Continuum and parcel-based approaches to dense granular rheology: model development and applications

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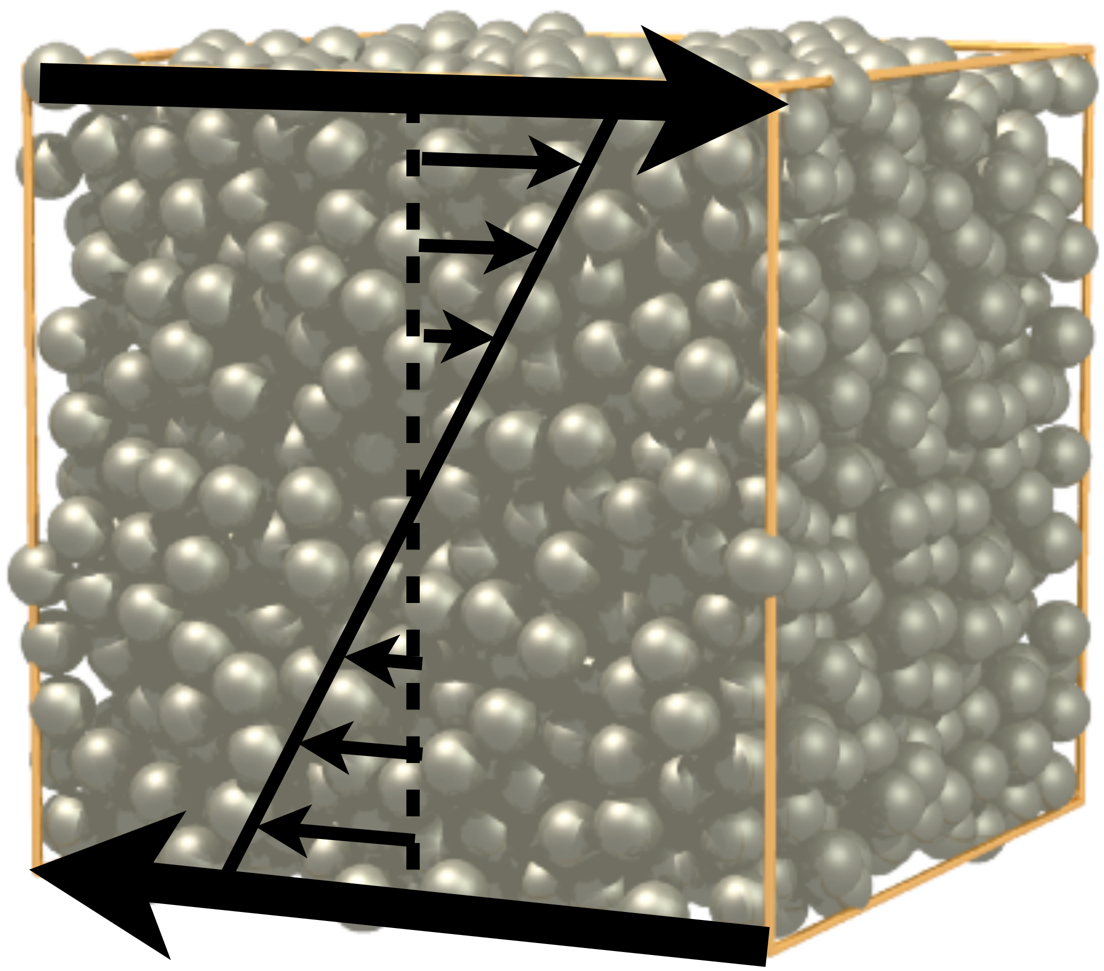
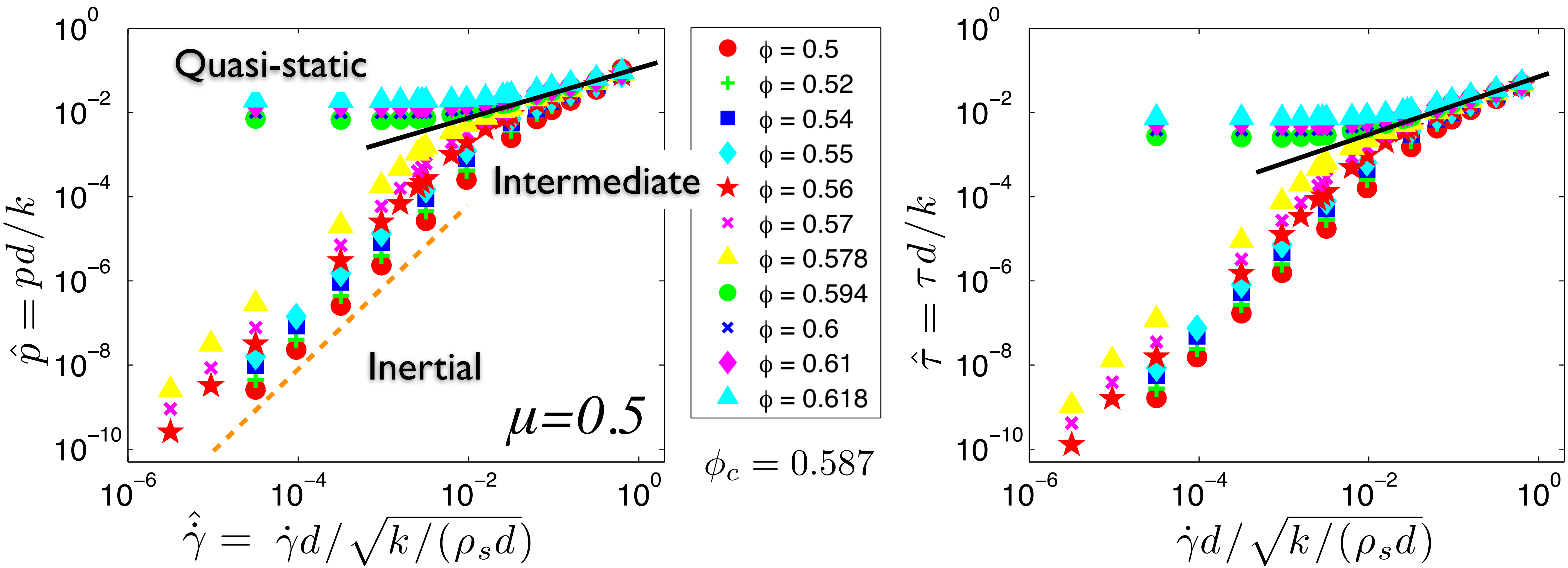
Discrete element method

- 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)

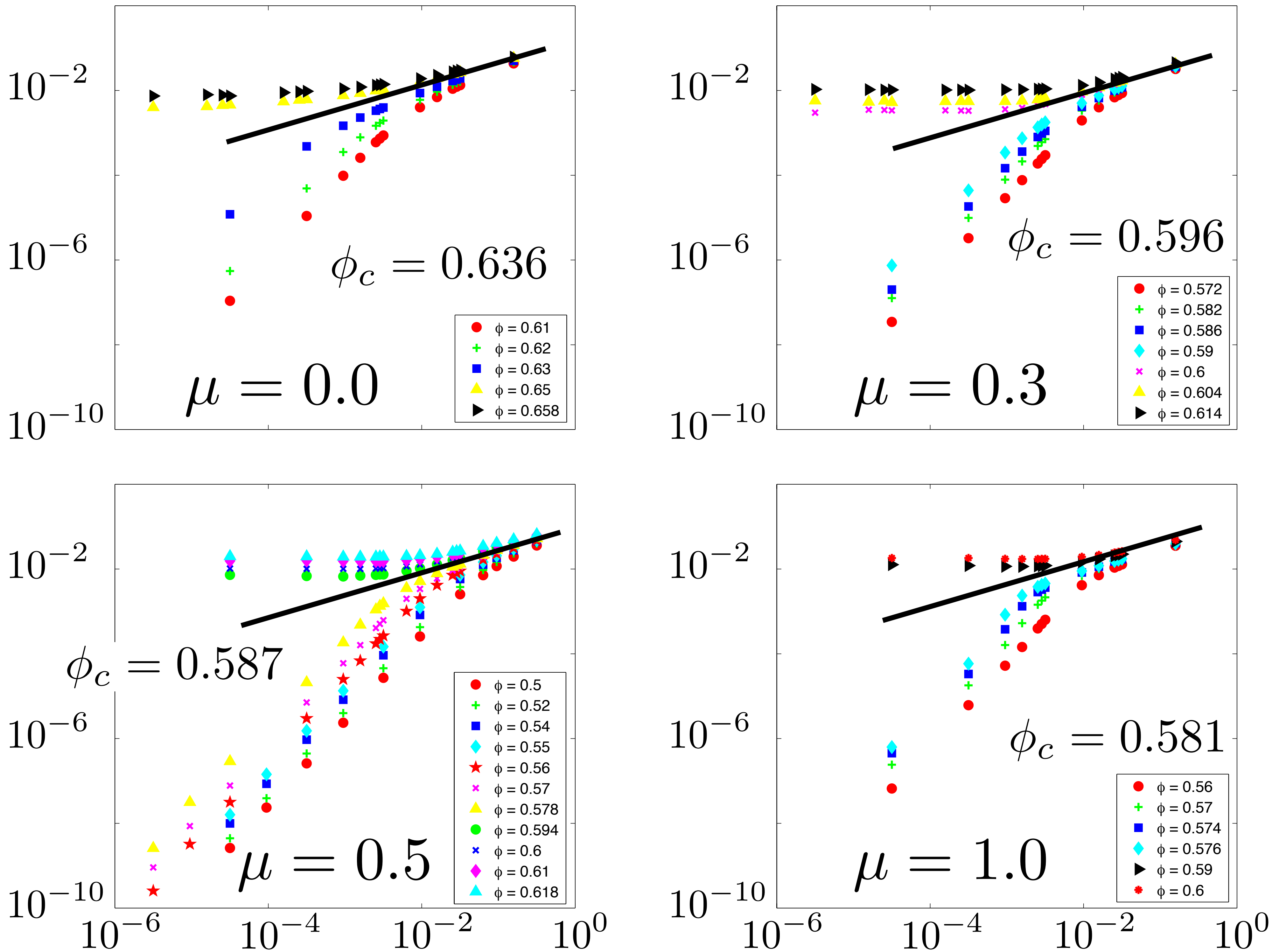
Flow map



- Flow curve at a critical volume fraction ϕ_c , $pd/k = \alpha \hat{\dot{\gamma}}^m$ distinguishes flow regimes: quasi-static, inertial, and intermediate.
- Quasi-static and inertial bands merge smoothly towards the critical scaling at high shear rates.

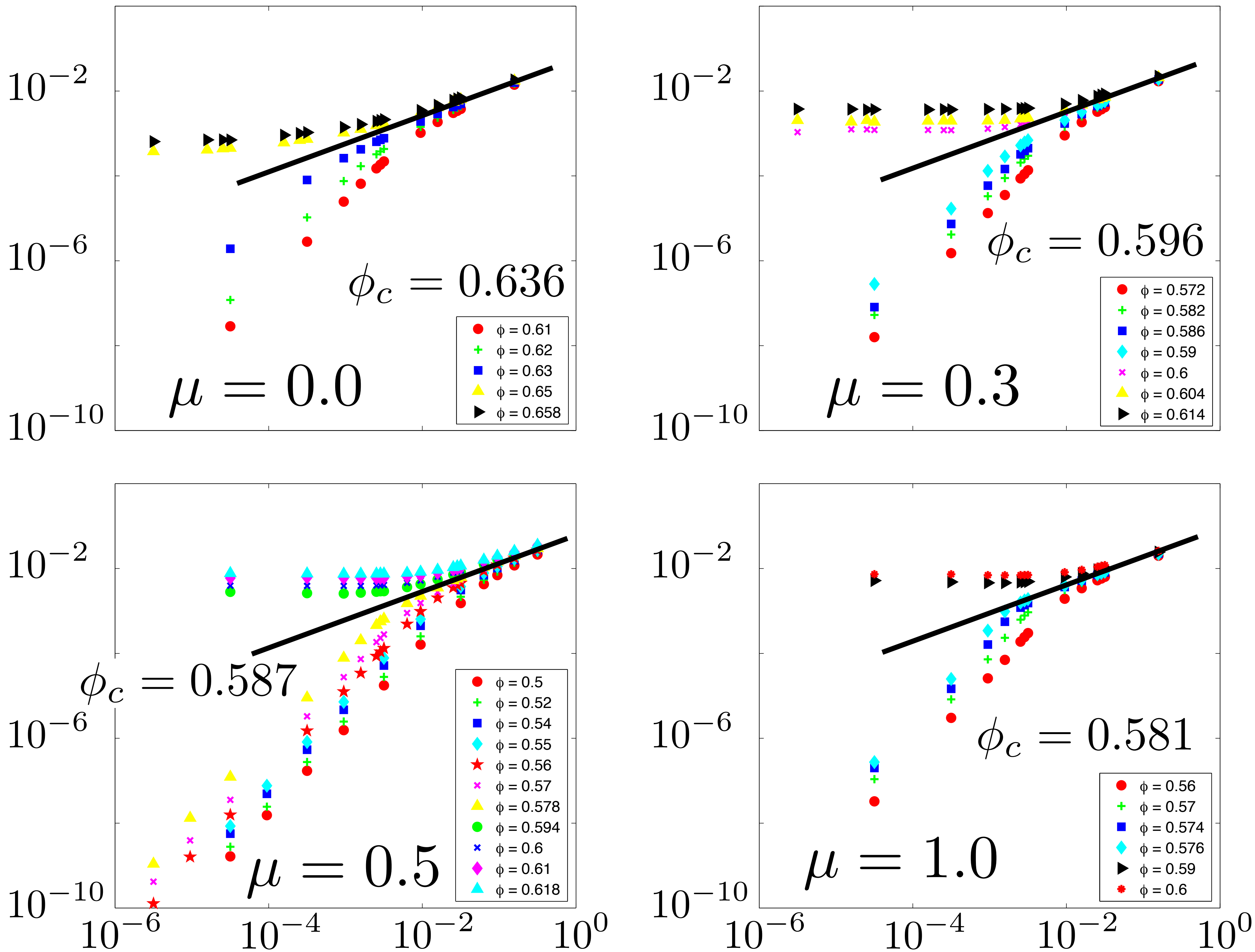
Effect of μ on rate dependence of pressure

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

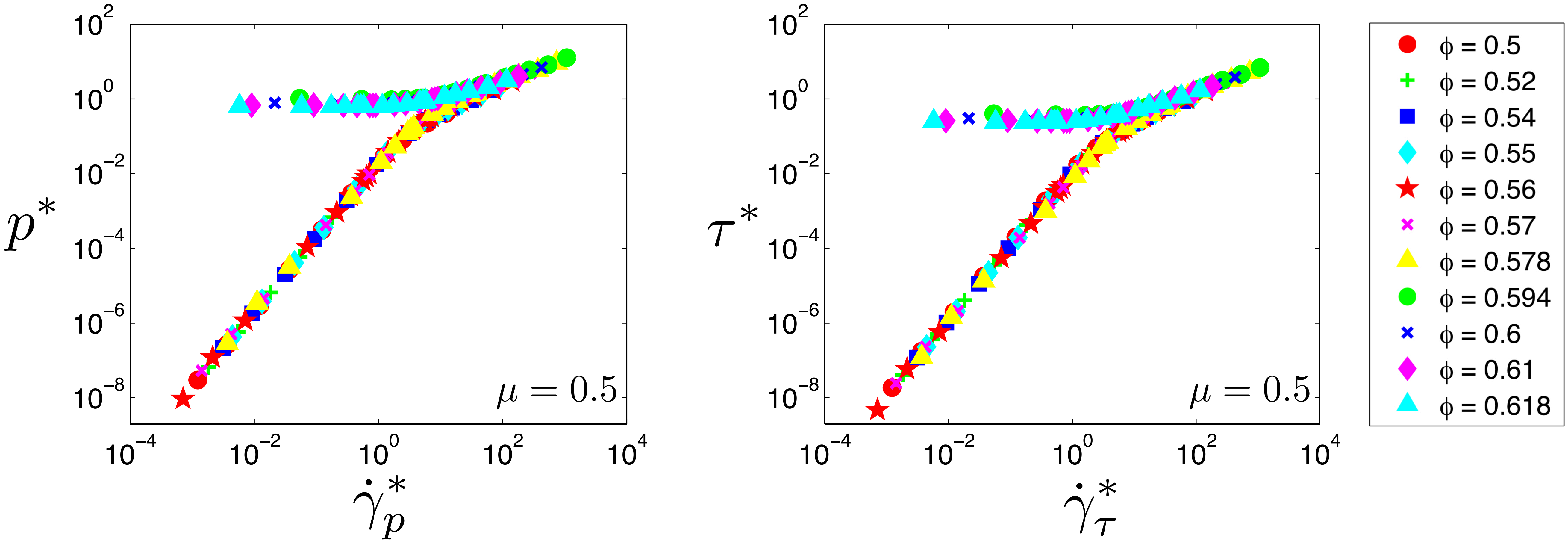


Effect of μ on rate dependence of shear stress

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



Stress scalings for frictional particles



$$p^* = \hat{p}/|\phi - \phi_c|^{a_1} \qquad \tau^* = \hat{\tau}/|\phi - \phi_c|^{a_2}$$

$$\dot{\gamma}_p^* = \hat{\dot{\gamma}}/|\phi - \phi_c|^{b_1} \qquad \dot{\gamma}_\tau^* = \hat{\dot{\gamma}}/|\phi - \phi_c|^{b_2}$$

- Quasi-static regime data $\Longrightarrow$ $a_1 = a_2 = 1$
- Inertial regime data $\Longrightarrow$ $b_1 = 1.5$, $b_2 = 1.4$

Proposed model: regime asymptotes

- Stresses in each regime asymptote can be written as a power-law functions of shear rate:

$$\frac{p_i}{|\phi - \phi_c|} = \alpha_i \left(\frac{\dot{\gamma}}{|\phi - \phi_c|^{1.5}} \right)^m$$

$$\frac{\tau_i}{|\phi - \phi_c|} = \beta_i \left(\frac{\dot{\gamma}}{|\phi - \phi_c|^{1.4}} \right)^n$$

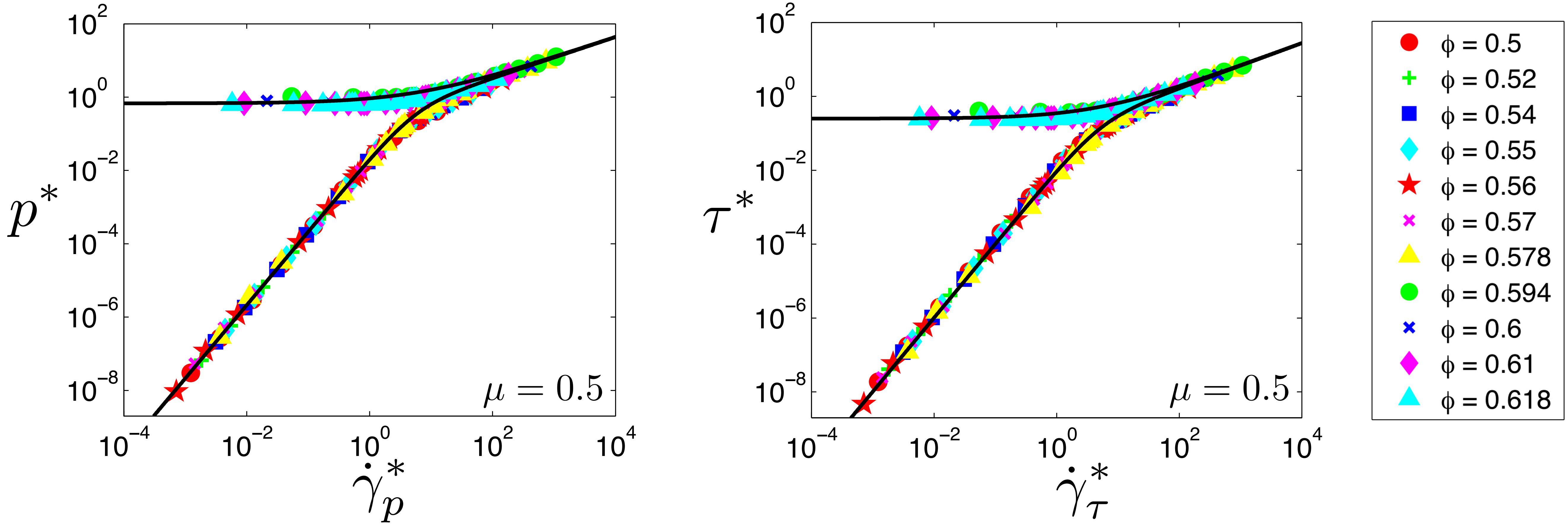
- Quasi-static: $m = n = 0$
- Inertial: $m = n = 2$
- Intermediate: $m = 2/3$
  $n = 5/7$

Proposed model: blending

- Transitions between regimes can be captured using a blending function of the form:

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

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



- Blended model provides fairly good agreement with DEM data.

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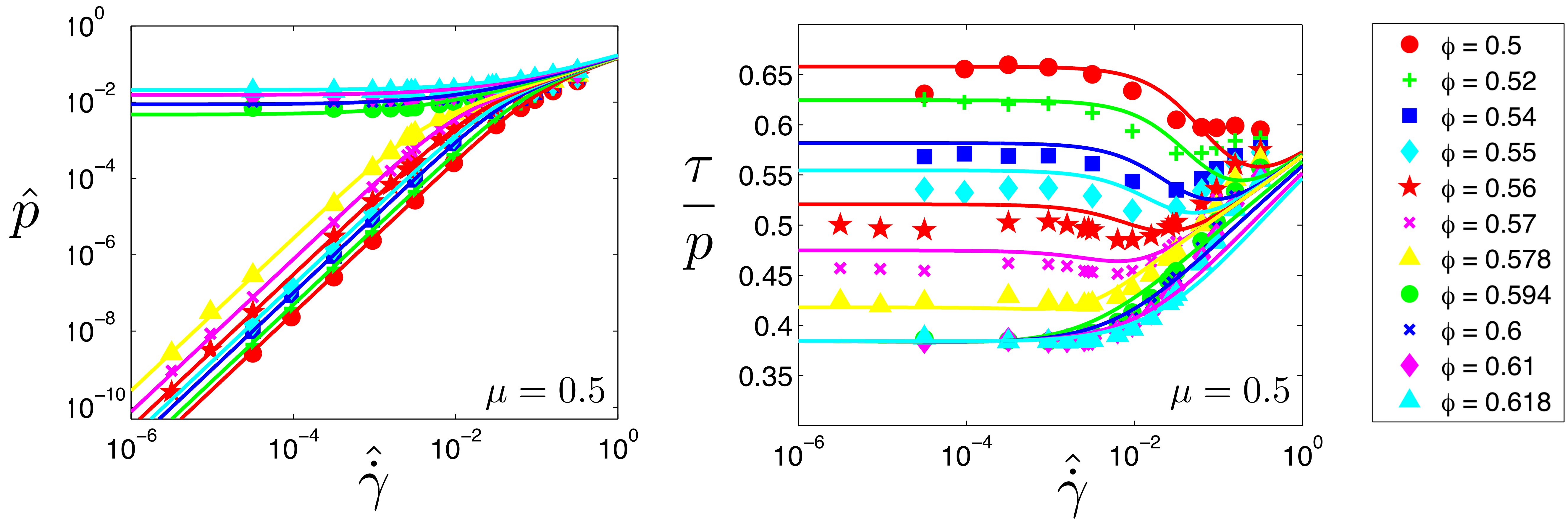

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Model summary

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

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

$$p_{QS} = \alpha_{QS}|\phi - \phi_c|$$

$$\tau_{QS} = \beta_{QS}|\phi - \phi_c|$$

$$p_{Int} = \alpha_{Int}\hat{\dot{\gamma}}^{2/3}$$

$$\tau_{Int} = \beta_{Int}\hat{\dot{\gamma}}^{5/7}$$

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

$$\tau_{Inert} = \frac{\beta_{Inert}\hat{\dot{\gamma}}^2}{|\phi - \phi_c|^{9/5}}$$

- Model features:
  - Captures behavior in all three flow regimes and the transitions them.
  - Continuous in shear rate – no arbitrary cutoffs.
  - Piecewise in volume fraction
  - $\alpha_{Inert}, \beta_{Inert} \sim (\phi/\phi_c)$ to ensure zero stresses in dilute limit.

