Interaction of Particles with Carrier Gas Revealed by Particle-resolved Direct Numerical Simulation: Improved Drag Laws and Models

Shankar Subramaniam

Department of Mechanical Engineering

Iowa State University

Sudheer Tenneti, Rahul Garg, K. Devendran, M. Mehrabadi, R.O. Fox, S. Sundaresan and C.M. Hrenya

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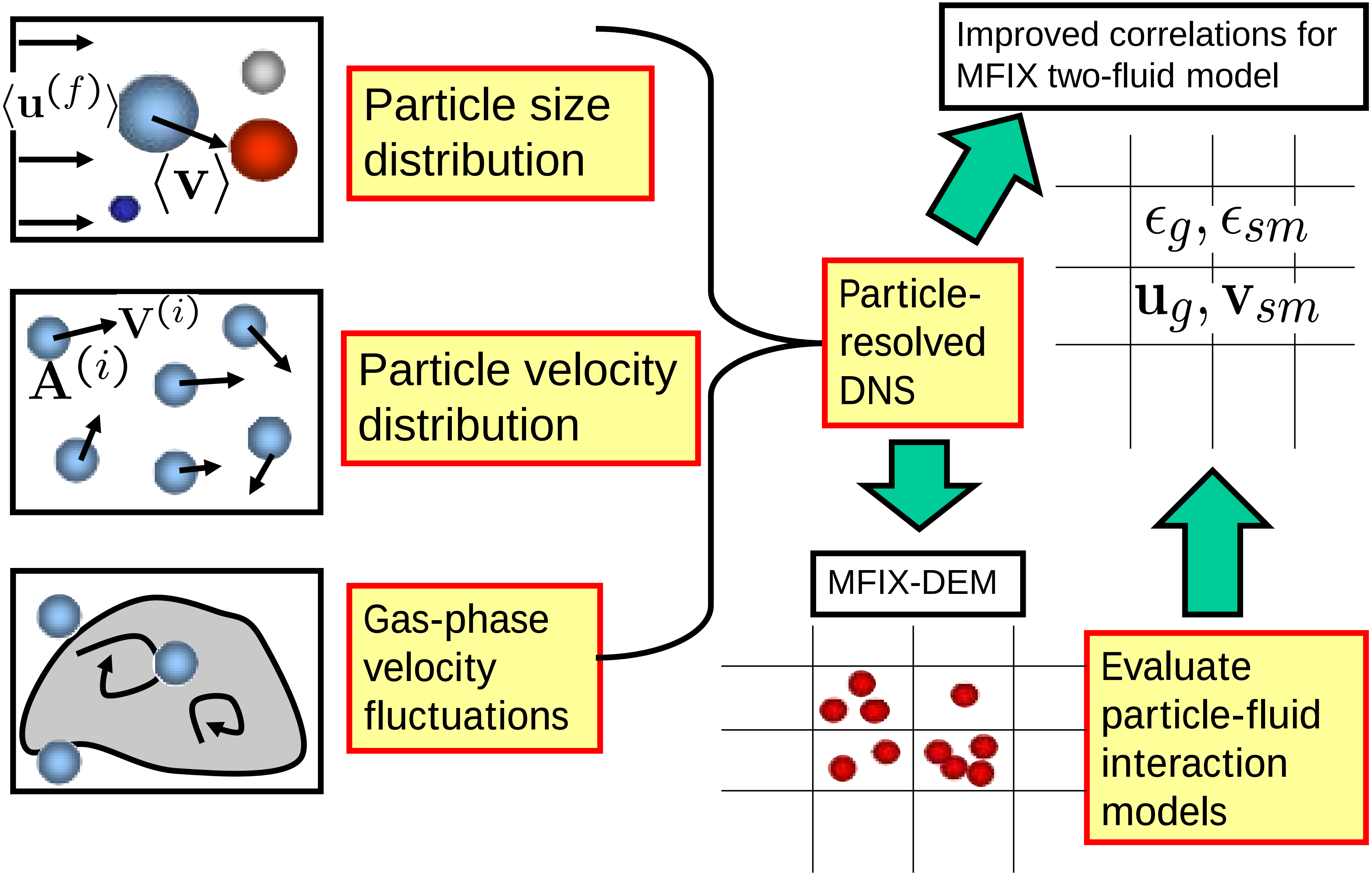
Outline

- Drag laws for monodisperse and bidisperse suspensions
- Particle velocity fluctuations
- Gas-phase velocity fluctuations

Modeling Polydisperse Gas-solid Systems



Approach: PUReIBM

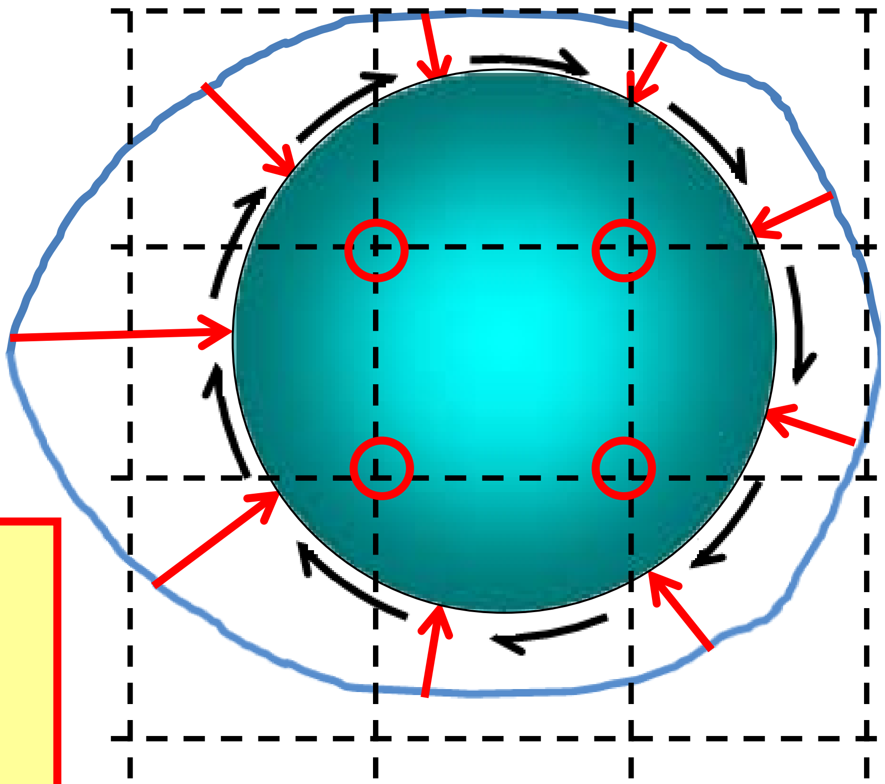
$$\partial_t \mathbf{u} + \nabla \cdot (\mathbf{u}\mathbf{u}) = -\frac{1}{\rho_f}\nabla p + \nu_f \nabla^2 \mathbf{u} + \mathbf{f}_{\mathbf{u}}$$

Particle-resolved

Uncontaminated-fluid

Reconcilable

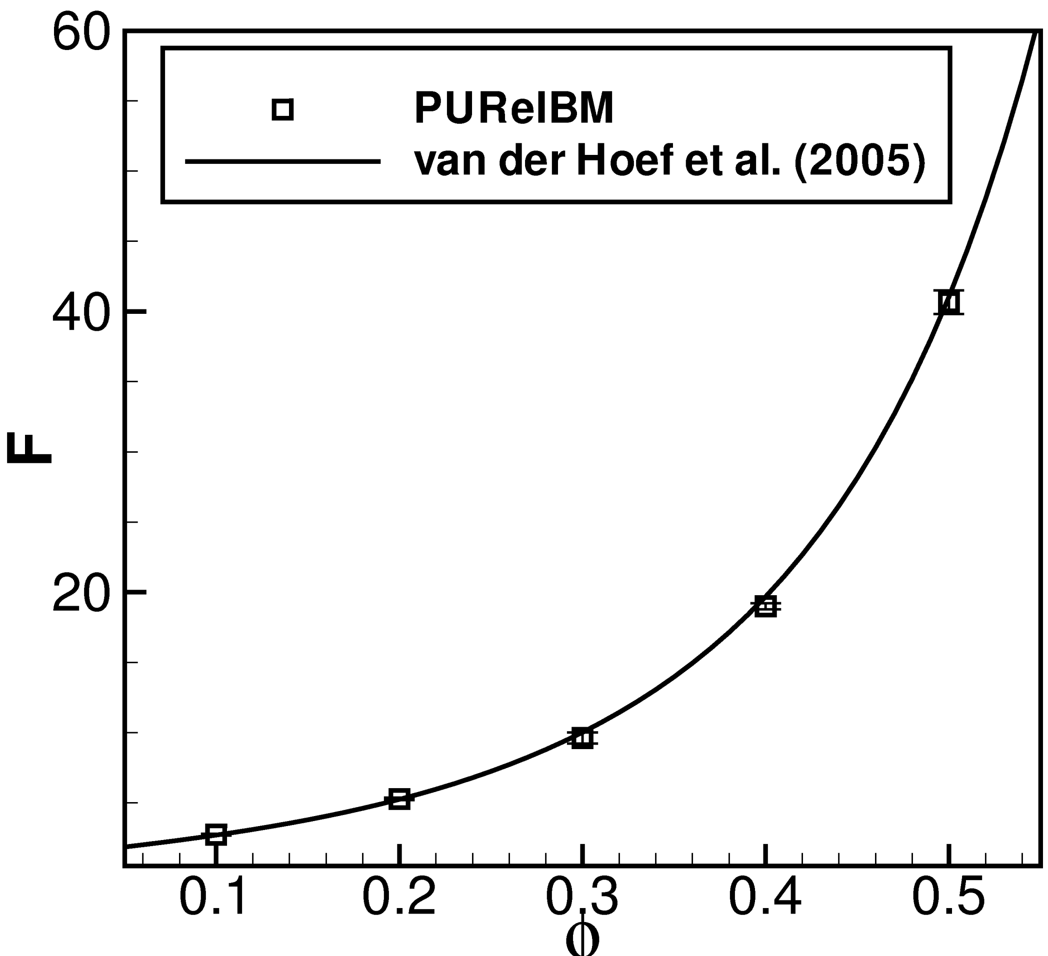
Immersed **B**oundary **M**ethod



Features:

