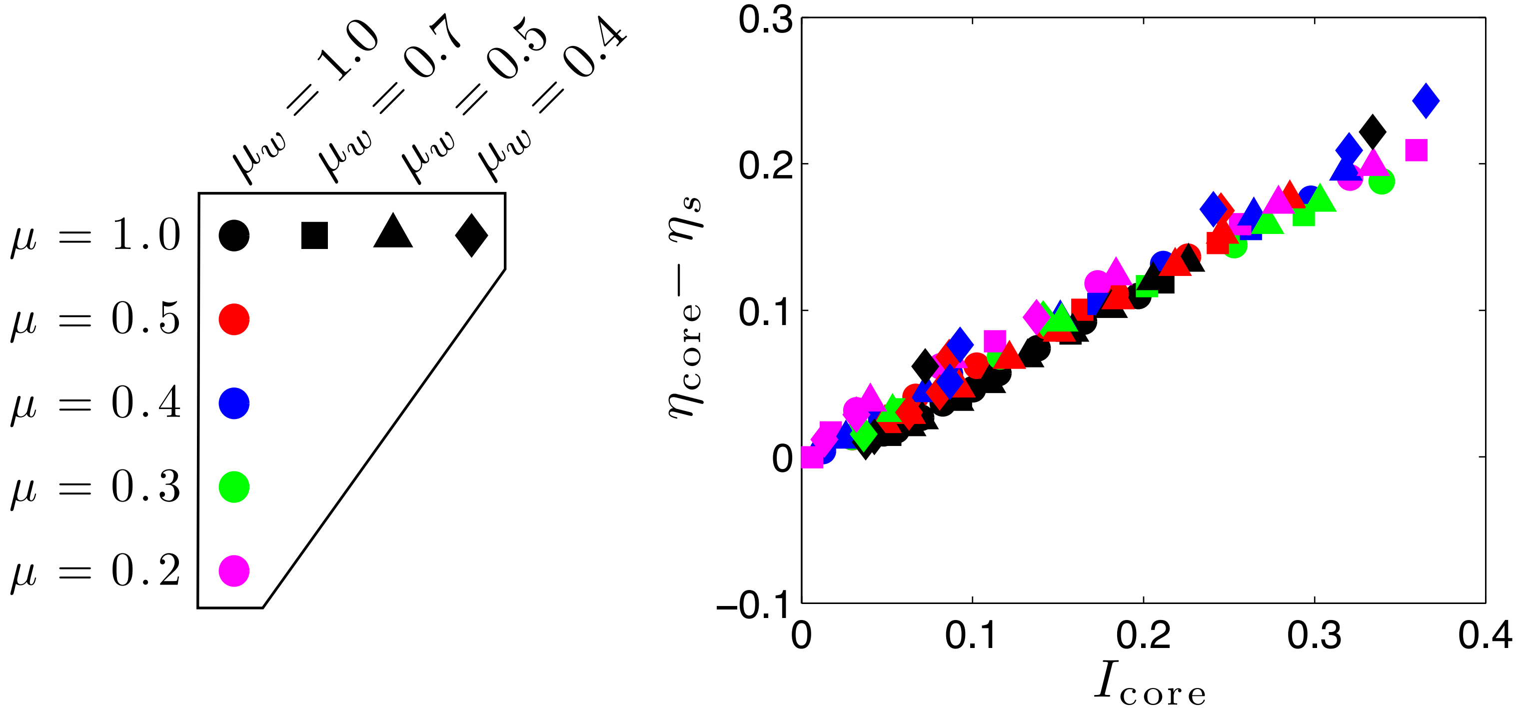
$$I_{\text{core}} \approx f(\phi) \text{ for } \phi < \phi_c(\mu)$$

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: $v_{\mathrm{slip}}^{(\cdot)} = v^{(\cdot)} - v_w$