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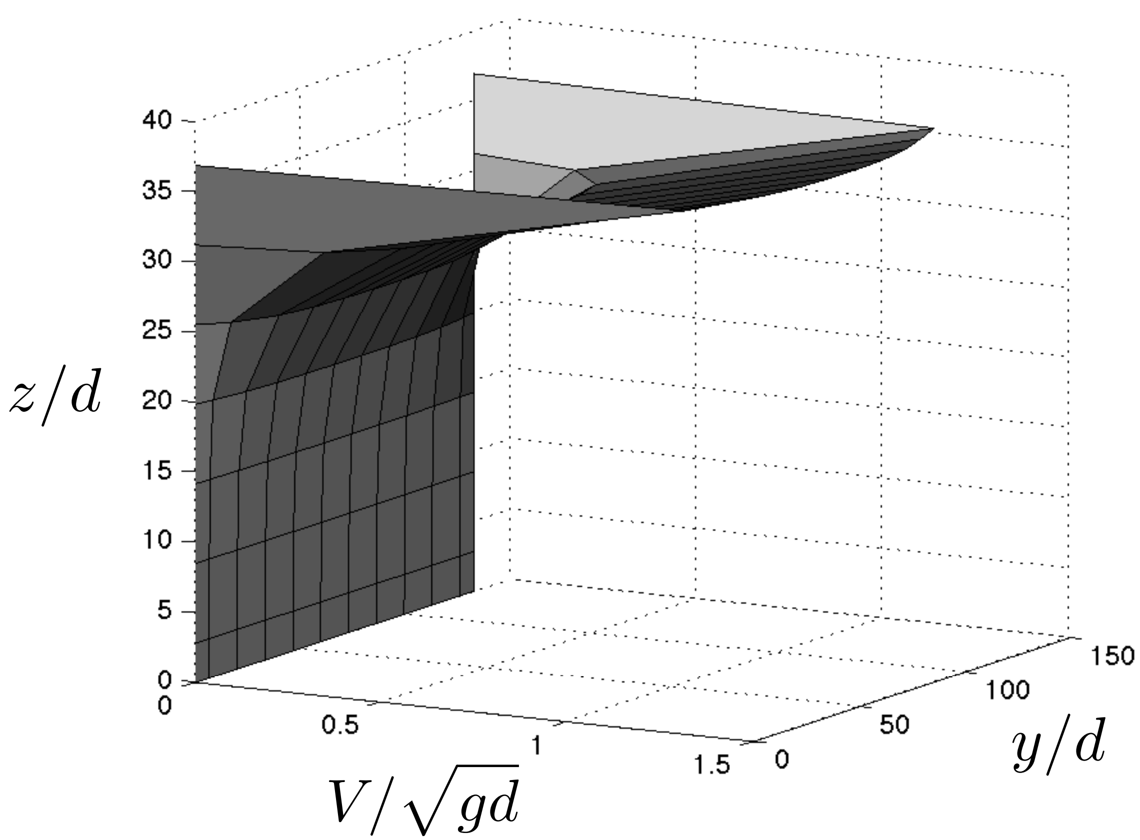
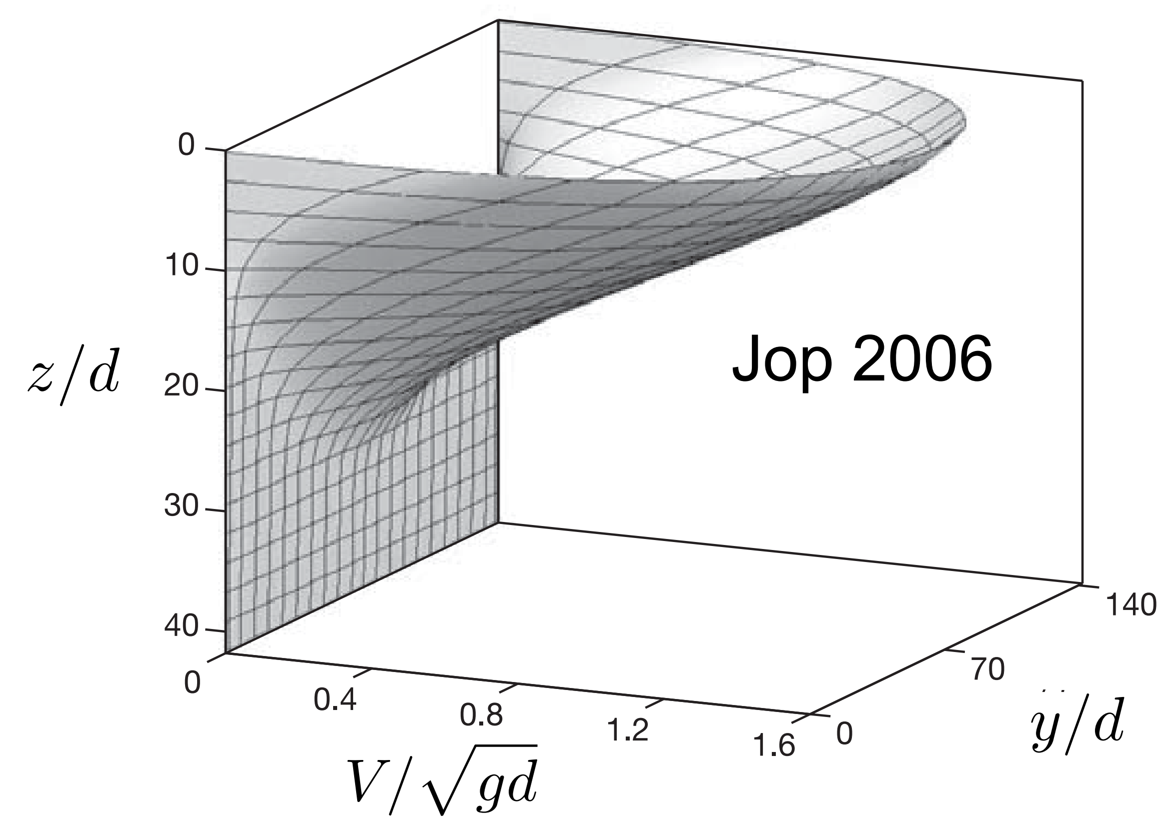
- Model features:
  - $\phi_c = \phi_c(\mu)$
  - α_{QS}, β_{QS} depend on μ
  - $\alpha_{Inert}, \beta_{Inert}$ depend on μ via effective restitution coefficient
  - $\alpha_{Int}, \beta_{Int}$ independent of μ

Continuum model application

- Stress model was implemented in MFIX
- Chute flow simulations were performed for comparison with existing experimental and computational data†.

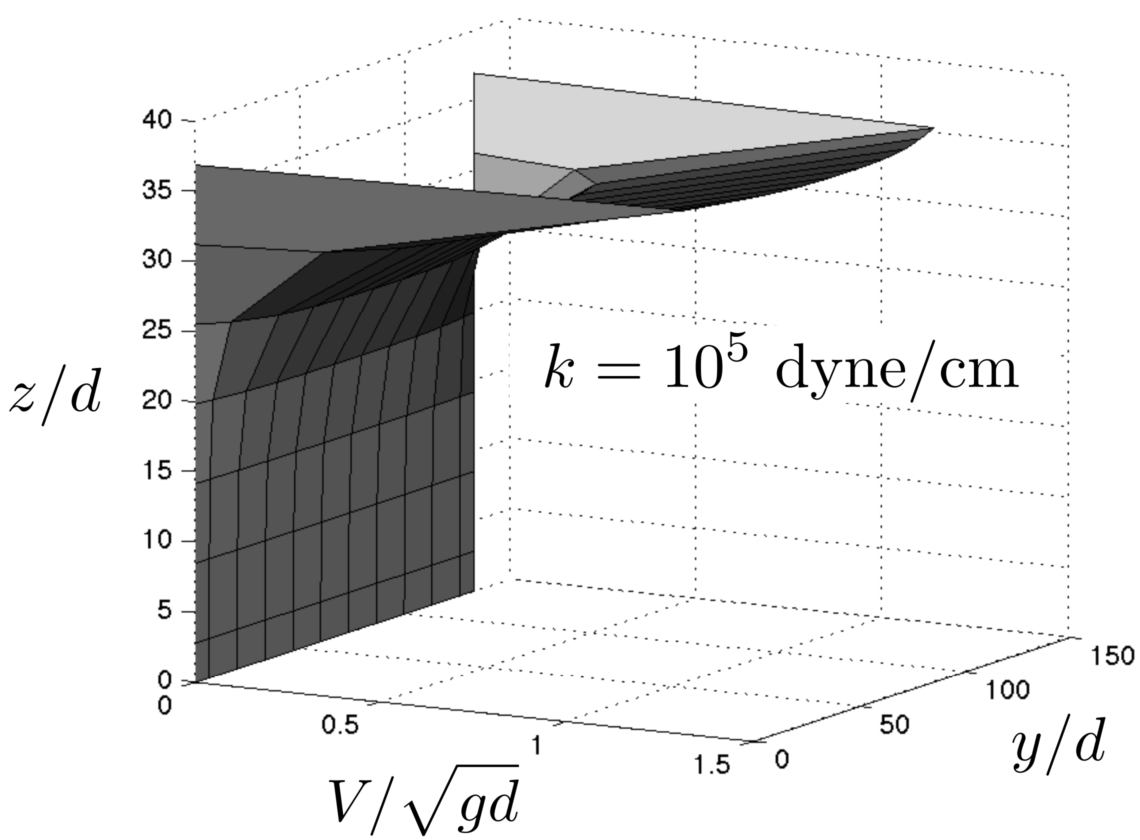


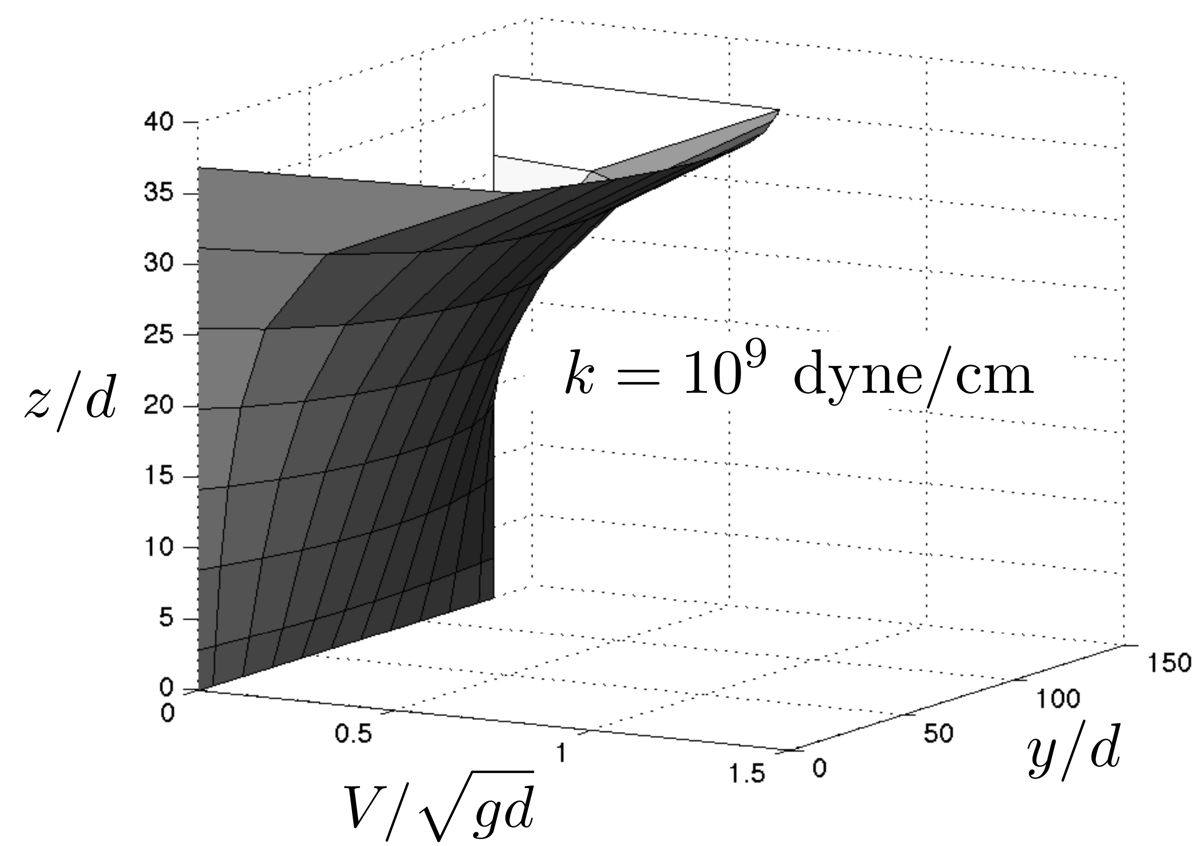


† P. Jop, Y. Forterre, and O. Pouliquen, Nature 441, 727 (2006).

Continuum model application

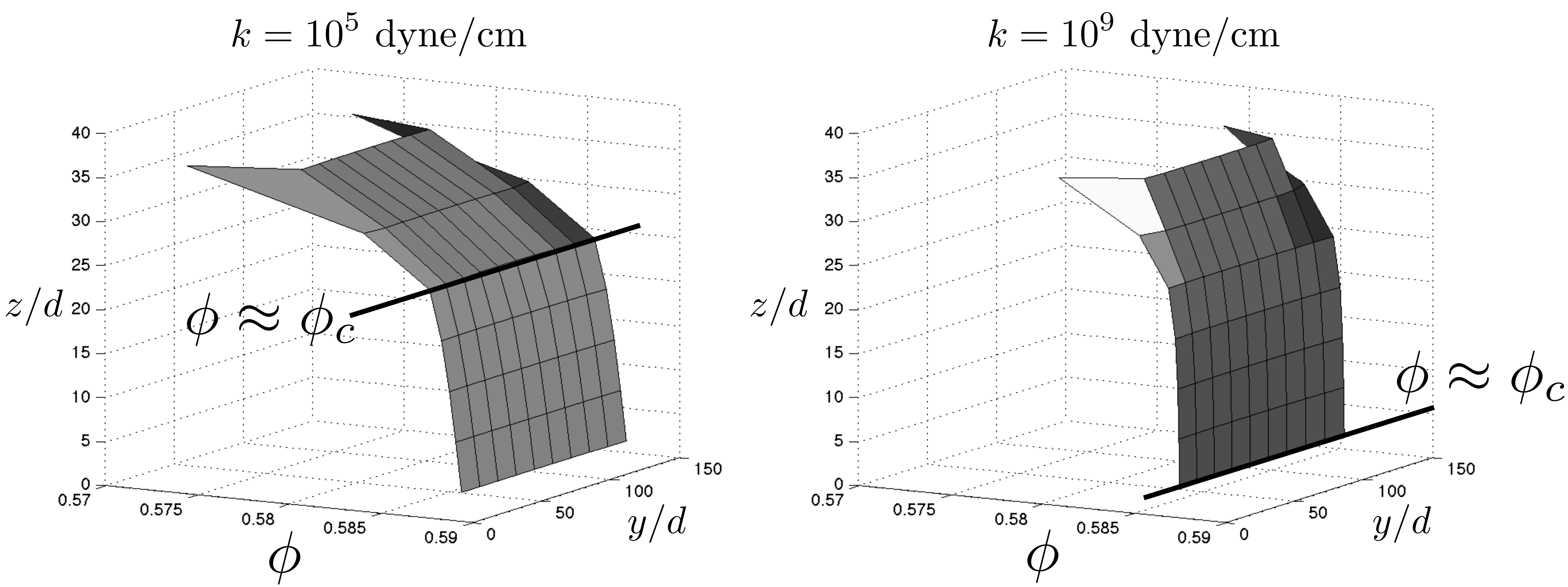
- Thickness of flowing and stagnant layers depends on particle stiffness *k*





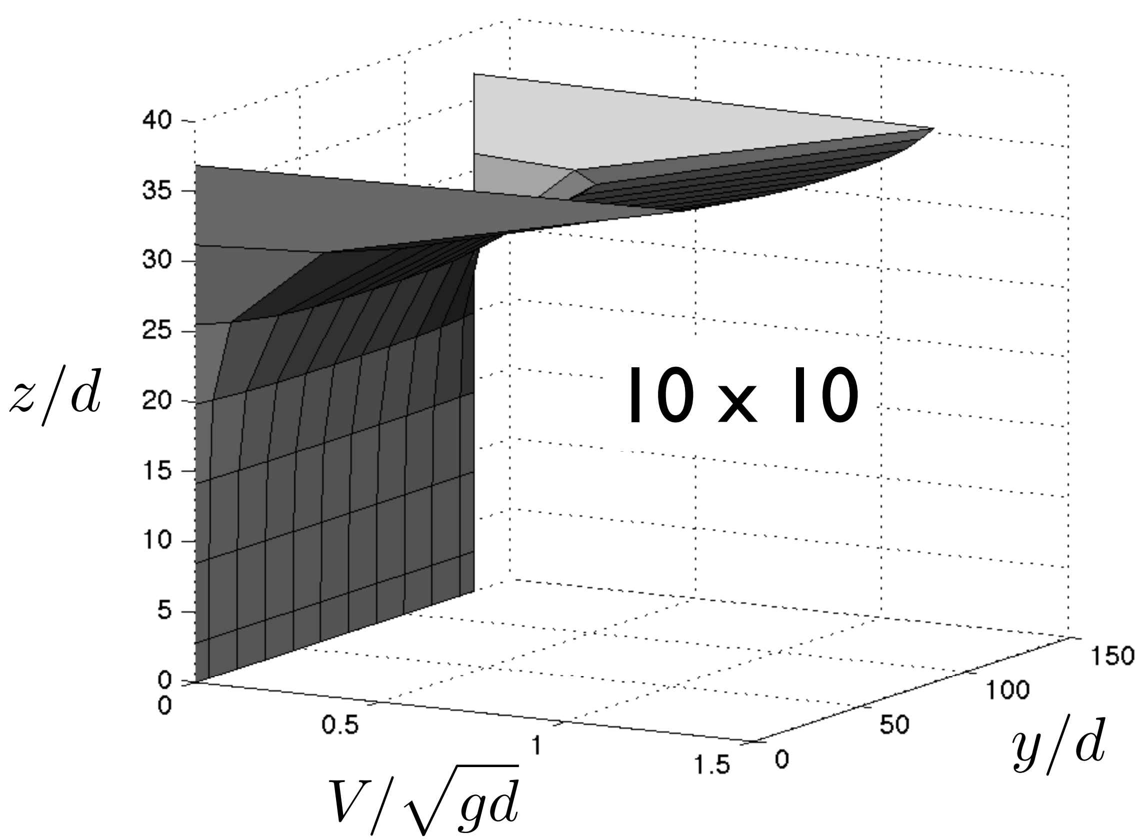
Continuum model application

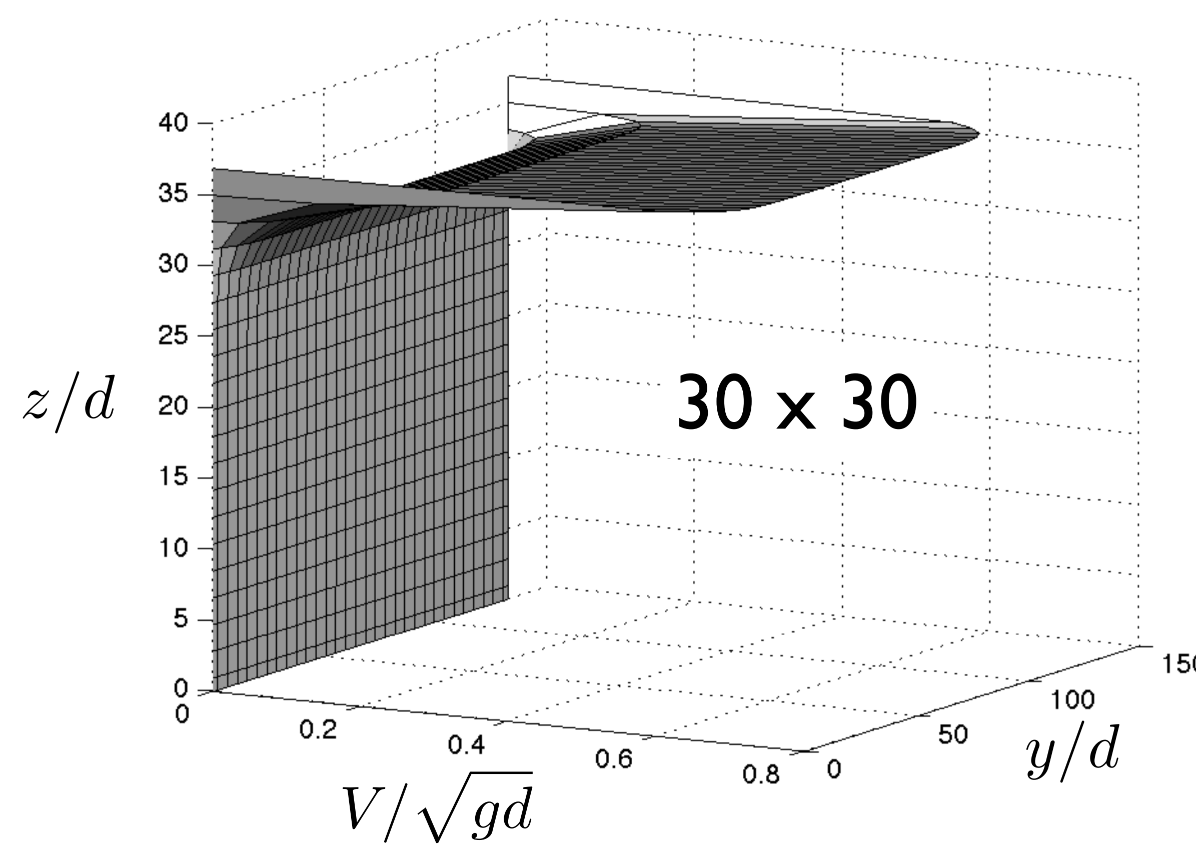
- Slight volume fraction variations around ϕ_c dictate regime of flow



Continuum model application

- Unresolved issues:
  - Flow profile depends on grid size
  - Flow profile is sensitive to initial volume fraction profile





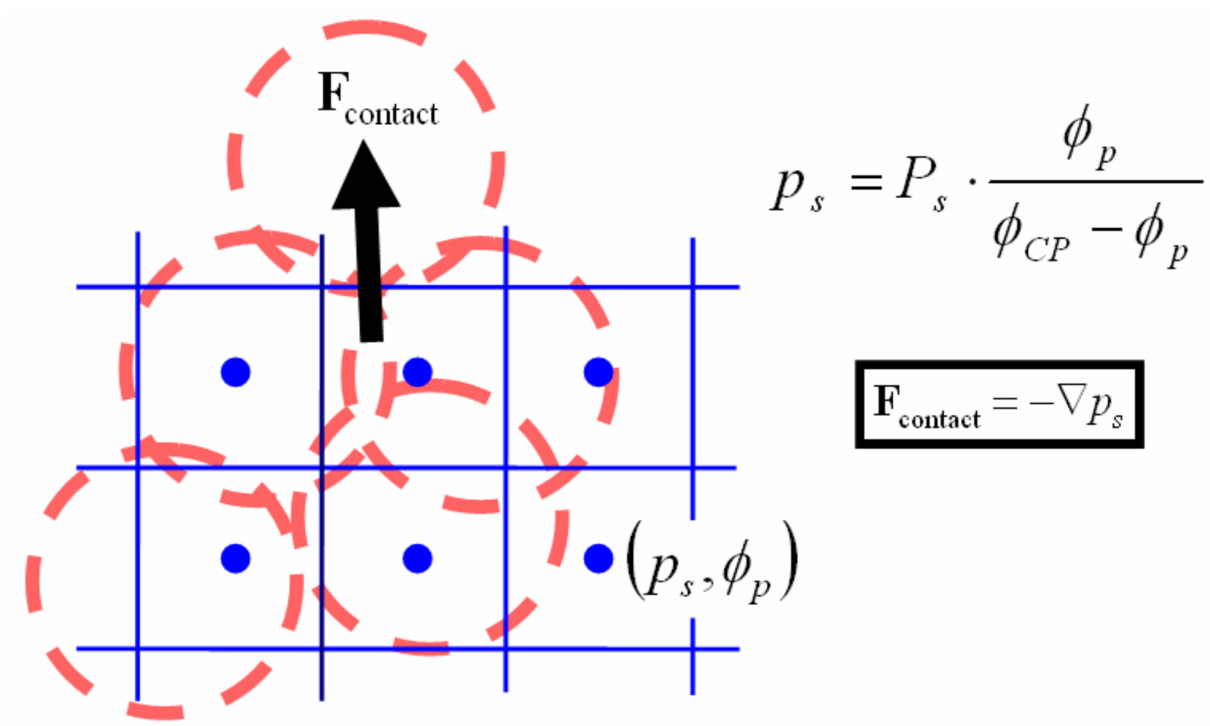
Parcel Based Methods

- Groups of particles
- Requires virtual contact forces to prevent overpacking

MP-PIC

Effective particle phase pressure

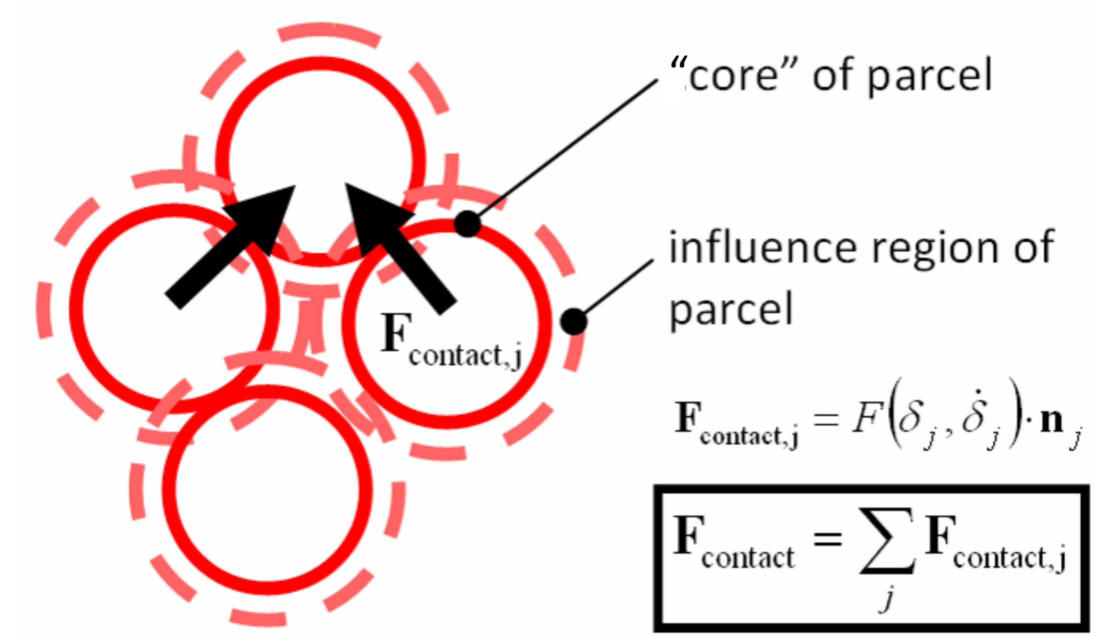
(Snider[1])



DPM

Parcel collisions

(Patankar and Joseph[2])



[1]Snider, ***JCP*** 170 (2001), 6014-6028. [2]Patankar and Joseph, ***IJMF*** 27 (2001), 1659-1684.