- Continuum Navier-Stokes Solver
- No contamination in fluid due to IB forcing
- Drag : integrating stress tensor at sphere boundary → consistent with two-fluid equations
- Accurate and Numerically Convergent

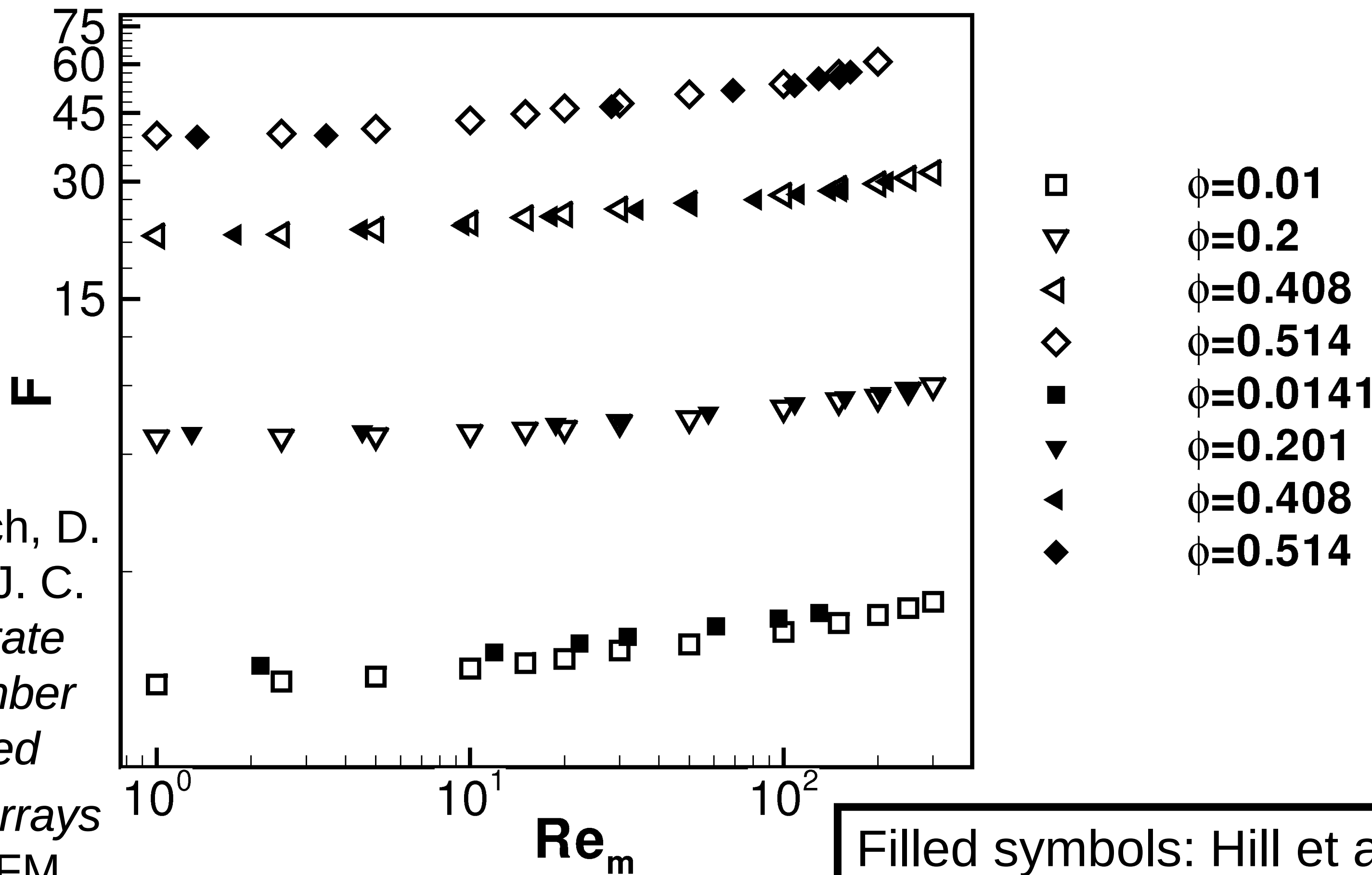
Validation Tests



van der Hoef, M. A., Beetstra, R. & Kuipers, J. A. M. 2005 "*Lattice-Boltzmann simulations of low-Reynolds-number flow past mono- and bidisperse arrays of sphere: results for the permeability and drag force*." JFM 528.

Stokes flow past random arrangement of monodisperse spheres

Validation Tests



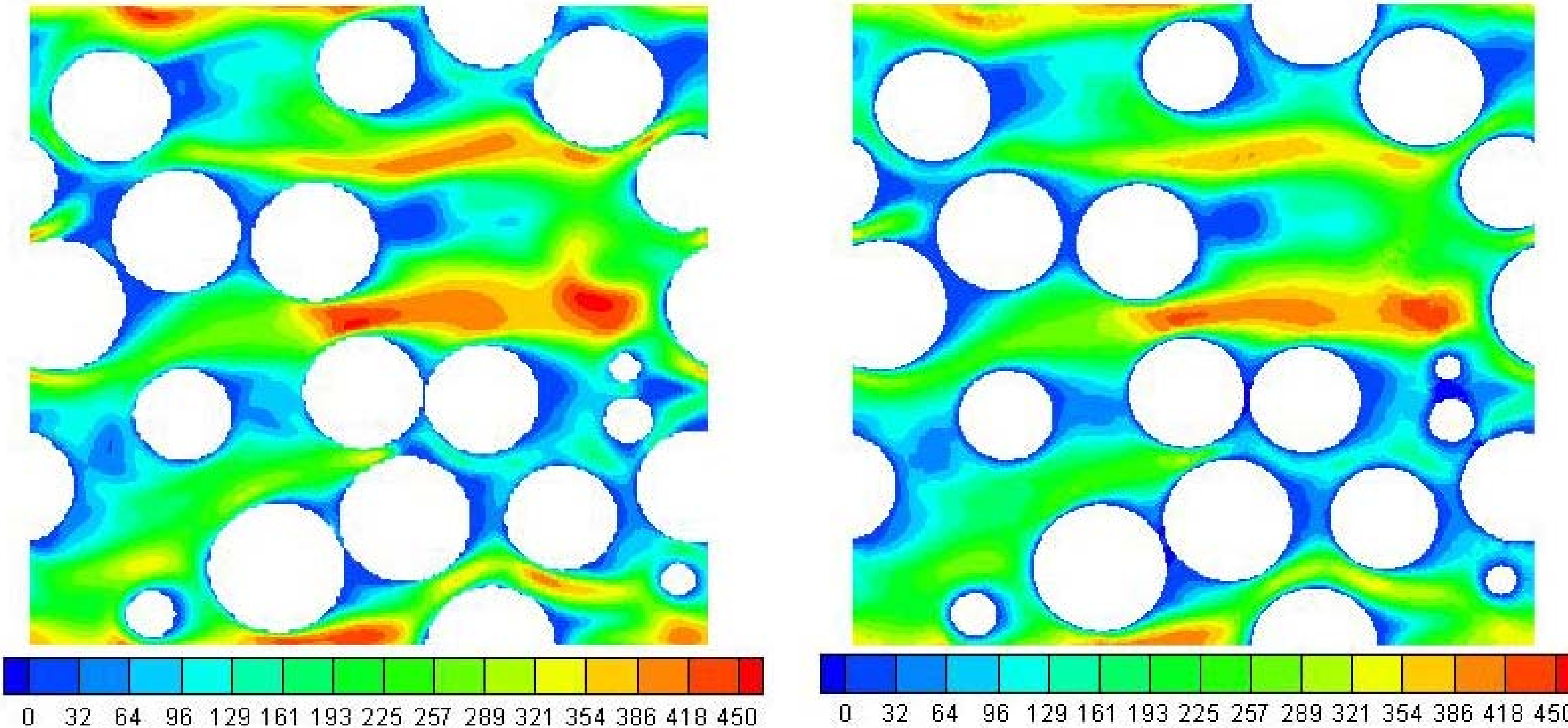
Hill, R. J., Koch, D. L. & Ladd, A. J. C. 2001*b* *“Moderate Reynolds number flows in ordered and random arrays of spheres*.” JFM 448