Some solids velocity at the wall

Velocity of wall

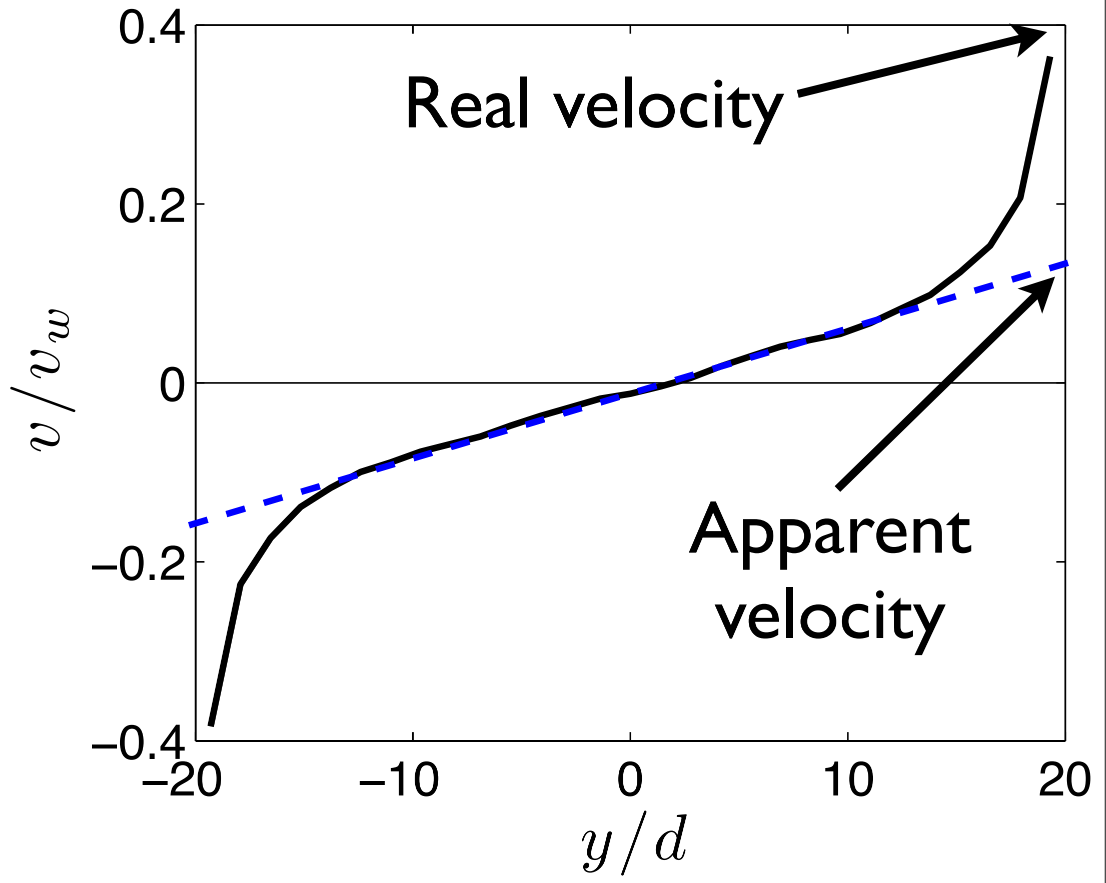
- Options for velocity $v^{(\cdot)}$:

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

$$v_{\mathrm{slip}}^{\mathrm{tr}} = v^{\mathrm{tr}} - v_w$$

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

$$v_{\mathrm{slip}}^{\mathrm{app}} = v^{\mathrm{app}} - v_w$$



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

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

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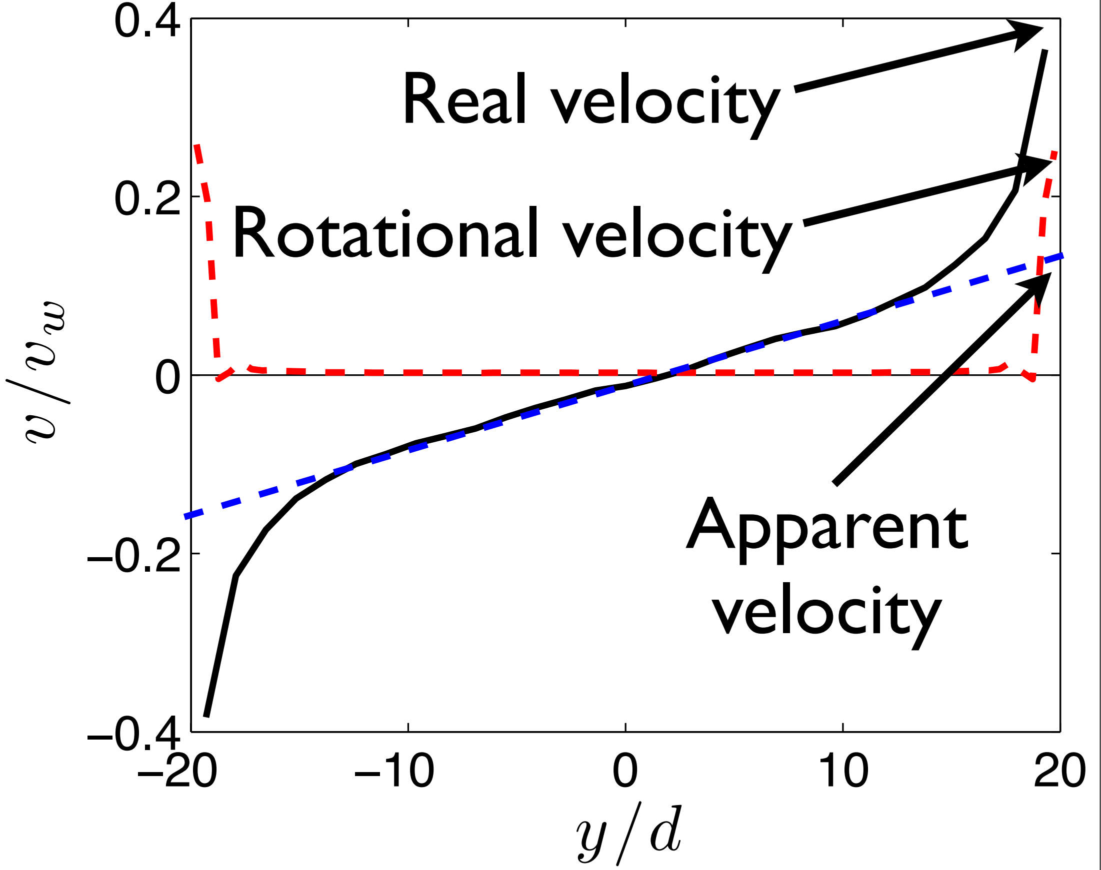
- Options for velocity $v^{(\cdot)}$:
  - c) 'Surface' slip velocity: based on relative velocity of particle surface at wall