Questions on DEM to DPM

1. Quasi-static flow regime
   - How should the particle interaction parameters in DEM be scaled for the DPM?
2. Inertial flow regime
   - Is the scaling identified in quasi-static flow sufficient?
   - If not, what additional model is needed?

Quasi-Static Regime Scaling

- Dimensional analysis of a linear spring-dashpot model requires:[3]

$$\left.\begin{array}{l}\Pi_1 = k_n \Big/ \left(R_i \cdot \rho_p \cdot v_0^{\,2}\right) \\ \Pi_2 = c_n \Big/ \left(R_i^{\,2} \cdot \rho_p \cdot v_0\right)\end{array}\right\} = const$$

c_n...damping coefficient

k_n...spring stiffness

R_i...radius of parcel i

v_0...char. impact velocity

ω...rotation rate

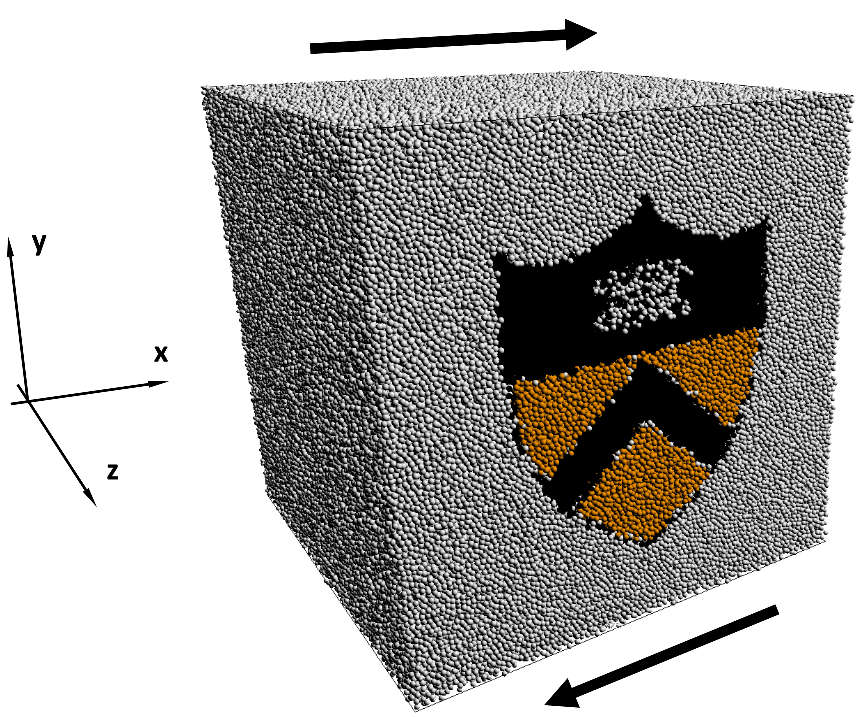
Π...dimensionless parameters

ρ_p...parcel density

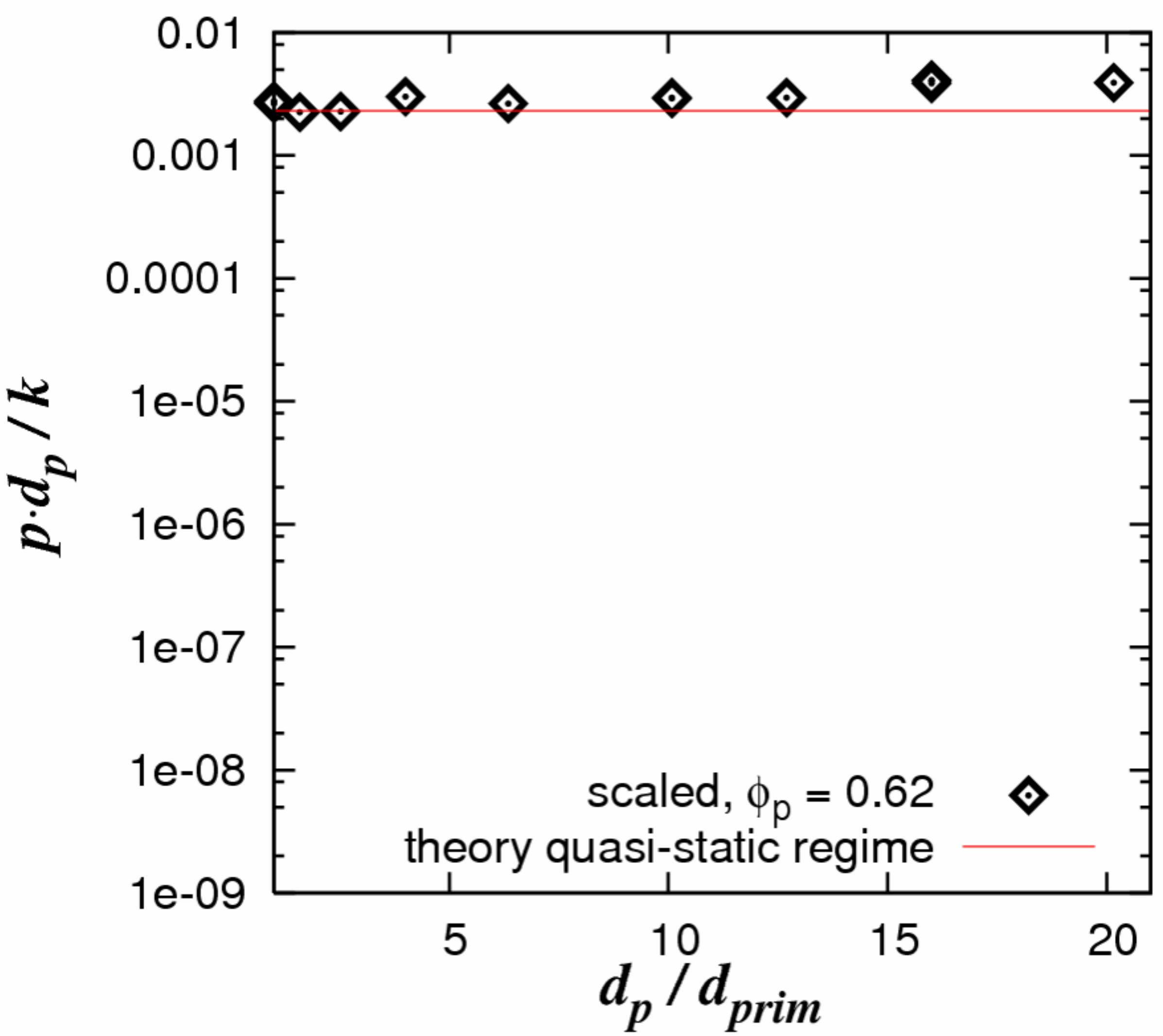
[3]Bierwisch, *PhD Thesis* (2009), University of Freiburg.

Simple shear in quasi-static regime

- Spring stiffness and damping coefficient are adjusted as stipulated by dimensional analysis.
- Stresses in the quasi-static regime (Φp = 0.62) are nearly constant.



Pressure



Inertial flow regime scaling

- Spring stiffness and damping coefficient are adjusted as stipulated by dimensional analysis
- Model unresolved collisions with BGK-like relaxation[4]
  - Try to achieve consistency with DEM by taking parcel-to-particle diameter ratio α into account.

$$1/\tau_{relax} = \underbrace{1/\tau_{coll}}_{} \underbrace{(1 - 1/\alpha)}_{}$$

collision time from kinetic theory

factor to guarantee consistency with DEM

α...ratio of parcel and primary particle diameter

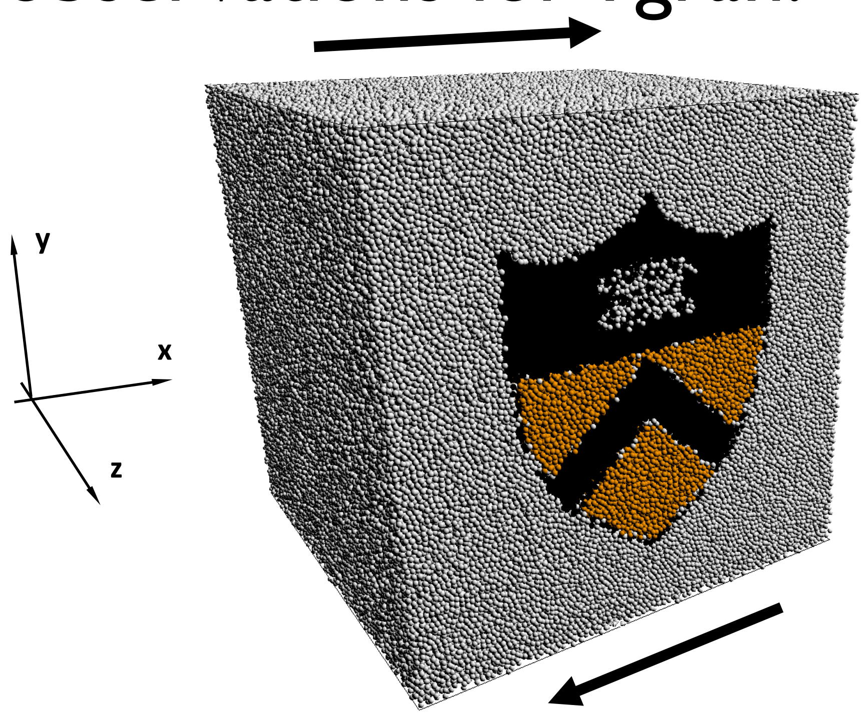
τ_{coll}...collision time

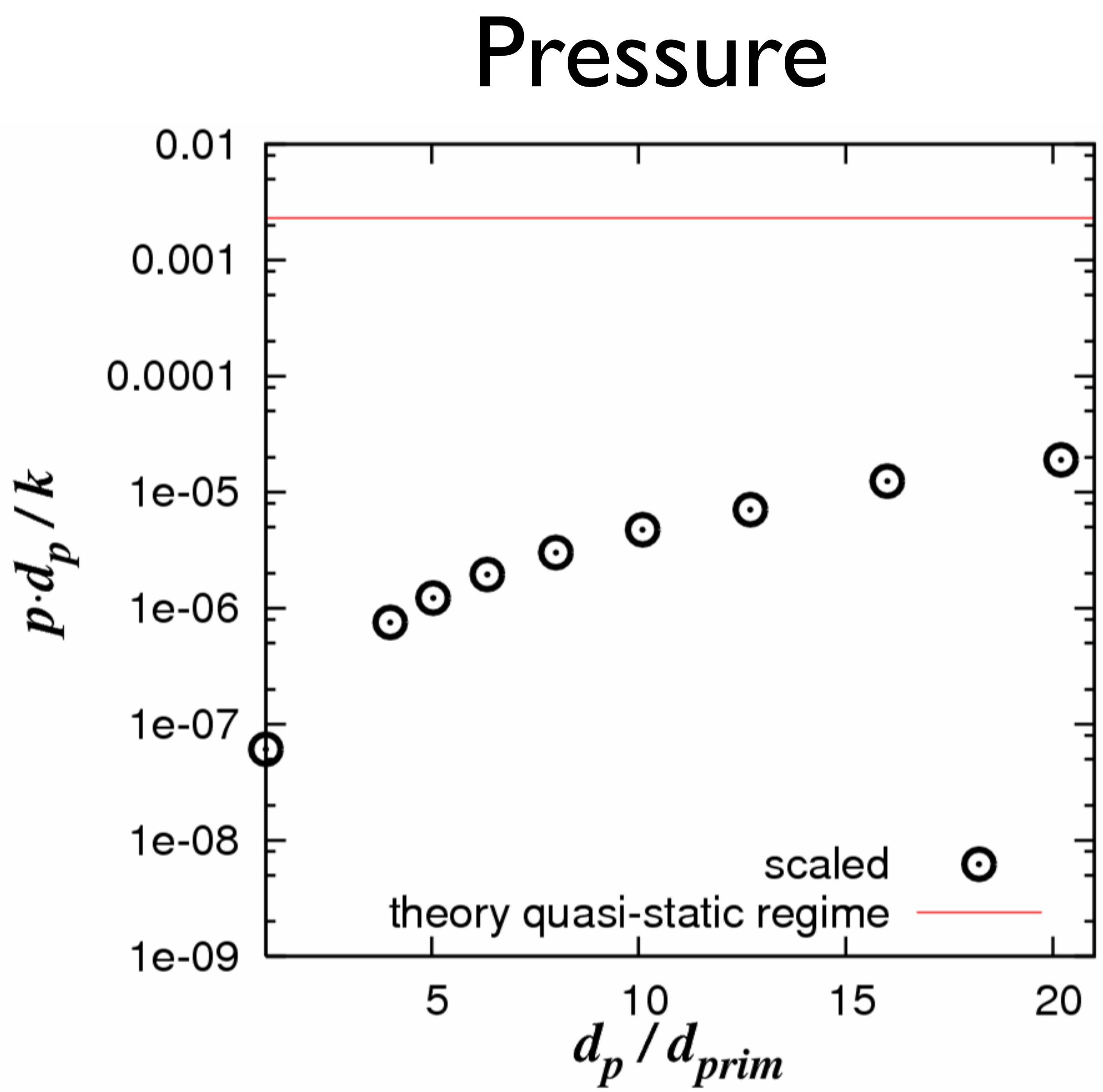
τ_{relax}...relaxation time

[4]O'Rourke and Snider, ***CES*** 65 (2010), 6014-6028

Simple shear in inertial regime

- Massive increase in stress in the inertial regime ($\Phi p = 0.55$). Similar observations for Tgran.[5]





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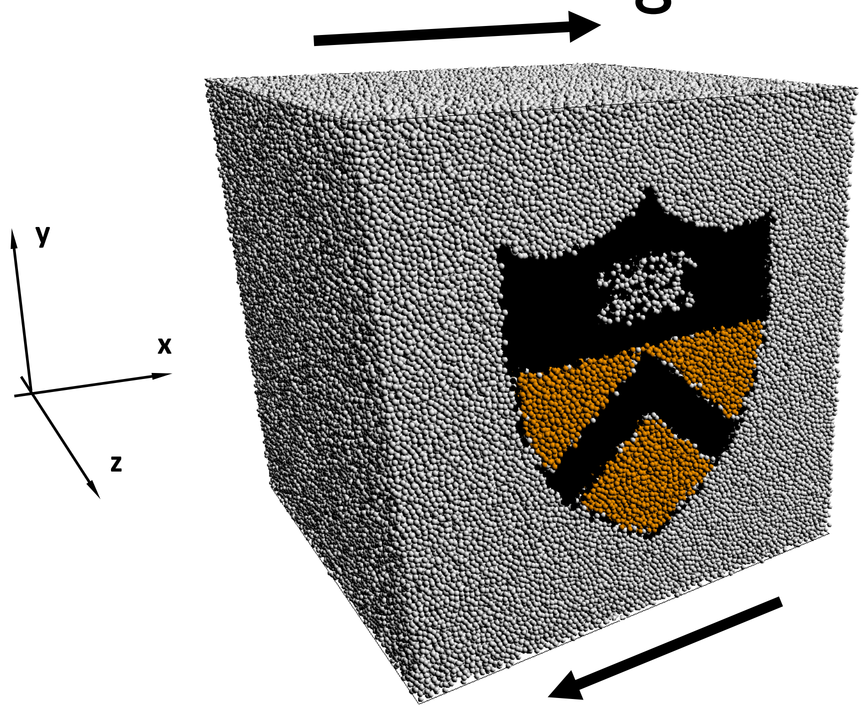

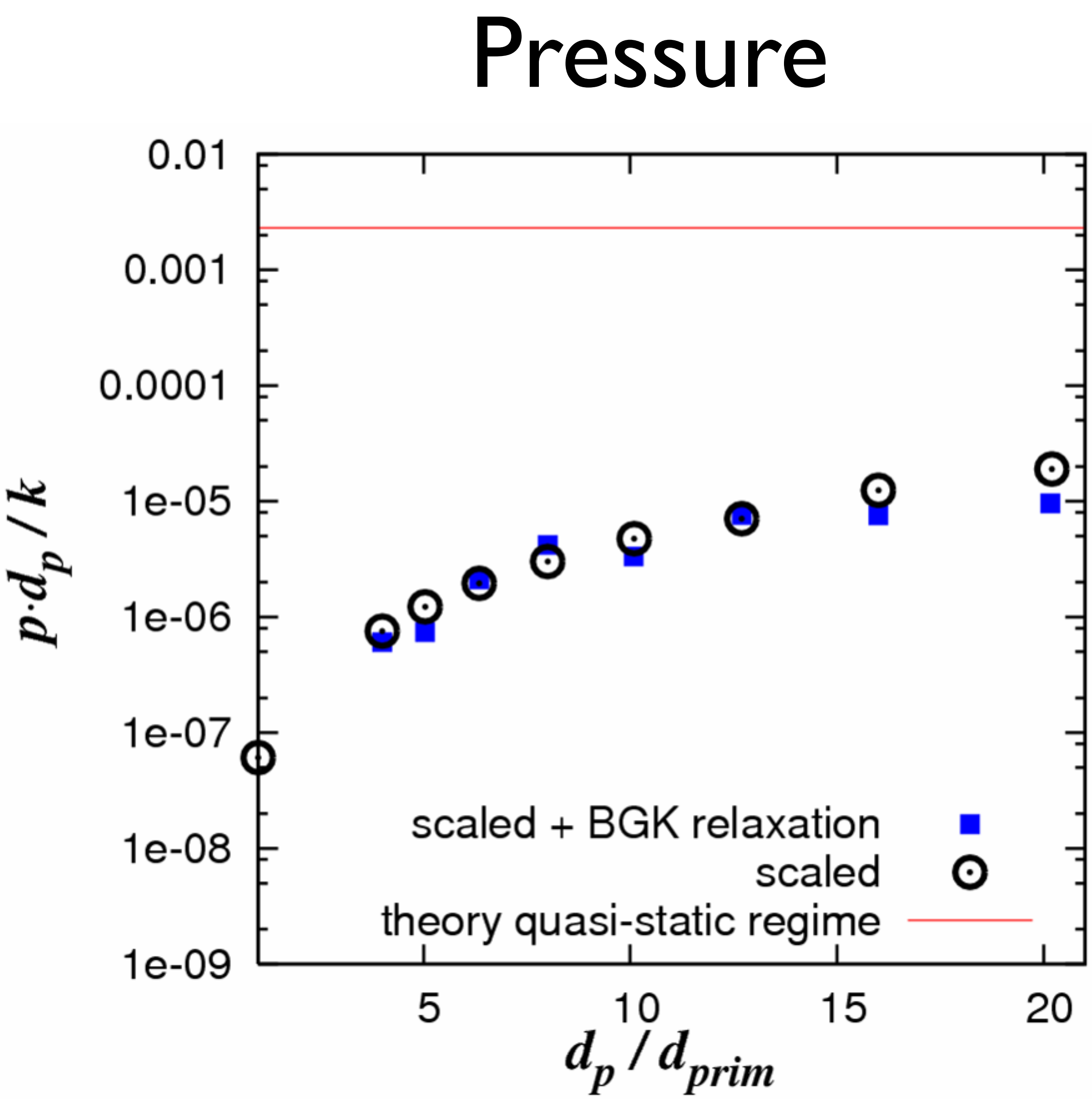

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Granular Jet

- Comparison of **scattering pattern** of particles with experiments.[5]

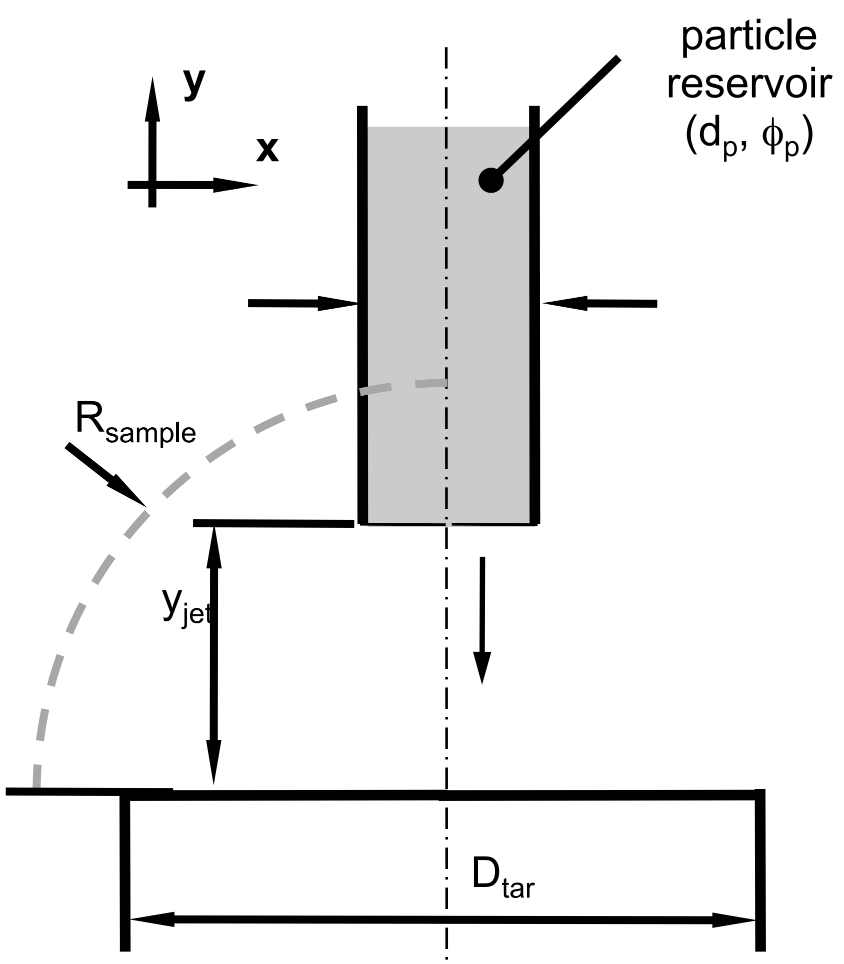


Figure: Setup used for the granular jet computations.