Filled symbols: Hill et al.
Open symbols: PUReIBM

Moderate Reynolds number flow past simple cubic arrays of monodisperse spheres

Validation Tests

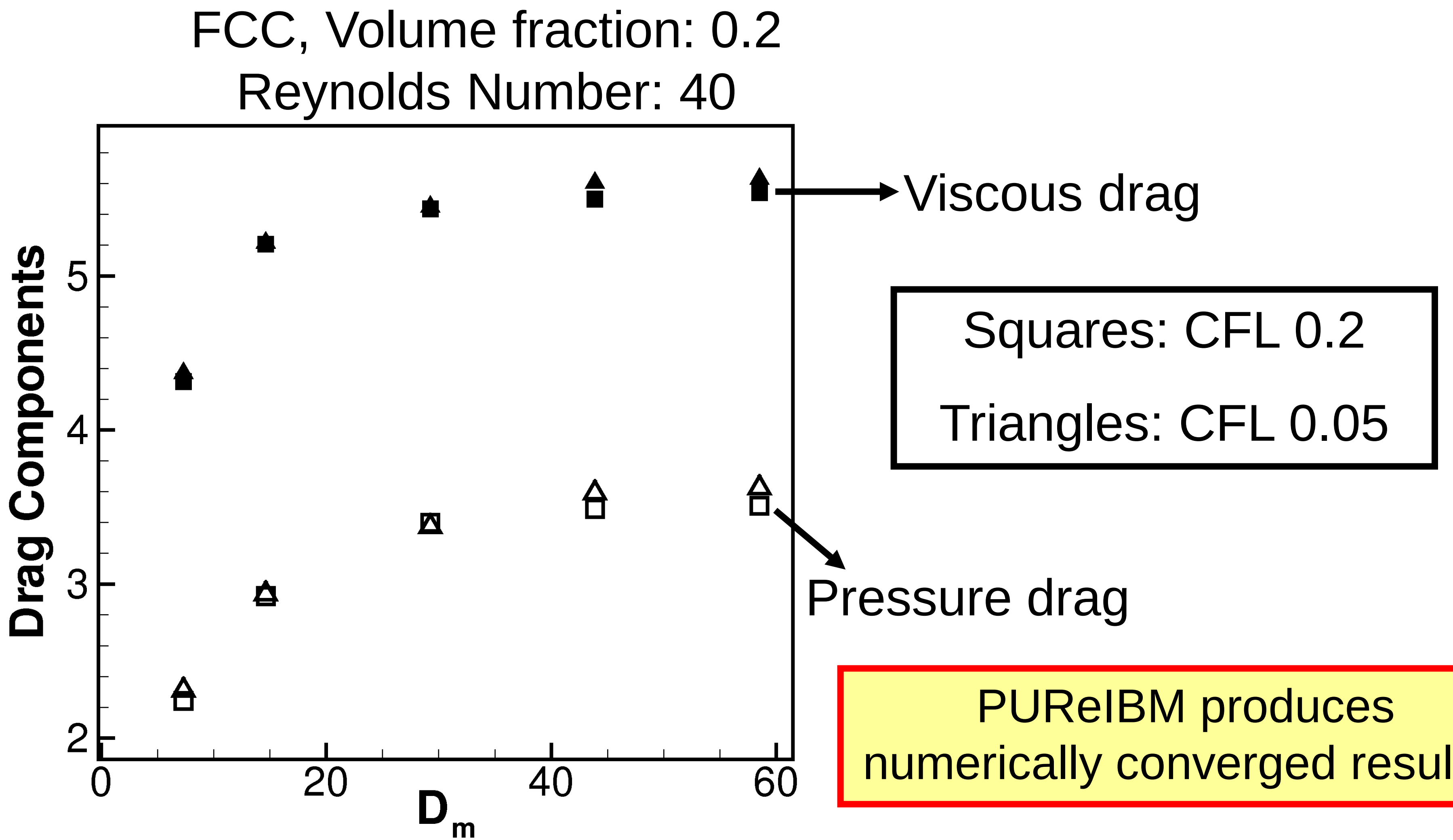
PUReIBM | ANSYS-FLUENT



Volume fraction: 0.4; Reynolds number: 100

High Reynolds number flow past random arrangement of monodisperse spheres

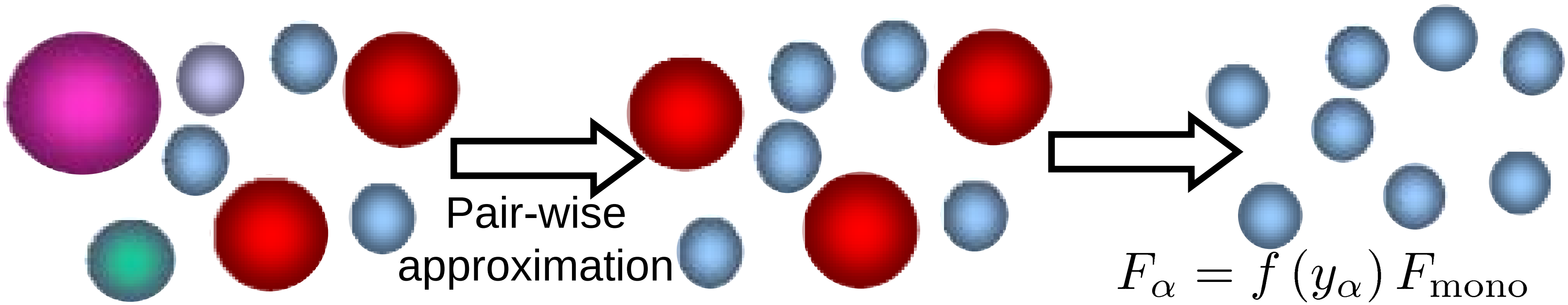
Numerical Convergence



PUReIBM produces numerically converged results*

* *Direct Numerical Simulation of Gas-Solids Flow based on the Immersed Boundary Method*, Garg et al. in Computational Gas-Solids Flows and Reacting Systems: Theory, Methods and Practice, eds S. Pannala, M. Syamlal and T. J. O'Brien (Accepted)

