Multiphase Flow Physics from Direct Simulation for Model Development

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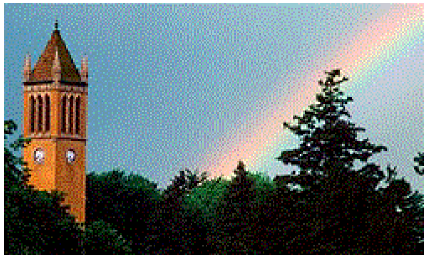


Part 1: Gas-phase fluctuations from Direct Numerical Simulation using PUReIBM

Graduate Assistants: Sudheer Tenneti, M. Mehrabadi

Collaborators: R.O. Fox, S. Sundaresan, and C.M. Hrenya

Funding: DE-FC26-07NT43098 (NETL AR)

Part 2: New Constitutive Model for Granular Stress using Discrete Element Simulations

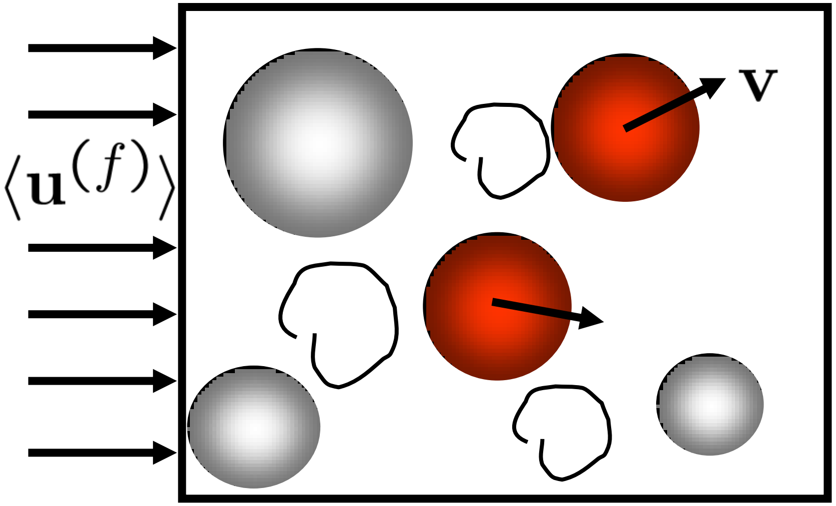
Graduate Assistant: Vidyapati

Collaborators: S. Sundaresan and G. Tardos

Funding: DE-FG26-07NT43070 (UCR)

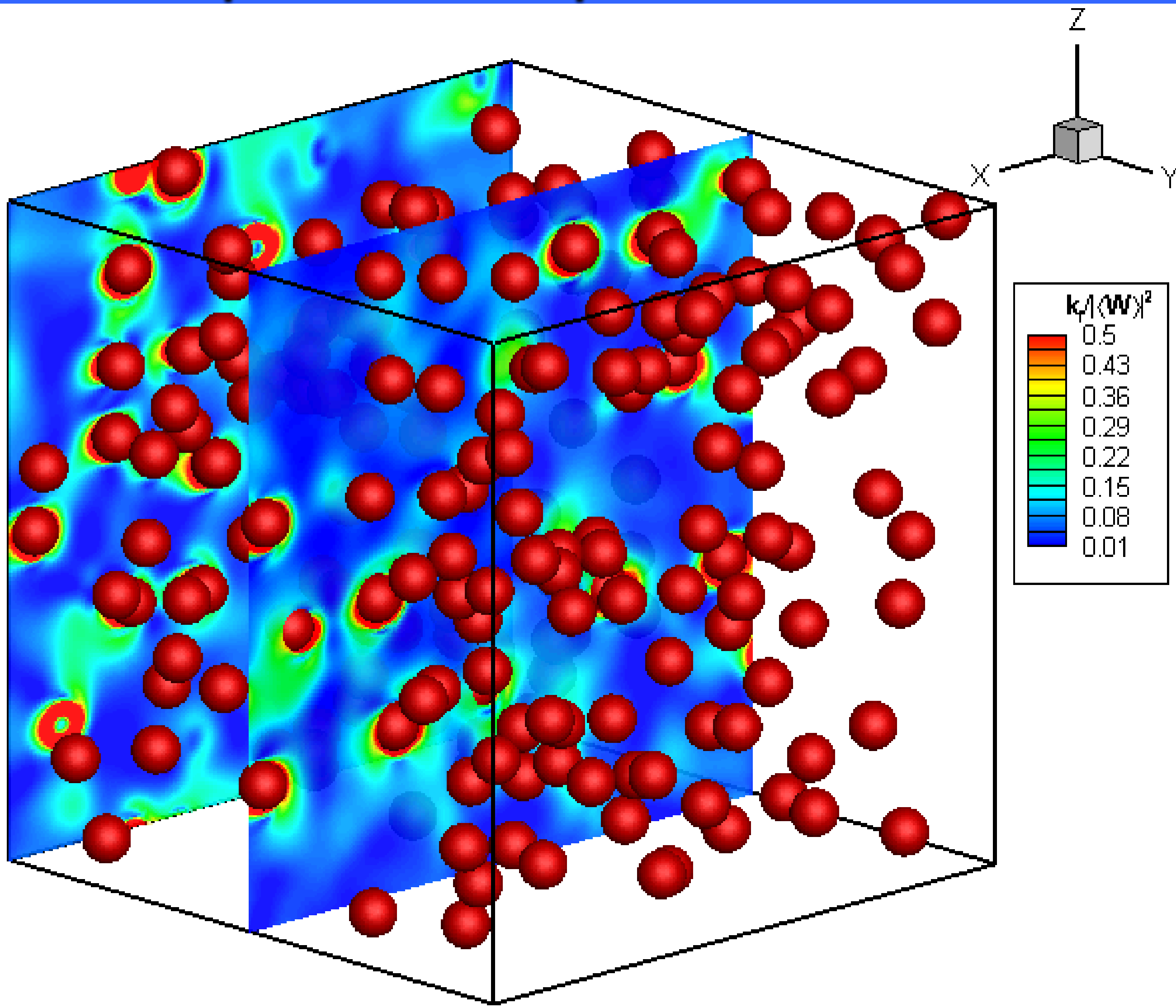
Regime Characterization

- Particles (100 to 500 micron) can be larger than the Kolmogorov scale of turbulence
- Large solid particles in a gas: high Stokes number *O*(100)
- Fixed particle assemblies are a reasonable approximation (verified by simulation)
- High solid volume fraction: not dilute
- Non-zero mean slip



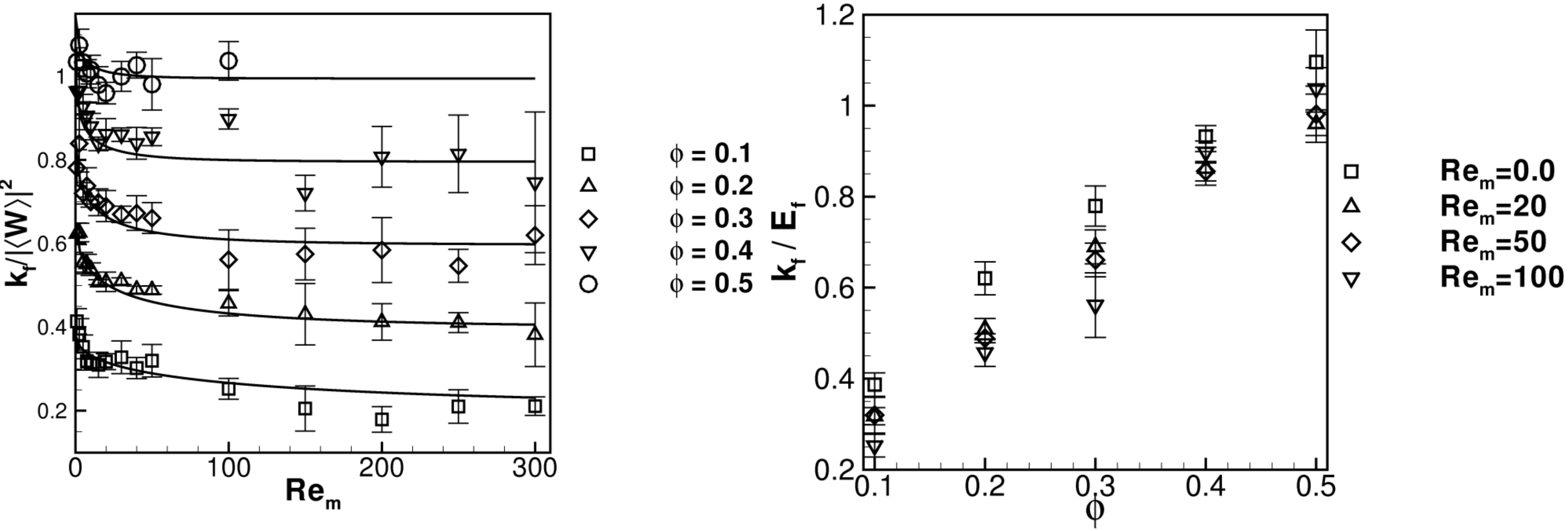
Significantly different from the well-documented dilute regime of small “sub-Kolmogorov size” particles of *O*(1) Stokes number in homogeneous, isotropic turbulence

Flow past fixed particle assemblies



Tenneti, S. Garg, R., Subramaniam, S., "Quantification of gas-phase velocity fluctuations in statistically homogeneous gas-solid flow using particle-resolved direct numerical simulation", *(in review)*

Steady State TKE

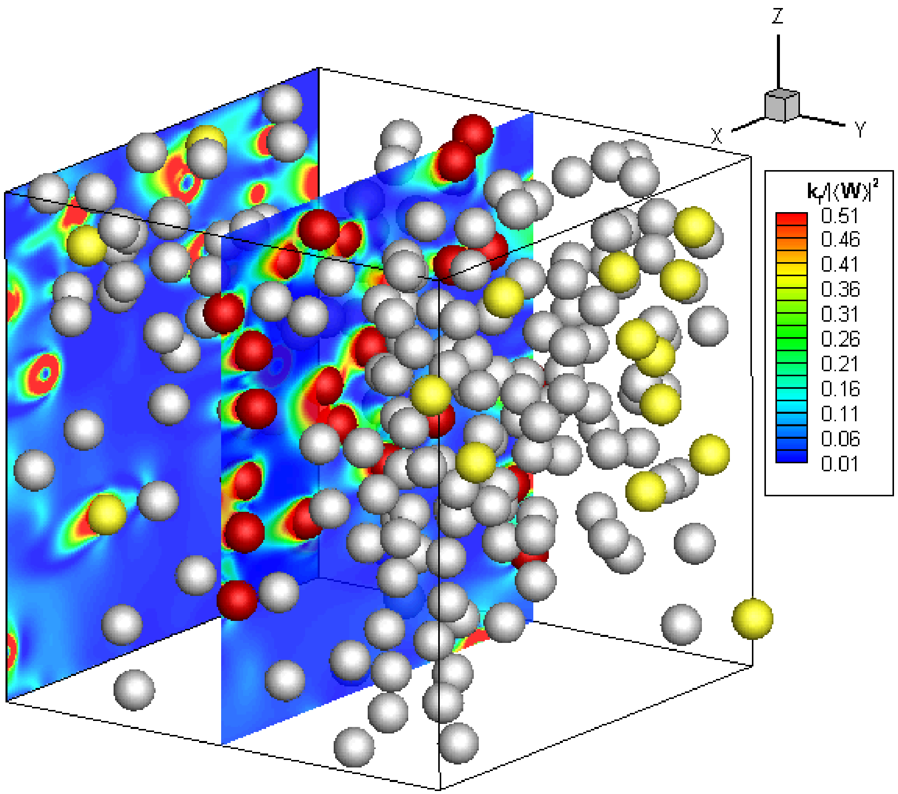


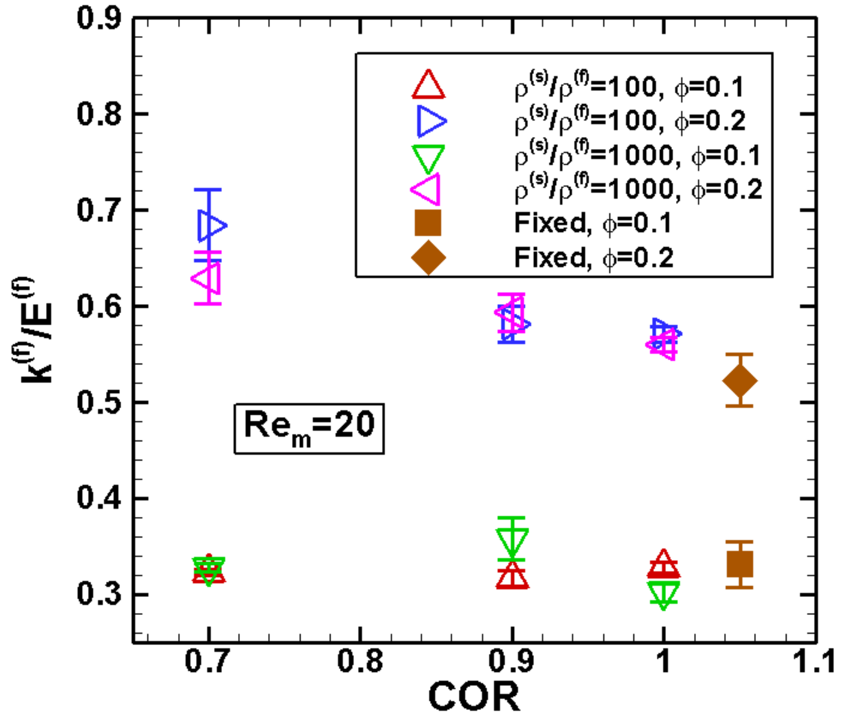
$$\frac{k_f}{|\langle \mathbf{W} \rangle|^2}(\phi, \mathrm{Re}_m) = 2\phi + 2.5\phi(1-\phi)^3 \mathrm{e}^{-\phi \mathrm{Re}_m^{1/2}}$$

Gas-phase velocity fluctuations show significant increase with volume fraction: implies transport of RS will be important

Freely evolving suspensions

Freely moving particles undergoing collisions (elastic and inelastic)





Gas-phase fluctuations in freely evolving suspensions are similar in magnitude to that in fixed particle assemblies because of low collisional dissipation

Anisotropy in gas-phase fluctuations

$$R_{ij}^{(f)} = \left\langle u_i''^{(f)} u_j''^{(f)} \right\rangle = f(\phi, Re_m)$$