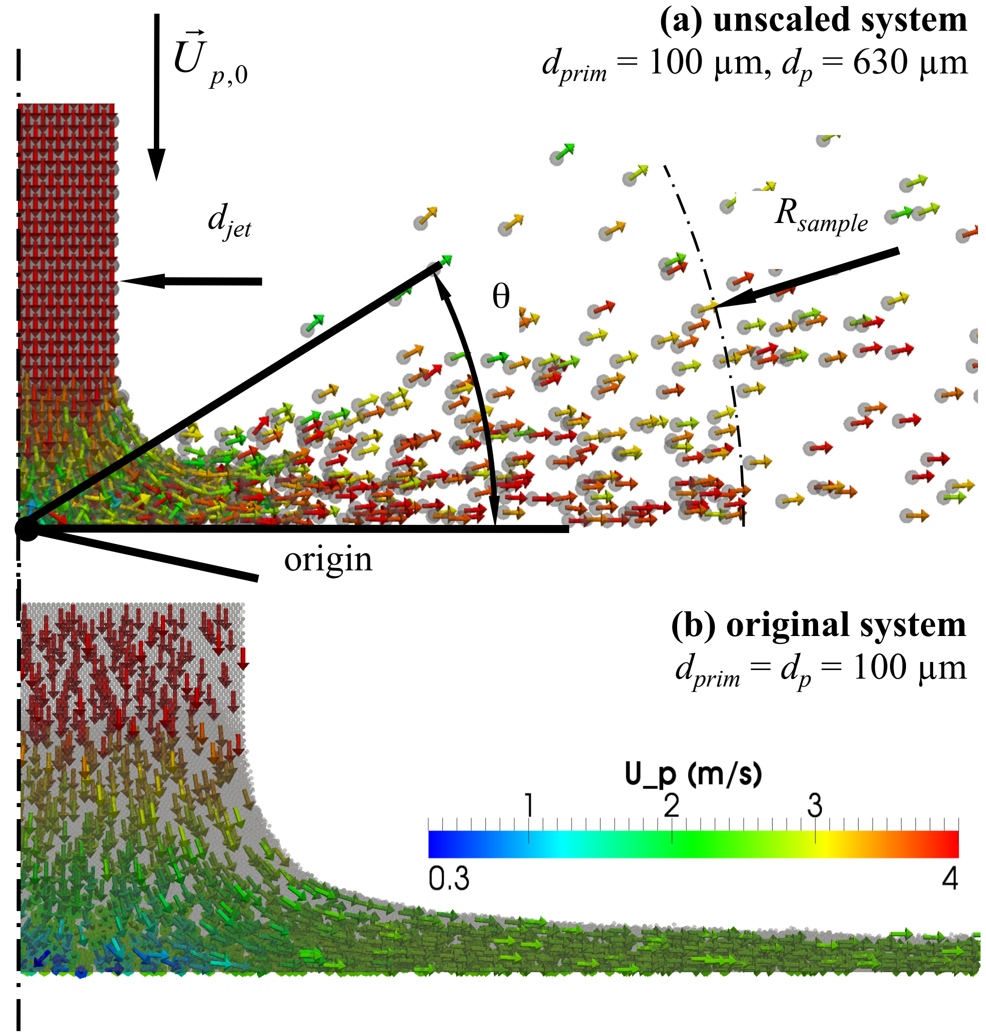
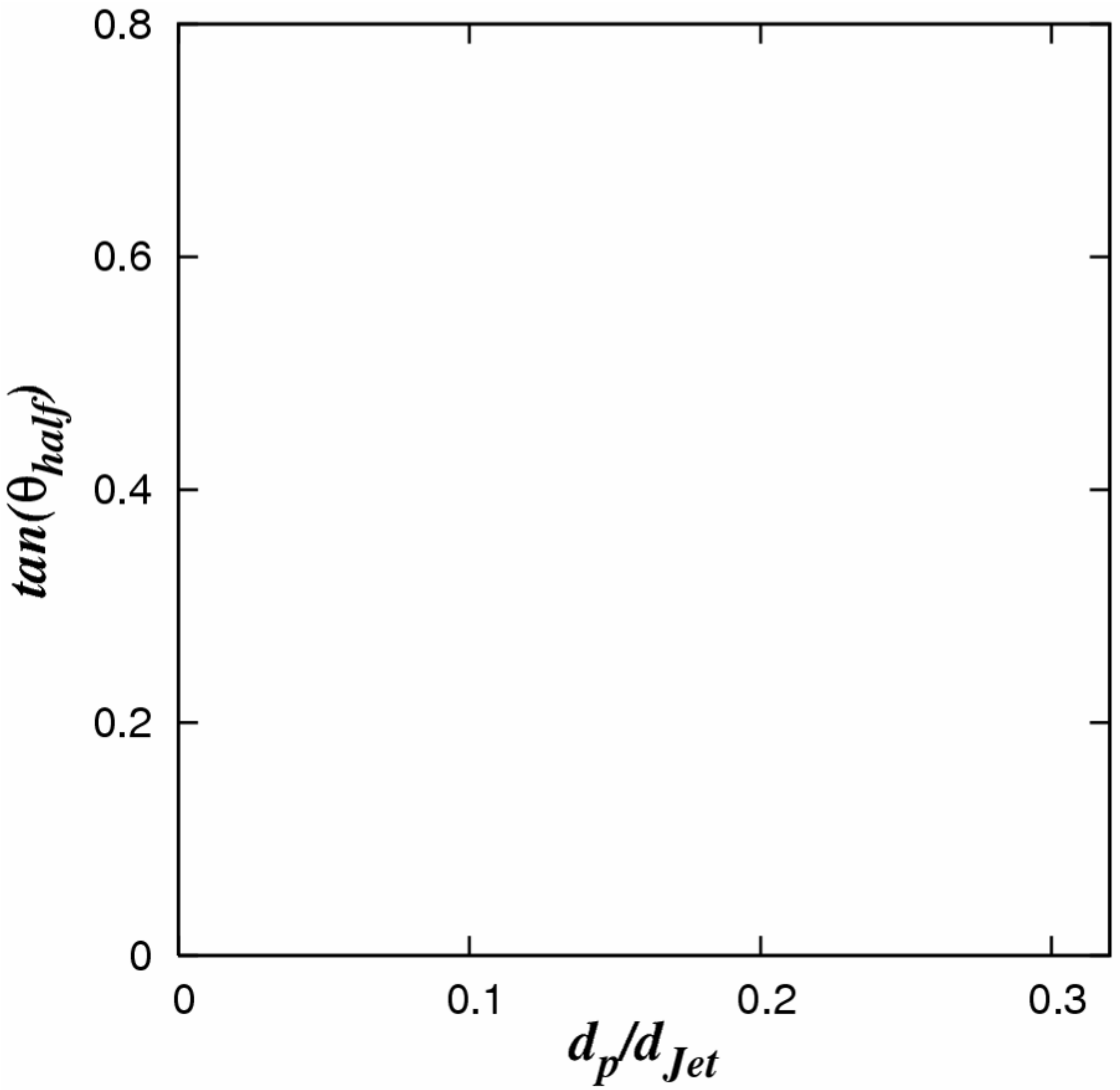


Figure: Particle velocities near the impact region of a granular jet.

[5]Cheng et al., ***PRL*** 99 (2007), 188001-188004.

Granular Jet

Scattering half angle θ_{half} $$\int_0^{\theta_{half}} P(\theta)\,d\theta = 0.5$$



P(θ)...Number density distribution of the scattering angle θ

Granular Jet

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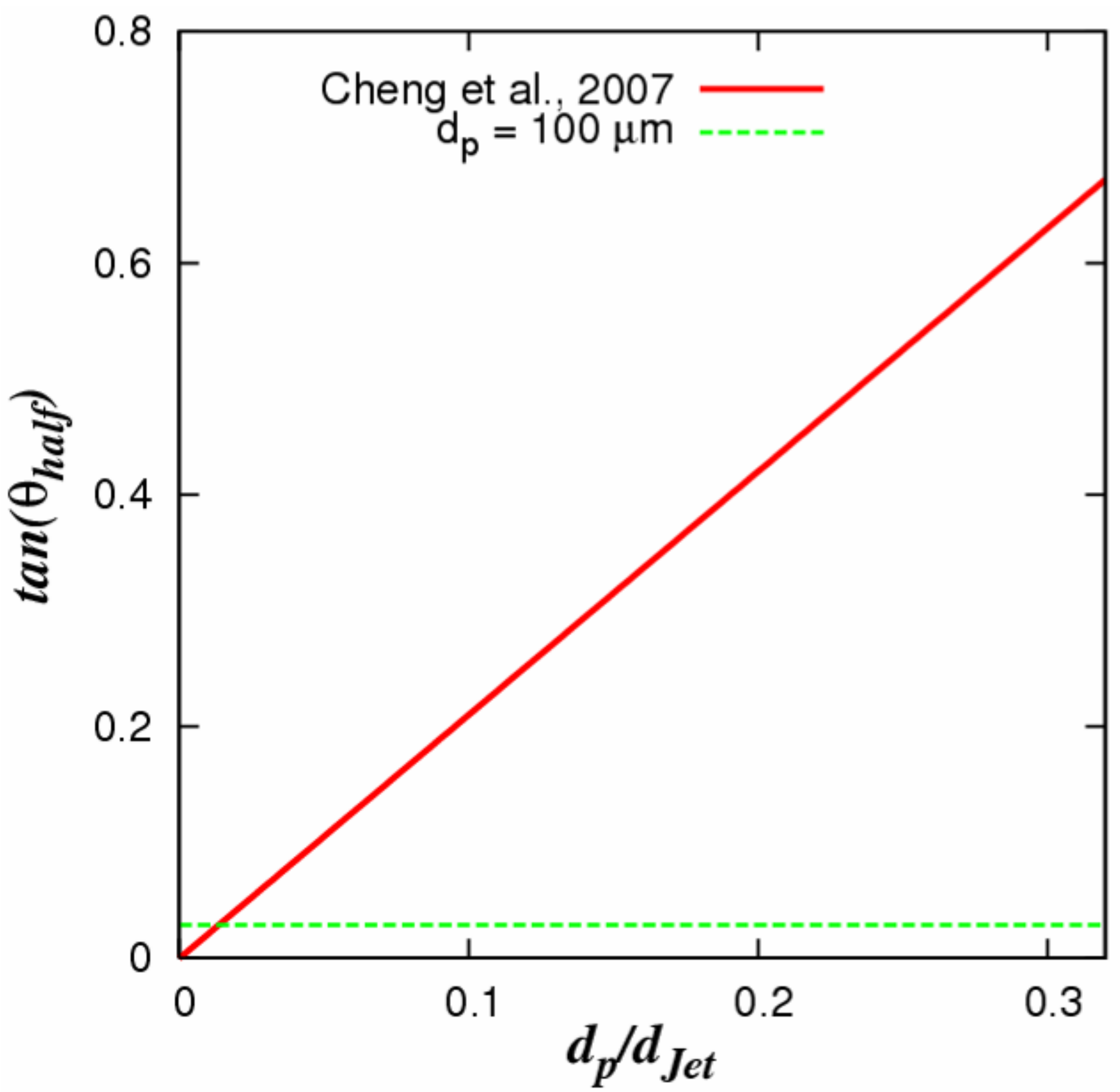

- **Cheng's** prediction:

$$\tan(\theta_{half}) = 2.1 \times d_p / d_{jet}$$

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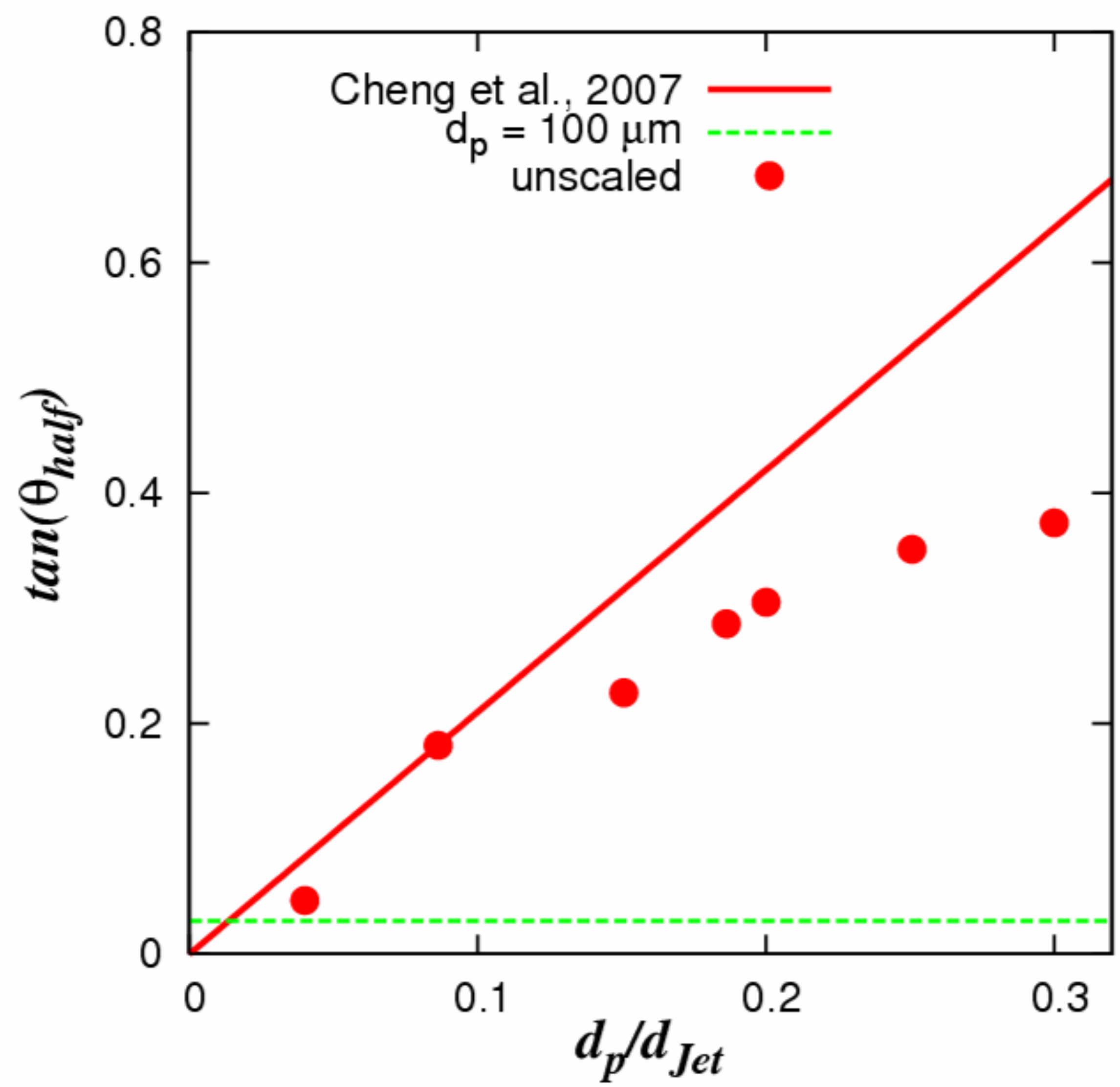

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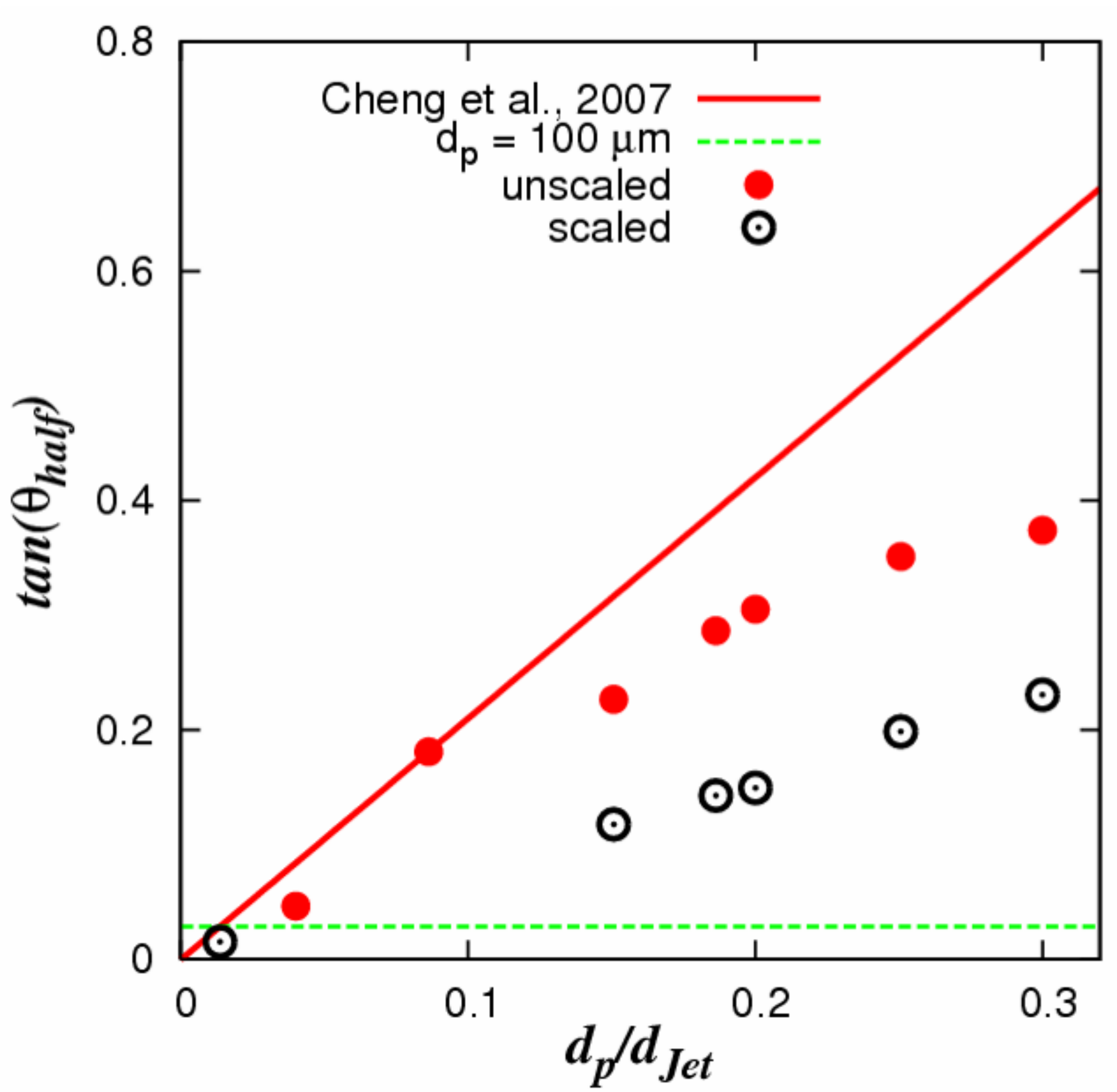

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- **Scaled system** also **overpredicts scattering angle.**

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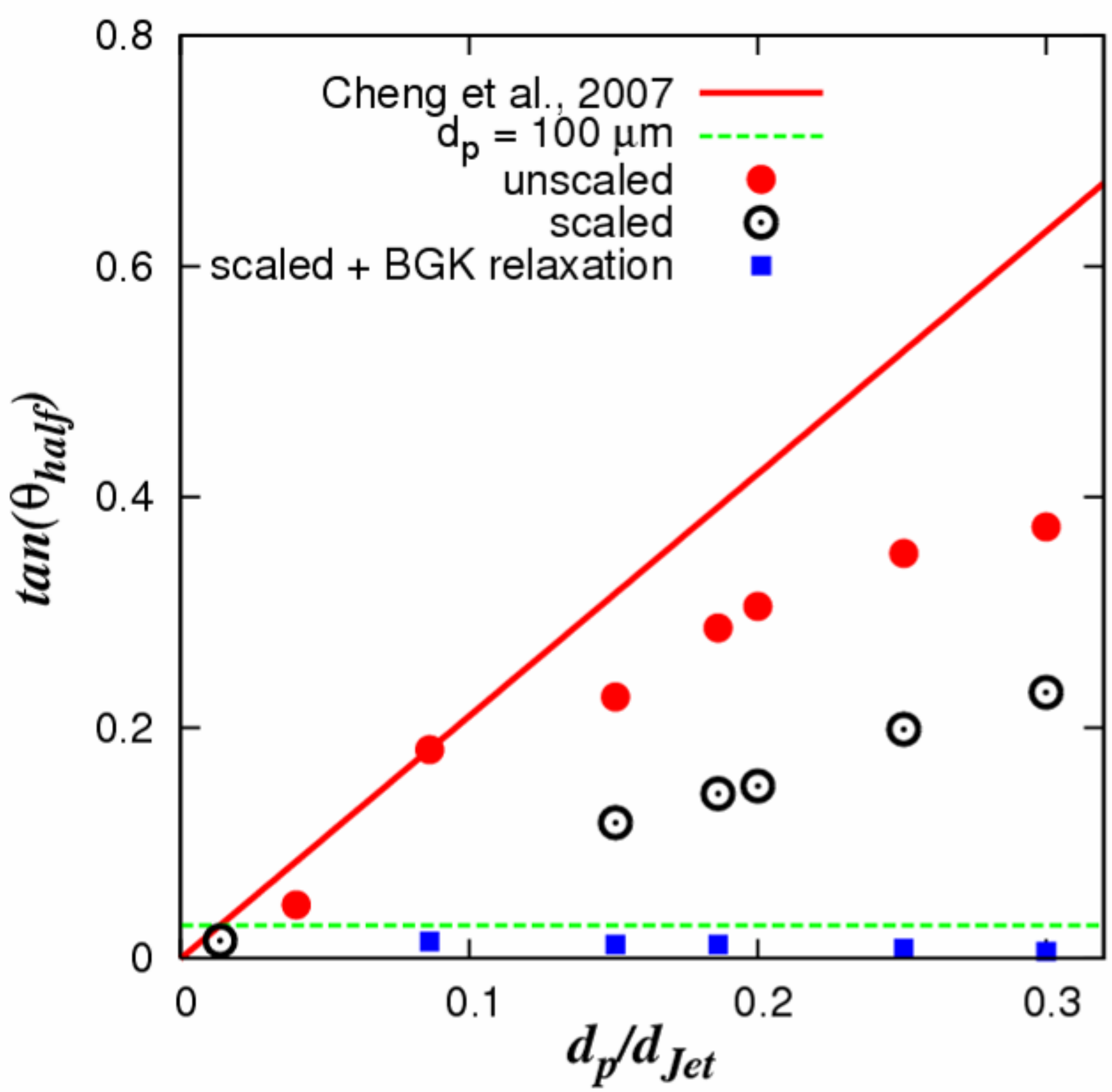

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- **Unscaled system** behaves like a system with **larger primary particles**.
- **Scaled system** also **overpredicts scattering angle.**
- **Improved agreement** when **BGK-like relaxation** is employed.