Effect of Particle Size Distribution



$$F_\alpha = f\left(y_\alpha\right) F_{\text{mono}}$$

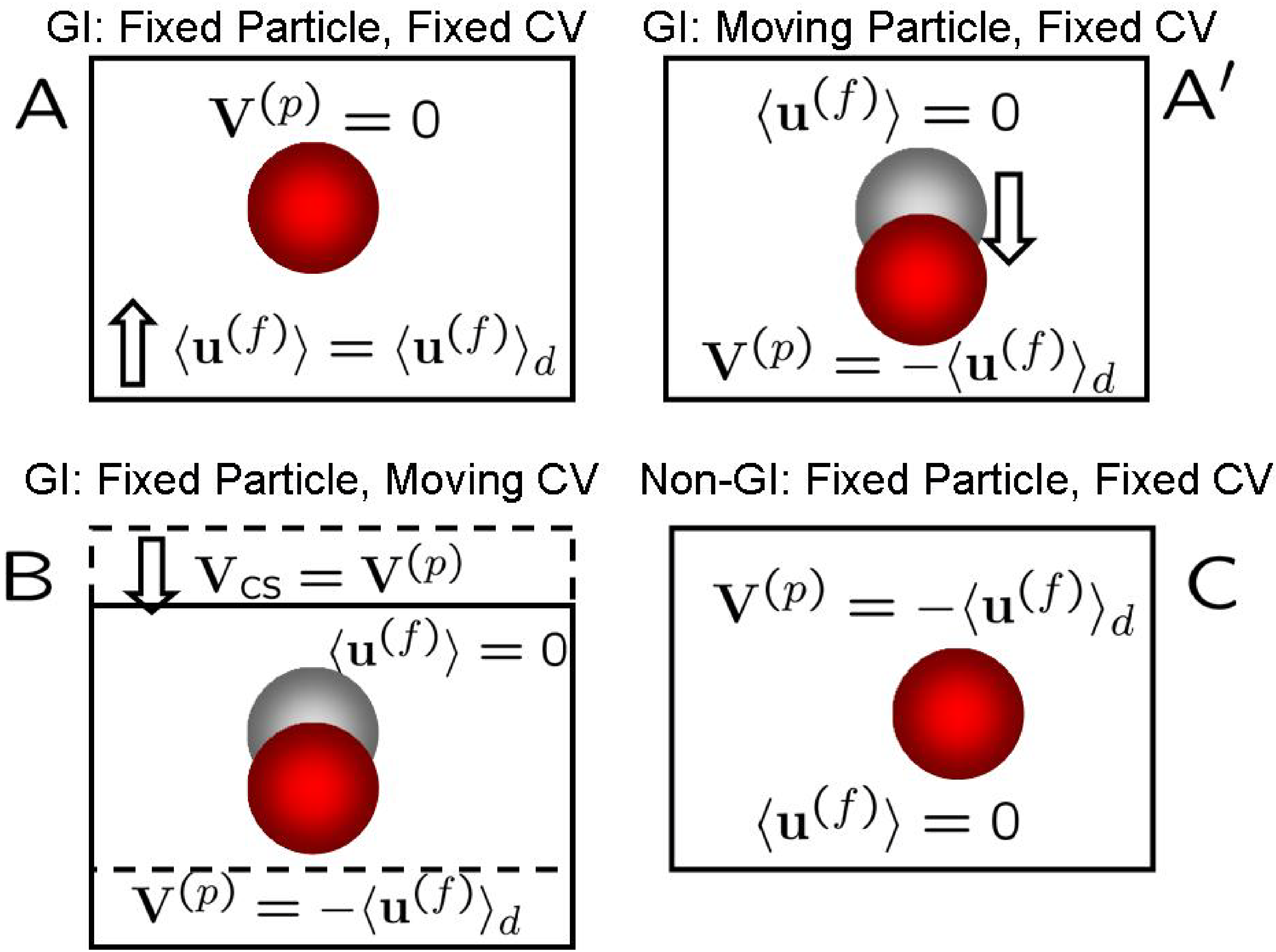
Poly-disperse suspension

Bi-disperse suspension

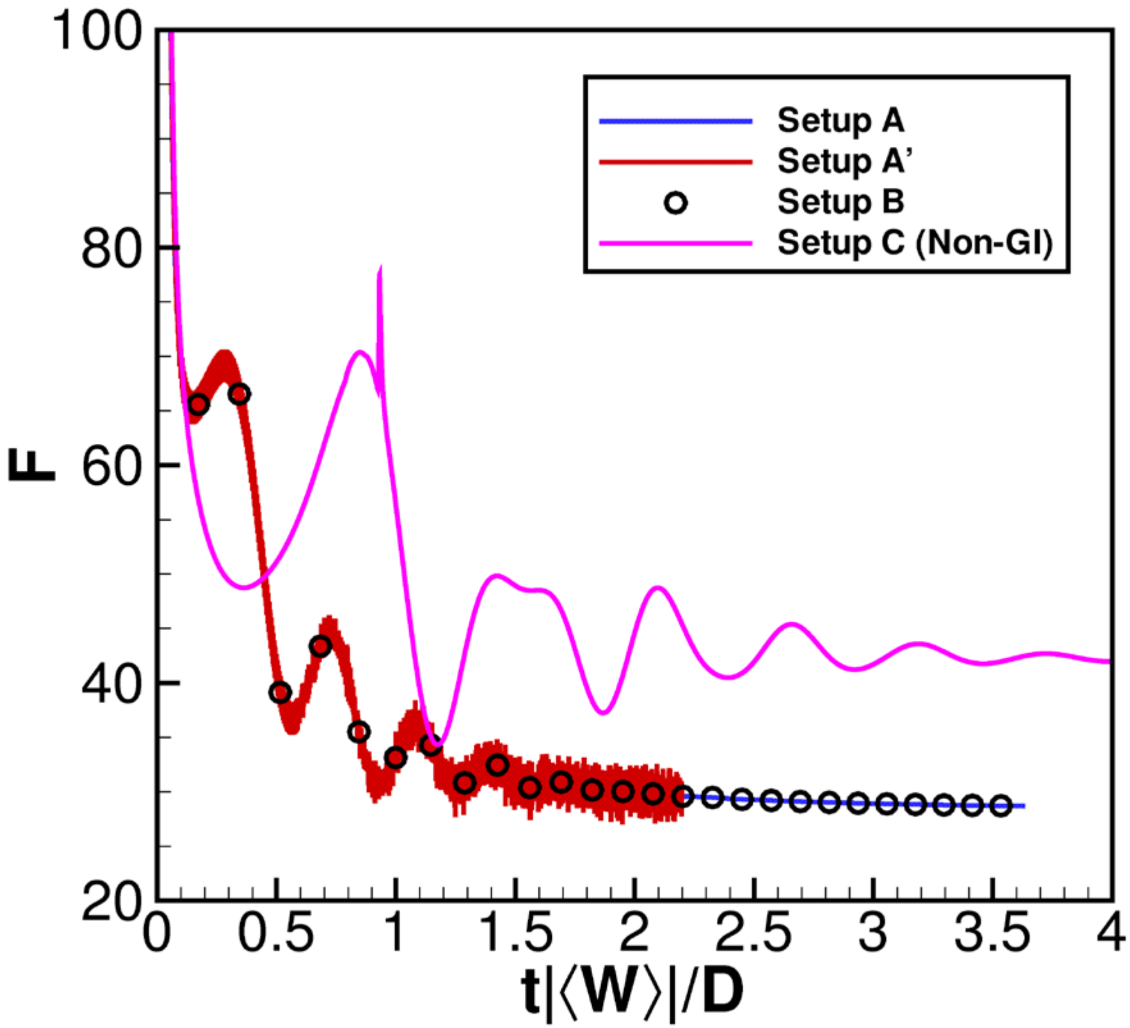
Equivalent mono-disperse suspension

- Drag laws for bi-disperse suspension depend on the accuracy of monodisperse drag law
- Correct development of computational drag laws requires the correct simulation setup
- Frozen particle simulations (FPS) are valid only when all particles have equal velocity
- FPS with unequal particle velocities are not Galilean Invariant

Comparison of Simulation Setups



Comparison of Simulation Setups



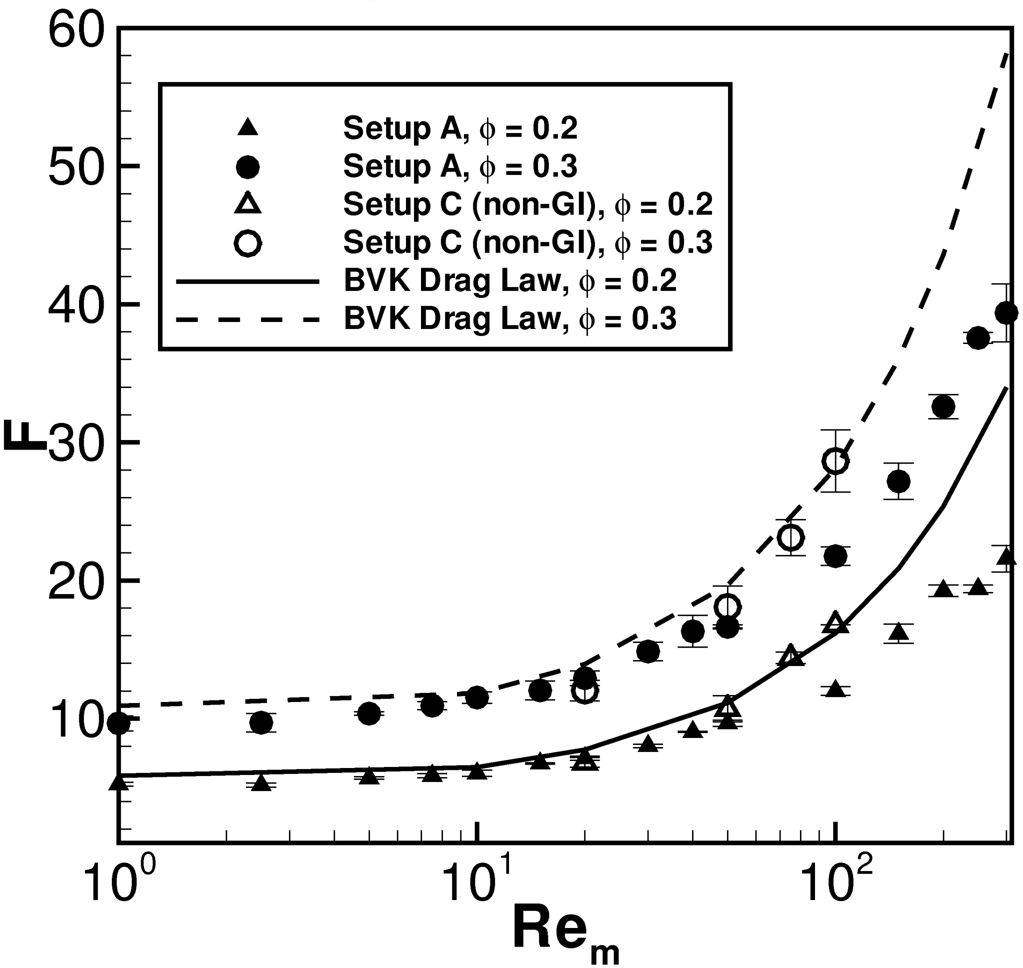
Simple Cubic

Volume fraction : 0.4

Reynolds number : 150

Non-GI setup gives erroneous results as the Reynolds number increases

Drag in Mono-disperse Suspensions



BVK : Setup A'