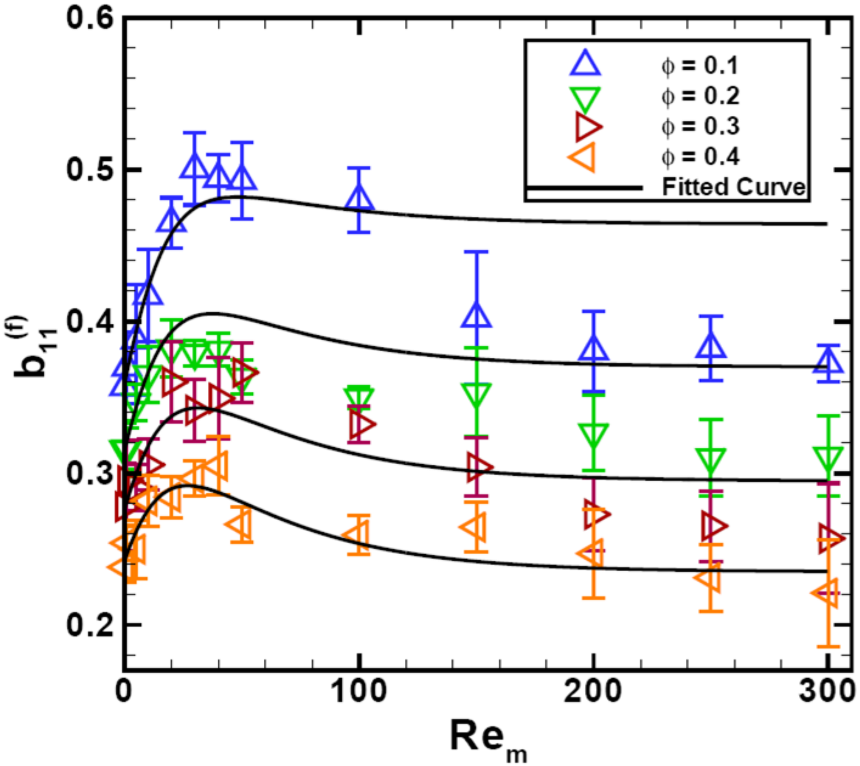
Decomposing Reynolds stress into isotropic and deviatoric part

$$b_{ij}^{(f)} = \frac{R_{ij}^{(f)}}{2k^{(f)}} - \frac{1}{3}\delta_{ij}$$

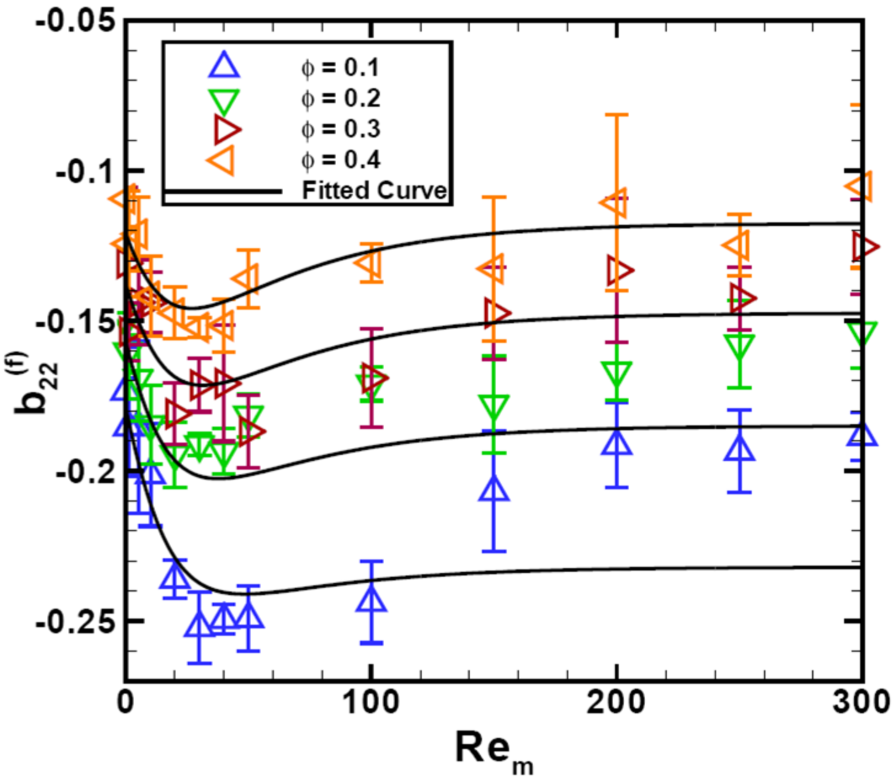
Velocity fluctuation components: parallel and perpendicular to mean flow

$$\begin{aligned} \mathbf{u}_{\parallel}'' &= \mathbf{u}'' \cdot \mathbf{e}_{\parallel} \\ \mathbf{u}_{\perp}'' &= \mathbf{u}'' \cdot \left(\mathbf{u}''/|\mathbf{u}''| - \mathbf{e}_{\parallel}\right) \end{aligned}$$

Parallel direction



Perpendicular plane



Anisotropy trends: length scale analysis

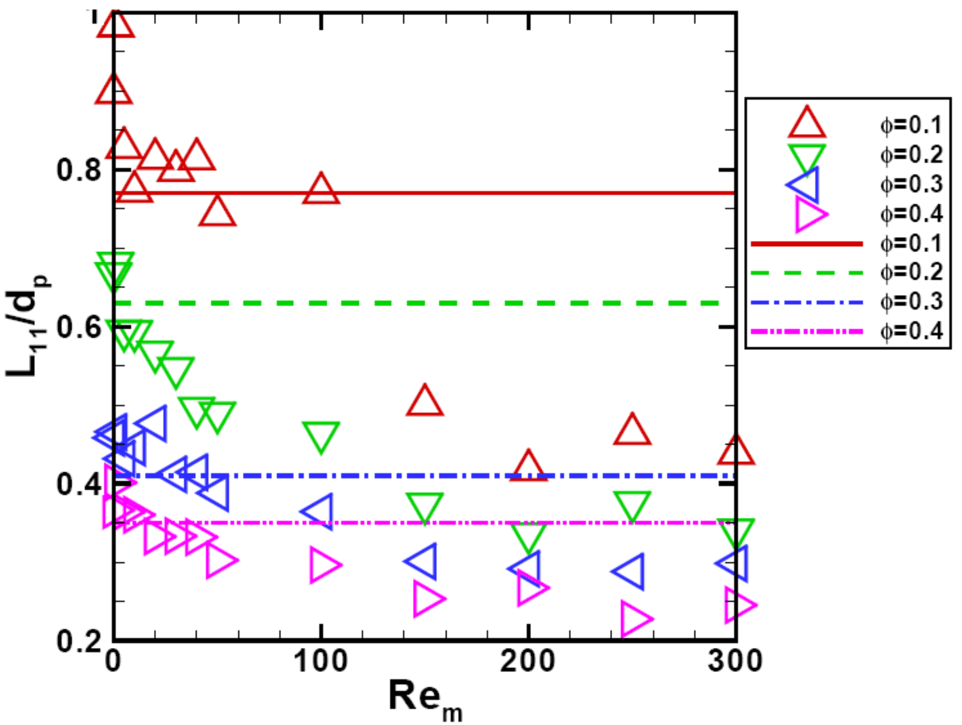
Integral length scale of gas-phase fluctuations

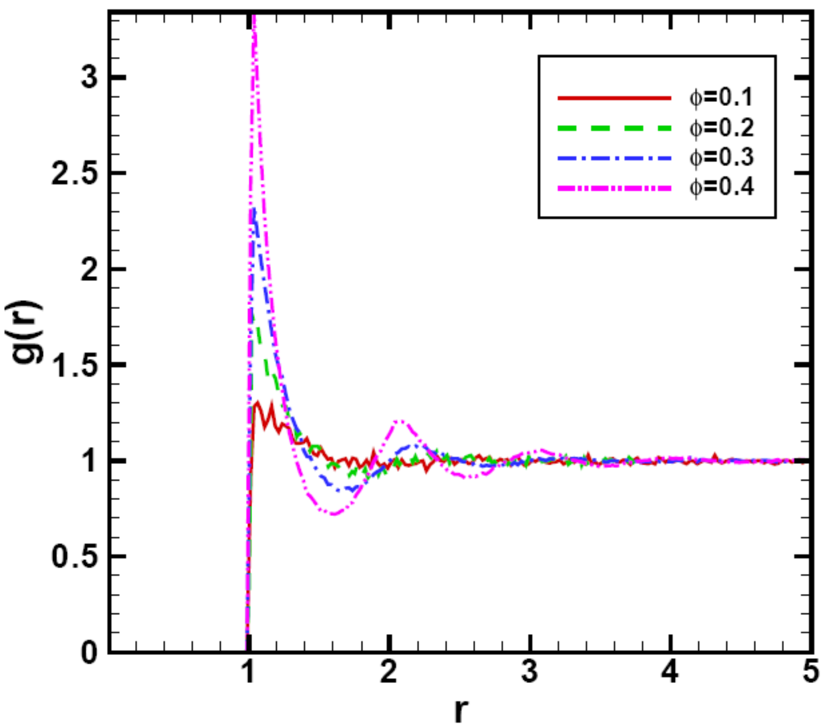
$$L_{\parallel} = \frac{1}{R_{\parallel}(0)} \int_0^{\infty} R_{\parallel}(r)dr$$

$$R_{\parallel}(r) = \int_{\mathcal{V}^{(f)}} u_{\parallel}^{\prime\prime(f)}(\mathbf{x}) u_{\parallel}^{\prime\prime(f)}(\mathbf{x}, r) d\mathbf{x}$$

Measure of inter-particle spacing: weighted average of neighbor particle distances

$$L_{int} = \frac{\int_0^{r_{eff}} \rho^{(2)}(r)dr}{\int_0^{r_{eff}} \frac{\rho^{(2)}(r)}{r}dr}$$





Multiphase Turbulence Model: Scaling Analysis

Fluid phase TKE equation (homogeneous case)

$$\frac{\partial}{\partial t}\left\{(1-\phi)\,\rho_f k_f\right\} = -\boxed{\left\langle {u_i}''^{(f)} \tau_{ji} n_j^{(s)} \delta\left(\mathbf{x}-\mathbf{x}^{(I)}\right)\right\rangle} - \boxed{2\mu_f \left\langle I_f S_{ij} S_{ij}\right\rangle}$$

Interphase TKE transfer

Dissipation

Source $\Pi_{k_f} = \langle \mathbf{W} \rangle \cdot \left\langle \mathbf{S}_M^{(f)} \right\rangle = \dfrac{18\phi\,(1-\phi)^2\,\mu_f}{D^2} F\left(\phi, \mathrm{Re}_m\right) \left|\langle \mathbf{W} \rangle\right|^2$

Steady state $\Pi_{k_f} = \rho_f\,(1-\phi)\,\varepsilon_f$

Scaling of TKE implies a scaling for dissipation: can verify existing models that use Kolmogorov scaling

Multiphase Turbulence Dissipation Models

$$\Pi_{k_f} \boxed{= \rho_f (1-\phi)\, \varepsilon_f}$$

Kolmogorov scaling

Taylor microscale

$$\varepsilon_f \sim k_f^{3/2} / l_{\text{diss}}$$

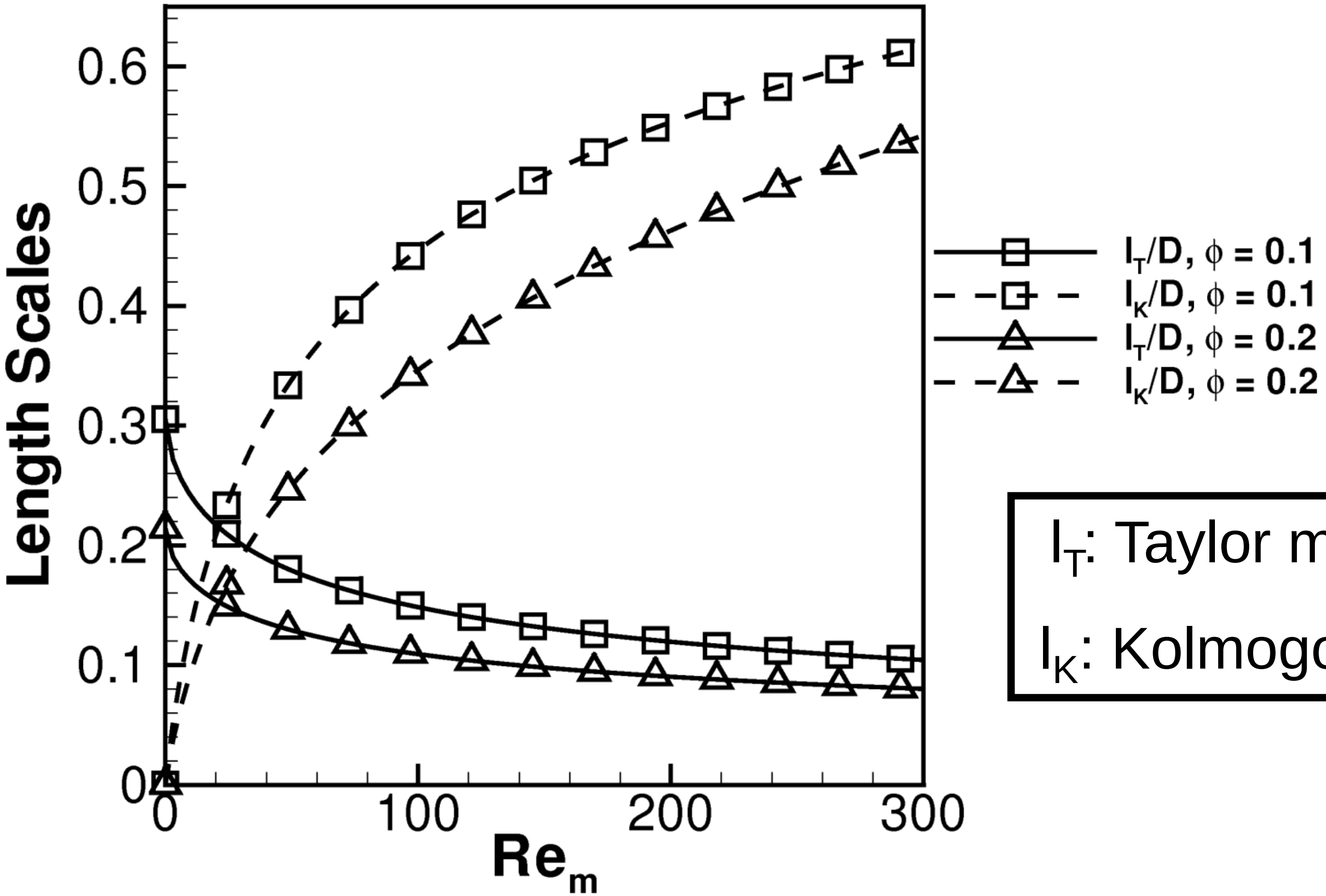
$$\varepsilon_f \sim 2\nu_f k_f / l_{\text{diss}}^2$$

$$\left(\frac{k_f}{E_f}\right)^{3/2} = \left(\frac{l_{\text{diss}}}{D}\right) 36\sqrt{2}\phi\,(1-\phi)^2\,\frac{F(\phi,\text{Re}_m)}{\text{Re}_m}.$$

$$\frac{k_f}{E_f} = \left(\frac{l_{\text{diss}}}{D}\right)^2 18\phi\,(1-\phi)\,F(\phi,\text{Re}_m)$$

Dissipation is assumed to take place on a length scale corresponding to l_{diss}

Implied Length Scales



l_T: Taylor microscale

l_K: Kolmogorov scale

Taylor microscale scaling is appropriate for gas-solid flows with finite sized particles

Summary

1. Presence of finite sized particles with mean slip velocity generate high level of *non-turbulent* gas-phase velocity fluctuations