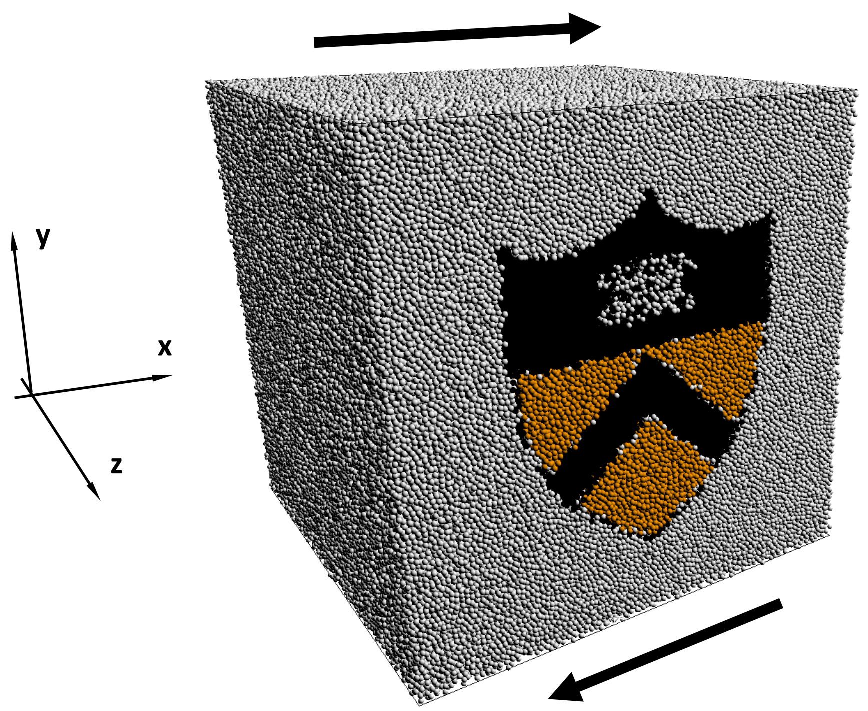
P(θ)...Number density distribution of the scattering angle θ

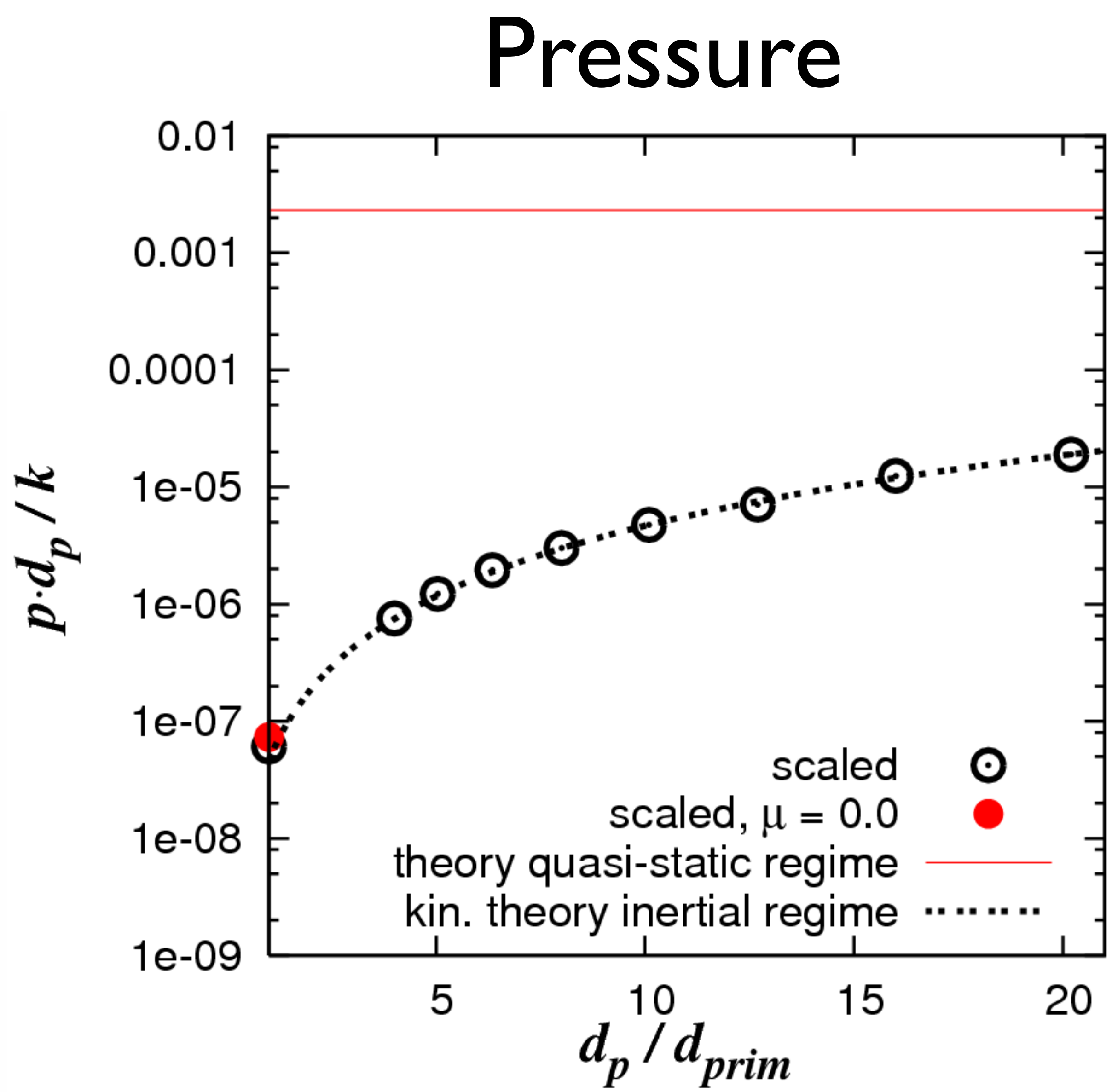
Summary

- Continuum model
  - We have formulated a continuum rheological model that spans all three regimes of flow and implemented in MFIX.
  - Preliminary results on chute flow have been obtained, but a systematic parametric study remains incomplete.
- Parcel-based simulation with collisions between parcels
  - Scaling DEM parameters for DPM in quasi-static flow regime readily follows from dimensional analysis.
  - Even with the addition of BGK-like relaxation, DPM cannot be made to yield the same stress as DEM in the inertial regime.
  - Particle jet data could be captured by DPM if BGK-like relaxation is included.

Simple shear in inertial regime

- Massive increase in stress in the inertial regime (Φp = 0.55).





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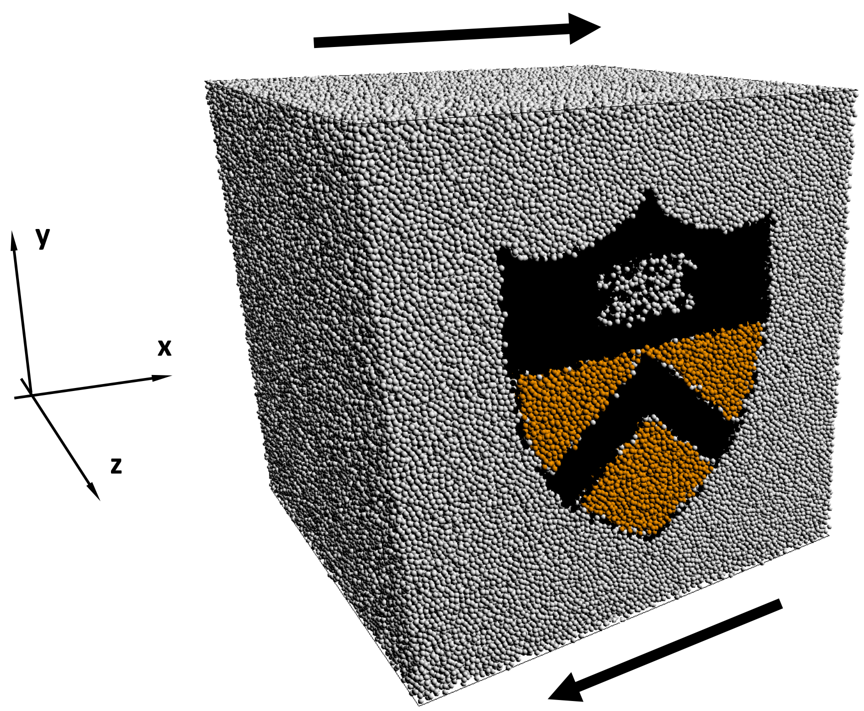

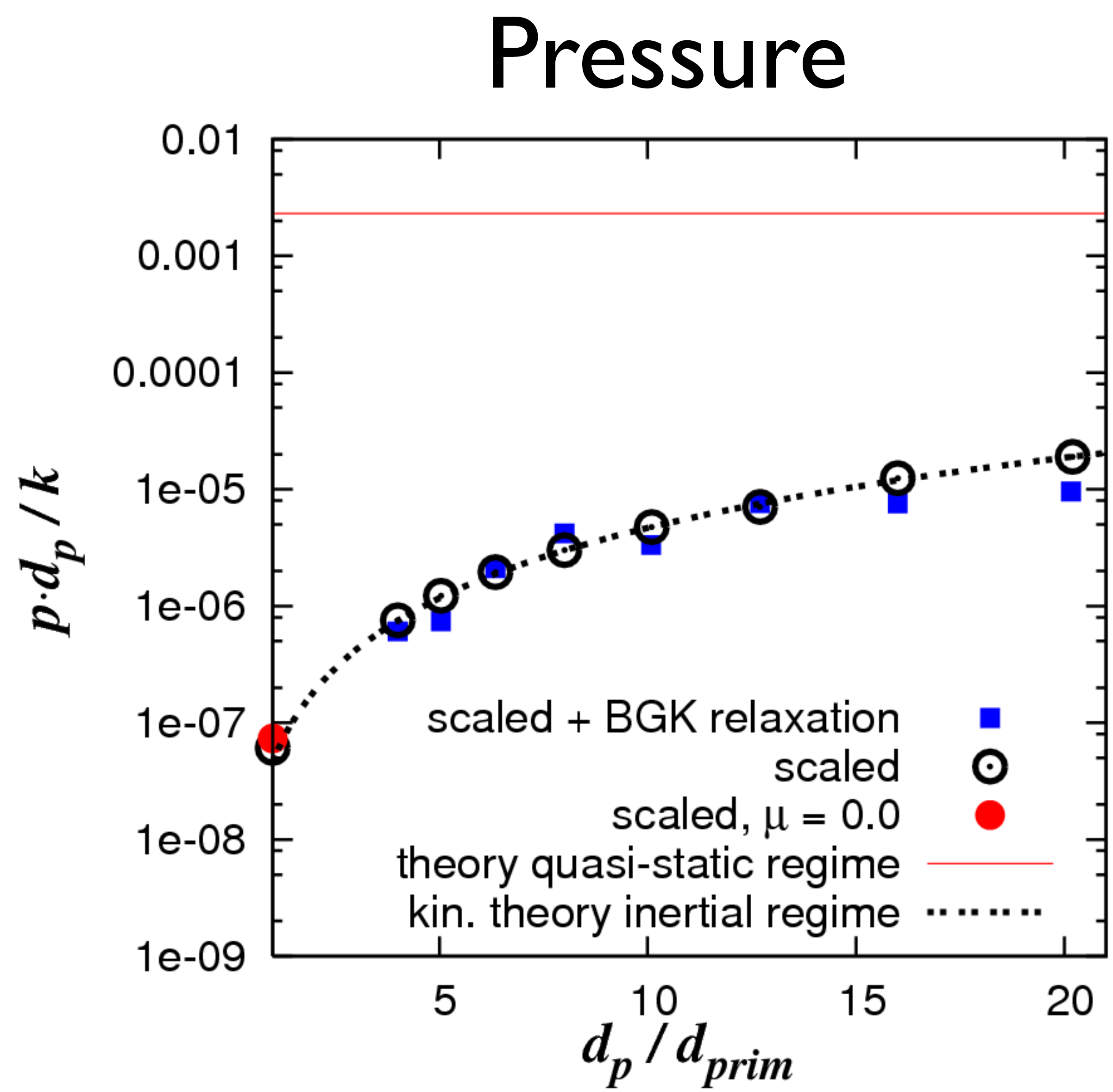

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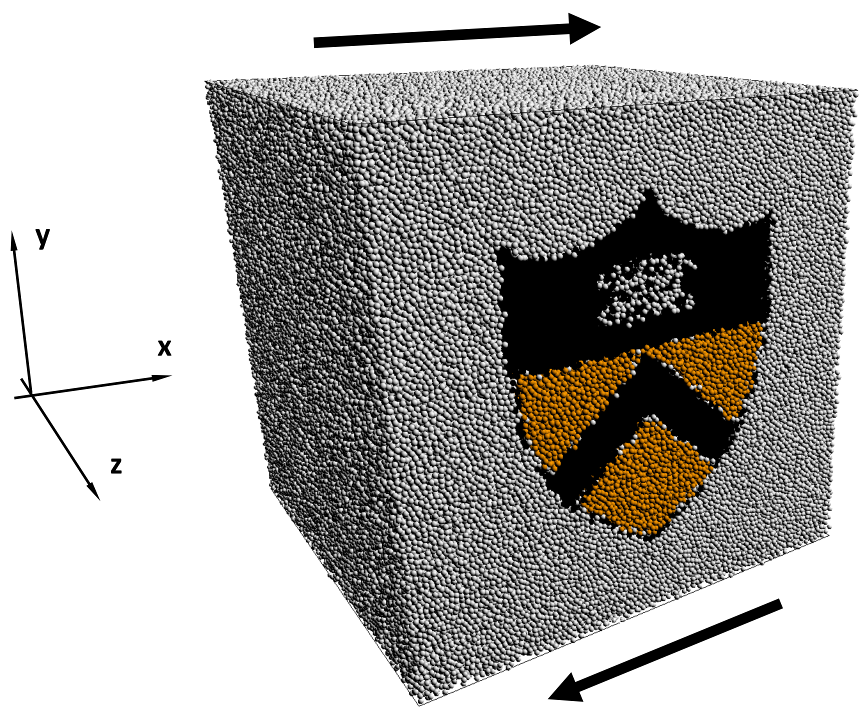

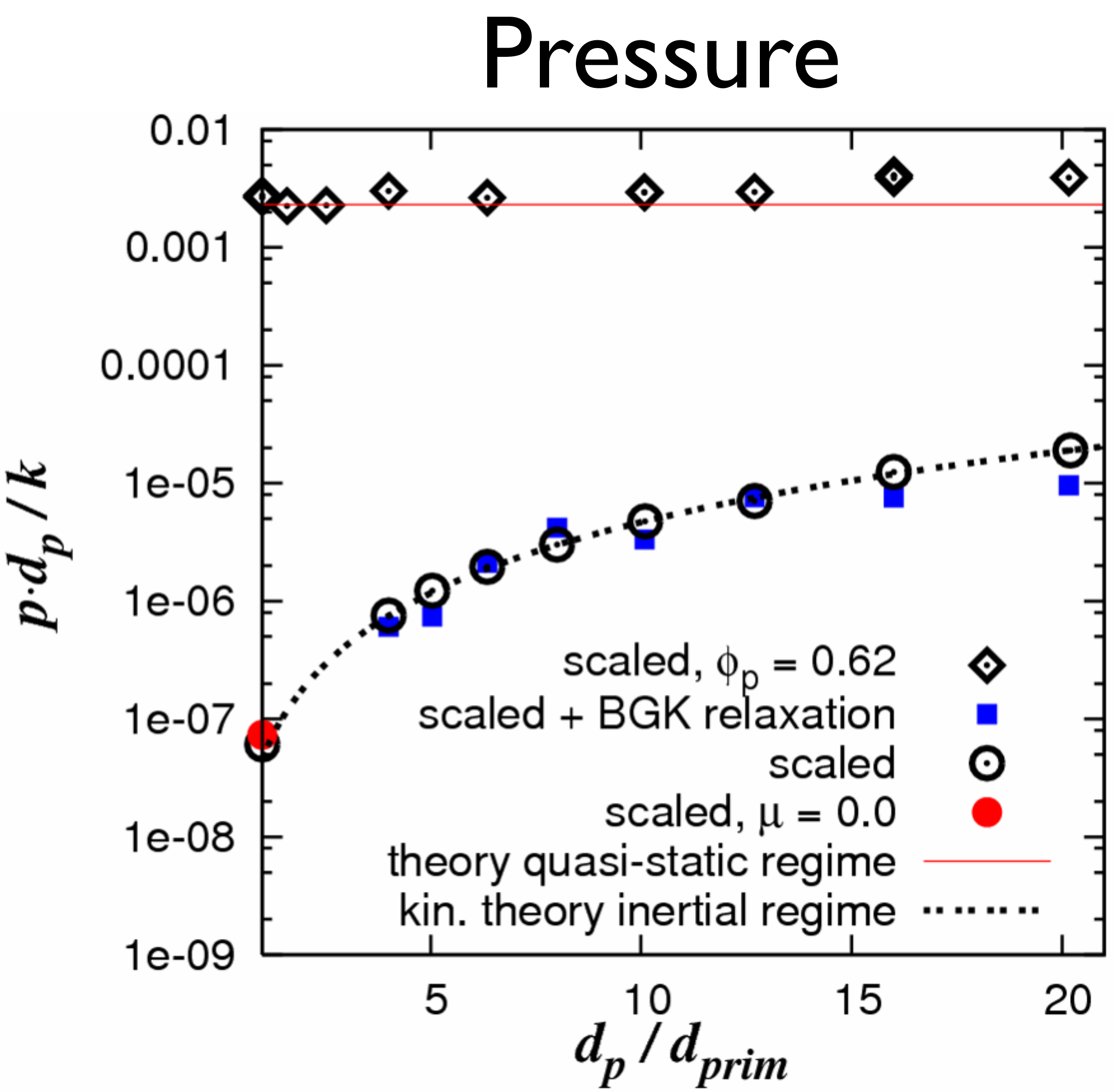

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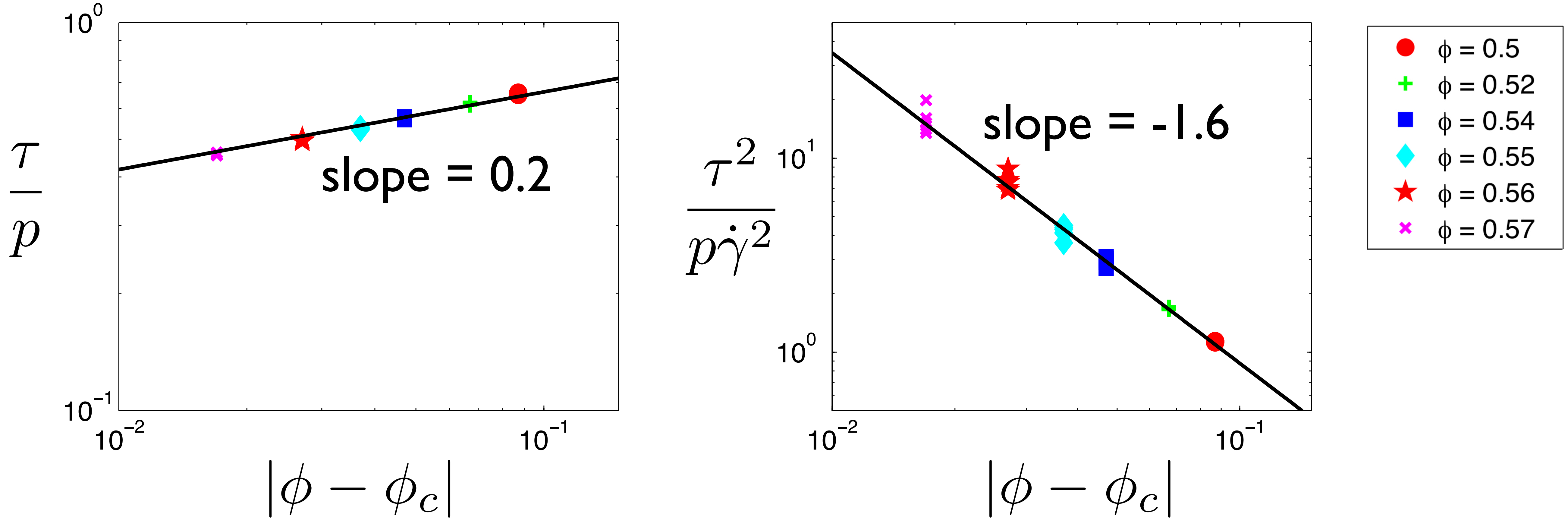
Work in progress

- Connect rheological behavior to changing microstructure.
- Refine the model for flows near bounding walls.
- Apply the model to
  - hopper and bin flows
  - shear bands

Stress scalings for frictional particles



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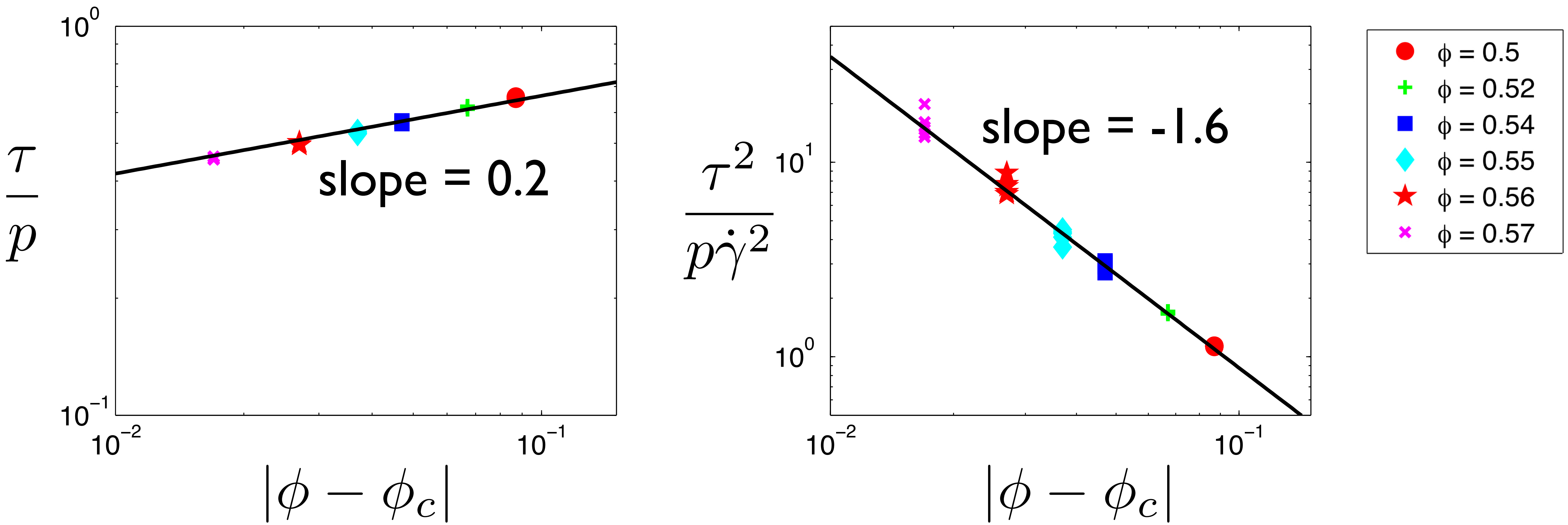

- From inertial regime data:

$$\frac{\tau}{p} \sim |\phi - \phi_c|^{0.2} \sim \frac{|\phi - \phi_c|^{a_2 - 2b_2}}{|\phi - \phi_c|^{a_1 - 2b_1}}$$

$$\frac{\tau^2}{p\dot{\gamma}^2} \sim |\phi - \phi_c|^{-1.6} \sim \frac{\left(|\phi - \phi_c|^{a_2 - 2b_2}\right)^2}{|\phi - \phi_c|^{a_1 - 2b_1}}$$

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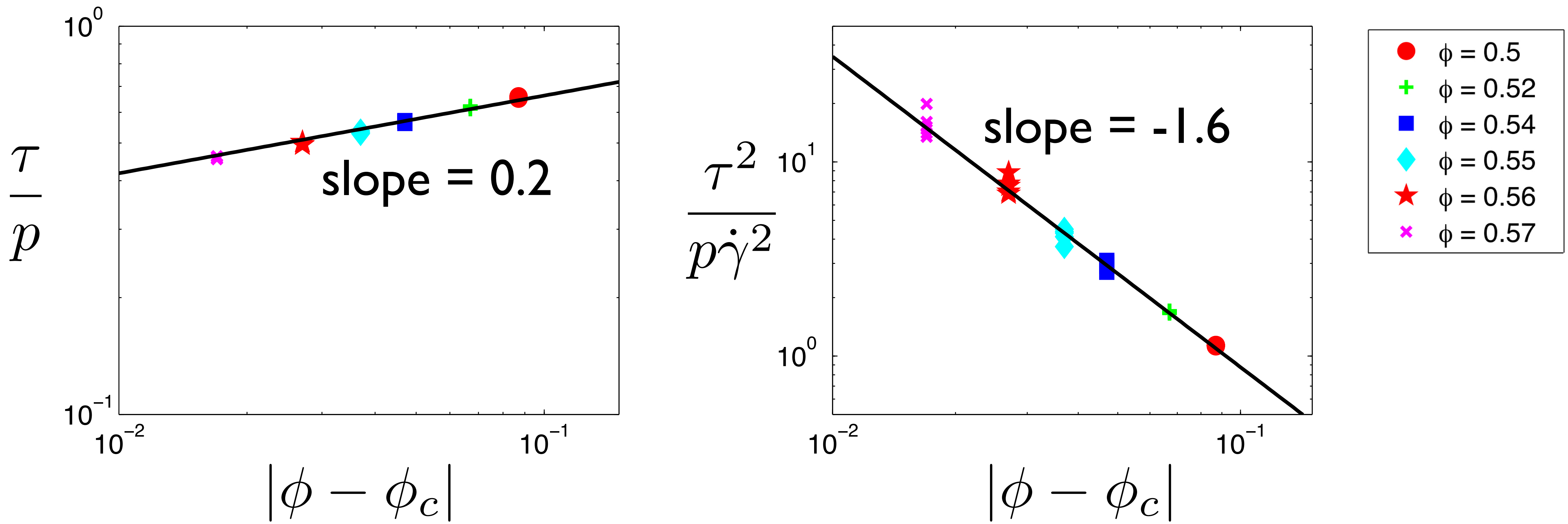