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

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



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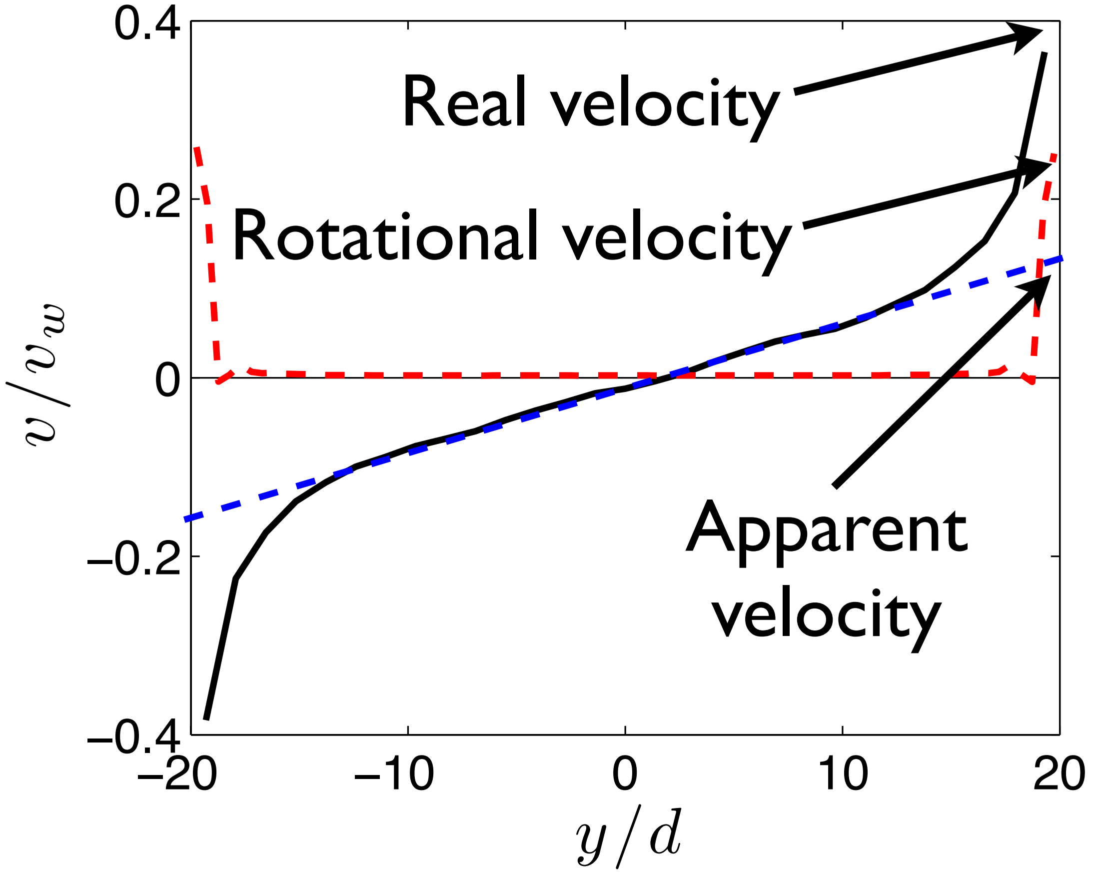


Question:

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

Velocity scales

- Dimensionless slip velocity:

$$I_{\mathrm{slip}}^{(\cdot)} = \frac{v_{\mathrm{slip}}^{(\cdot)}}{v_{\mathrm{char}}}$$

← 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).**

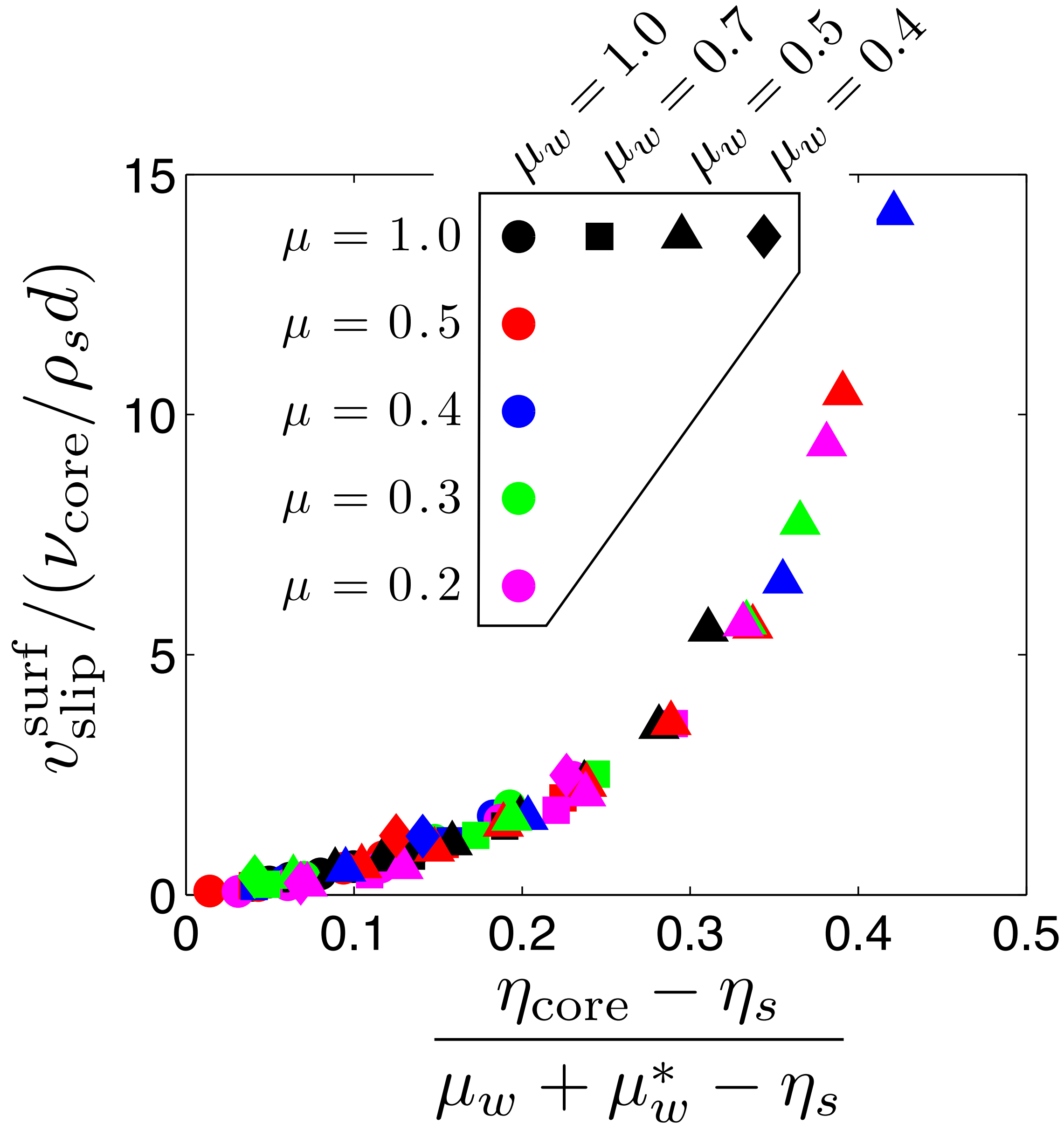
***Artoni et al. PRE 79, 031304 (2009).**