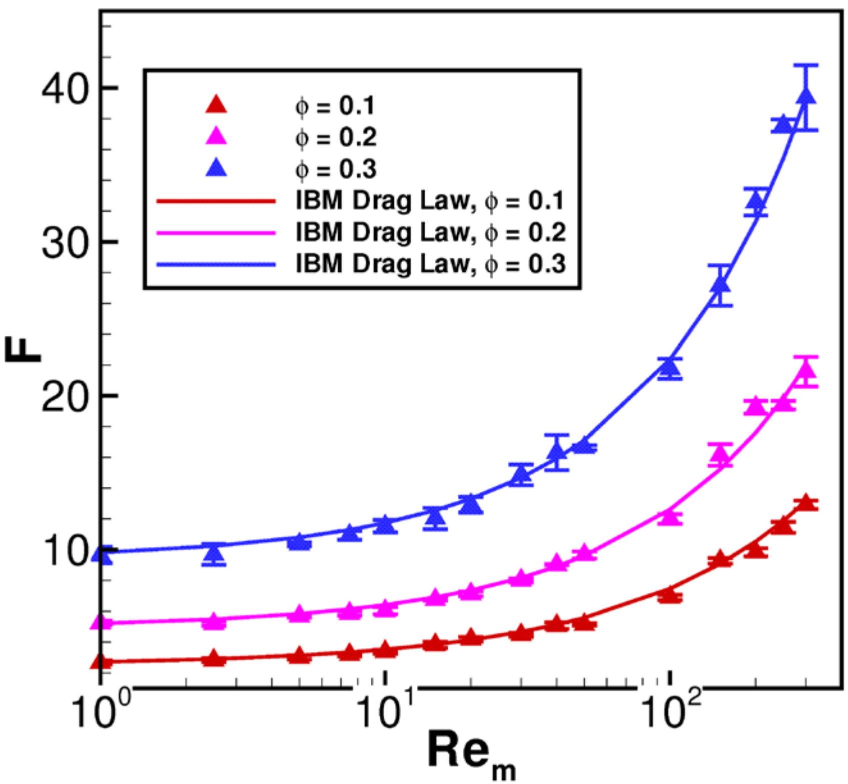
PUReIBM : Setup A

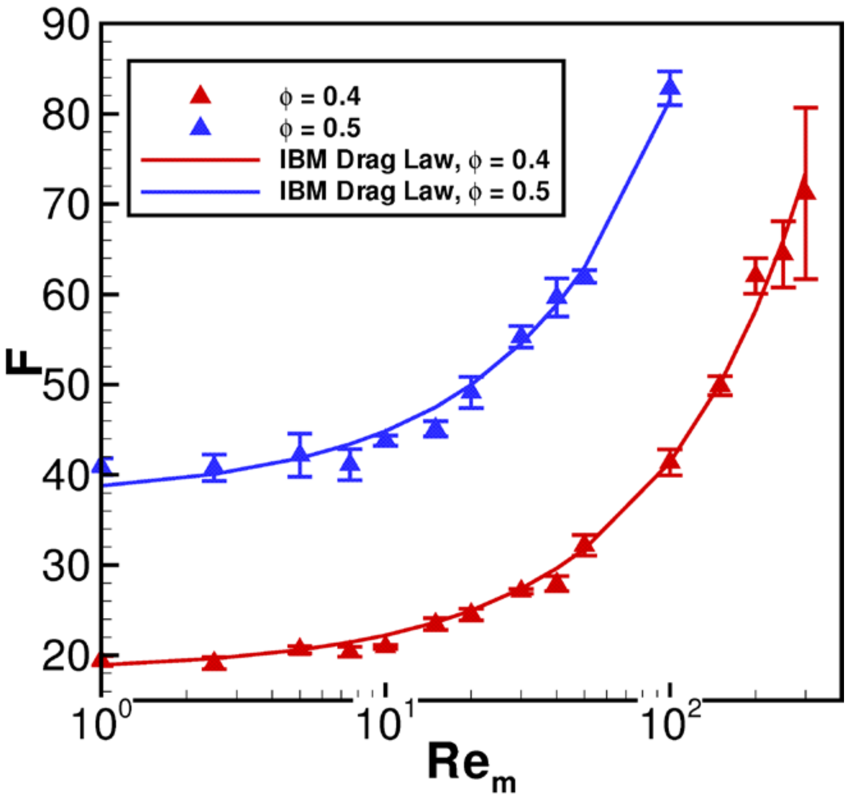
Beetstra, R., van der Hoef, M. A. & Kuipers, J. A. M. 2007. *Drag force of intermediate Reynolds number flows past mono and bidisperse arrays of spheres.* AIChEJ. 53, 489.

PUReIBM drag data differ from Beetstra et al.'s drag law by more than 20% for Re_m > 100

Drag from a non-GI setup matches well with BVK's drag law

IBM Monodisperse Drag law





New IBM drag law fits the PUReIBM data well with an average deviation of less than 2%

PUReIBM Monodisperse Drag law

$$F(\phi, \mathrm{Re}_m) = \frac{F^{\mathrm{Isol}}(\mathrm{Re}_m)}{(1-\phi)^3} + F_\phi(\phi) + F_\phi^{\mathrm{Re}_m}(\phi, \mathrm{Re}_m)$$

Single sphere drag law (Schiller-Naumann)

Purely a function of volume fraction

Separable function Linear in Reynolds number

Hill et al. (JFM, 2001):

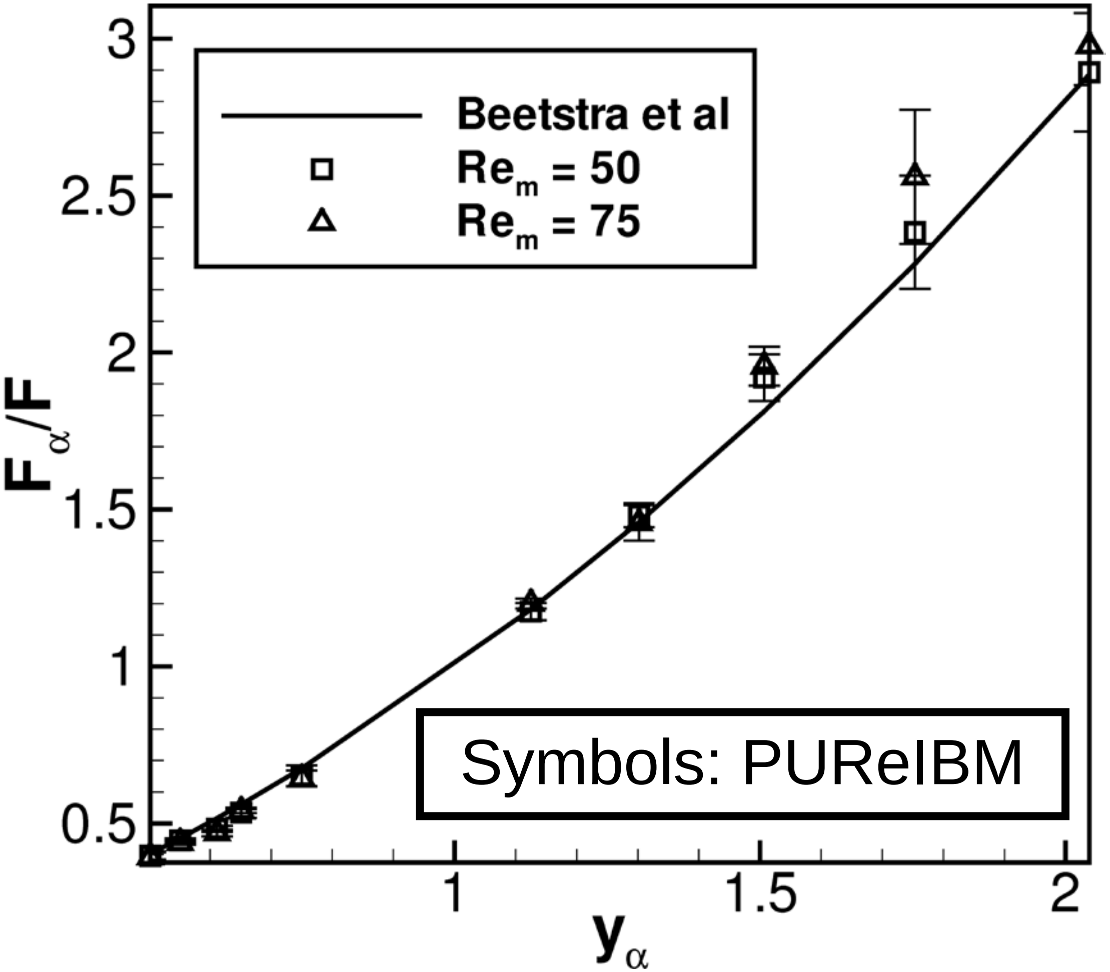
- ➢Pressure drag varies linearly with Reynolds number ($\mathrm{Re}_m > 40$)
- ➢Viscous drag is independent of Reynolds number

PUReIBM DNS:

- ✓Pressure drag varies linearly with Reynolds number ($\mathrm{Re}_m > 40$)
- ❖Viscous drag is **NOT** independent of Reynolds number*

* *Drag law for monodisperse gas-solid systems using particle-resolved direct numerical simulation.* Tenneti, S., Garg, R. & Subramaniam, S. (In preparation)