2. Developed a correlation for kinetic energy for monodisperse suspensions

3. Strong anisotropy: depends on Re & volume fraction

4. From scaling analysis it is found that Taylor microscale type scaling for the dissipation of TKE is appropriate for gas-solid flows with finite sized particles

5. Correlation and the turbulence model extend to bidisperse suspensions in terms of SMD (not shown)

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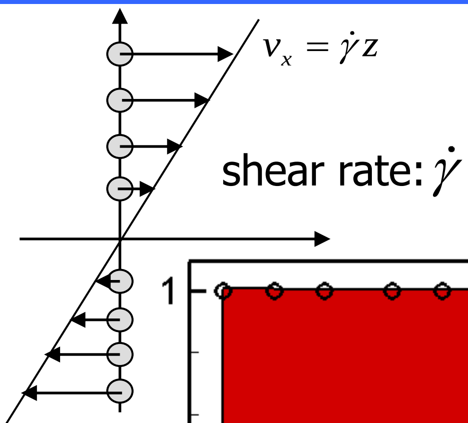
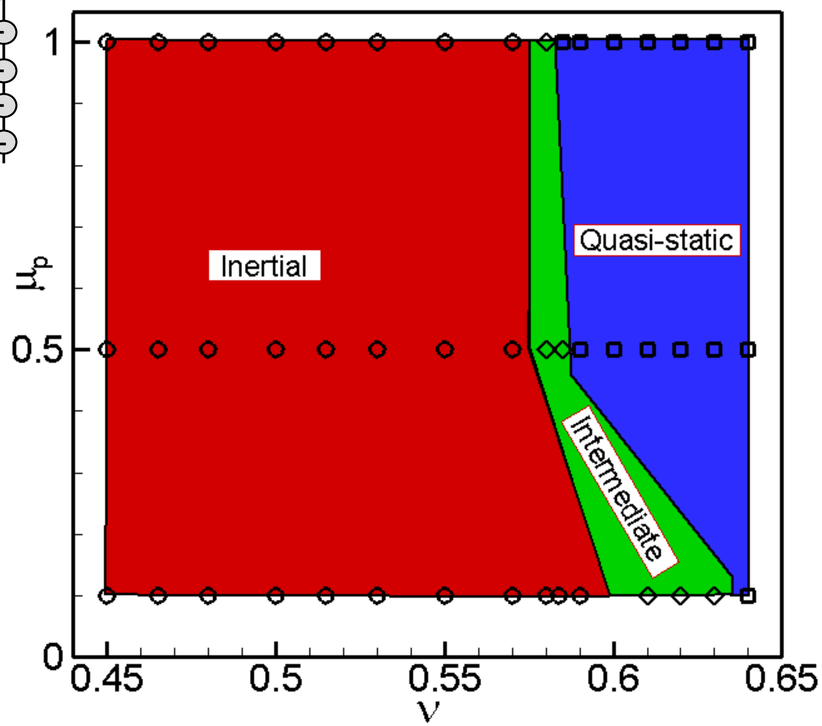
Existence of different regimes using DEM

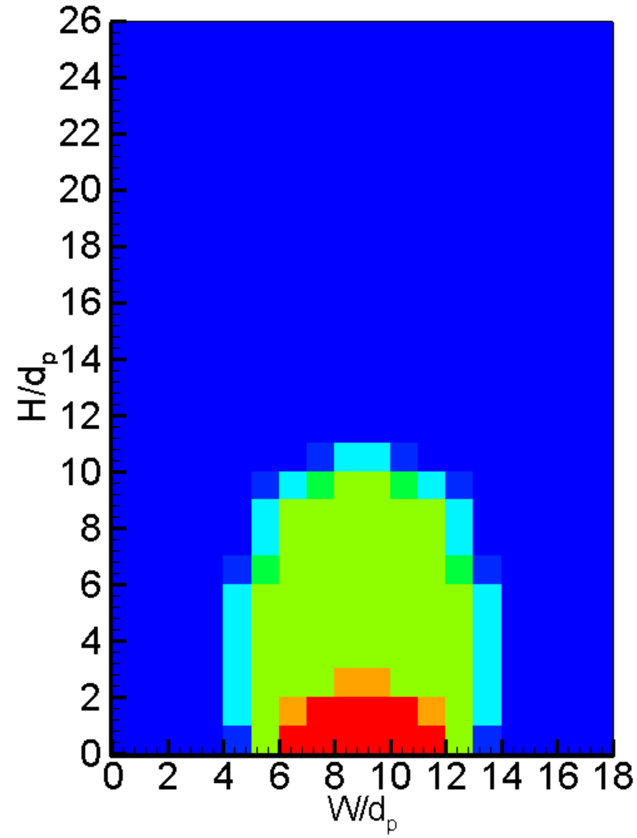




Regime map is established from DEM data of homogeneously sheared granular flow

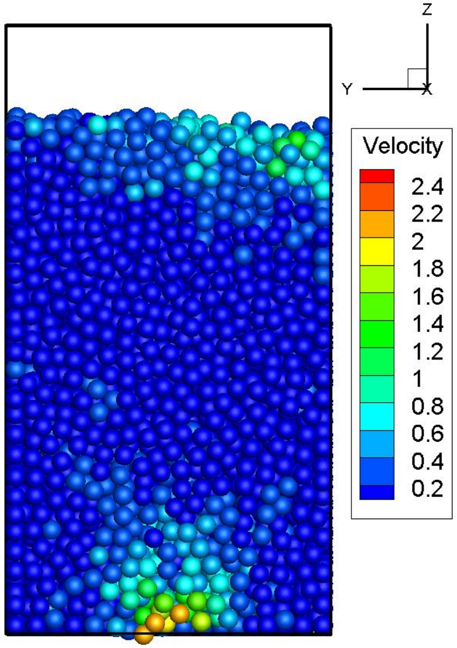
3D DEM simulation of flat bottomed silo

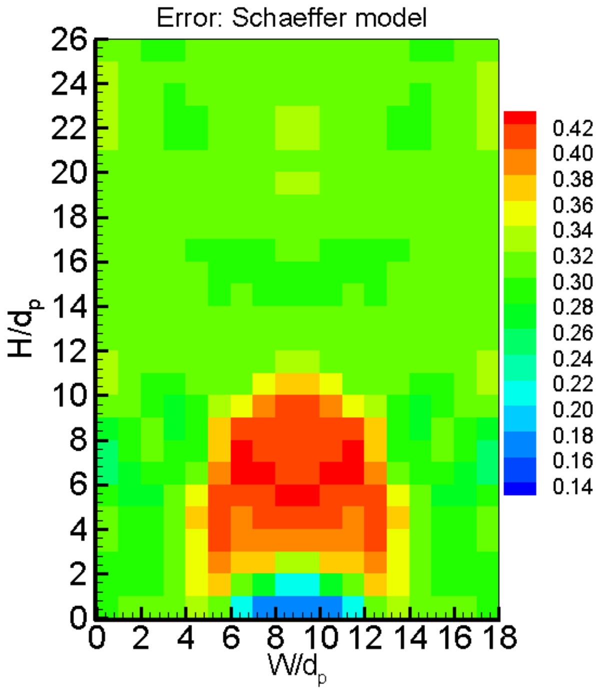
Regime classification: Red = Inertial regime; Blue = Quasi-static regime

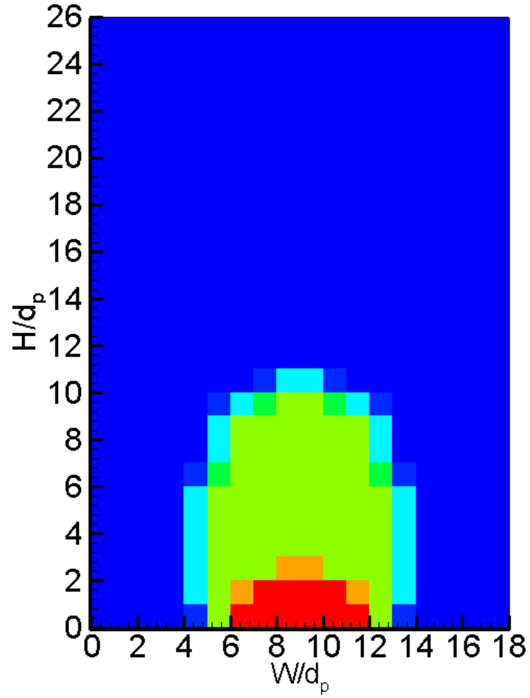


Even in a simple problem such a discharge from a silo, different regimes coexist

Challenges for continuum models

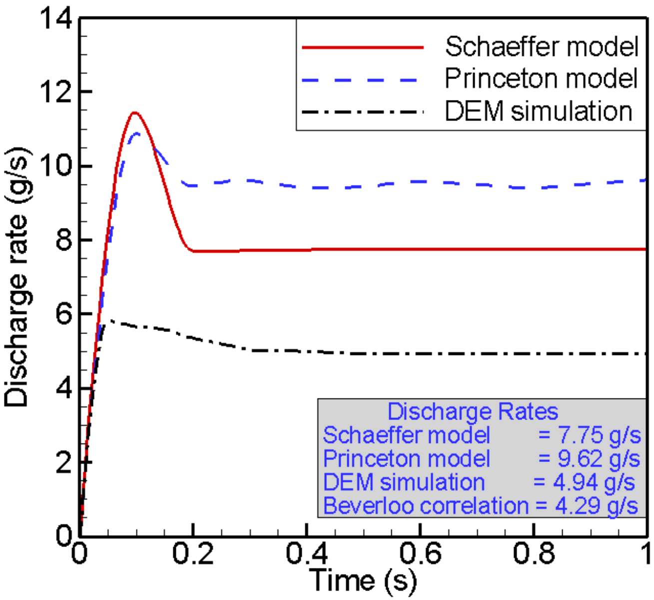






Error in stress prediction: Schaeffer model

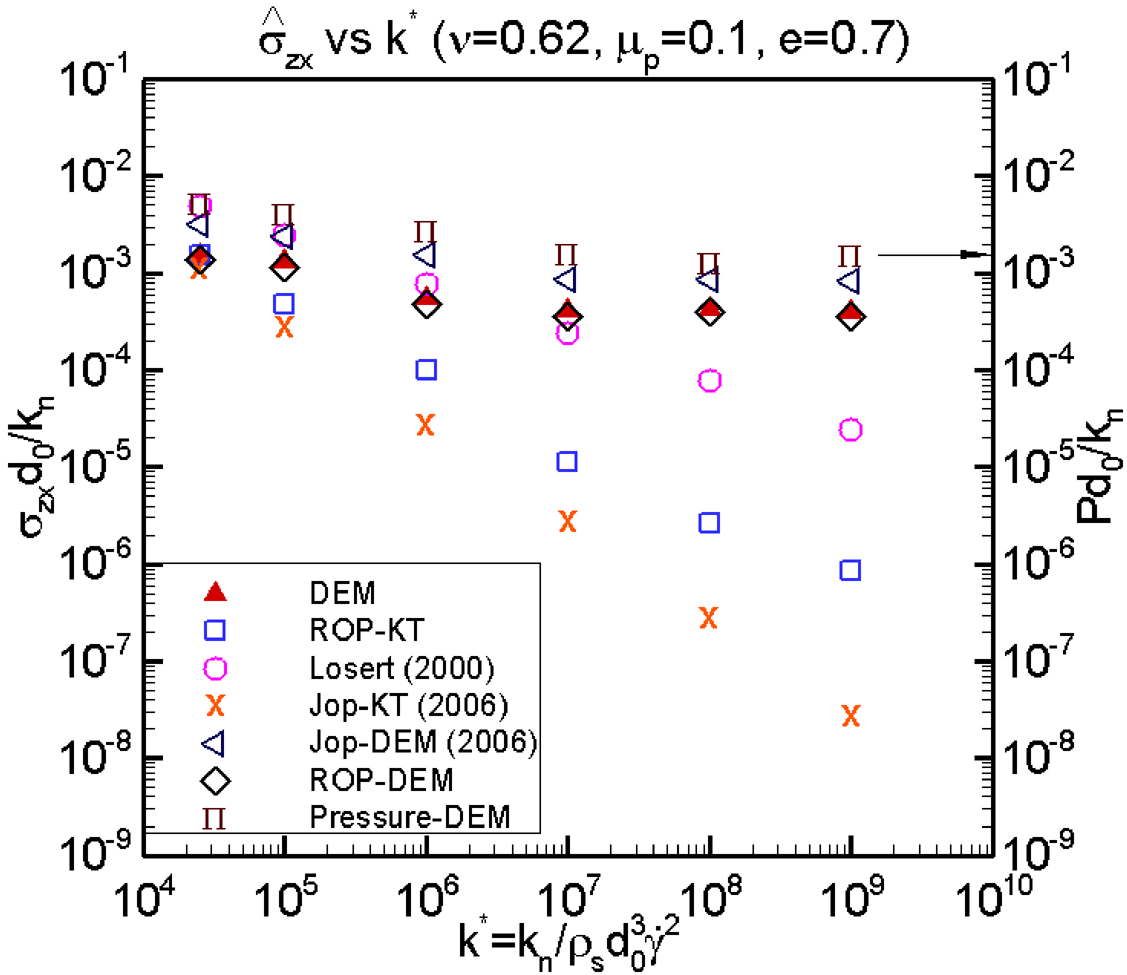
Spatial extent of different regimes in a silo



$$Error = \frac{\left\| \left(\sigma_{ij}\right)_{model} - \left(\sigma_{ij}\right)_{DEM} \right\|_2}{\left\| \left(\sigma_{ij}\right)_{DEM} \right\|_2}$$

Vidyapati and Subramaniam, S.,"*Granular flow in Silo discharge: DEM simulations and model assessment*", (in prep)

Model assessment in intermediate regime



- The different constitutive models evaluated are,
  - ROP-KT: ROP model coupled with kinetic theory of granular flows (KTGF)
  - Losert (2000): Model proposed in Losert et al., *PRL*, 85(7), 2000
  - Jop-KT (2006): Isotropic pressure computed using kinetic theory
  - Jop-DEM (2006): Isotropic pressure specified using data from DEM simulation
  - ROP-DEM: ROP model coupled with DEM for fluidlike

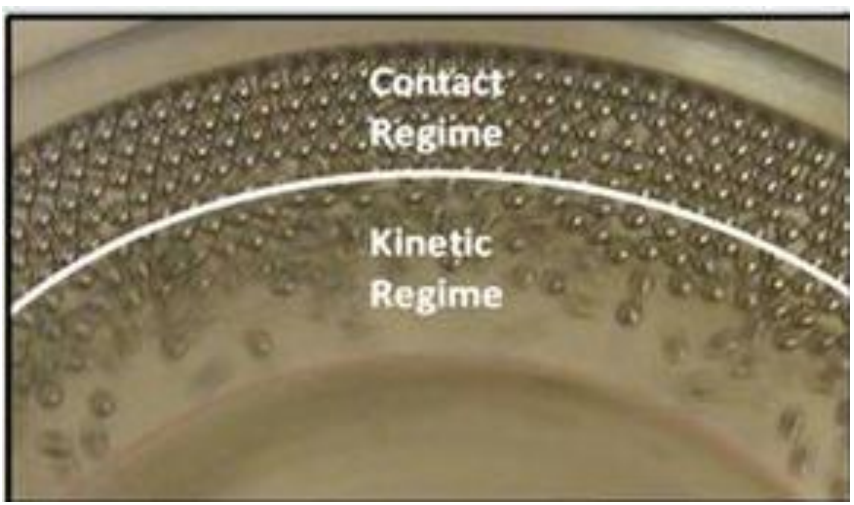
None of these models captures the correct scaling of shear stress with shear rate in the intermediate regime