DEM results: dimensionless slip velocity

- Full collapse achieved by scaling of $\eta_{\rm core} - \eta_s$:
  - $\eta_{\rm wall} = \mu_w + \mu_w^*$
  - 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



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

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

Dense phase rheology: Summary

- Flow regime map: (completed)
- Rheological models
  - Steady state models that bridge various regimes (completed)
  - Modified kinetic theory (completed)
- Wall Boundary conditions (manuscript under preparation)
- Implementation of modified kinetic theory in MFIX/openFOAM

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

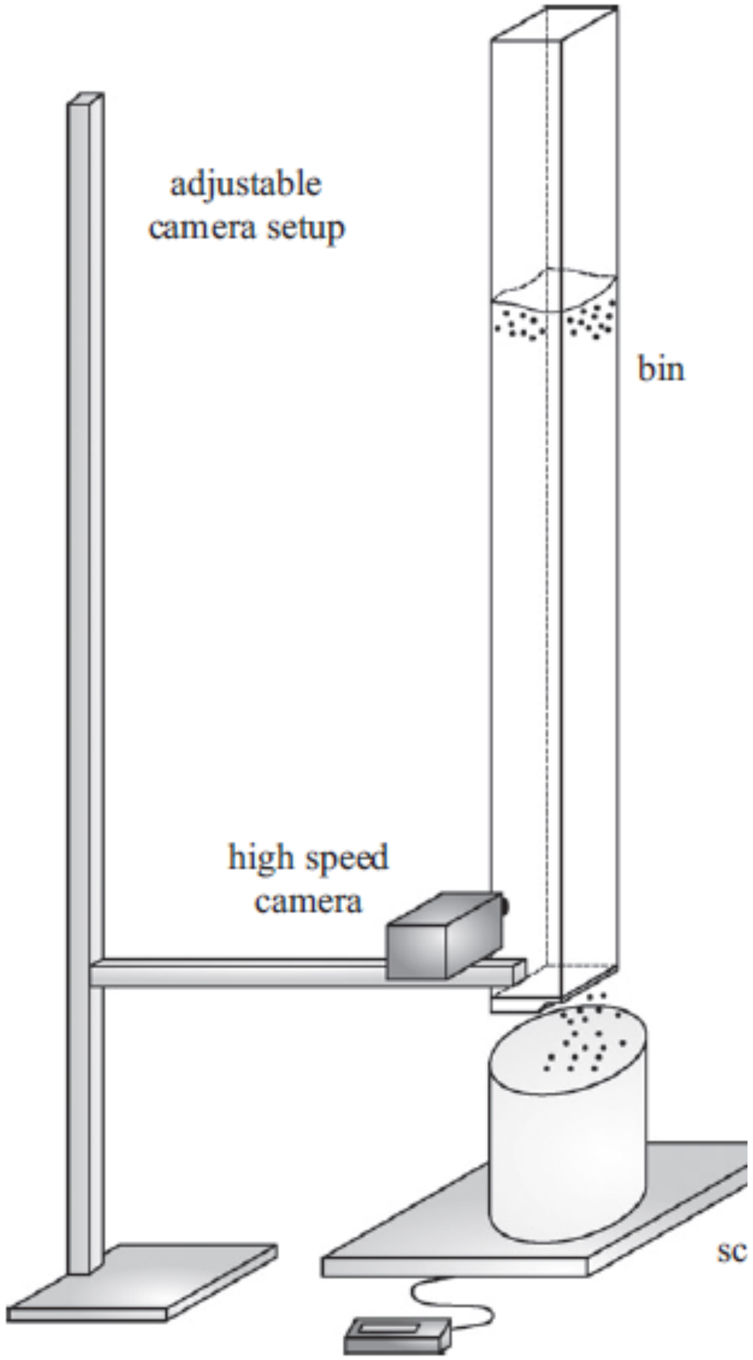
S. Chialvo & S. Sundaresan, Phy. of Fluids, 25, 070603 (2013).