Extension of Monodisperse Drag Law to Bidisperse



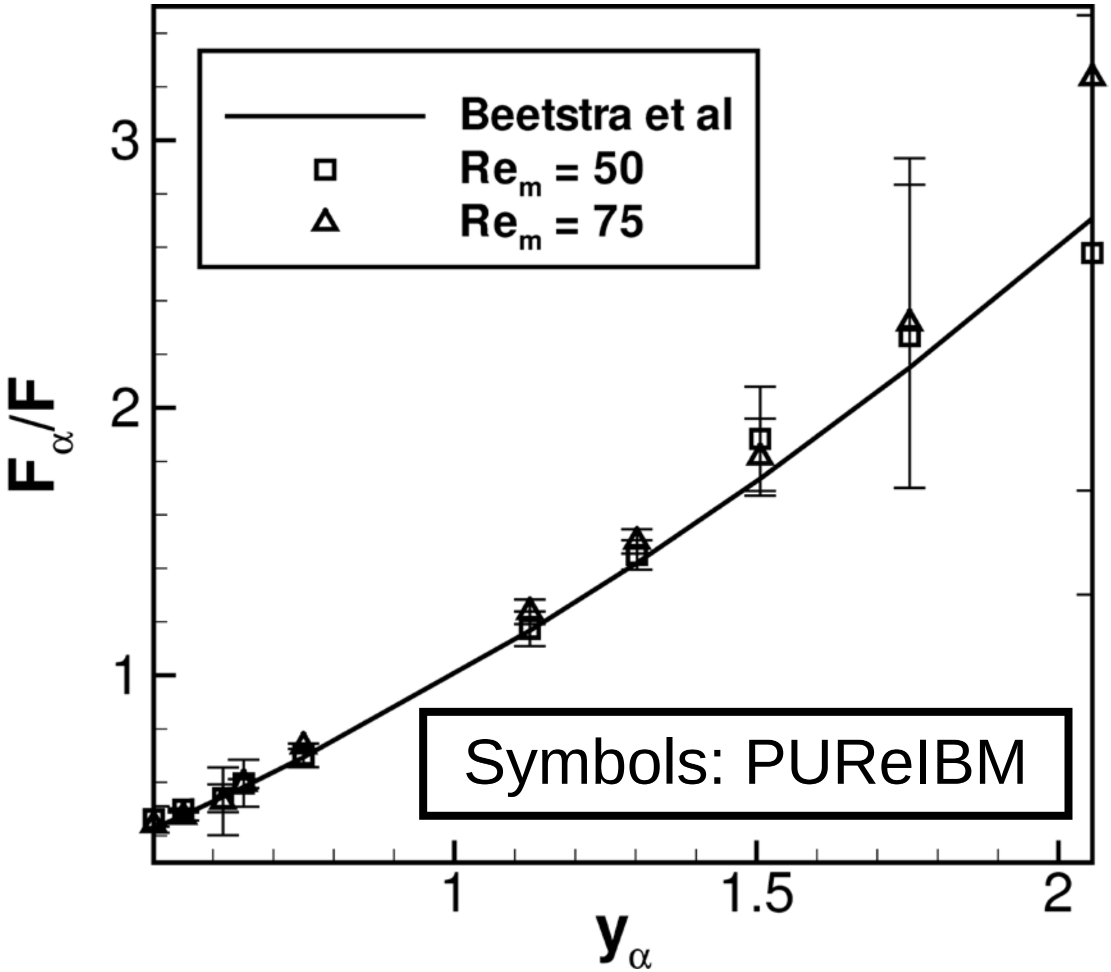
Volume fraction : 0.4

Beetstra *et al*'s extension of monodisperse drag law to bidisperse drag holds even at moderate Reynolds number

$$y_\alpha = \frac{D_\alpha}{\langle D \rangle}$$

$$\frac{F_\alpha(\phi, \mathrm{Re}_m)}{F(\phi, \mathrm{Re}_m)} = y_\alpha (1 - \phi) + y_\alpha^2 \phi$$

Extension of Monodisperse Drag Law to Bidisperse



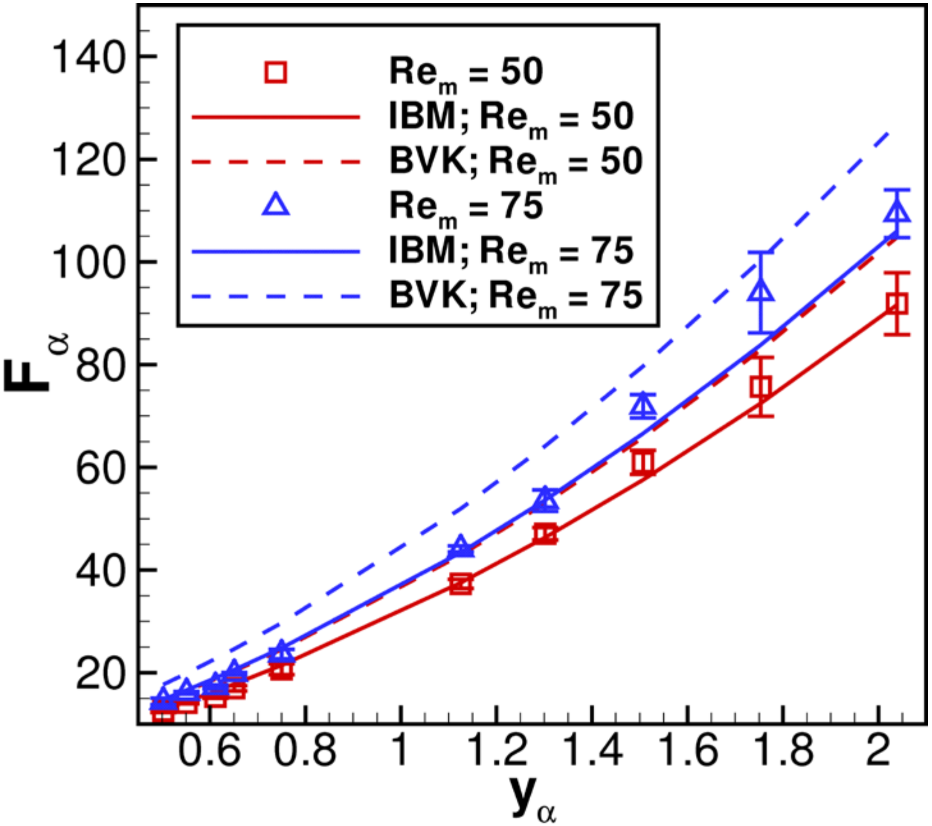
Volume fraction : 0.3

Beetstra *et al*'s extension of monodisperse drag law to bidisperse drag holds even at moderate Reynolds number

$$y_\alpha = \frac{D_\alpha}{\langle D \rangle}$$

$$\frac{F_\alpha(\phi, \mathrm{Re}_m)}{F(\phi, \mathrm{Re}_m)} = y_\alpha (1 - \phi) + y_\alpha^2 \phi$$

Bidisperse Drag Law



Volume fraction : 0.4

Solid lines : Using PUReIBM monodisperse drag law

Dashed lines : Using Beetstra *et al*'s monodisperse drag law

$$F_\alpha^{\mathrm{BVK}}(\phi, \mathrm{Re}_m) = [\quad f(y_\alpha, \phi) \quad] F_{\mathrm{mono}}^{\mathrm{BVK}}(\phi, \mathrm{Re}_m)$$

Data Not same — Same function — Not same

$$F_\alpha^{\mathrm{IBM}}(\phi, \mathrm{Re}_m) = [\quad f(y_\alpha, \phi) \quad] F_{\mathrm{mono}}^{\mathrm{IBM}}(\phi, \mathrm{Re}_m)$$

Summary

- Drag laws for mono- and bi-disperse suspensions
  - Mono-disperse drag law is improved for high Reynolds numbers
  - Data for F_α from PUReIBM DNS corrects earlier data from Beetstra et al
  - Form of the drag law to account for dependence on polydispersity is verified
- Particle velocity fluctuations
- Gas-phase velocity fluctuations

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Effect of Particle Velocity Fluctuations

- Particle velocity fluctuations affect the mean drag
- Particle velocity fluctuations correlate with particle acceleration fluctuations to generate source for granular temperature
- Tenneti *et al*[*] showed that simple extensions of mean particle acceleration models do not recover the correct acceleration-velocity covariance obtained from DNS

* S. Tenneti, R. Garg, C.M. Hrenya, R.O. Fox and S. Subramaniam. *Direct numerical simulation of gas-solid suspensions at moderate Reynolds number: Quantifying the coupling between hydrodynamic forces and particle velocity fluctuations*. Powder Tech. Journal. Spl. Issue 2010. Ed: Ron Breault

Instantaneous Particle Acceleration Model

$$dv_i = -\beta_{(i)} \langle W_i \rangle dt - \gamma_{ij} v''_j dt + B_{ij} dW_j$$