Granular phase transition: Order Parameter

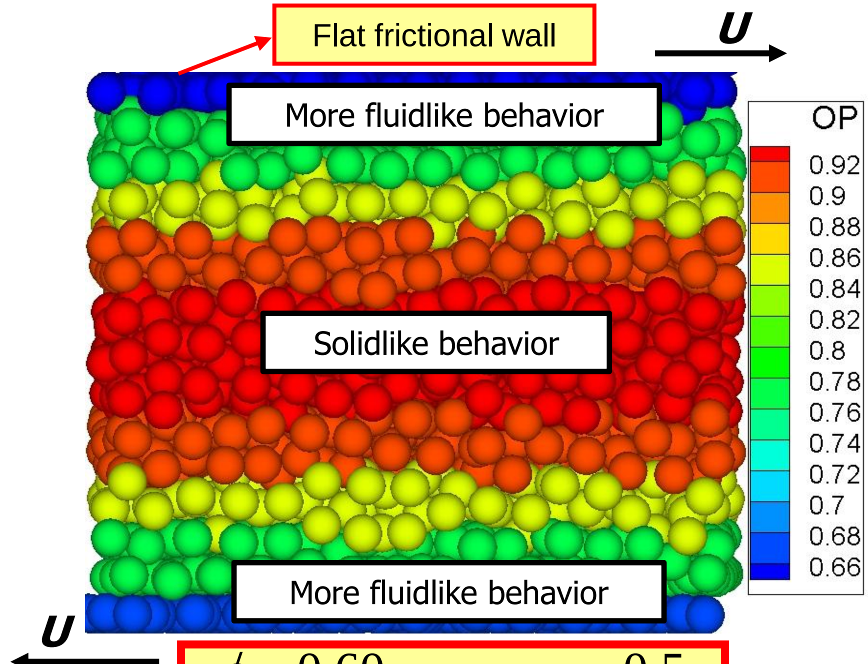
$$\mathrm{OP} = \frac{\langle \overline{Z_s} \rangle}{\langle \overline{Z} \rangle}$$

Number of solid contacts

Total number of contacts



Different regimes in granular shear cell (GSC) experiment[1]



$\phi = 0.60, \mu_p = \mu_w = 0.5$

DEM Simulations[2]

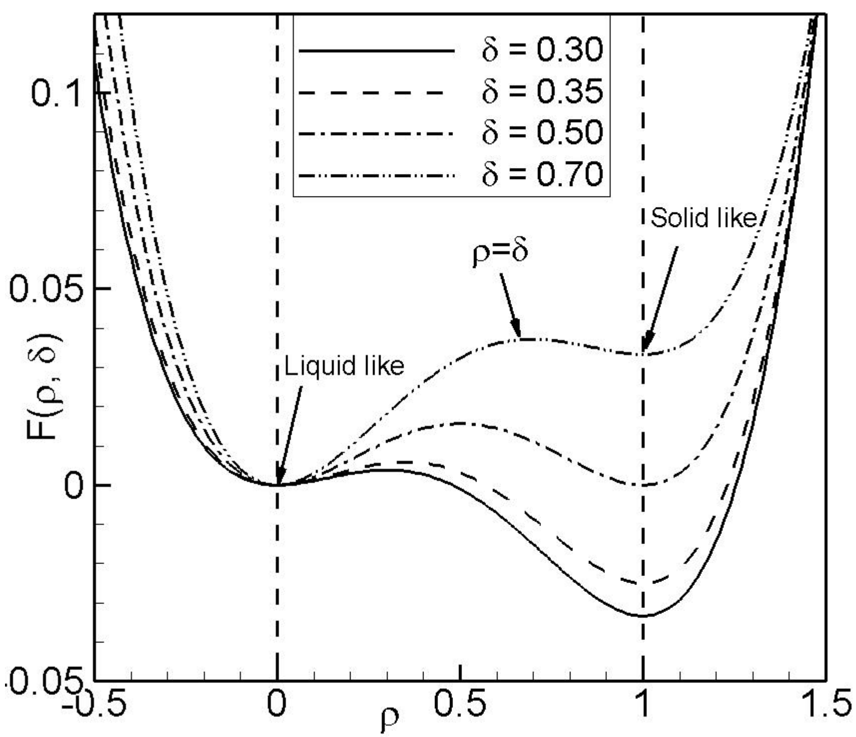
Order Parameter is indeed capable of capturing granular 'phase' transition from solidlike to fluidlike behavior

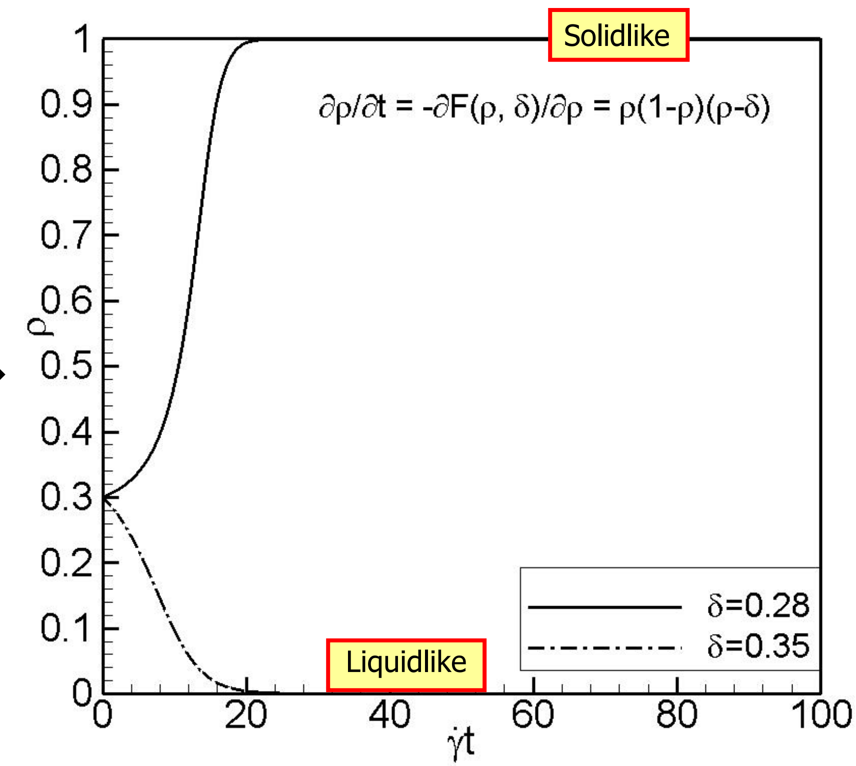
[1]McCarthy et al., *Powder Technology*, vol. 203, 70-77 (2010)

[2]Vidyapati and Subramaniam, S., "*Granular rheology and phase transition: DEM simulations and order-parameter based constitutive model*", (preprint)

Aranson's free energy density function

It was postulated[1] that free energy density function has two local minima at $\rho = 1$ (completely solidlike) and $\rho = 1$ (completely fluidlike)





$$F(\rho,\delta) = \int_{o}^{\rho} \rho(\rho-1)(\rho-\delta)\,d\rho$$

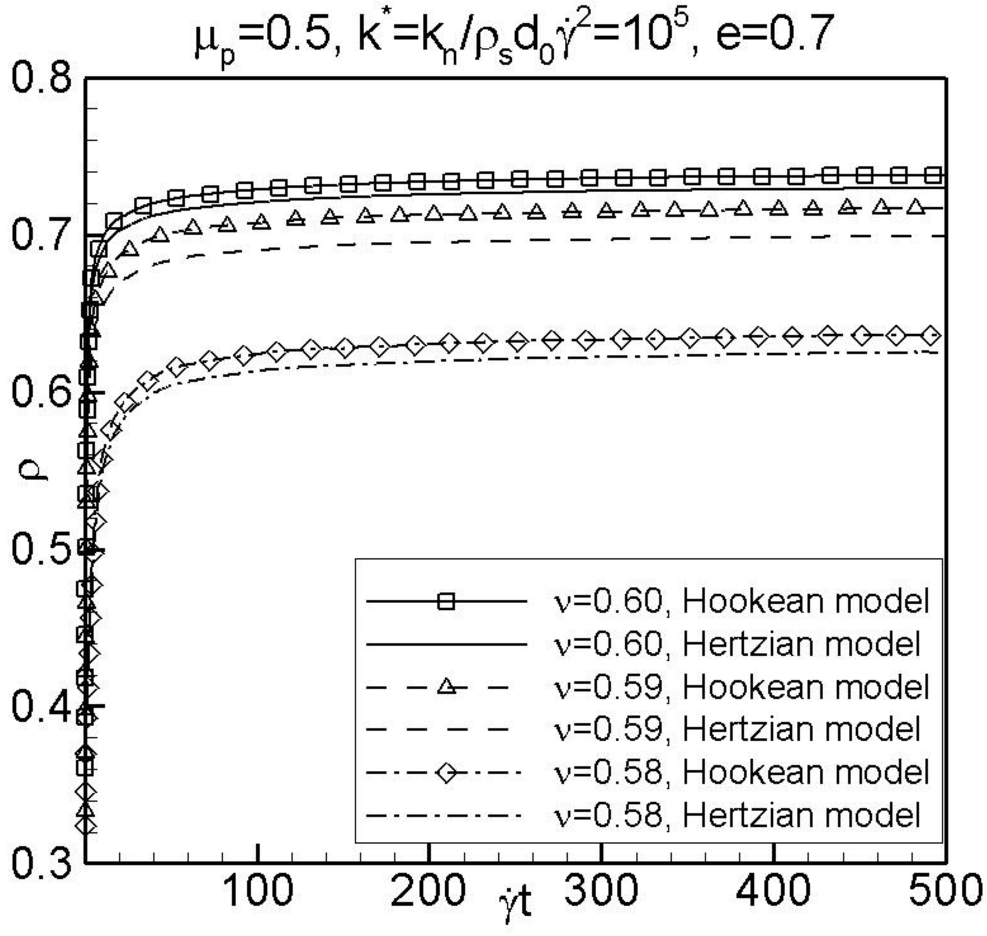
$$\frac{D\rho}{Dt} = D_c \nabla^2 \rho - \frac{\partial F(\rho,\delta)}{\partial \rho}$$

[1]Aranson et al., *Phys. Rev. E*, vol. 65, 061303 (2001)

OP dynamics from DEM simulations

OP extracted from DEM simulations using two different contact models

- Hooke
- Hertzi



$$\boldsymbol{F}_{n_{ij}} = f(\delta_{ij}/d)(k_n\delta_{ij}\boldsymbol{n}_{ij} - \gamma_n m_{eff} v_{n_{ij}})$$

$$\boldsymbol{F}_{t_{ij}} = f(\delta_{ij}/d)(-k_t u_{t_{ij}} - \gamma_t m_{eff} v_{t_{ij}})$$

Hookean contact model:

$$f(\delta_{ij}/d) = 1$$

Hertzian contact model:

$$f(\delta_{ij}/d) = \sqrt{\delta_{ij}/d}$$

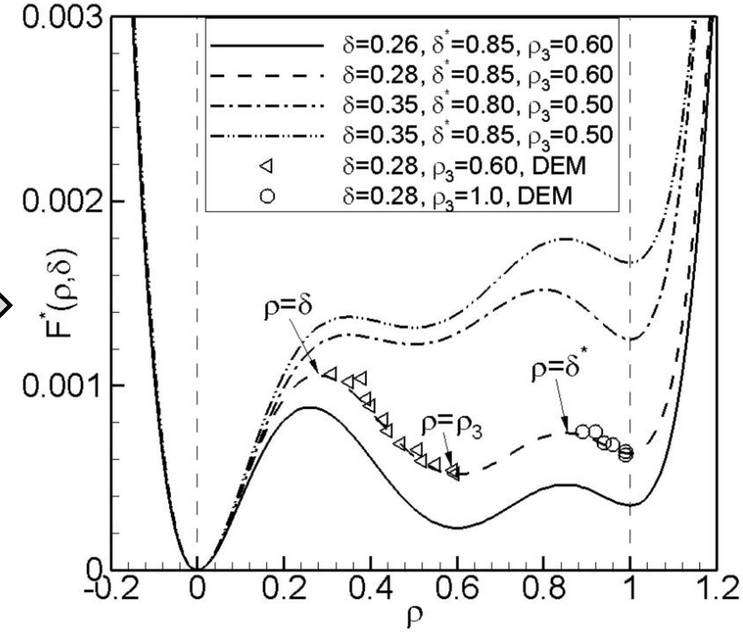
Discovered existence of a third stable granular phase which is neither completely solidlike nor completely fluidlike

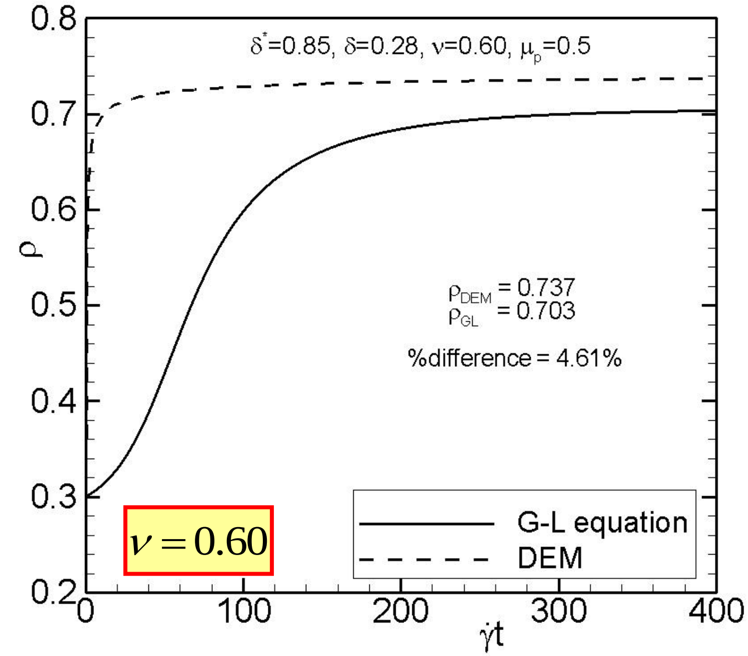
New formulation of free energy density function

$$F^*(\rho,\delta)=\int_o^{\rho}\rho(\rho-1)(\rho-\rho_3)(\rho-\delta)(\rho-\delta^*)\,d\rho$$

ρ_3 **third stable phase of granular material**

$$\frac{D\rho}{Dt}=D_c\nabla^2\rho-\frac{\partial F^*(\rho,\delta)}{\partial\rho}$$