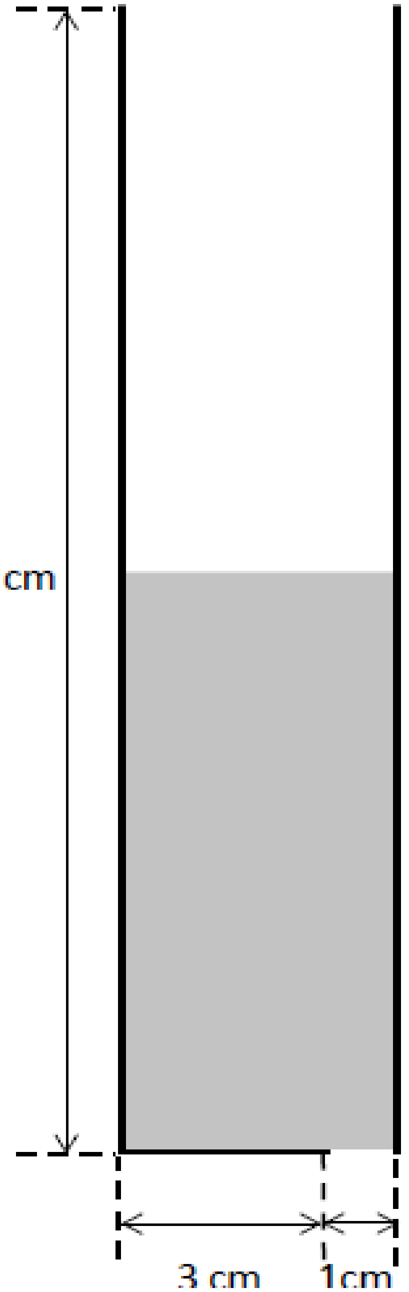
Y. Gu et al., PRE 90, 032206 (2014).

MKT Model implemented in openFOAM

- Implemented modified kinetic theory in MFIX
  - Ran into convergence issues
- Implemented MKT in openFOAM
  - After a few months of efforts, resolved convergence issues
  - Model solves for both gas and particles
  - Algebraic form of MKT
  - Will show sample findings in the next few slides
- Will return to MFIX implementation soon

Granular Discharge





Default material properties. Alternative values also explored here are included in parentheses.

Property	Value	Units
Particle diameter, d_p	0.875 (2, 4)	mm
Particle friction coefficient, μ	0.3 (0.1)	-
Particle restitution coefficient, e_p	0.8	-
Particle density, ρ_s	2500	$kg\ m^{-3}$
Gas viscosity, μ_g	1.78e-5	$kg\ m^{-1}s^{-1}$
Gas density, ρ_g	1.224	$kg\ m^{-3}$

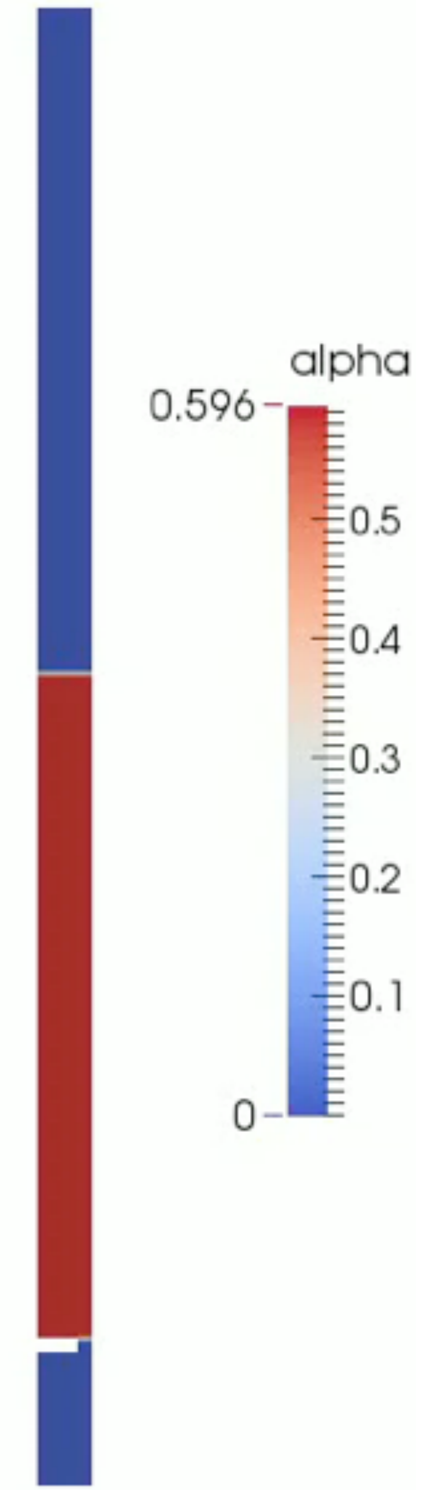
S. Schneiderbauer, A. Aigner, S. Pirker, *Chemical Engineering Science,* **80**, 279-292, (2012)

Granular Discharge

- Unphysical results with free-slip BC. Meaningful trends with no-slip BC.