Mean slip

Velocity fluctuations

Wiener process

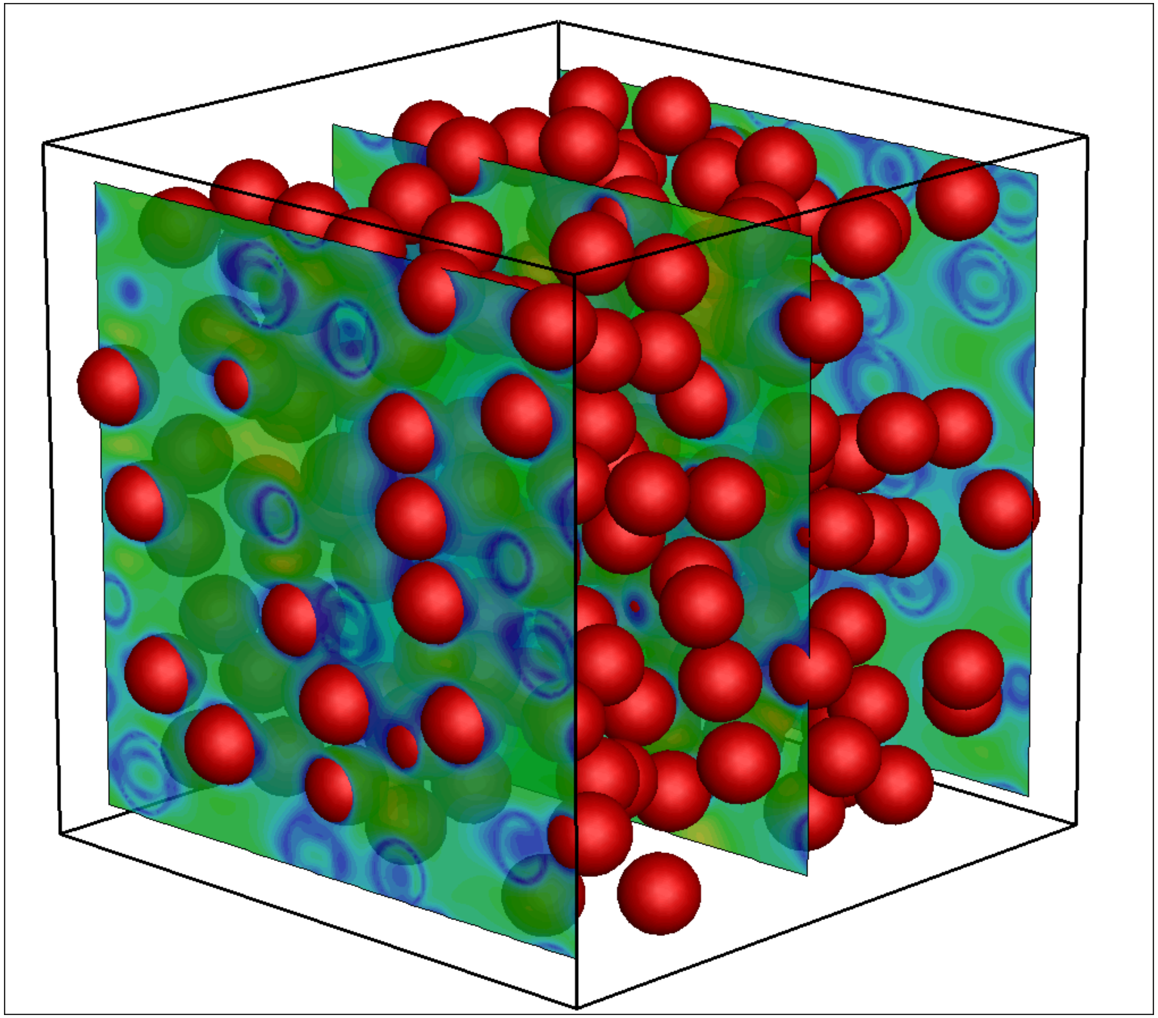
(effect of neighbouring particle)

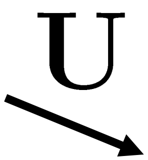
γ_{ij}

- inverse of Lagrangian particle velocity autocorrelation time
- How long particle retains memory of initial velocity
- function of Stokes number

Simulation of freely evolving suspensions necessary to extract the model coefficients as a function of Stokes number and granular temperature

Freely Evolving Suspensions



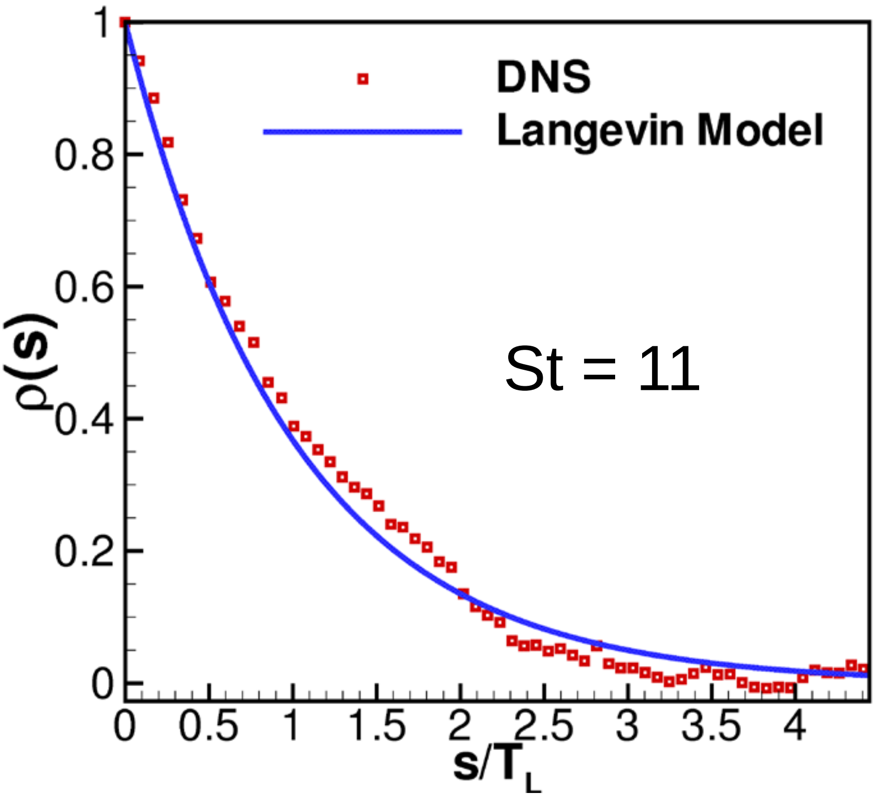


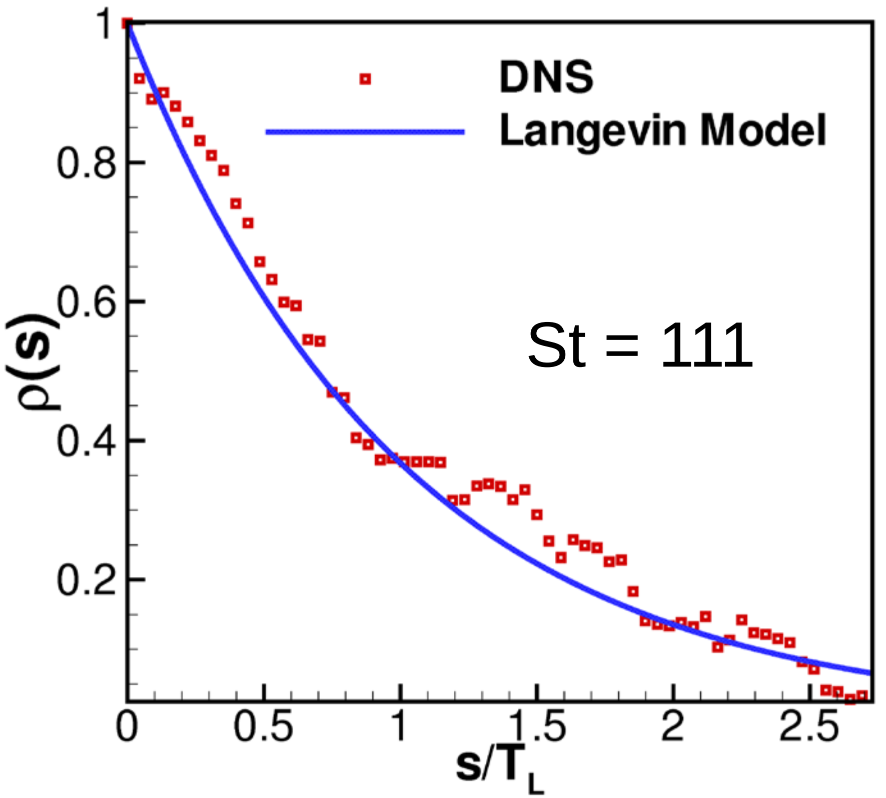
$Re_m = 20$

$\phi = 0.2$

$St = 11$

Verification of Langevin Model





$$T_L = \int_0^\infty \rho(s)ds$$

Langevin model ⇨ $\rho(s) = e^{-s/T_L}$

Evolution of the autocorrelation function obtained from DNS matches with the exponential function predicted by the Langevin equation

Specification of Langevin model coefficients

STATISTICALLY HOMOGENEOUS

ZERO MEAN VELOCITY GRADIENTS

ELASTIC COLLISIONS

$$\frac{dT}{dt} = \frac{2}{3}\left\langle A_i''v_i''\right\rangle$$

Koch (1990)

$$\frac{dT}{dt} = S - \Gamma_v$$

Langevin Model

$$\frac{dT}{dt} = B^2 - 2\gamma T$$

Kinetic theory for a monodisperse gas-solid suspension. Koch, D. L, *Phys. Fluids* 1990