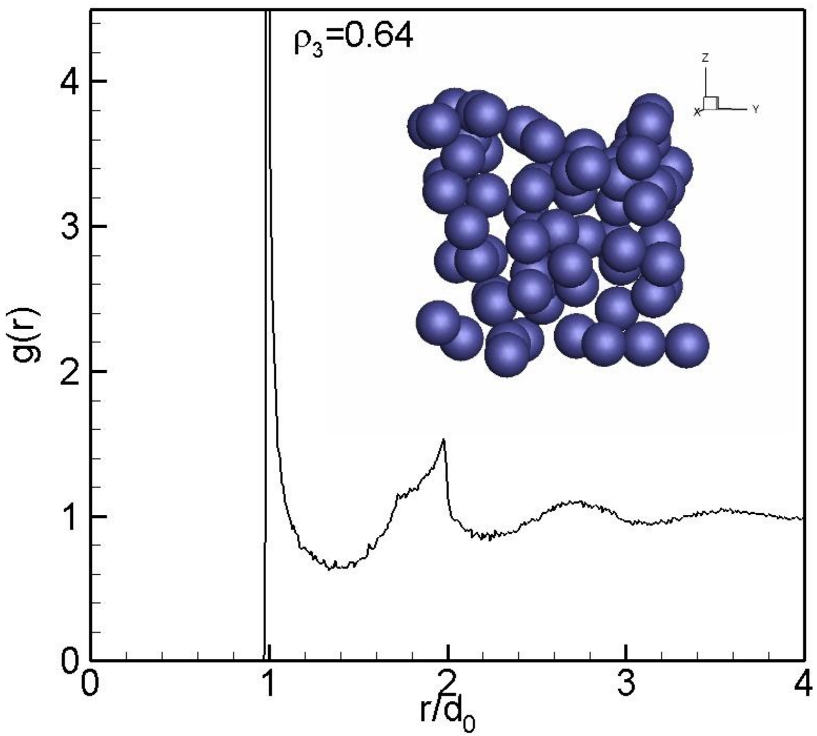




$\nu=0.60$

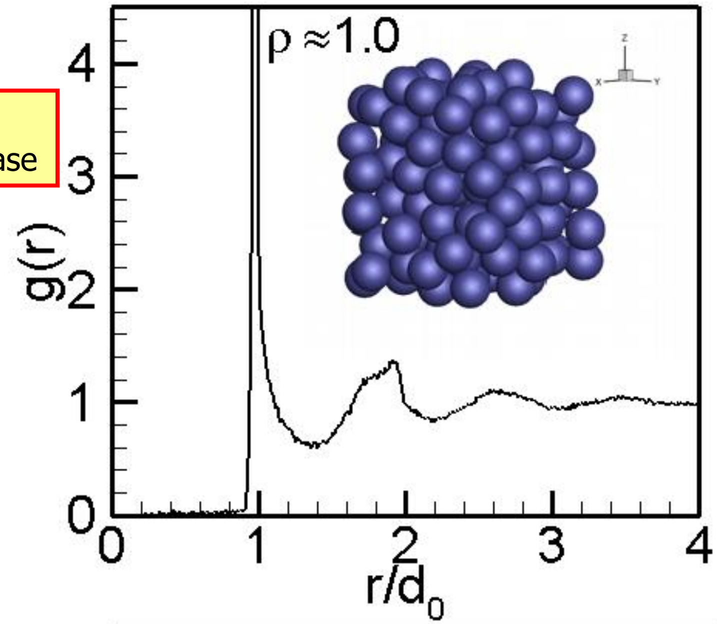
Quantification of third phase

The third stable granular phase is quantified using structural quantity such as pair correlation function

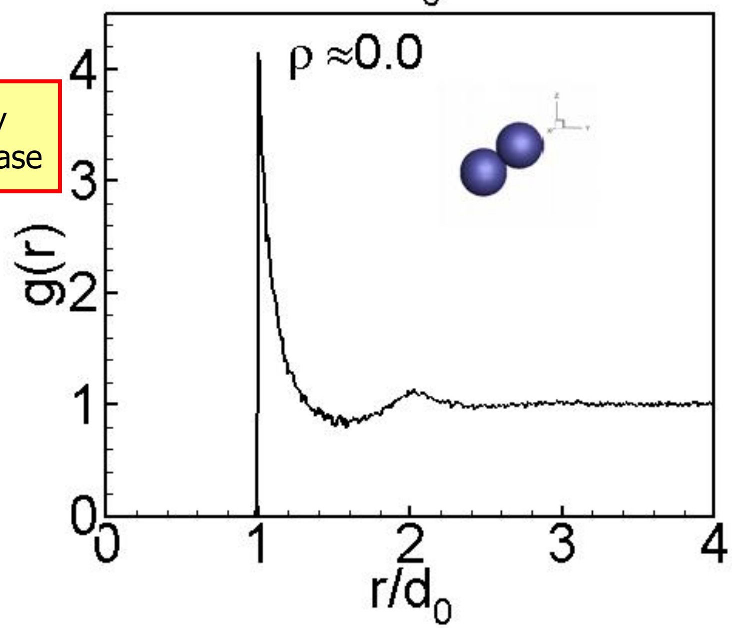


Pair correlation function and internal structure of solidlike contacts (in Inset) at third stable granular phase

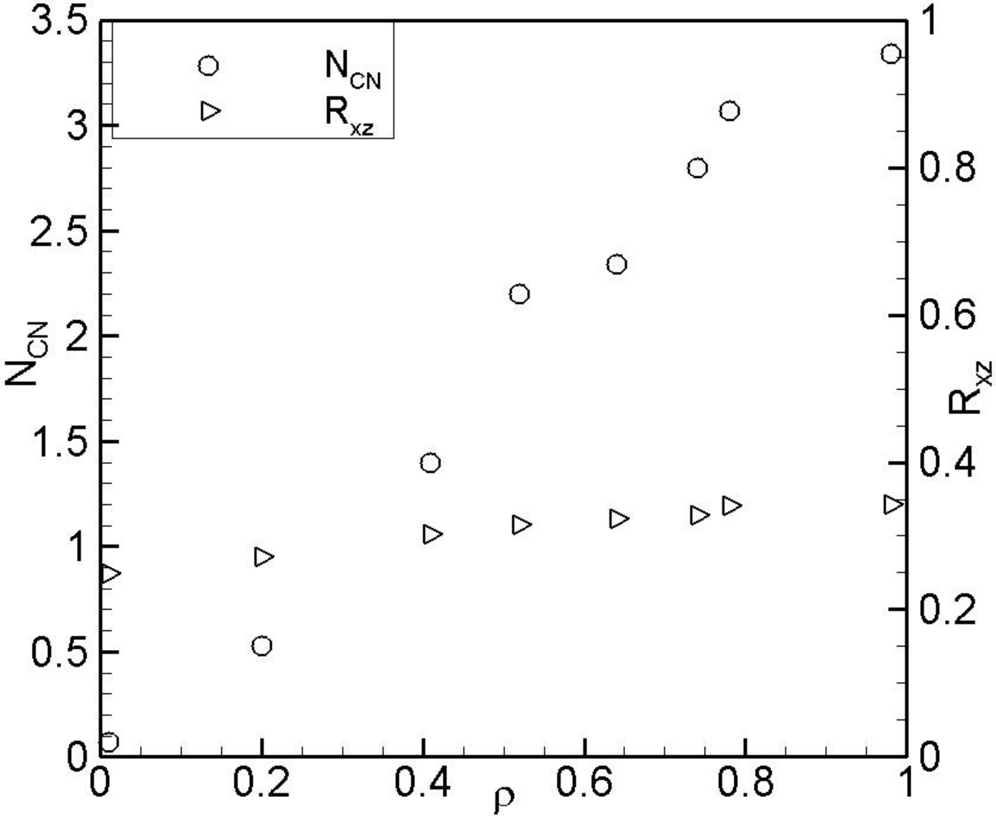
Completely solidlike phase



Completely fluidlike phase



Quantification of third phase



Average coordination number is more sensitive to the phase change as indicated by stable OP values, than the fabric tensor

Stress tensor in granular media

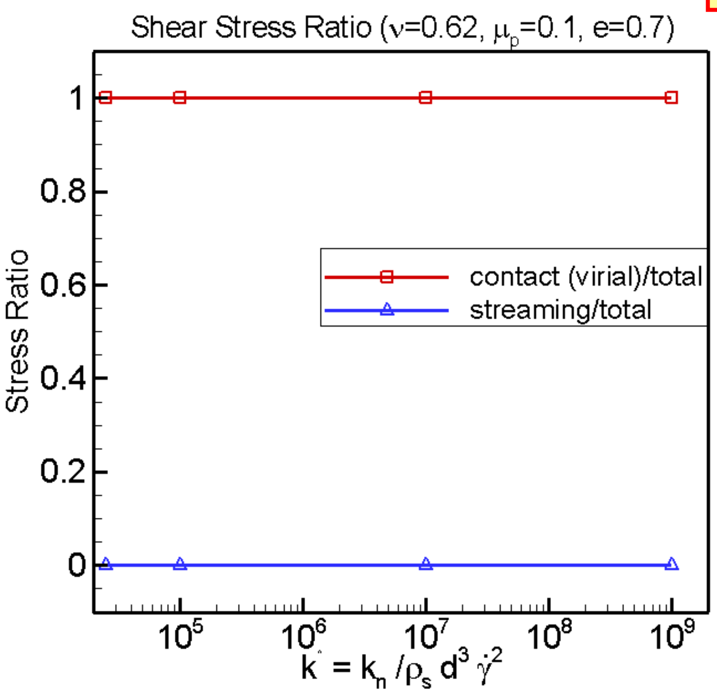
$$\sigma_{\alpha\beta}^{tot} = \frac{1}{V}\left[\sum_i m^{(i)} v_\alpha^{(i)} v_\beta^{(i)} + \sum_i \sum_{j,j\neq i} \frac{1}{2} r_\alpha^{(i)(j)} f_\beta^{(i)(j)}\right]$$

Streaming stress

Contact (virial) stress

DEM reveals that streaming part of the total stress is negligible (<3%) in the intermediate and dense regimes

streaming stress << contact stress



Accurate modeling of contact (virial) stress is critical in the intermediate regime

Developed the ***Relative Acceleration*** model: a statistical model based on evolution of the pair-correlation

Relative acceleration concept

- The term $\left\langle r_\alpha^{(i)(j)} \Delta A_\beta^{(i)(j)} \right\rangle$ can be computed using the idea of relative acceleration

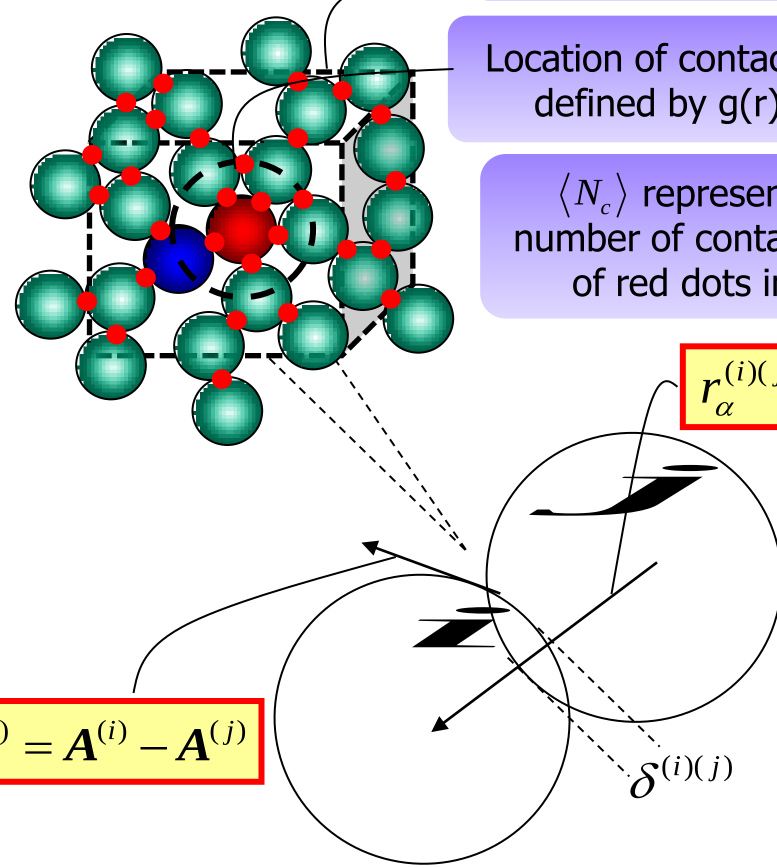
$$\boxed{\left\langle \Delta \boldsymbol{A}^{(i),(j)} \mid \boldsymbol{r}, \boldsymbol{w} \right\rangle = \left\langle \boldsymbol{A}^{(i)} \mid \boldsymbol{r}, \boldsymbol{w} \right\rangle - \left\langle \boldsymbol{A}^{(j)} \mid \boldsymbol{r}, \boldsymbol{w} \right\rangle = \left\langle \boldsymbol{A} \mid \boldsymbol{r}, \boldsymbol{w} \right\rangle}$$

$$\boldsymbol{r} = \boldsymbol{r}^{(i)} - \boldsymbol{r}^{(j)} \qquad \boldsymbol{w} = \boldsymbol{v}^{(i)} - \boldsymbol{v}^{(j)}$$

- The conditional relative acceleration can be decomposed as

$$\boxed{\left\langle \Delta \boldsymbol{A} \mid \boldsymbol{r}, \boldsymbol{w} \right\rangle = \left\langle \Delta \boldsymbol{A} \mid \boldsymbol{r} \right\rangle + \left\langle \Delta \boldsymbol{A} \mid \boldsymbol{w} \right\rangle}$$

- In LD (Langevin dynamics), the term $\left\langle \Delta \boldsymbol{A} \mid \boldsymbol{w} \right\rangle$ can be modeled in terms of inelasticity and damping