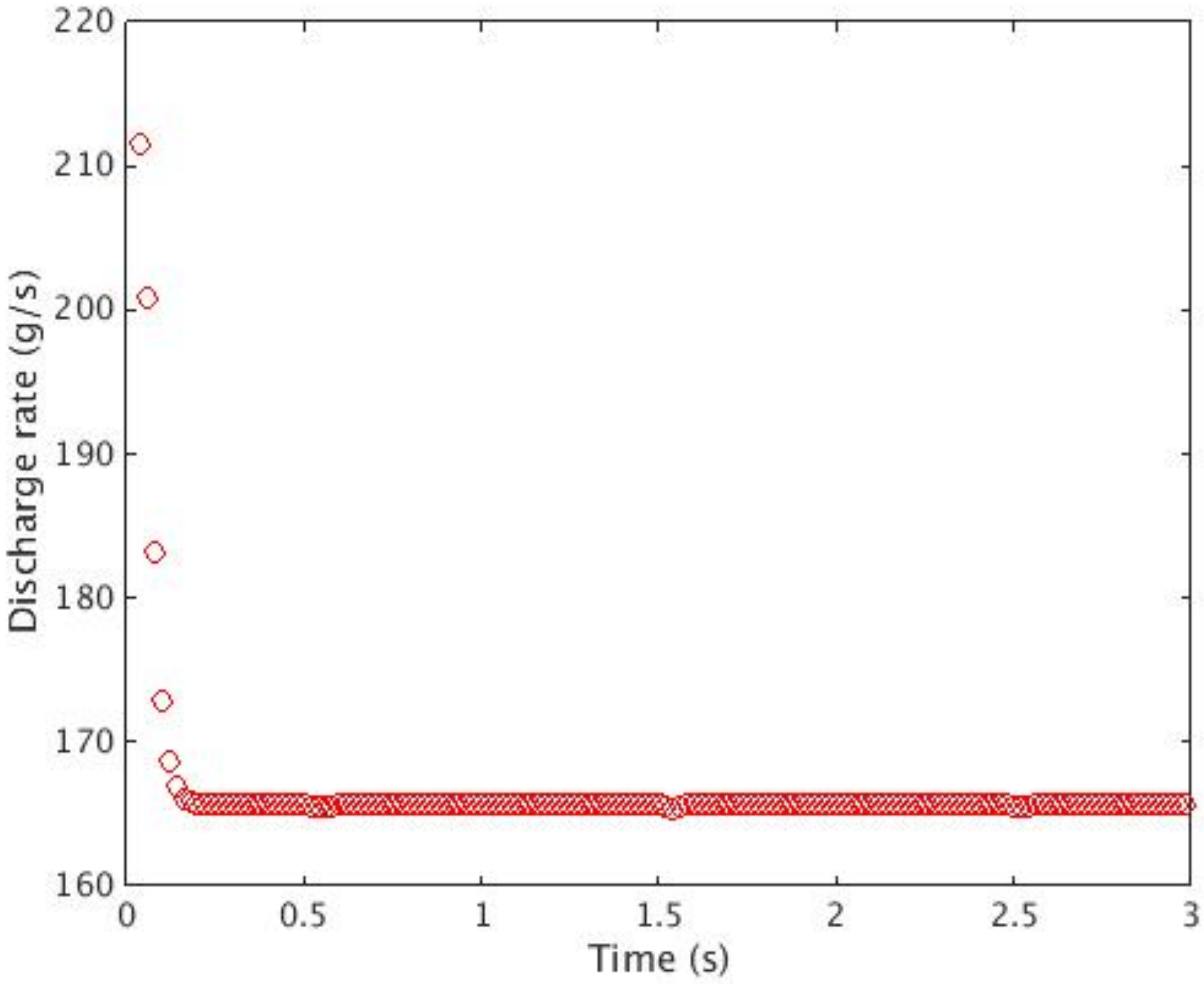
Granular Discharge

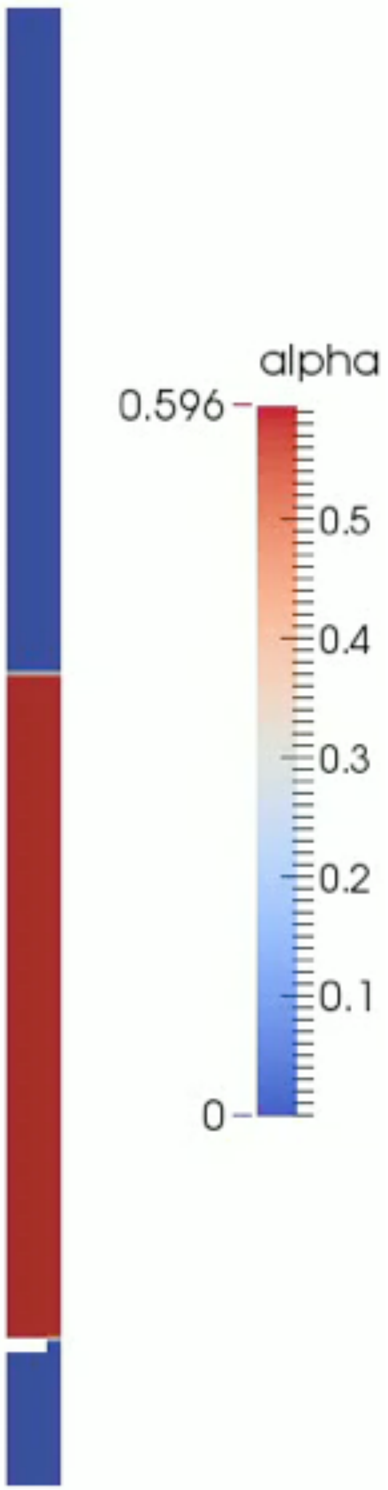
- Unphysical results with free-slip BC. Meaningful trends with no-slip BC.