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$$\Rightarrow \quad b_1 = 1.5, \quad b_2 = 1.4$$

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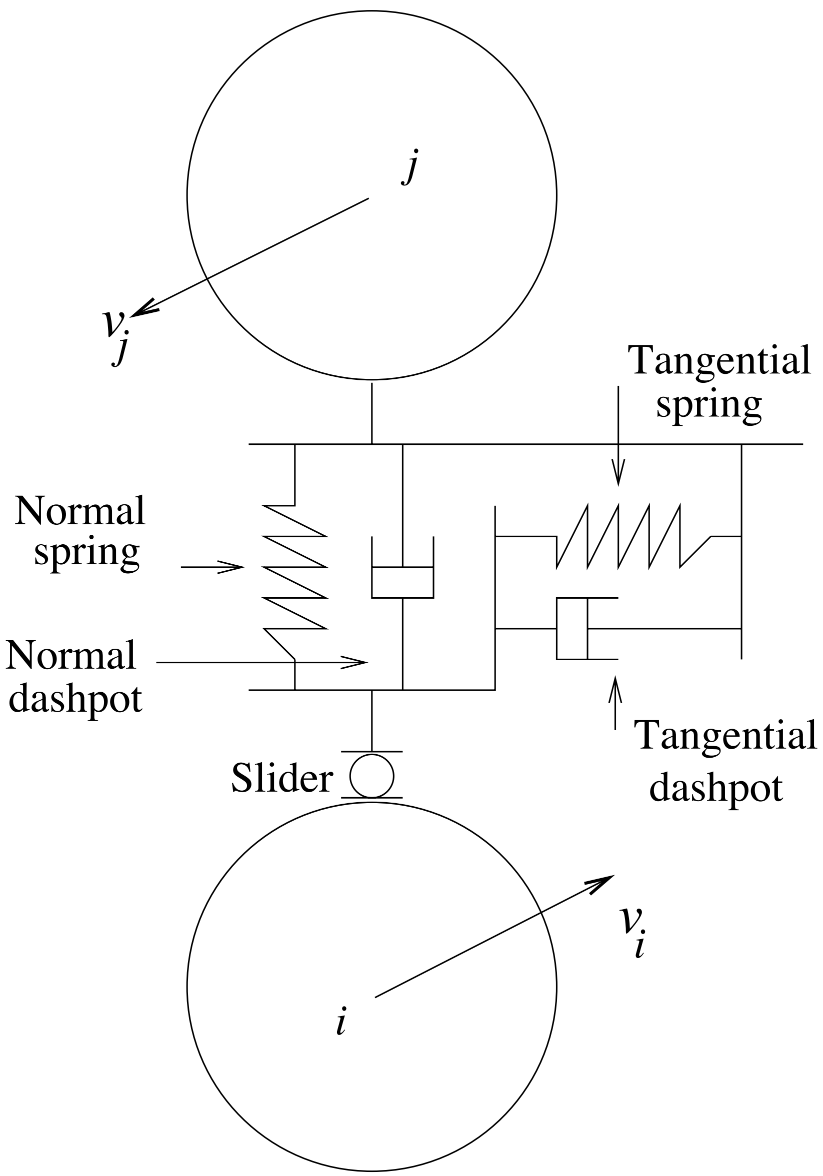

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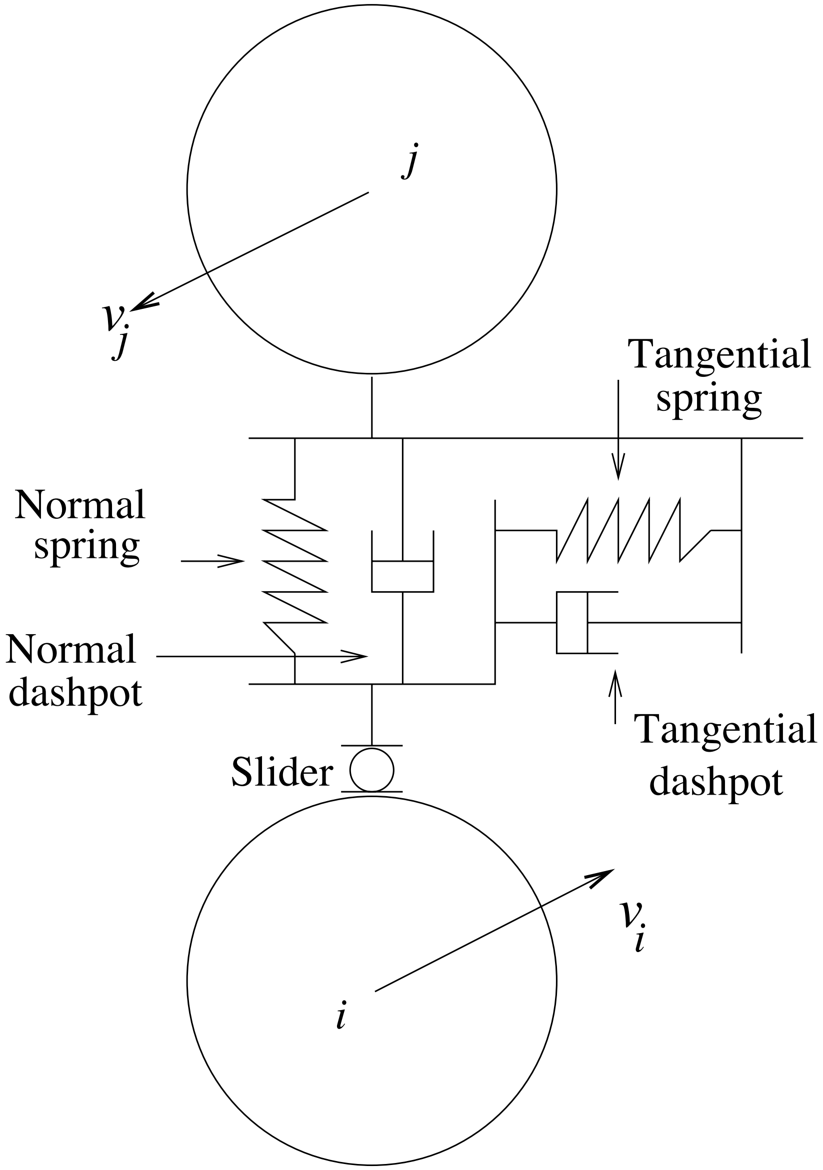
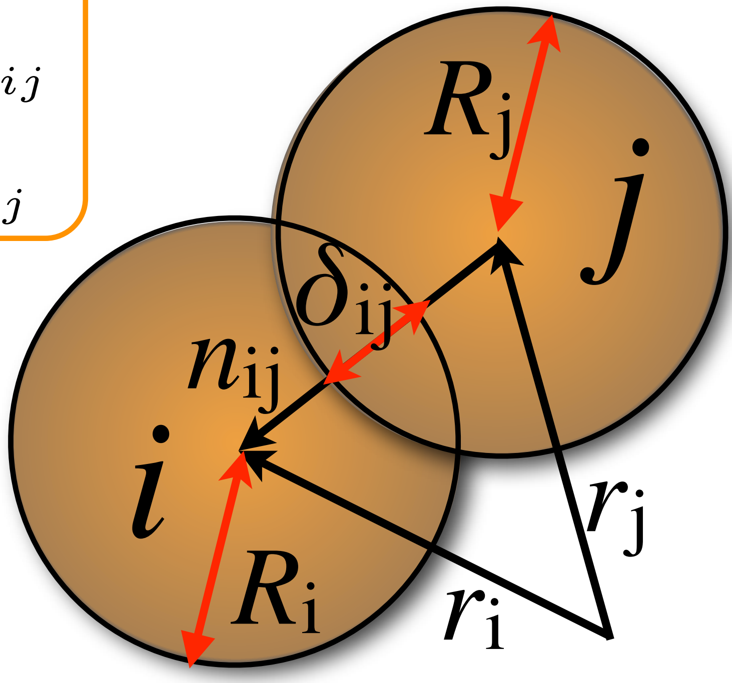


Linear (Hookean) model:

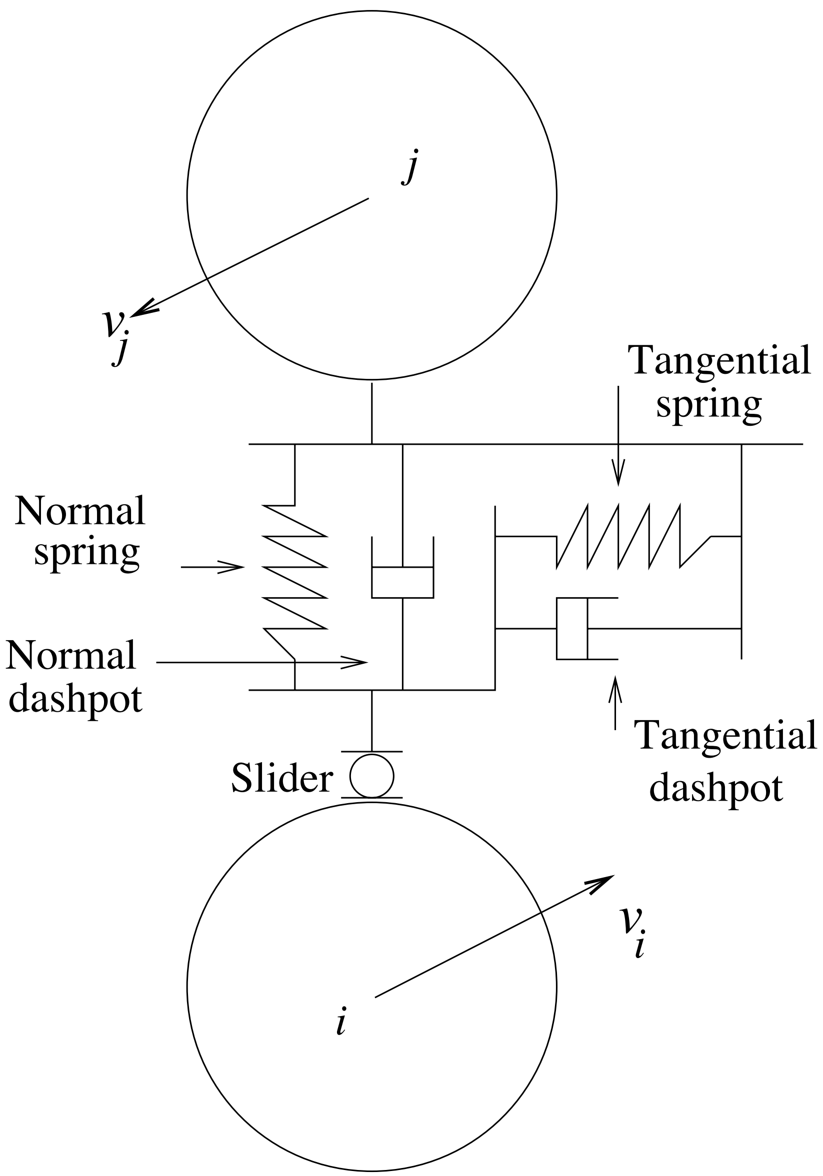
$$\mathbf{F}_{\mathrm{n}_{ij}} = k_{\mathrm{n}}\delta_{ij}\mathbf{n}_{ij} - \gamma_{\mathrm{n}} m^* \mathbf{v}_{\mathrm{n}_{ij}}$$
$$\mathbf{F}_{\mathrm{t}_{ij}} = -k_{\mathrm{t}}\mathbf{u}_{\mathrm{t}_{ij}} - \gamma_{\mathrm{t}} m^* \mathbf{v}_{\mathrm{t}_{ij}}$$



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

Discrete element method

- Numerically integrate equations of motion for every particle
- Short range ($r_c = d$) repulsive force based on spring-dashpot model



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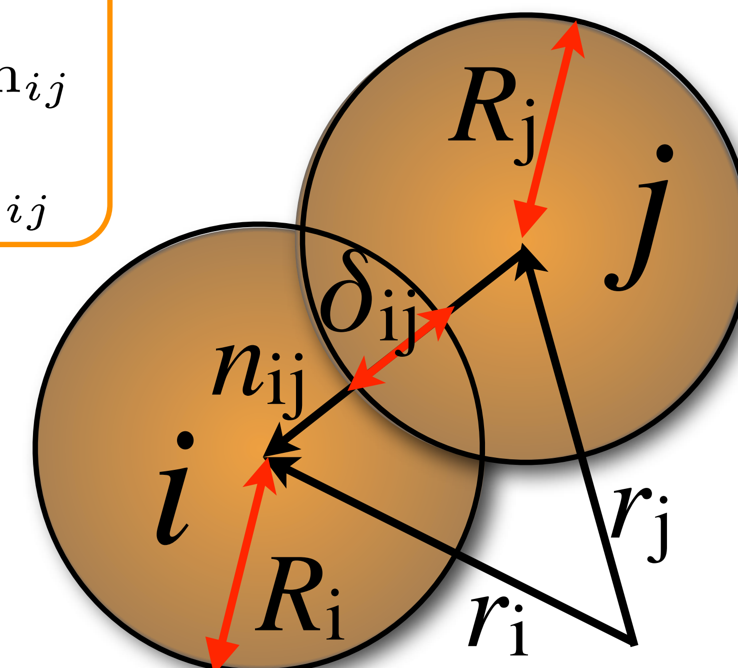

Non-linear (Hertzian) model:

$$\mathbf{F}_{ij\mathrm{HZ}} = \sqrt{\delta_{ij} R^*} \mathbf{F}_{ij\mathrm{HK}} \quad R^* = \frac{R_i R_j}{R_i + R_j}$$

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

Stress and microstructure

- Stress $\boldsymbol{\sigma} = \frac{1}{V}\sum_{i}^{N}\left[\sum_{j,j\neq i}\frac{1}{2}\mathbf{r}_{ij}\mathbf{F}_{ij} + m_i\mathbf{C}_i\mathbf{C}_i\right]$

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Exclude particles with zero or one contact

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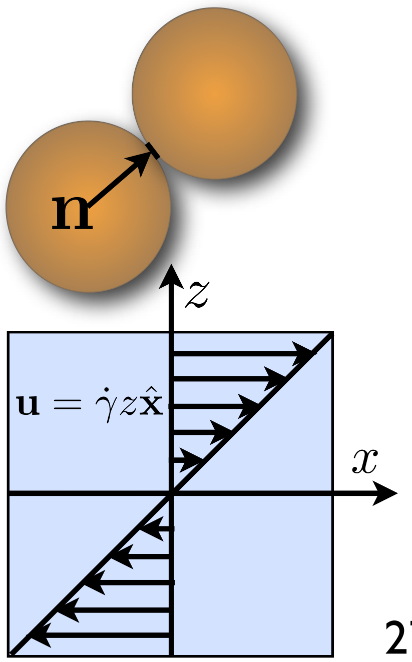
Exclude particles with zero or one contact

- Fabric tensor: average of dyadic product of unit contact normals

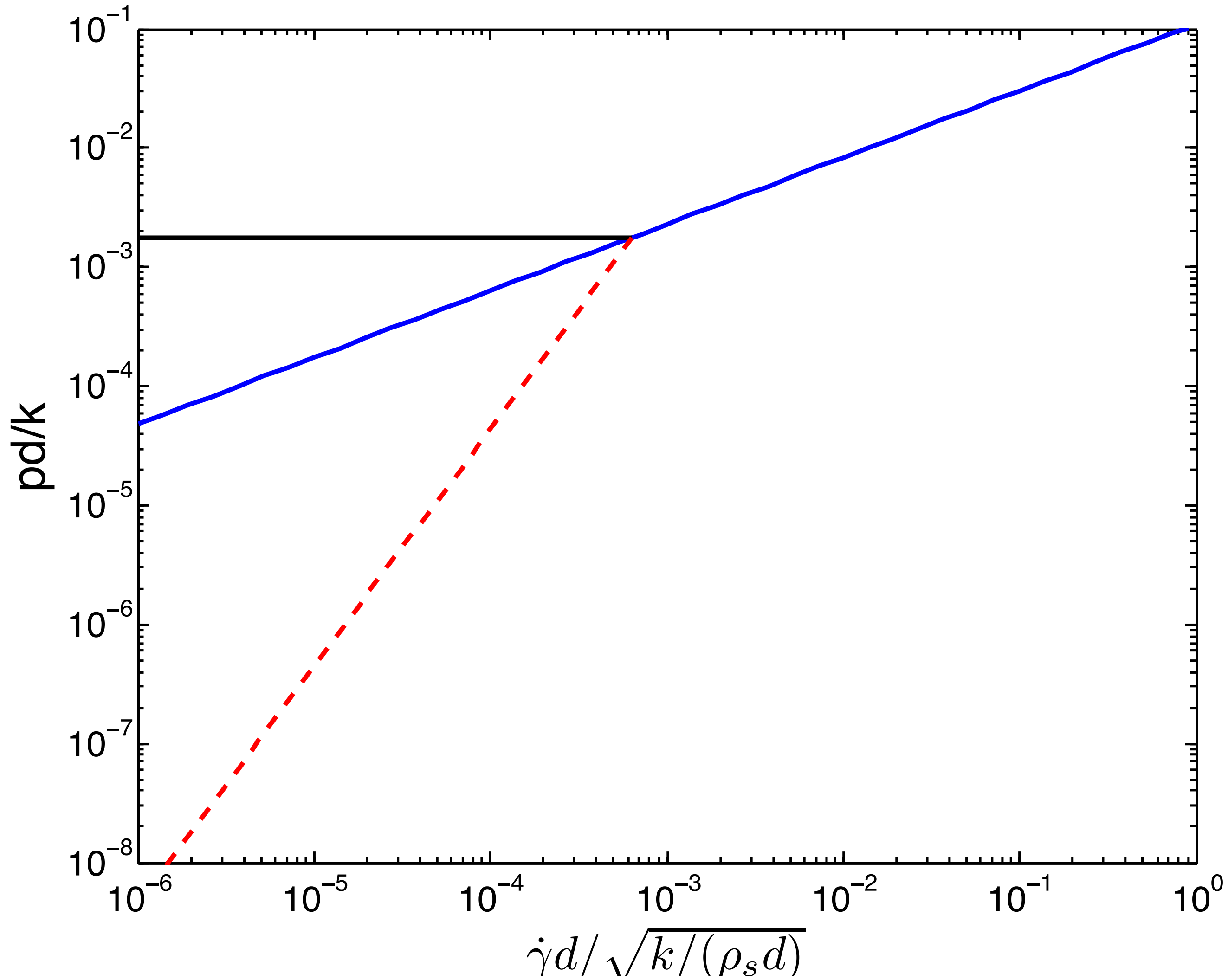
$$\mathrm{A} = \frac{1}{N_c}\sum_{\alpha=1}^{N_c}\mathbf{n}^{\alpha}\mathbf{n}^{\alpha} - \frac{\mathbf{1}}{\mathbf{3}}\mathrm{I}$$

N_c: number of contacts



A_{xz} magnitude indicates the microstructure anisotropy strength for simple shear flows; sign indicates the anisotropy direction for simple shear flows.

Bridging the regimes



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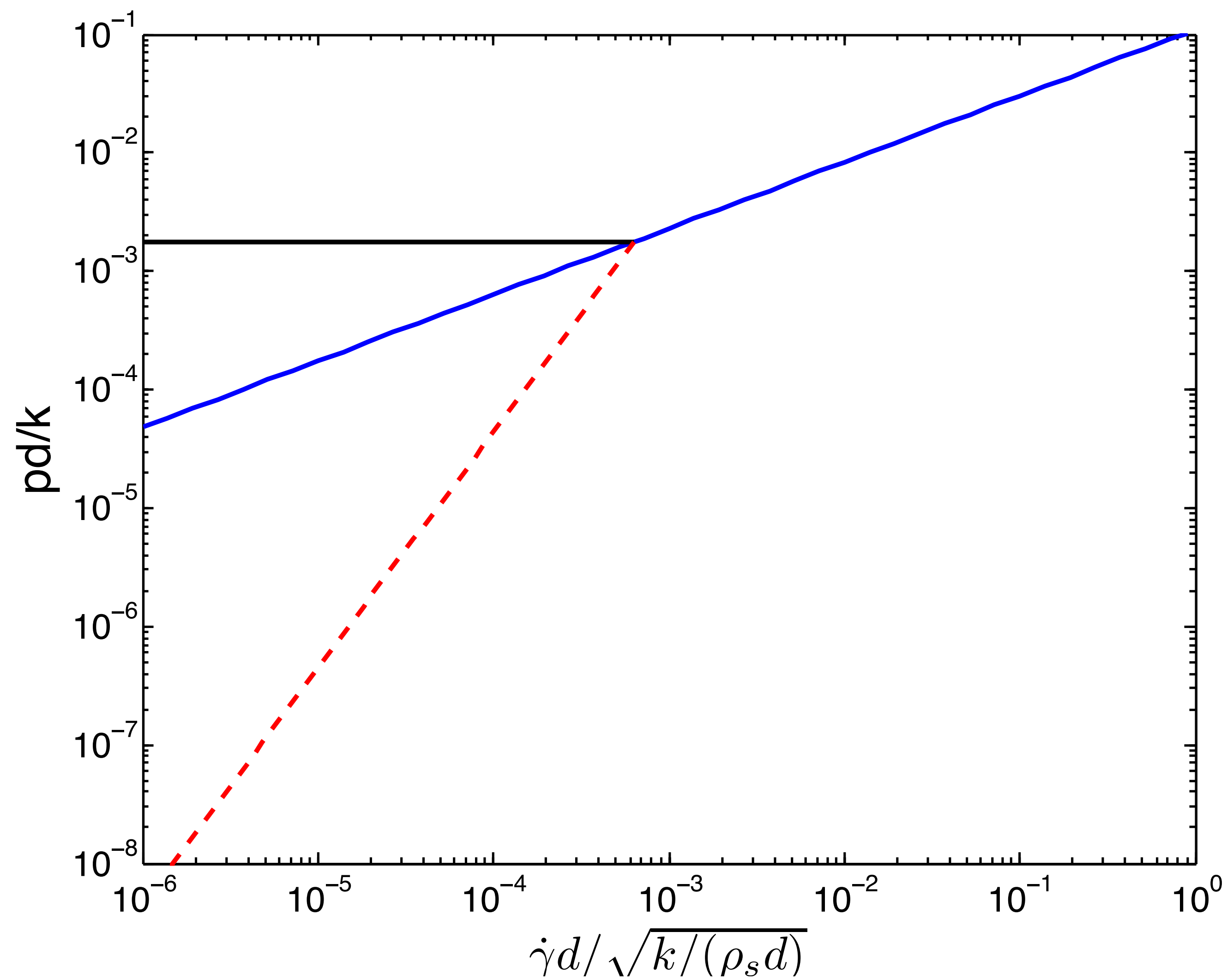

- Regime transitions can be modeled using a simple function to "blend" the asymptotes: $f = (f_1{}^m + f_2{}^m)^{1/m}$, $m = 1$ or -1 for quasi-static and inertial to intermediate transitions, respectively.