Relative acceleration model

- RA model for normal component of contact stress

$$\boxed{\sigma_{\alpha\beta} = \frac{1}{2V} N_{CN} \left\langle N\left(V\right)\right\rangle k_n R_{\alpha\beta} \int_0^{r_c} r^{(i)(j)} \delta^{(i)(j)} g\left(\mathbf{r}\right) d\mathbf{r}}$$

$$r^{(i)(j)} = d - \delta^{(i)(j)}$$

for small normal overlaps one can write the contact stress as

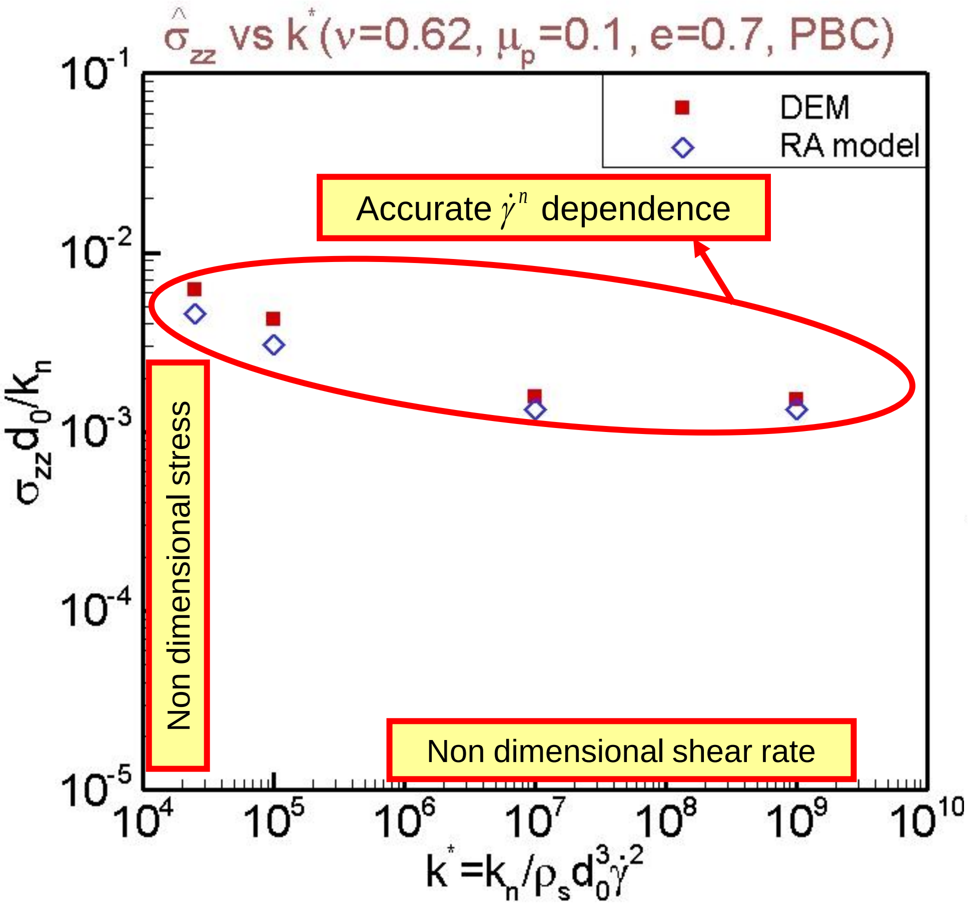
$$\boxed{\sigma_{\alpha\beta} = \frac{1}{2V} N_{CN} \left\langle N\left(V\right)\right\rangle k_n R_{\alpha\beta} d \int_0^{r_c} \delta^{(i)(j)} g\left(\mathbf{r}\right) d\mathbf{r}}$$

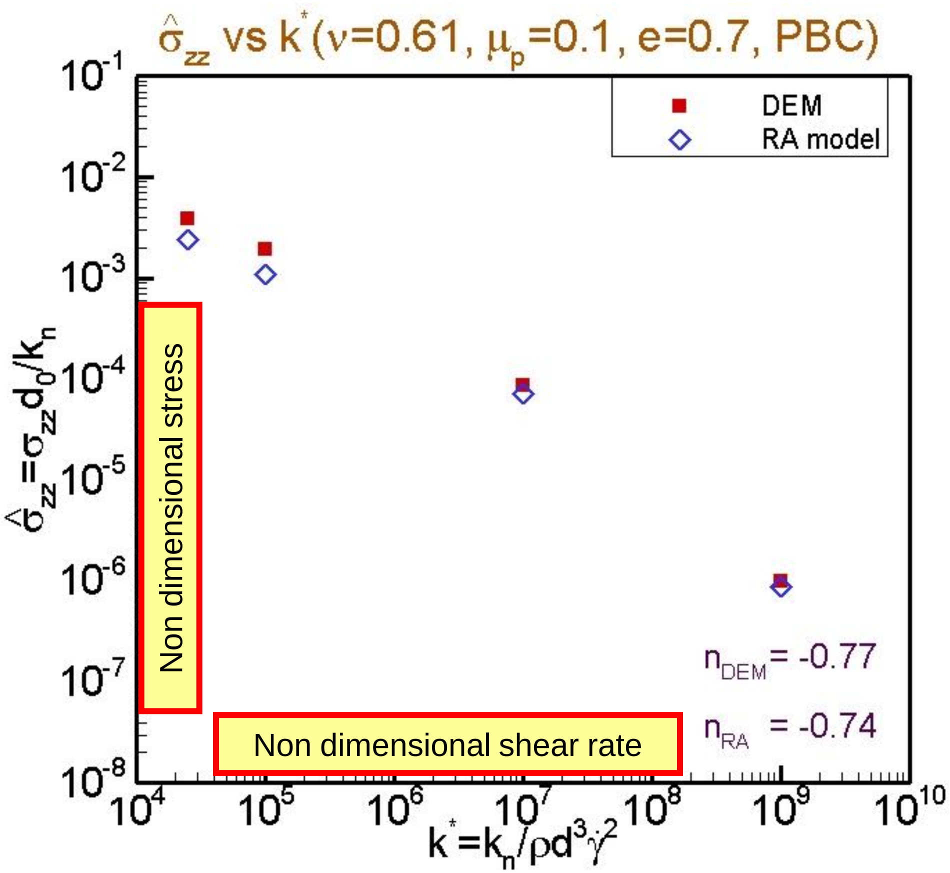
Model Inputs:

1. Average coordination number
2. Fabric tensor
3. Pair Correlation ($r<r_c$) or Force PDF

Preliminary model prediction using DEM data

- Model inputs $(N_{CN}, R_{\alpha\beta}, \delta^{(i)(j)}, g(\mathbf{r}))$ directly taken from data of DEM



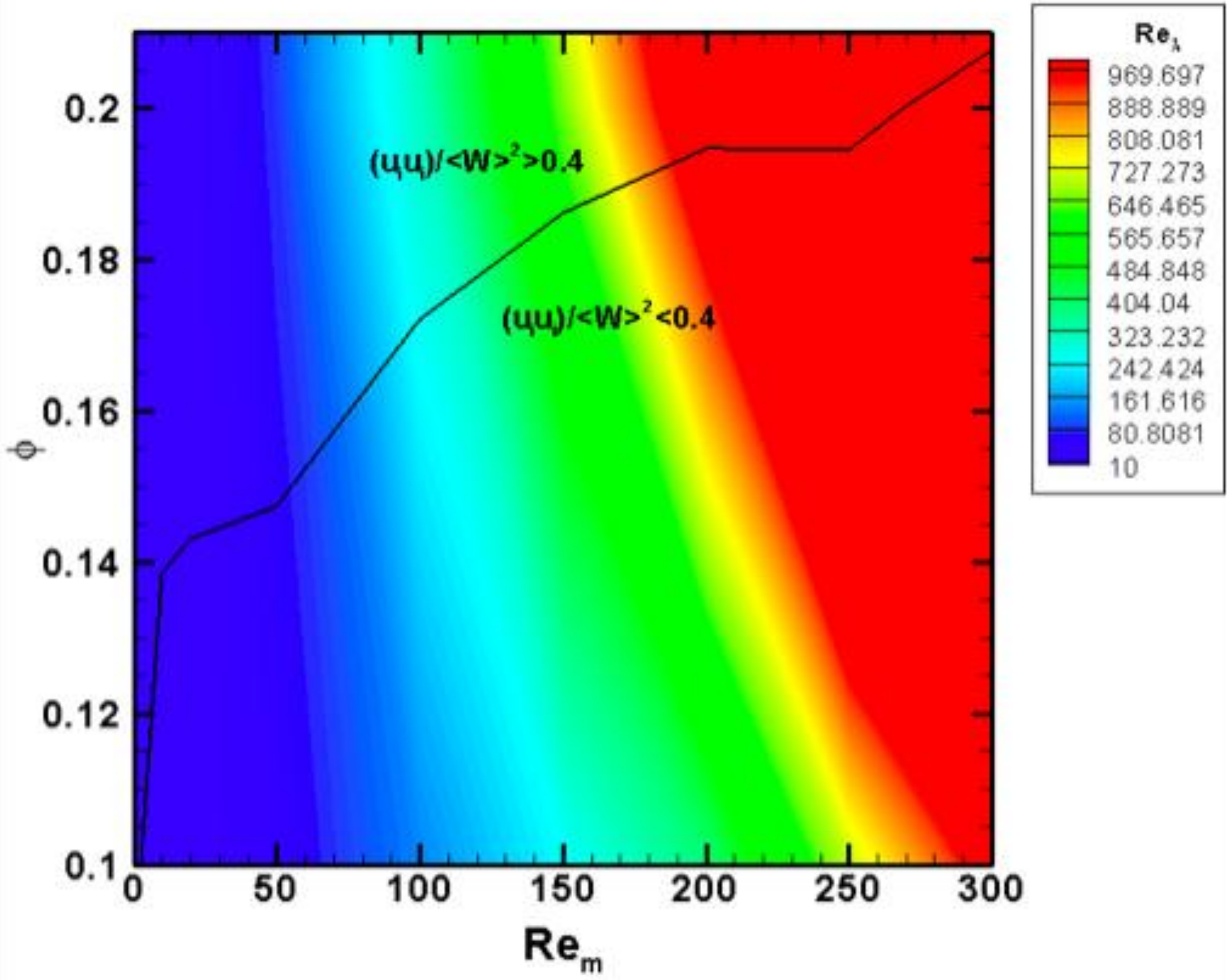


Preliminary results confirm the correct scaling of stress-strain scaling in intermediate regime

Conclusion

Particle-resolved Direct Numerical Simulation for gas-solid flows, and Discrete Element Simulations for granular flows, are useful approaches for understanding *multiphase flow physics* and for *model development*

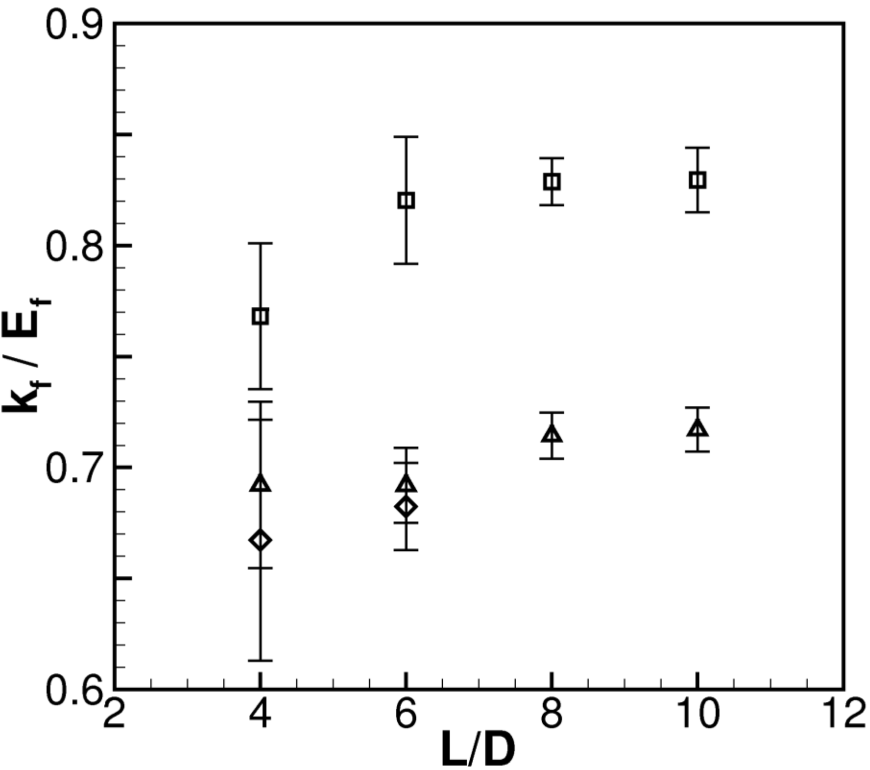
Turbulent and non-turbulent fluctuations



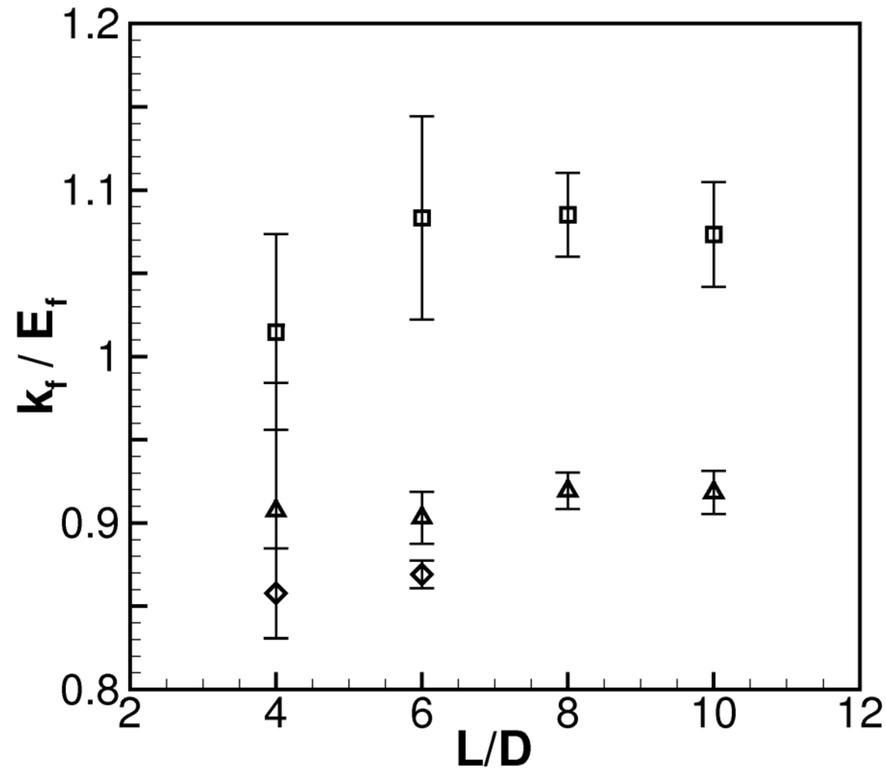
Contour plot of equivalent R_λ generating the same energy in velocity fluctuations as the non-turbulent fluctuations arising from the presence of particles in gas-solid flow