Granular Discharge

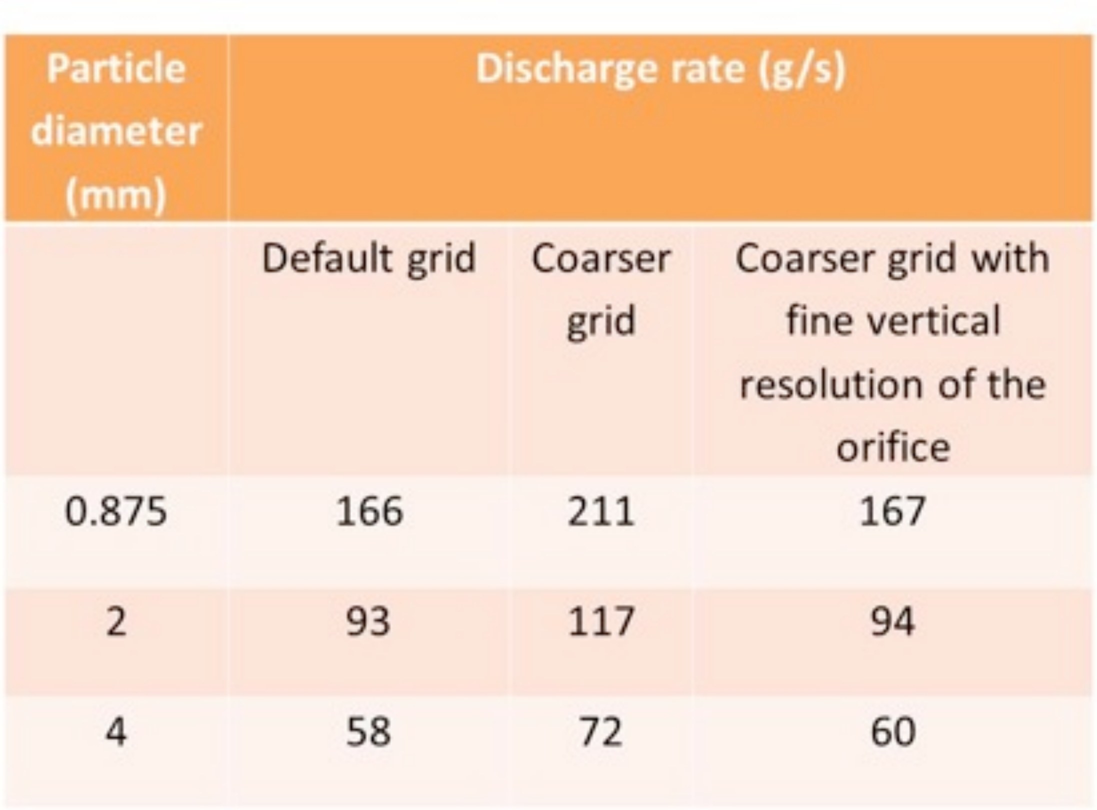
- Unphysical results with free-slip BC. Meaningful trends with no-slip BC.