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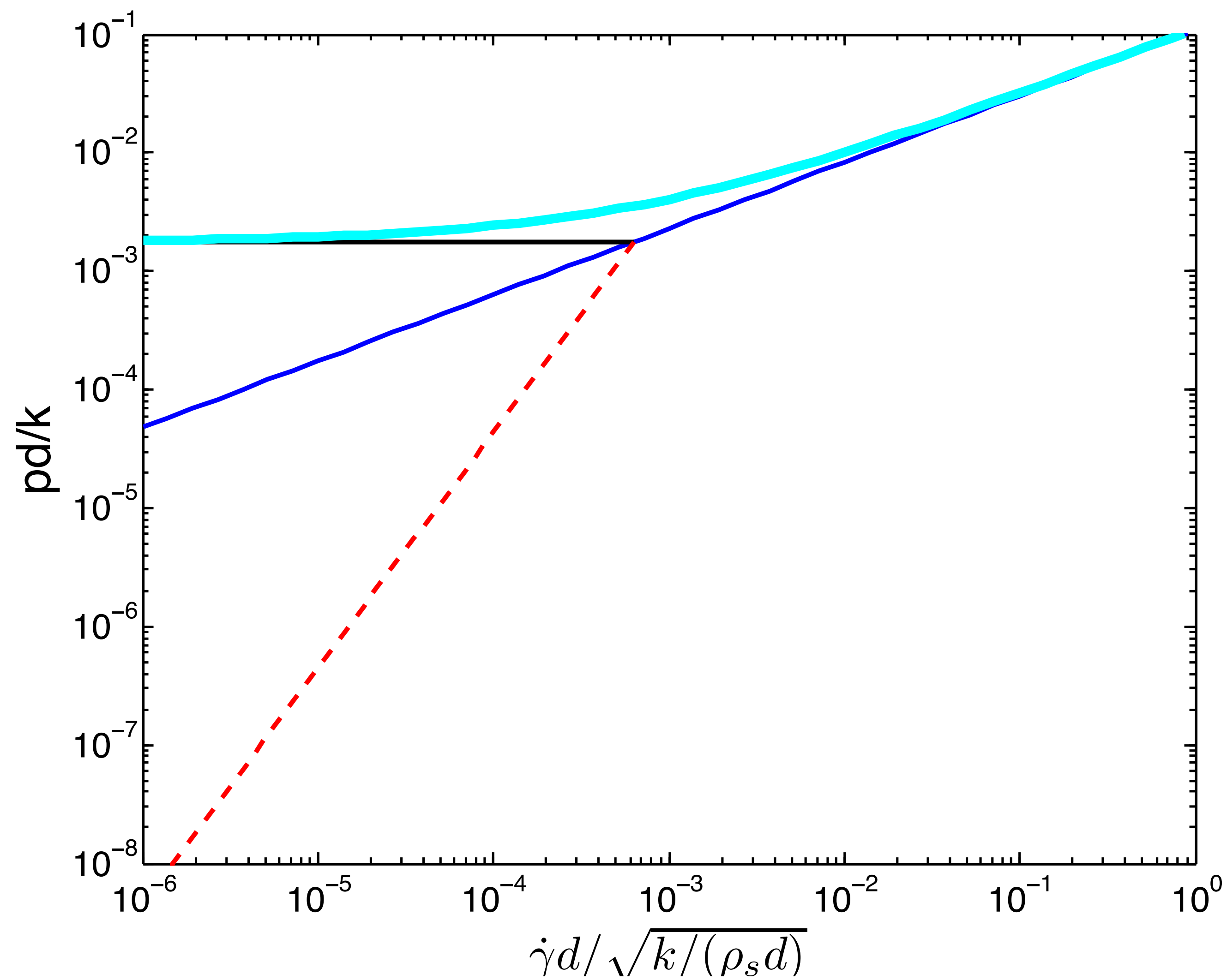

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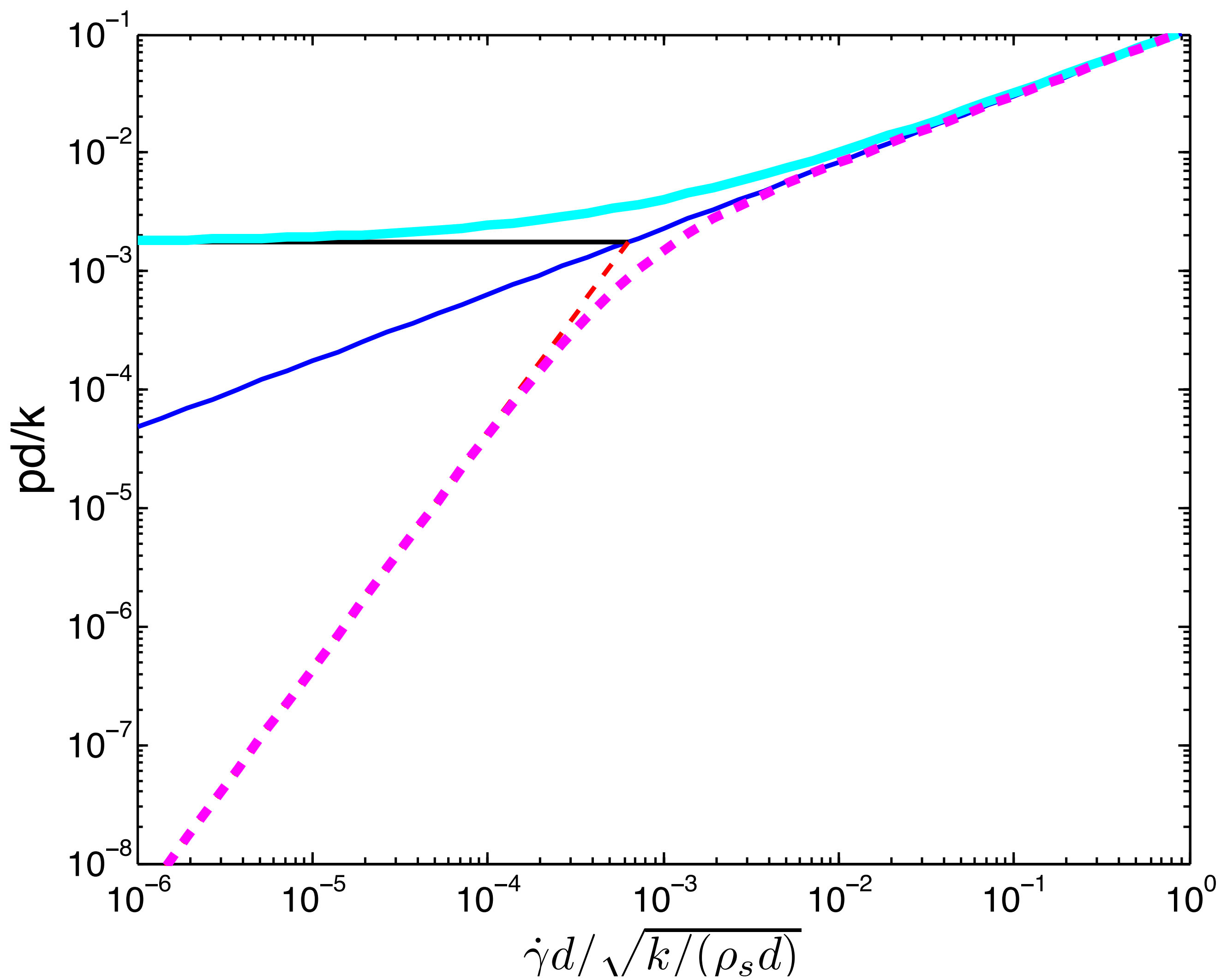

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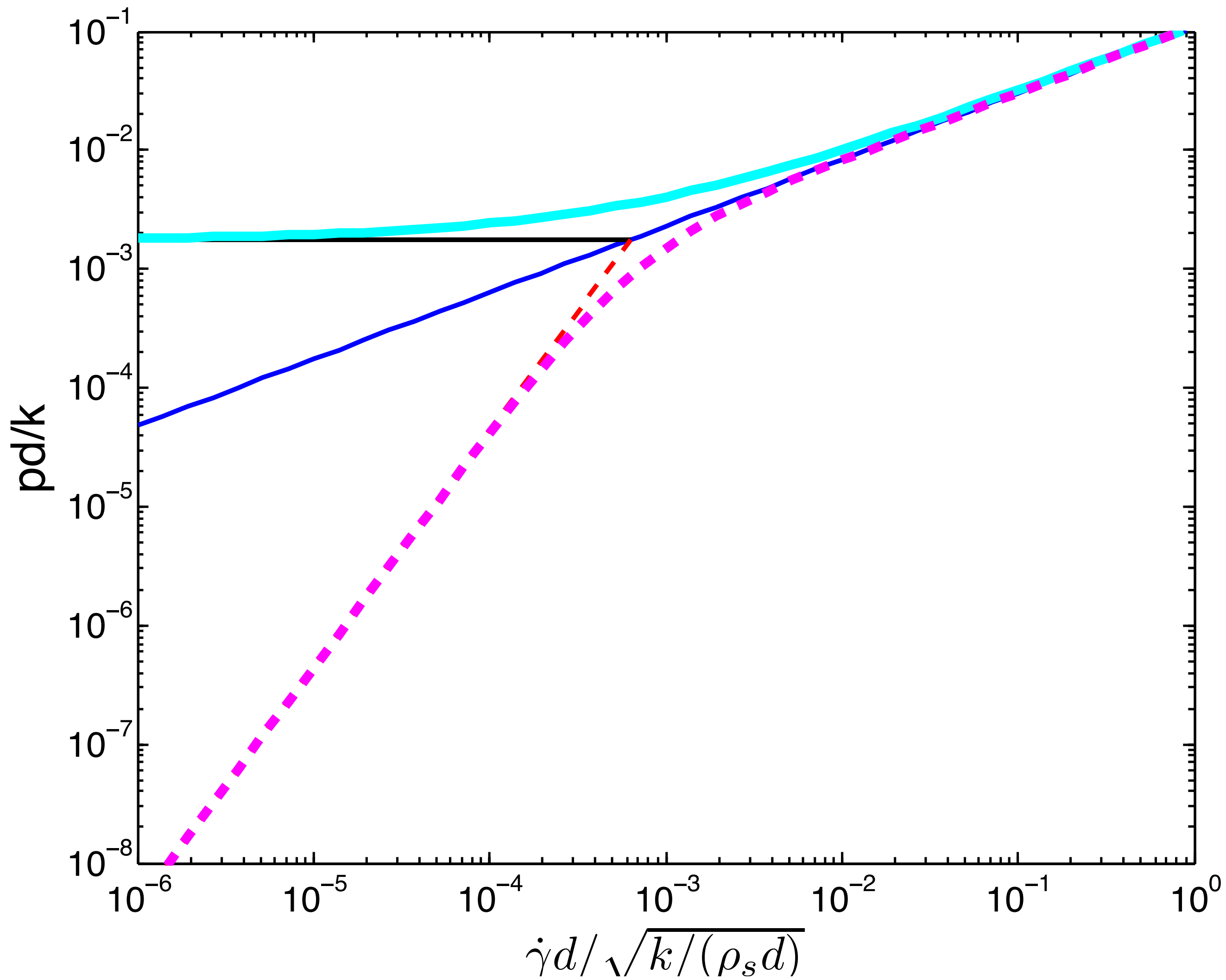

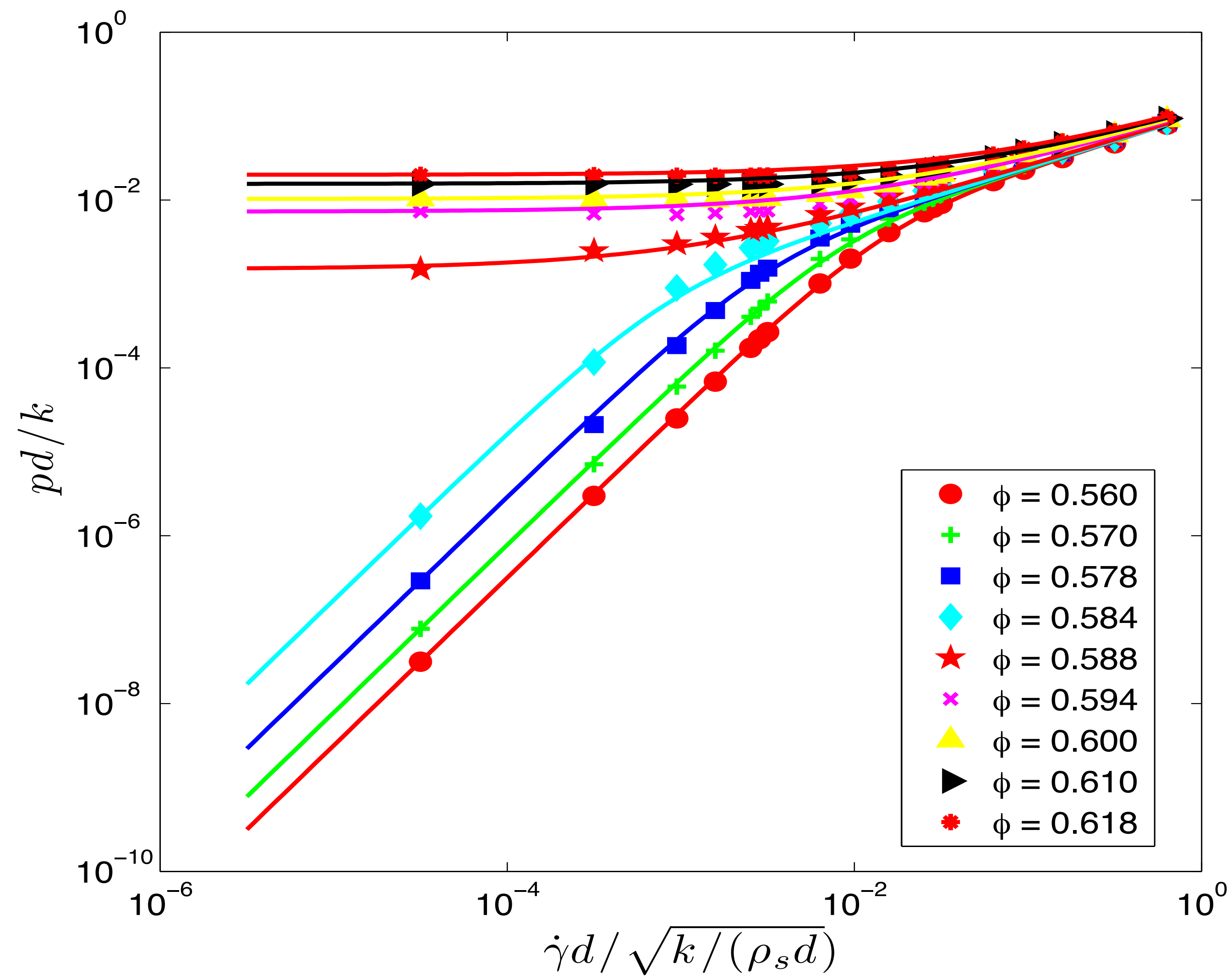

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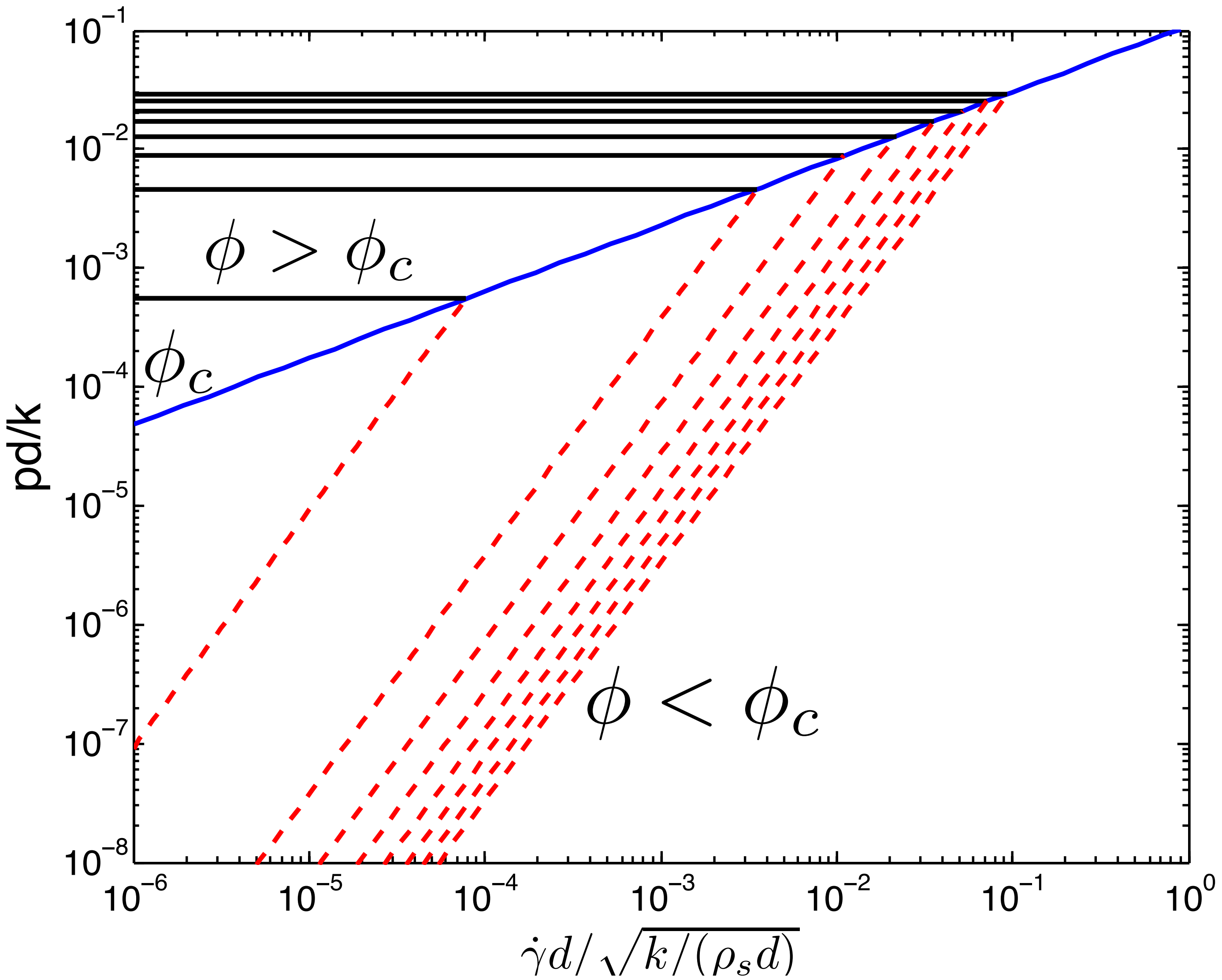
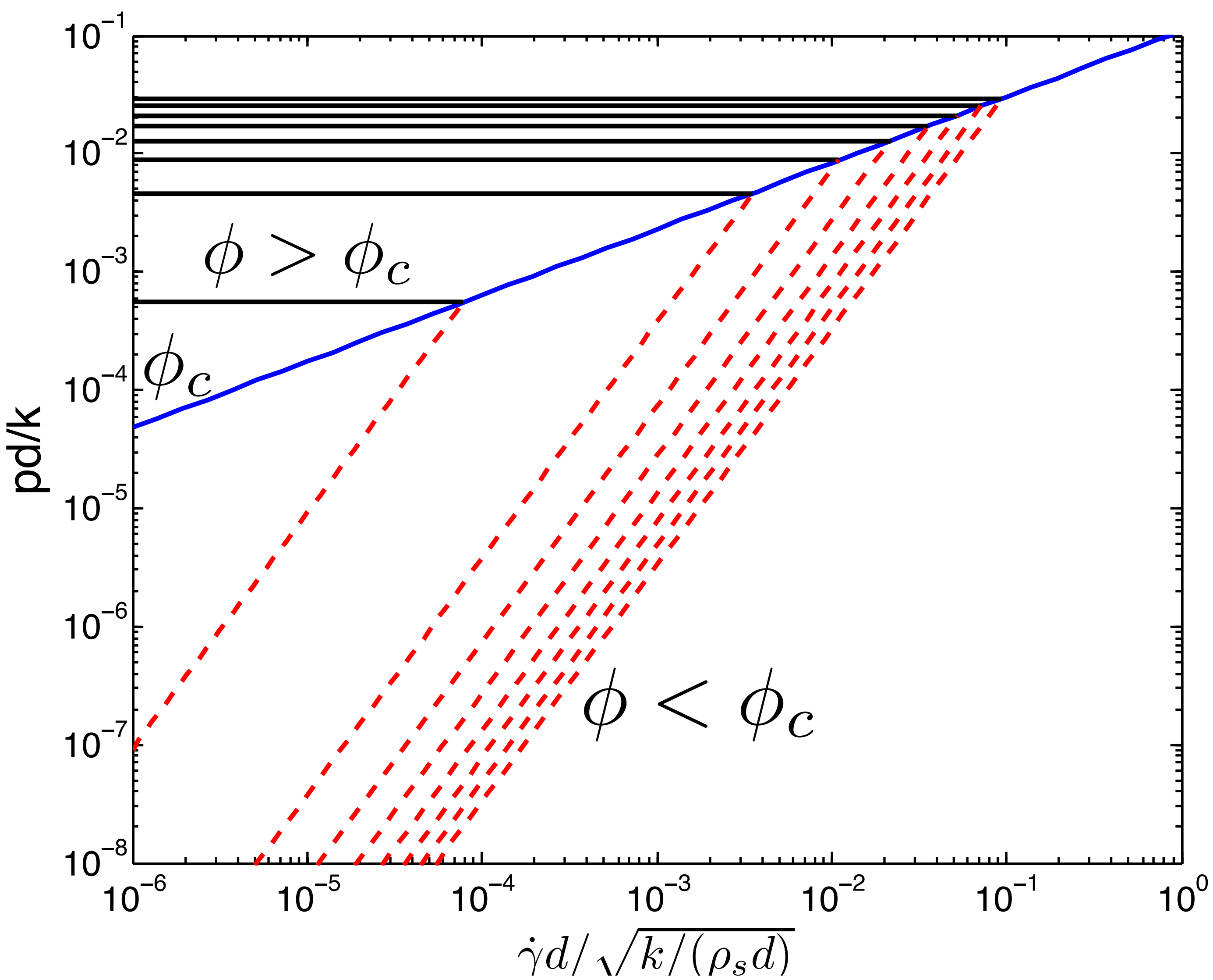
- Agree reasonably well with DEM data

Flow regime map

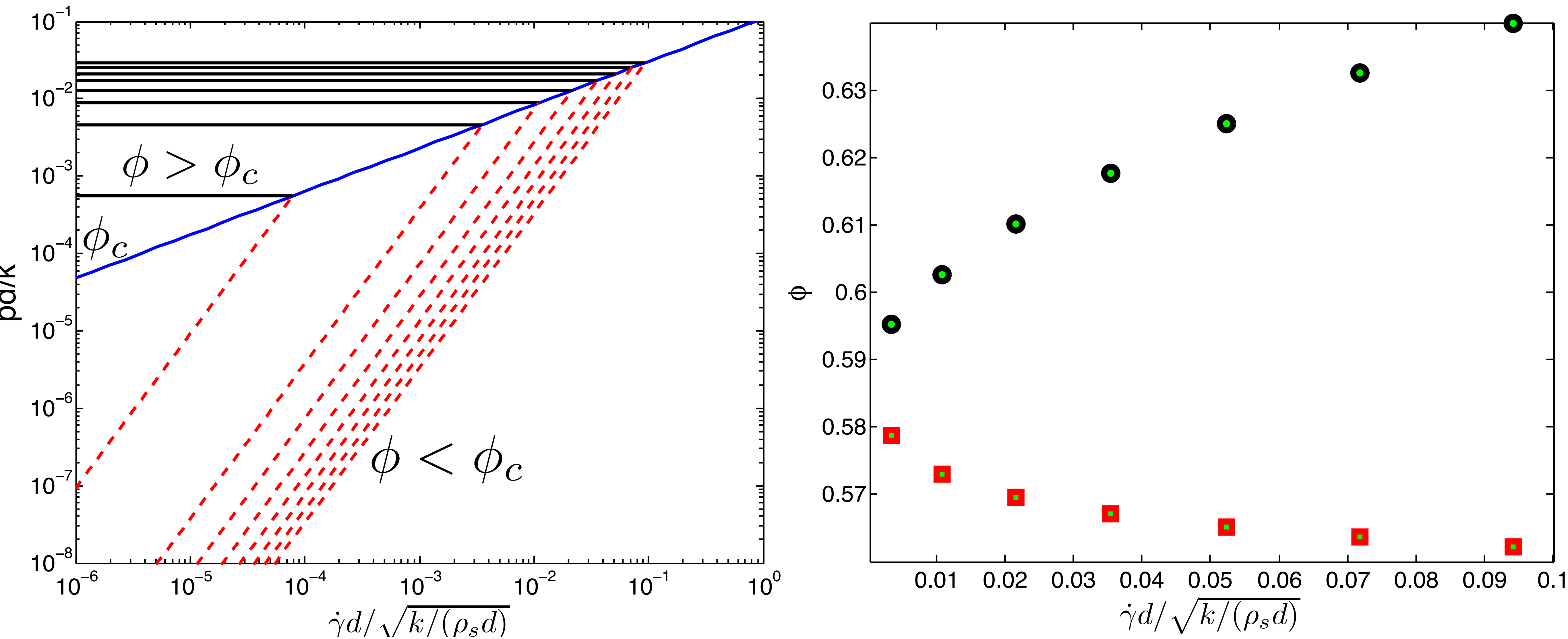


Flow regime map



- Estimate the volume fractions and shear rates at boundaries between regimes using the asymptotic flow curves