Convergence of k_f at Re_m =

Volume fraction: 0.3



Volume fraction: 0.4

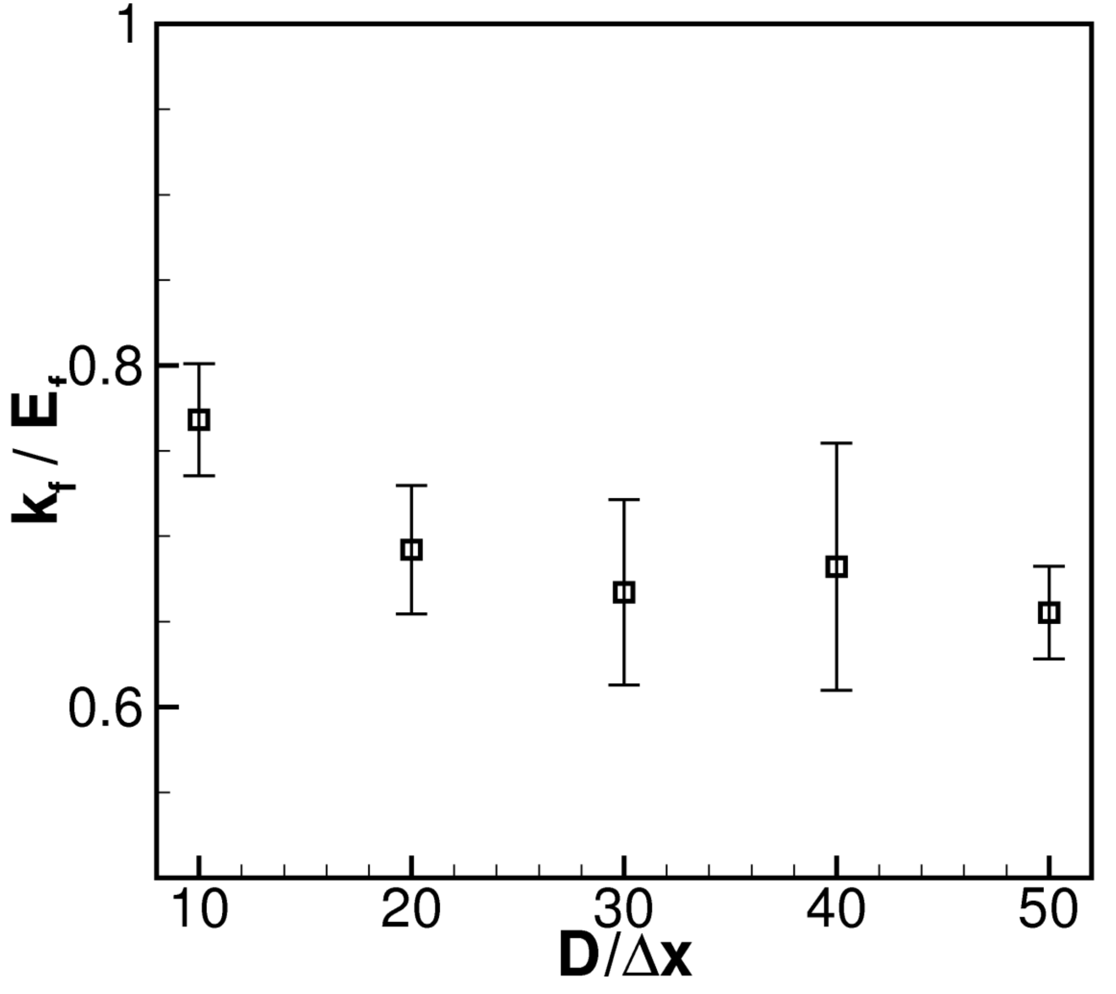


Squares : D_m = 10

Triangles : D_m = 20

Diamonds : D_m = 30,

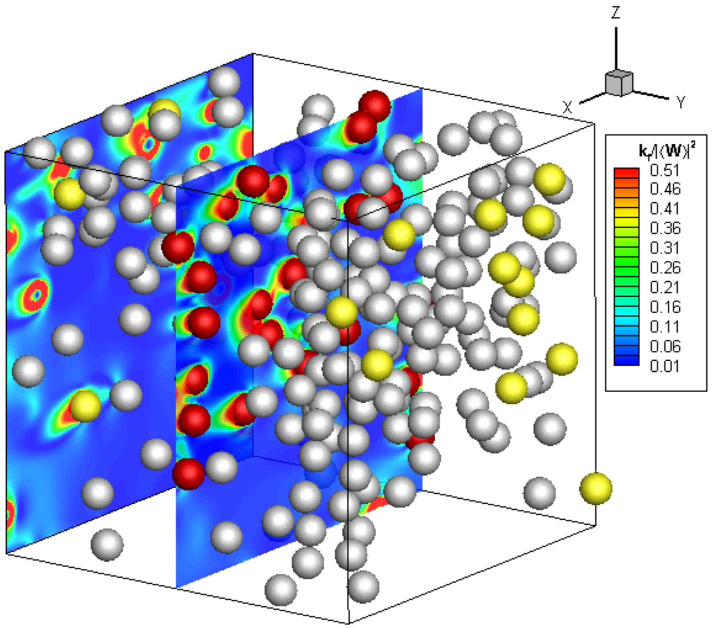
Convergence of k_f at Re_m =

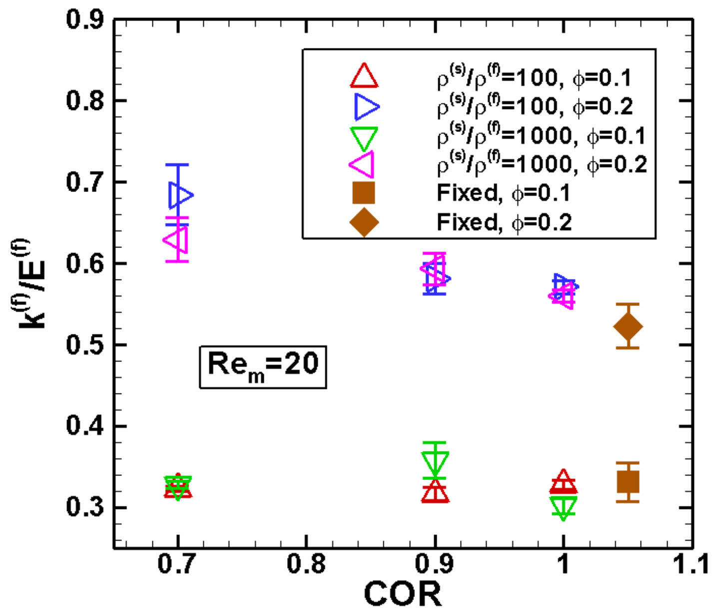


Volume fraction: 0.3

Freely evolving suspensions

Freely moving particles with inelastic collisions





Similarity of $k^{(f)}$ among fixed and moving particles

$$\underbrace{\cancel{\left\langle I^{(f)}\rho^{(f)}\right\rangle \frac{d}{dt}k^{(f)}}}_{\text{unsteady term}} = \underbrace{\langle W_i\rangle \left\langle \tau_{ji} n_j^{(s)} \delta\left(\mathrm{x}-\mathrm{x}^{(\mathrm{I})}\right)\right\rangle}_{(\mathrm{I})} - \underbrace{\cancel{\left\langle u_i^{\prime\prime(s)} \tau_{ji} n_j^{(s)} \delta\left(\mathrm{x}-\mathrm{x}^{(\mathrm{I})}\right)\right\rangle}}_{(\mathrm{II})} - \underbrace{2\mu^{(f)}\left\langle I^{(f)} S_{ij}S_{ij}\right\rangle}_{\text{Viscoud dissipation}}$$

$$\underbrace{\cancel{\left\langle I^{(s)}\rho^{(s)}\right\rangle \frac{d}{dt}k^{(s)}}}_{\text{unsteady term}} = \underbrace{\left\langle u_i^{\prime\prime(s)} \tau_{ji} n_j^{(s)} \delta\left(\mathrm{x}-\mathrm{x}^{(\mathrm{I})}\right)\right\rangle}_{\text{interphase TKE transfer}} + \underbrace{\Gamma_{coll}^{(s)}}_{\text{onal dissipation}}$$

Small compared to others

Evolution equation the same as fixed beds

Reynolds stress model

Cross correlations are almost zero

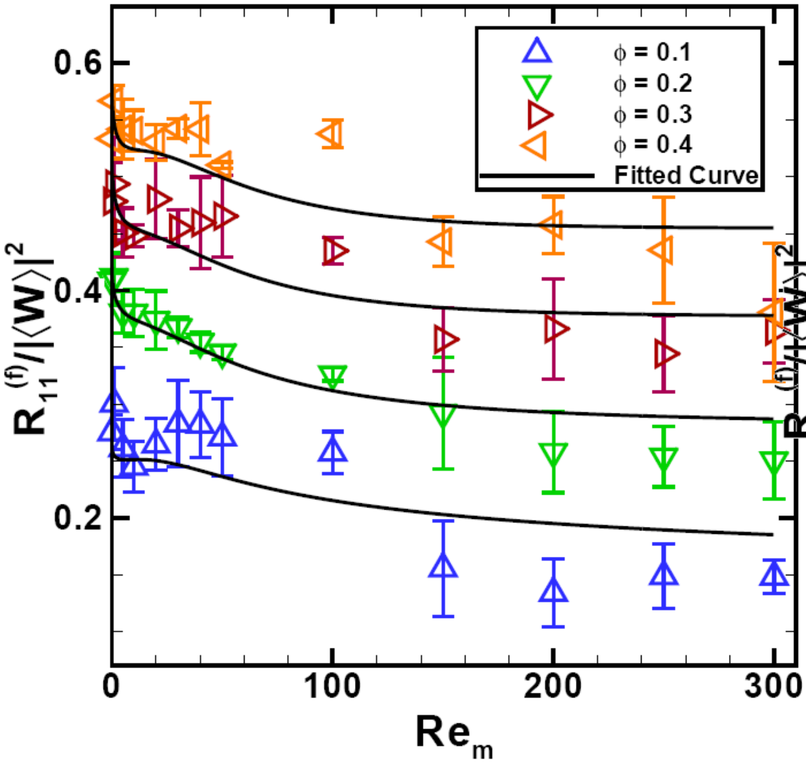
Anisotropy is along mean flow direction

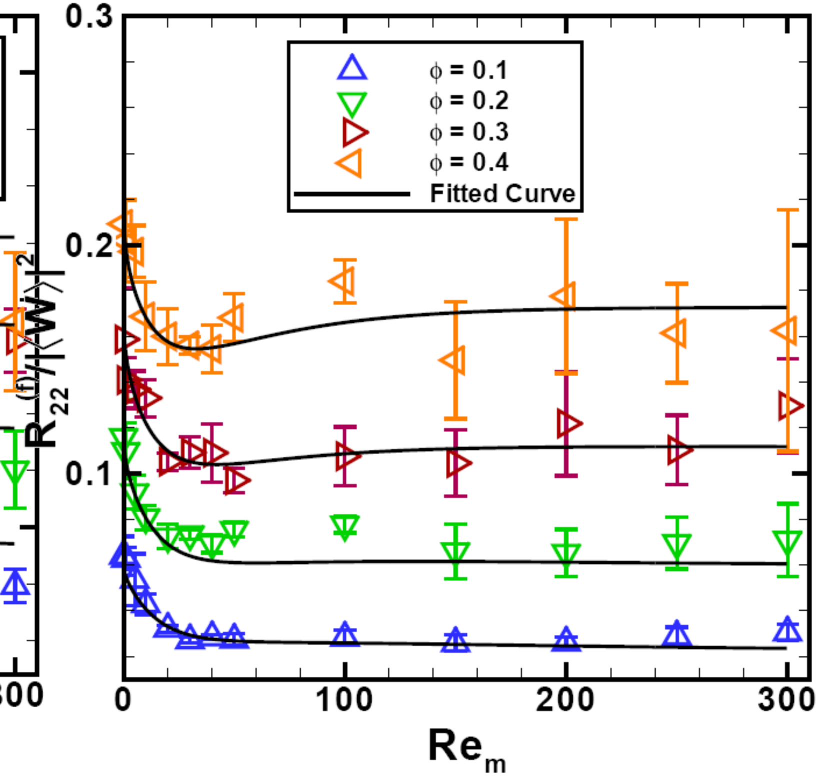
The normal correlations in perpendicular plane are similar

Reynolds stress is axi-symmetric along the mean flow

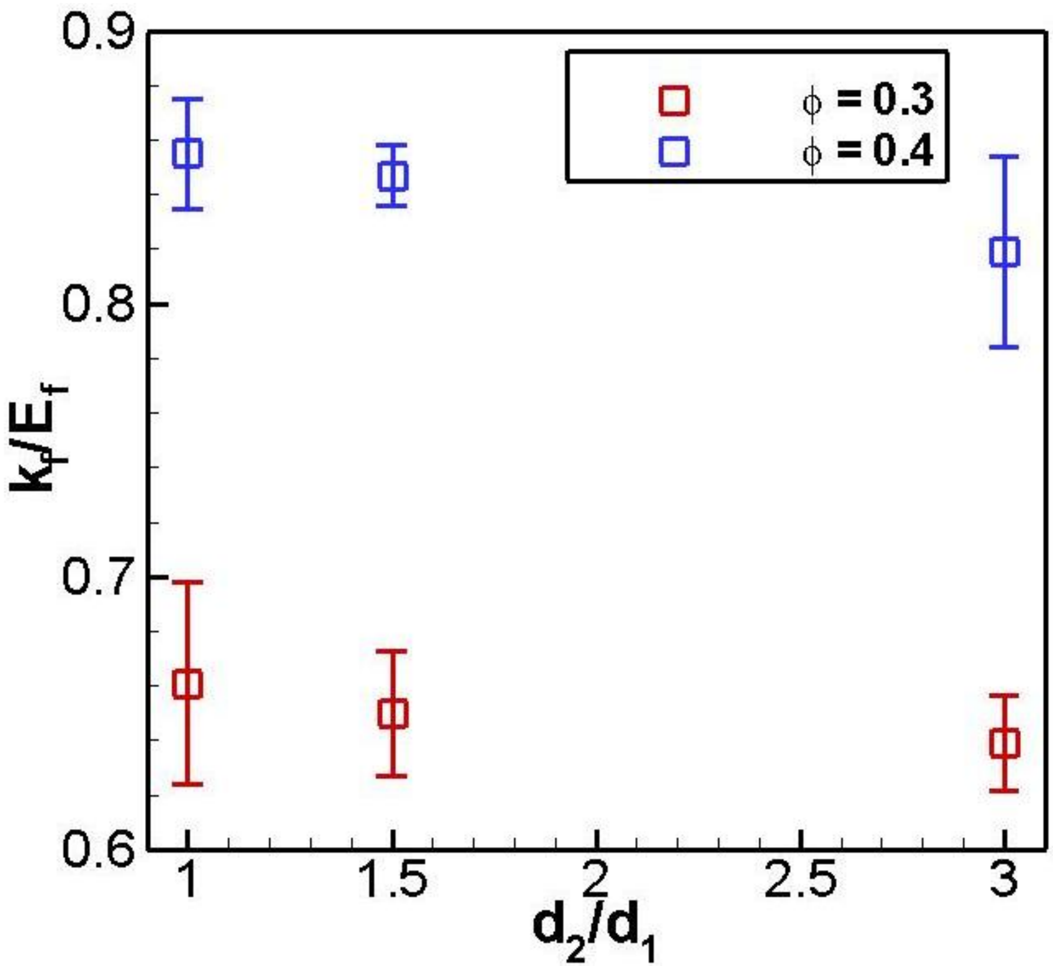
$$
\begin{cases}
b_{11}^{(f)}(Re_m,\phi) = \frac{a}{1+b\mathrm{e}^{-cRe_m}}\mathrm{e}^{-d\phi/(1+e\mathrm{e}^{-fRe_m})} \\
b_{22}^{(f)}(Re_m,\phi) = b_{33}^{(f)}(Re_m,\phi) = -\frac{b_{11}^{(f)}(Re_m,\phi)}{2} \\
b_{ij}^{(f)}(Re_m,\phi) = 0, \quad i \neq j
\end{cases}
$$

$$
\begin{cases}
a = 0.523 \\
b = 0.303 \\
c = 0.114 \\
d = 3.526 \\
e = 1.809 \\
f = 0.005
\end{cases}
$$





Gas-phase Velocity Fluctuations: Bidisperse



Strength of gas-phase velocity fluctuations depend strongly on only the total solid volume fraction and the Reynolds number based on Sauter mean diameter