Effect of grid resolution

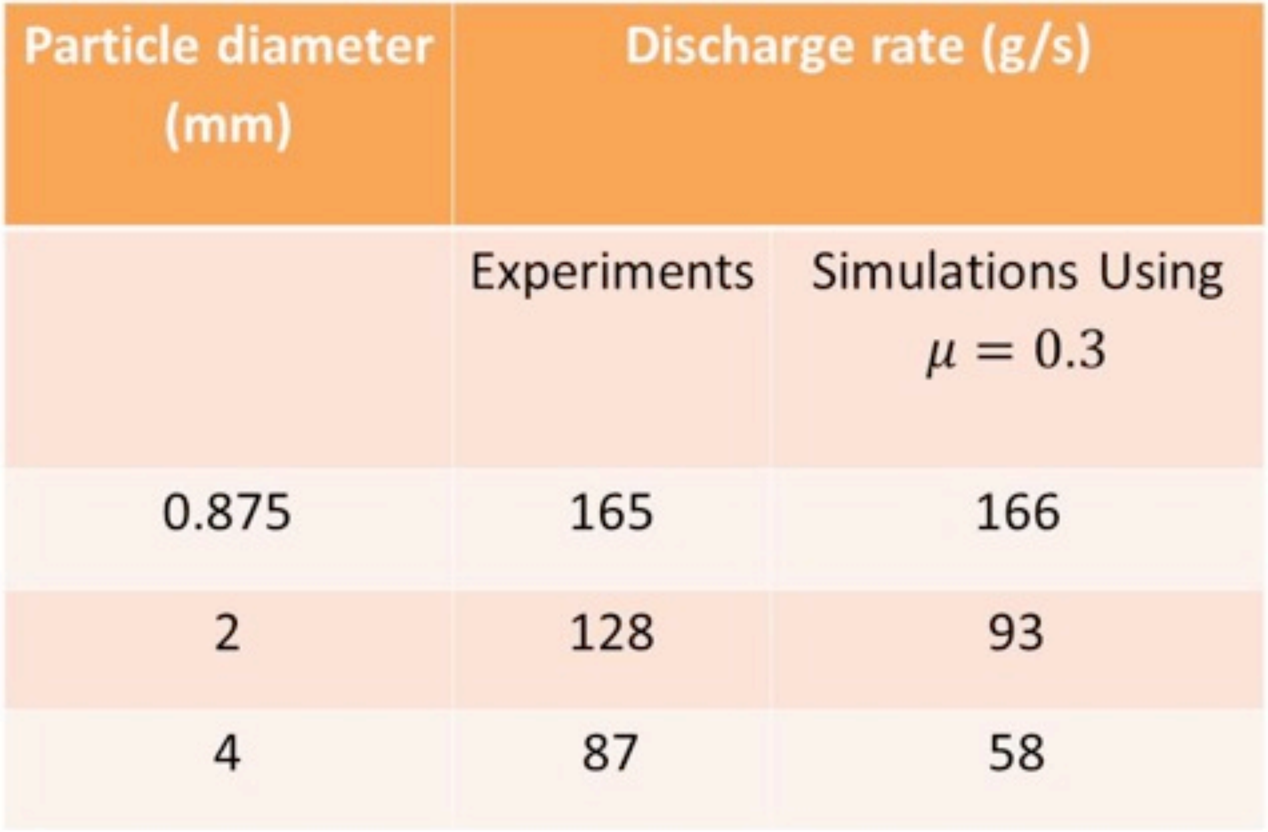
- Default grid:
  - The horizontal resolution
    - 1.25 mm in the direction of the width of the rectangular orifice
    - 2.5 mm in the direction of the length of the orifice.
  - The vertical resolution is 2.5 mm.
- Coarser grid: Coarsened by a factor of 2 in each direction
- Coarser grid with fine vertical resolution of the orifice:
  - All grids are coarsened except for the vertical resolution of the orifice



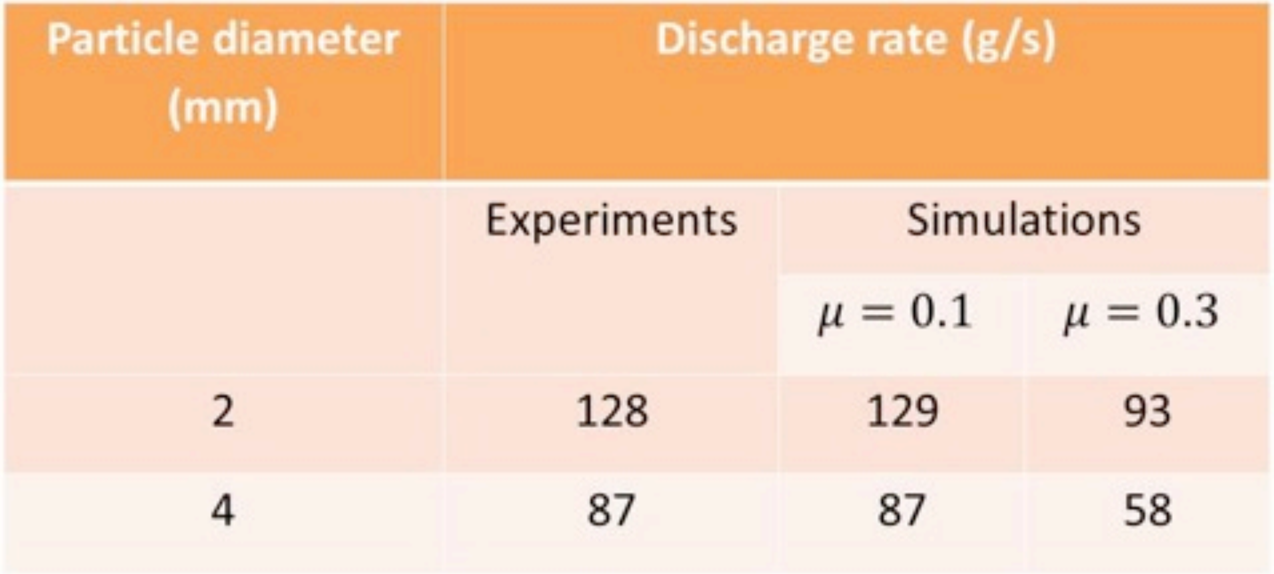
Particle diameter (mm)	Discharge rate (g/s)		
	Default grid	Coarser grid	Coarser grid with fine vertical resolution of the orifice
0.875	166	211	167
2	93	117	94
4	58	72	60

Comparison with experimental data

- For 0.875 mm particles, excellent agreement with friction coefficient of 0.3
- Discharge rate varies significantly with friction coefficient
- For the 2 and 4 mm particles, good agreement if the friction coefficient is chosen to be 0.1.
- Granular discharge experiments may be a simple way of tuning friction coefficient!



Particle diameter (mm)	Discharge rate (g/s)	
	Experiments	Simulations Using $\mu = 0.3$
0.875	165	166
2	128	93
4	87	58



Particle diameter (mm)	Discharge rate (g/s)		
	Experiments	Simulations	
		$\mu = 0.1$	$\mu = 0.3$
2	128	129	93
4	87	87	58

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 effective boundary conditions for dense flows
- Implementation in openFOAM completed; implementation in MFIX is ahead of us.