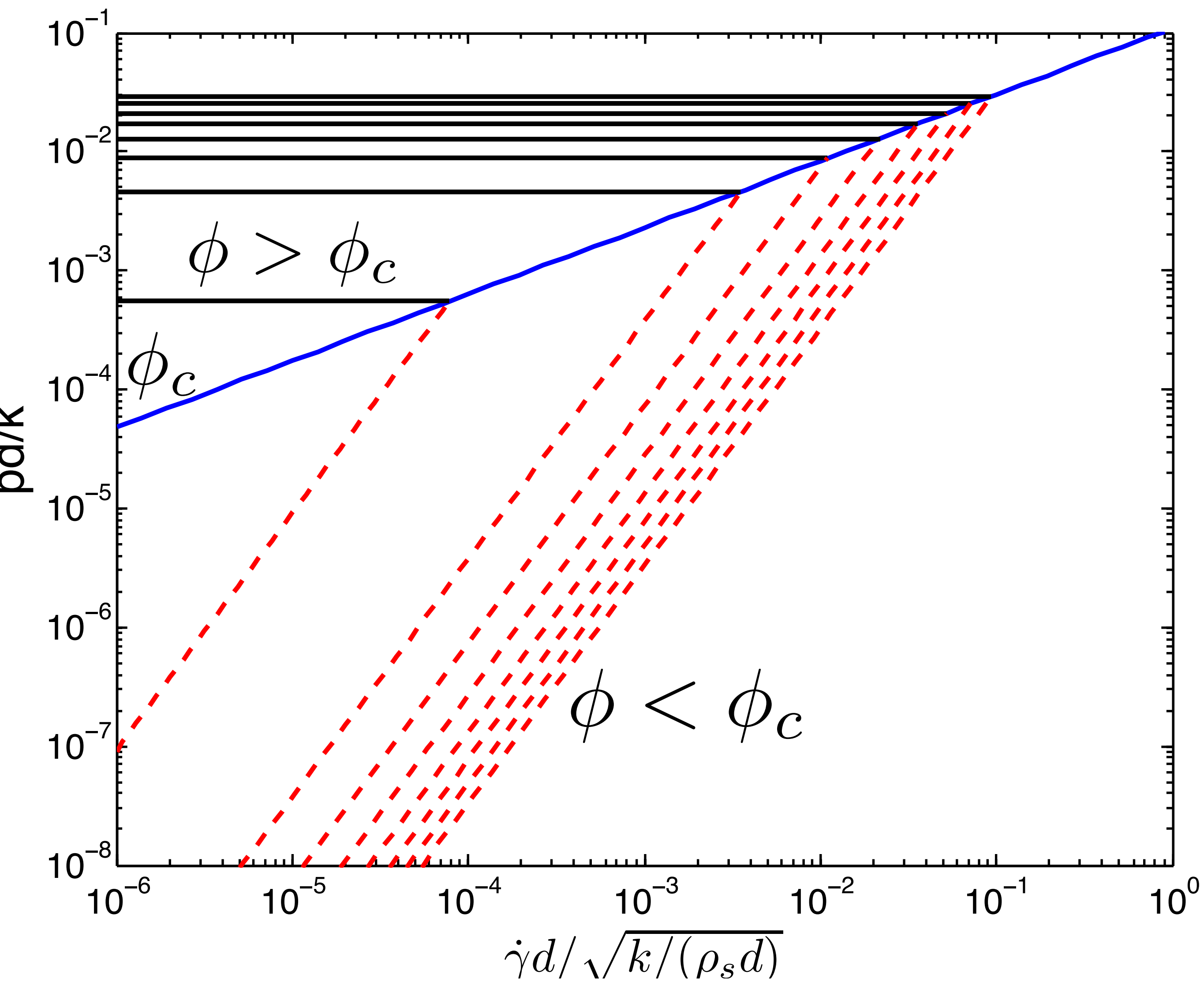
Flow regime map

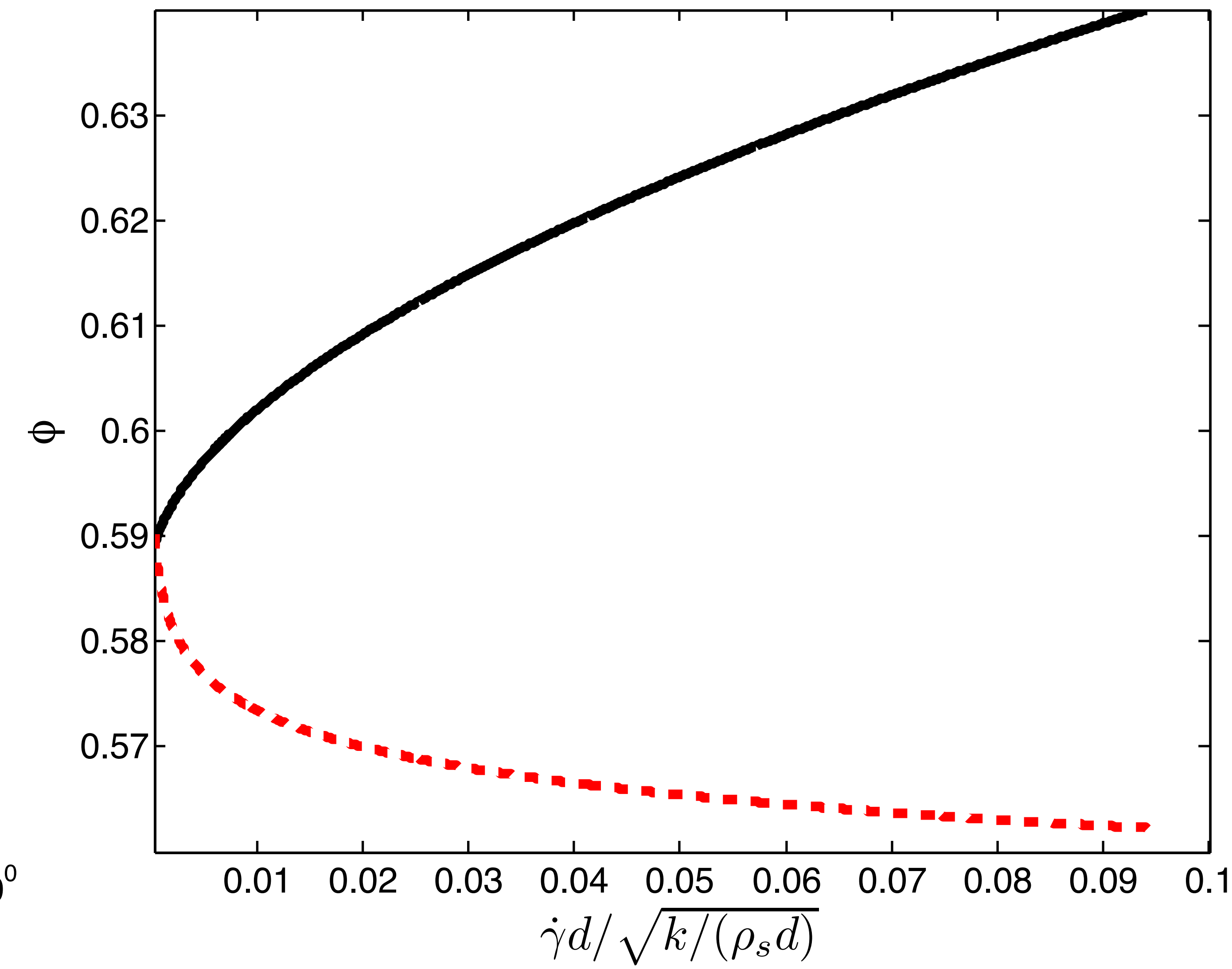


- Estimate the volume fractions and shear rates at boundaries between regimes using the asymptotic flow curves

- Obtain regime map in (volume fraction)-(shear rate) space

Flow regime map





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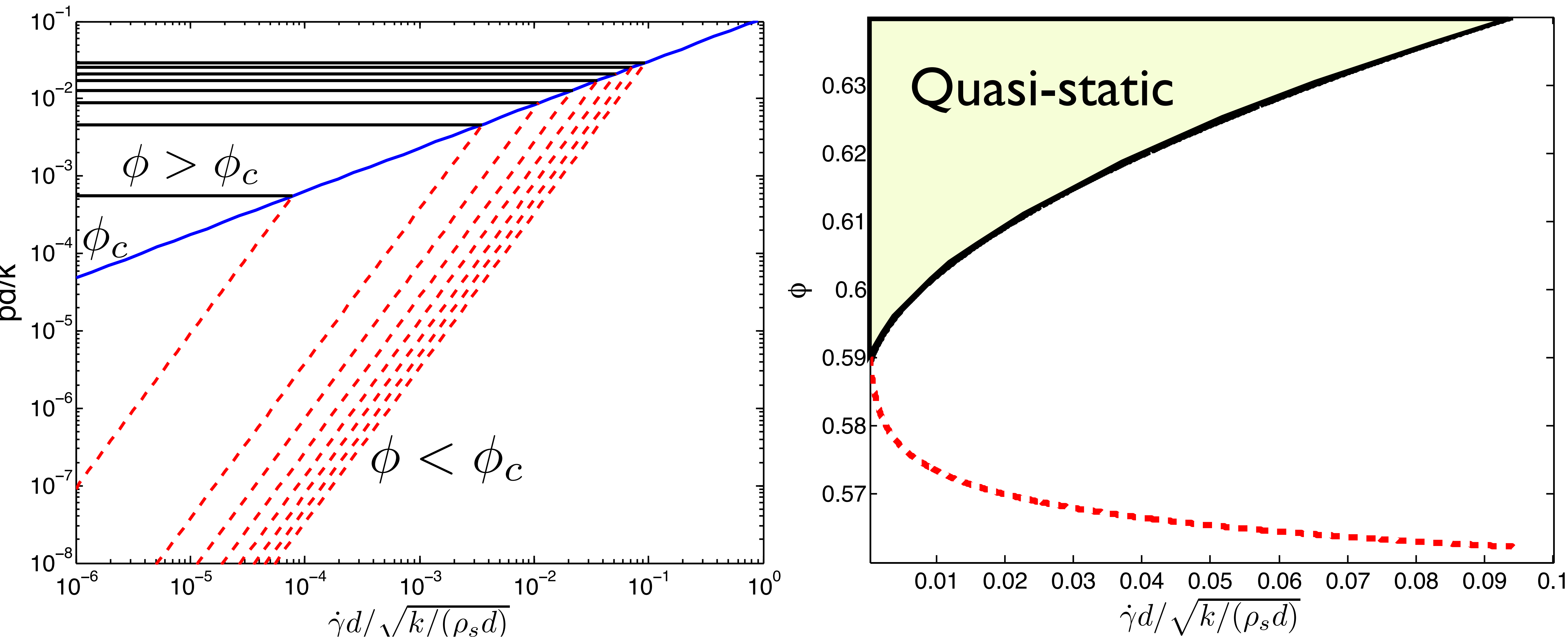

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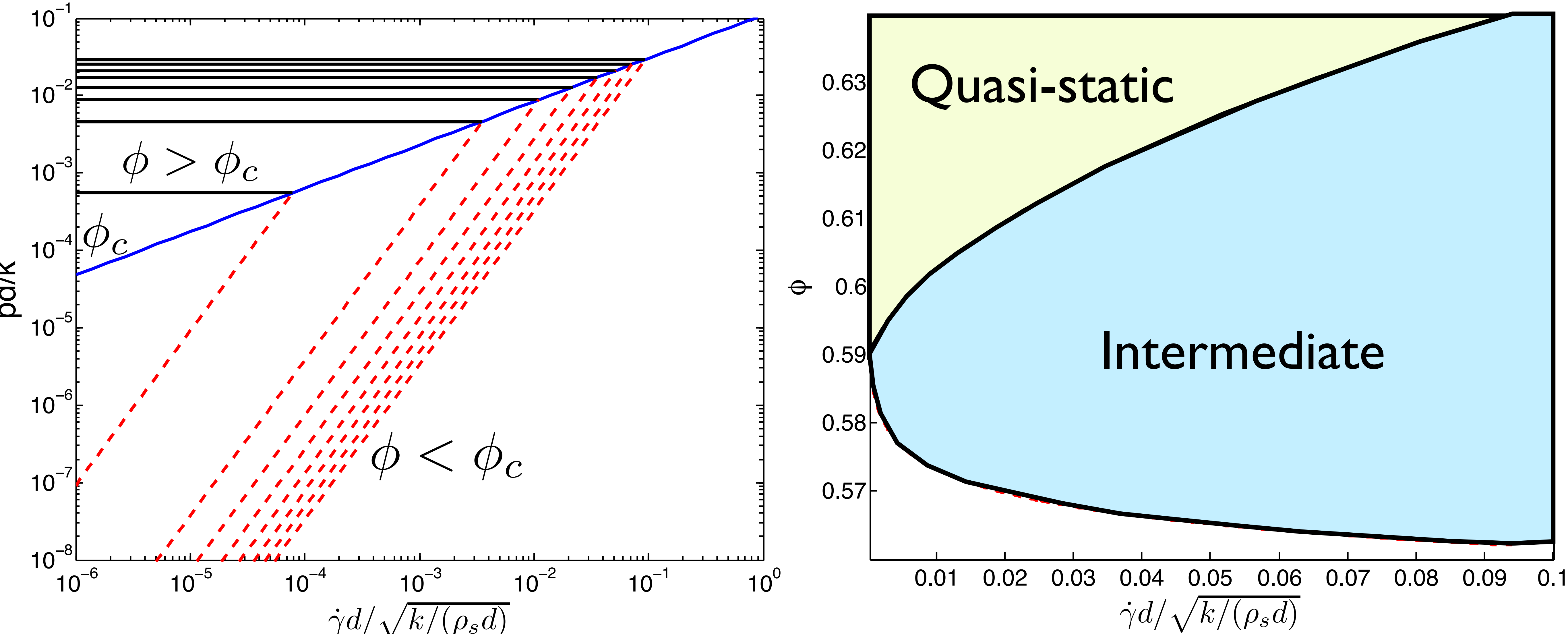

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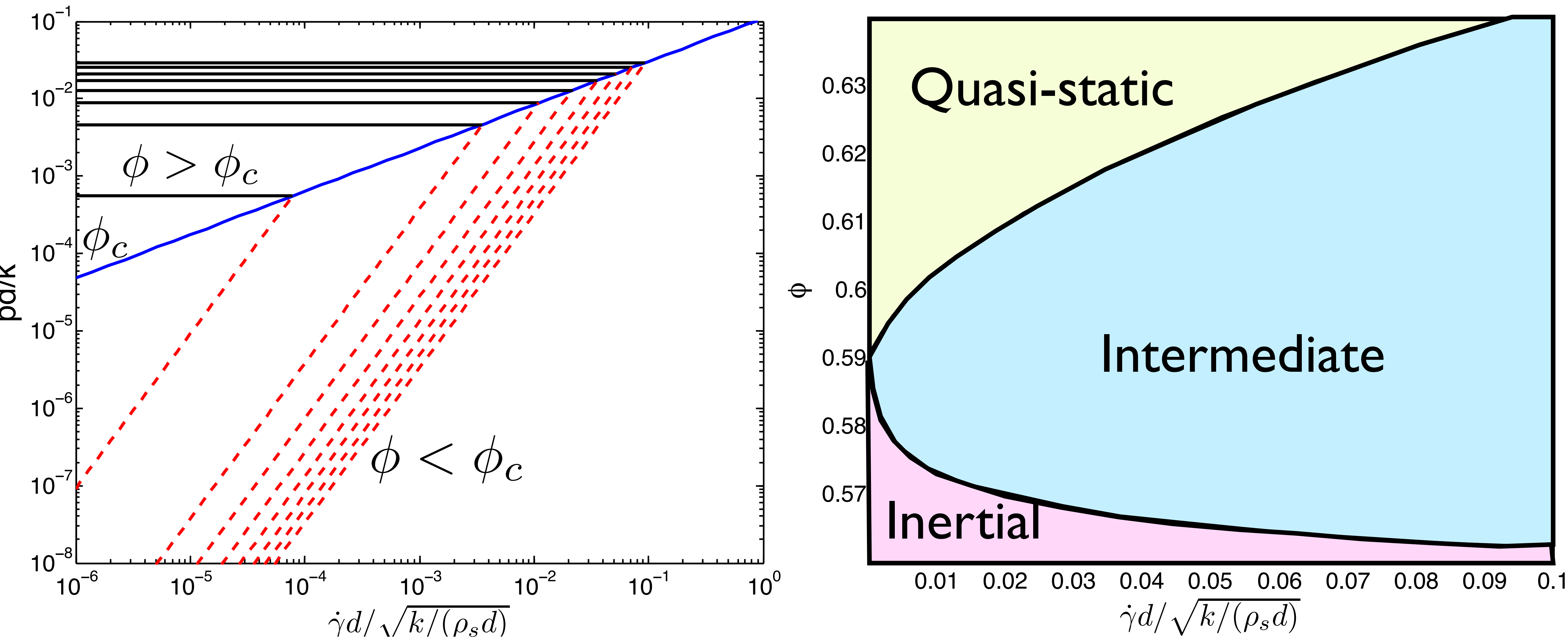

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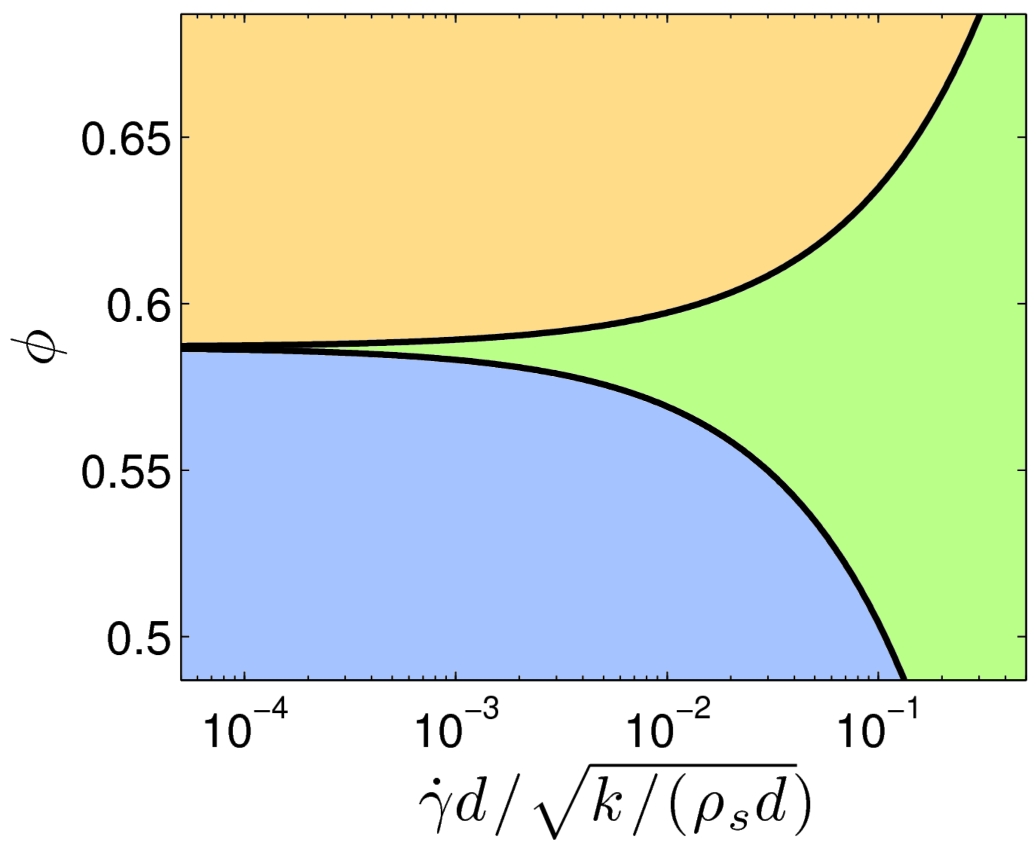
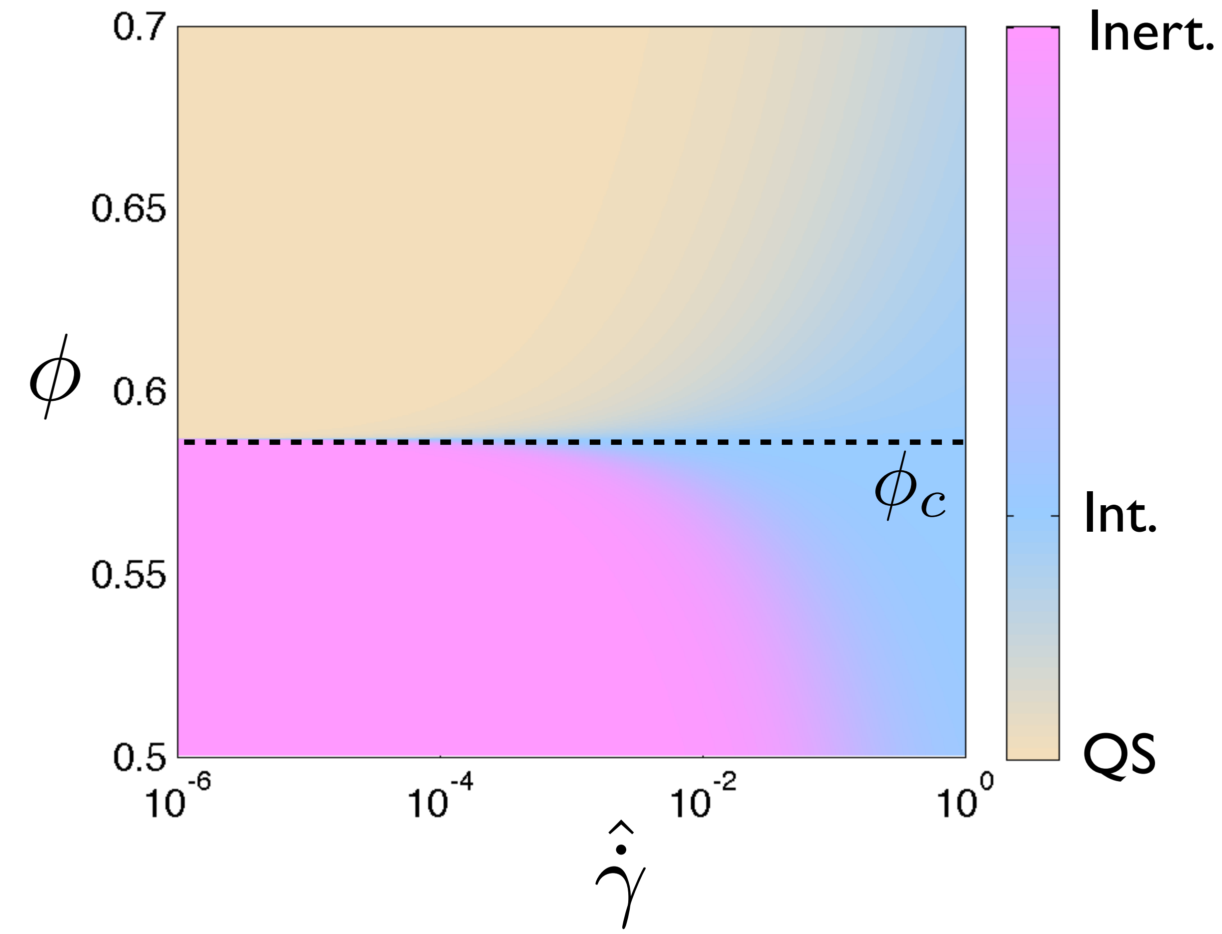
[1] C. S. Campbell. Journal of Fluid Mechanics, 465:261–291, 2002.
[2] G. Lois and J. M. Carlson. Europhysics Letters, 80(5):58001–1–5, 2007.

Regime maps





$$p = \begin{cases} B(p_{QS}, p_{Int}) & \text{for } \phi \geq \phi_c \\ B(p_{Inert}, p_{Int}) & \text{for } \phi < \phi_c \end{cases}$$

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Outline

- Introduction
- Models for different flow regimes
- Bridging across flow regimes
- Summary and future work