Multiphase Flow Turbulence Model

Mean momentum equation: fluid phase

$$\frac{\partial}{\partial t}\left\{\rho_f\left(1-\phi\right)\left\langle {u_i}^{(f)}\right\rangle\right\}+\frac{\partial}{\partial x_j}\left\{\rho_f\left(1-\phi\right)\left\langle {u_i}^{(f)}\right\rangle\left\langle {u_j}^{(f)}\right\rangle\right\}$$
$$=-\left(1-\phi\right)\left\langle g_i^{(f)}\right\rangle-\frac{\partial}{\partial x_j}\boxed{\left\{\rho_f\left\langle I_{\mathsf{f}} u_i^{\prime\prime(f)} u_j^{\prime\prime(f)}\right\rangle\right\}}$$
$$+\boxed{\left\langle \tau_{ji} n_j^{(s)}\delta\left(\mathbf{x}-\mathbf{x}^{(I)}\right)\right\rangle}.$$

Turbulence model

$$(1-\phi)\rho_f\frac{k_f^2}{\varepsilon_f}\frac{\partial}{\partial x_j}\langle u_i^{(f)}\rangle$$

Drag law

Existing multiphase turbulence models are extensions of single-phase turbulence models

Back-Up

Granular phase transition: Order parameter

- Characterizes the phase or "state" of the granular material

$\mathrm{OP} = 0$ → Pure fluid

$\mathrm{OP} = 1$ → Pure solid

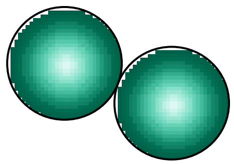
- Order parameter is defined by[1]

$$\mathrm{OP} = \frac{\langle \overline{Z_s} \rangle}{\langle \overline{Z} \rangle}$$

$\langle \overline{Z_s} \rangle$ → Number of solid contacts

$\langle \overline{Z} \rangle$ → Total number of contacts

Solidlike contacts[1]



$F_t < \mu_t F_n$ → eliminates long lasting sliding contacts

$t^* > 1.1 t_{bc}$ → excludes short term collisions

- Solidlike stress
  - *stress from solidlike contacts*
- Fluidlike stress
  - *stress from fluidlike contacts + streaming stress*

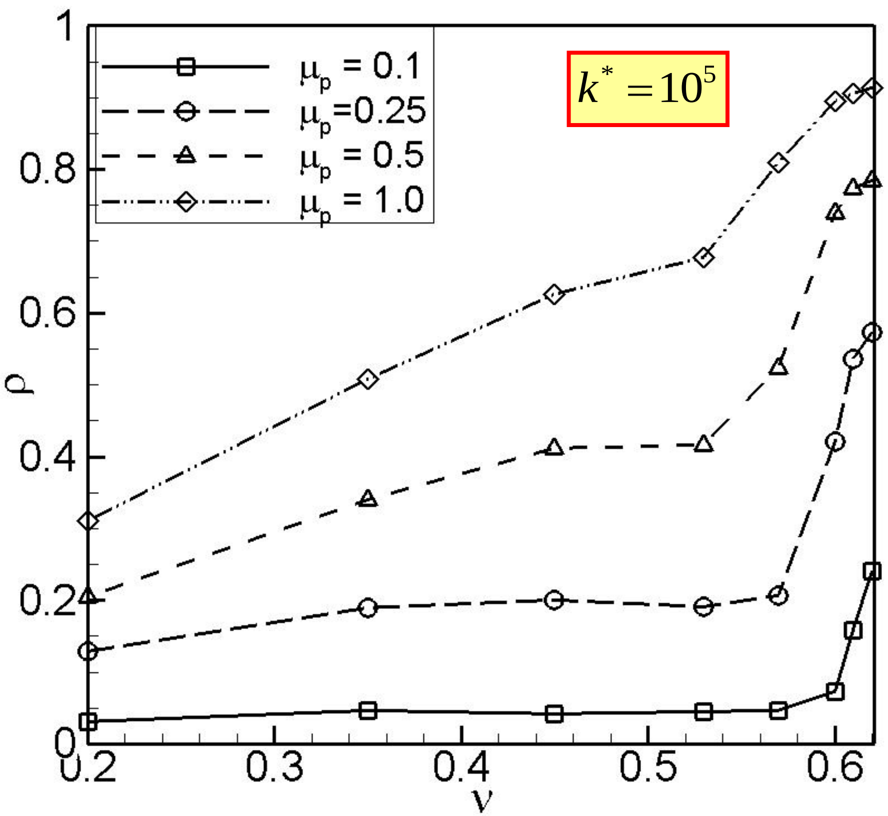
Total granular stress

↓

Solidlike stress + Fluidlike stress

[1]Volfson et al., *Phys. Rev. E*, vol. 68, 021301 (2003)

OP from DEM



A fit for steady values of ρ_3 OP with solid volume fraction and friction coefficient is proposed based on the data obtained from DEM simulations

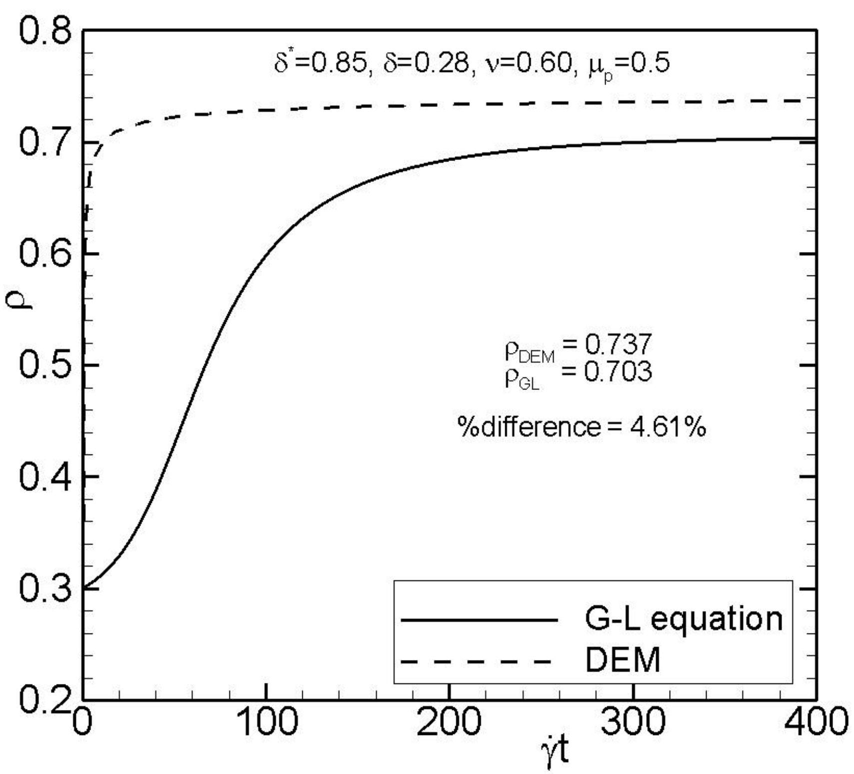
$$\rho_3 = \begin{cases} a\sin(b\pi\nu\mu_p) & 0 < \nu \le \nu^* \\ A\log(B\nu^2\mu_p) + C\exp(\nu^2 - \mu_p) & \nu^* < \nu < \nu_{max} \end{cases}$$

$a = 0.804$, b=0.678, A=0.5547, B=6.769, C=0.6847

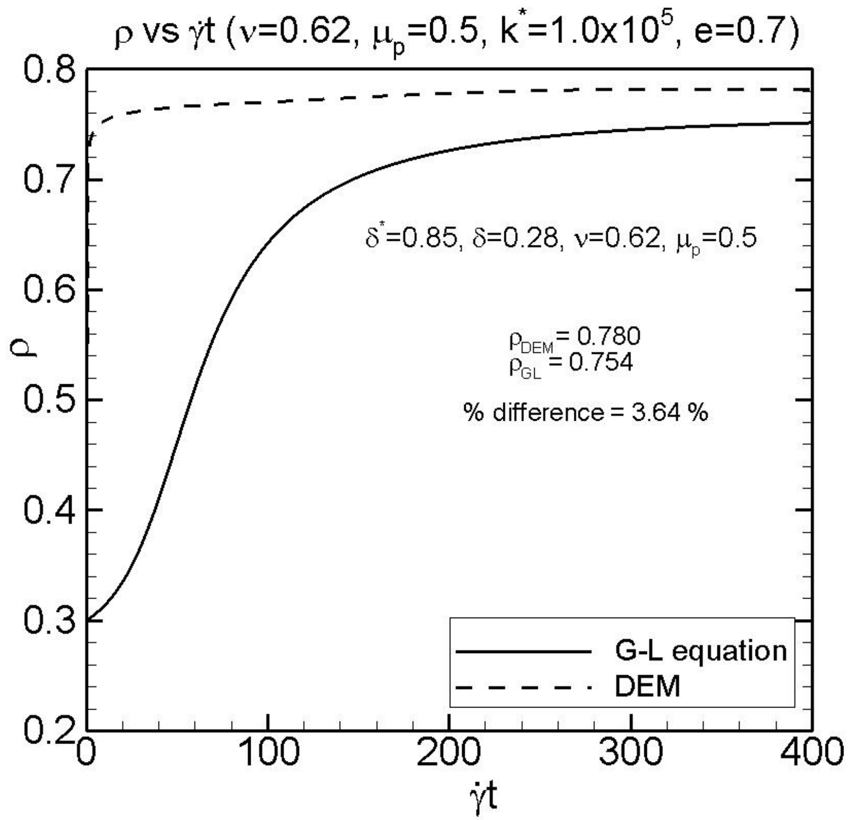
Assessment of proposed hypothesis

$$\frac{D\rho}{Dt} = D_c \nabla^2 \rho - \frac{\partial F^*(\rho,\delta)}{\partial \rho}$$

$$F^*(\rho,\delta) = \int_o^\rho \rho(\rho-1)(\rho-\rho_3)(\rho-\delta)(\rho-\delta^*)\,d\rho$$



$\nu = 0.60$



$\nu = 0.62$

Quantification of third phase

Co-ordination number (N_{CN}): average number of contacts par particle

$$N_{CN} = \frac{\sum_i N_c^{(i)}}{N}$$

$N_c^{(i)}$: number of contacts for i[th] particle

N: total number of particles

Fabric tensor R_{ij} : describes the anisotropy of the contact distribution in granular media

$$R_{ij} = \frac{1}{N_c} \sum_{c \in V} n_i n_j$$

Pair correlation function (g(**r**)): probability of finding a particle at a distance r away from given reference particle

$$g(\boldsymbol{r}) = \frac{N_r}{N \times V_r \times n}$$

$$V_r = 4\pi r^2 dr$$

n :Number density

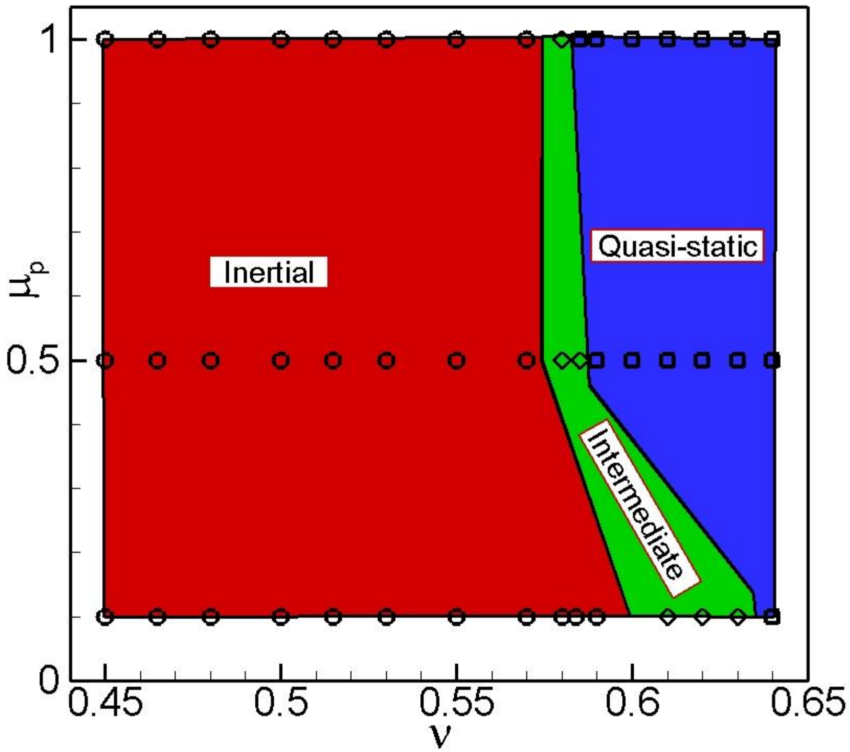
Regime map

Regime classified based on relationship between stress-strain

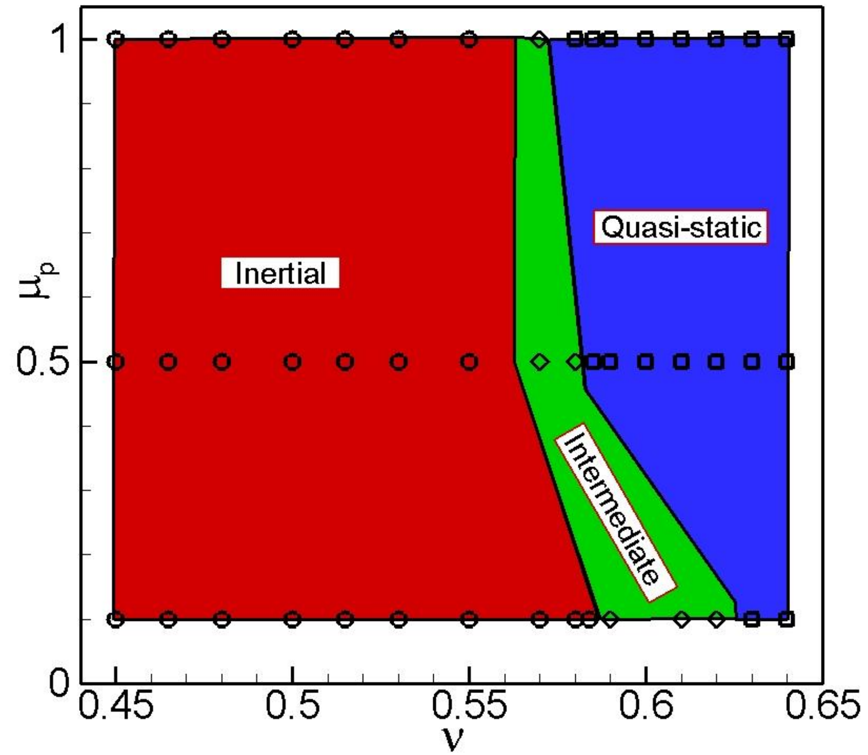
Inertial regime: $\sigma \propto \dot{\gamma}^2$

Intermediate regime: $\sigma \propto \dot{\gamma}^n, 0 < n < 2$

Quasi-static regime: $\sigma \neq f(\dot{\gamma})$



$k^* = k_n / \rho_s d_0^3 \dot{\gamma}^2 = 2.5\times10^4$



$k^* = k_n / \rho_s d_0^3 \dot{\gamma}^2 = 10^9$