Devised a novel approach to uniquely identify the source and dissipation of granular temperature from DNS

Acceleration Model for Dilute Suspensions in Stokes flow

- For dilute suspensions of highly massive and perfectly elastic monodisperse particles in Stokes flow, the evolution of granular temperature *T* is given by (Koch,1990):

$$\frac{dT}{dt} = -\frac{2R}{\tau}T + \frac{2S_I}{3} = S - \Gamma$$

- Comparison with Koch's model yields the coefficients of the Langevin model as

$$\gamma = \frac{R}{\tau} = \frac{1}{\tau}\left(1 + \frac{3}{\sqrt{2}}\phi^{1/2}\right)$$

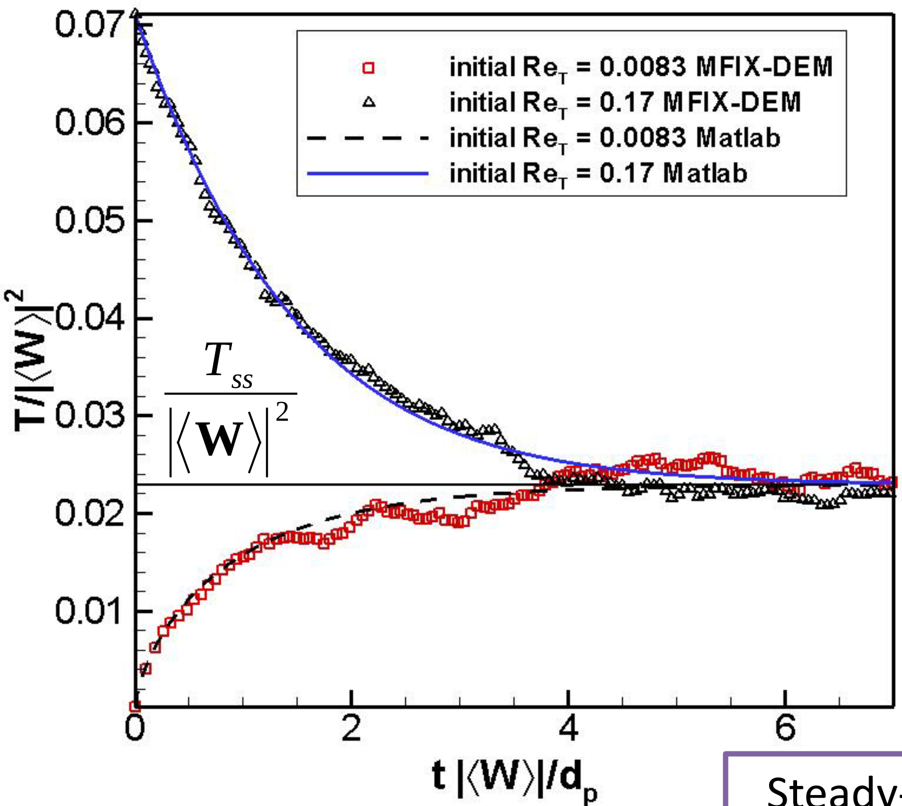
$$B^2 = \frac{2S_I}{3} = \frac{1}{3\sqrt{\pi}}\frac{a\left|\langle \mathbf{W} \rangle\right|^2}{\tau^2 T^{1/2}}$$

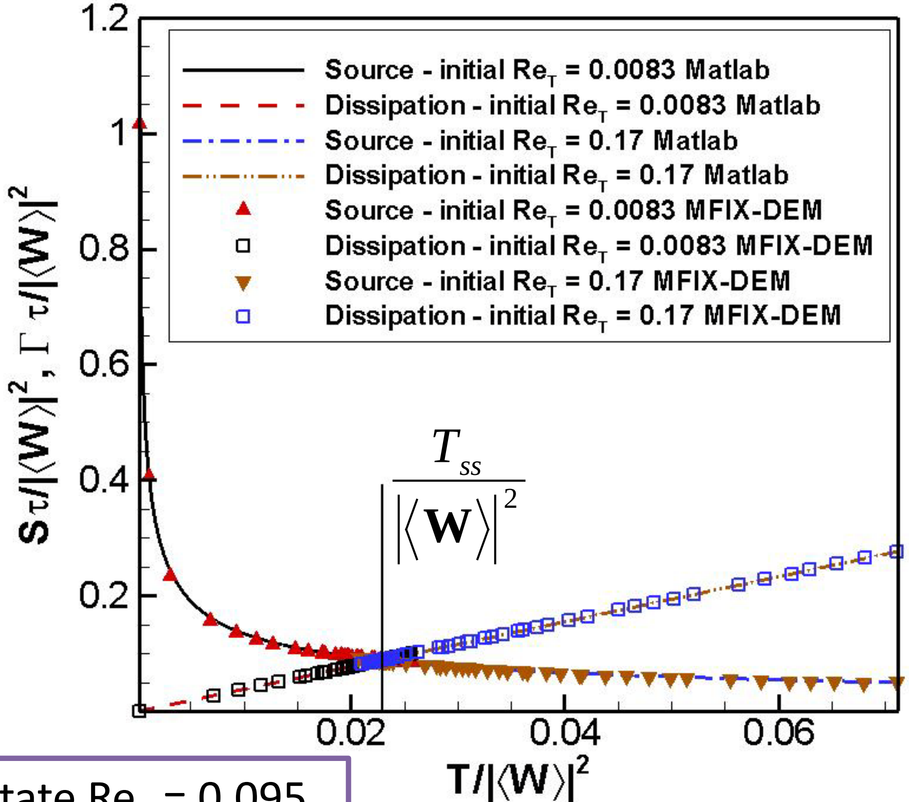
- At steady state $S = \Gamma$

$$T_{ss} = \left[\frac{\left(a\left|\langle \mathbf{W} \rangle\right|^2\right)}{6\tau\sqrt{\pi}\left(1 + 3\phi^{1/2}/\sqrt{2}\right)}\right]^{2/3}$$

Model Validation Using MFIX-DEM

MFIX-DEM: $\phi = 0.2$; $L/d_p = 7.5$; $Re_m = 0.5$; $\rho_p/\rho_f = 200$
Matlab: Granular Temperature Evolution ODE with Koch's coefficients





Steady-state $Re_T = 0.095$

- MFIX-DEM and Matlab results match well
- Granular temperature reaches a steady state when the source and dissipation balance each other and it is independent of the initial conditions

Summary

- ❑ Drag laws for mono- and bi-disperse suspensions
- ❑ Particle velocity fluctuations

  - ➢ We propose a Langevin model for the particle acceleration that can accurately model the granular temperature evolution
  - ➢ ISU acceleration model for Stokes flow implemented in MFIX-DEM and validated
  - ➢ For moderate Reynolds numbers we developed a method to uniquely determine the source and dissipation from the DNS of freely evolving suspensions*

- ❑ Gas-phase velocity fluctuations

* *Instantaneous particle acceleration model for gas-solid suspensions at moderate Reynolds numbers.* Tenneti, S., Fox, R.O., & Subramaniam, S. ICMF 2010, Tampa, FL

Summary

- Drag laws for mono- and bi-disperse suspensions
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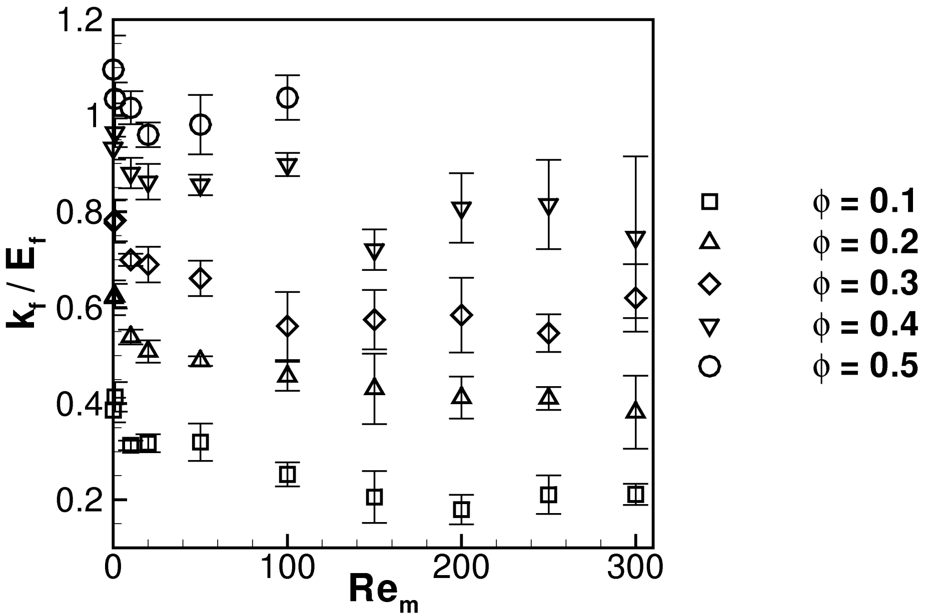
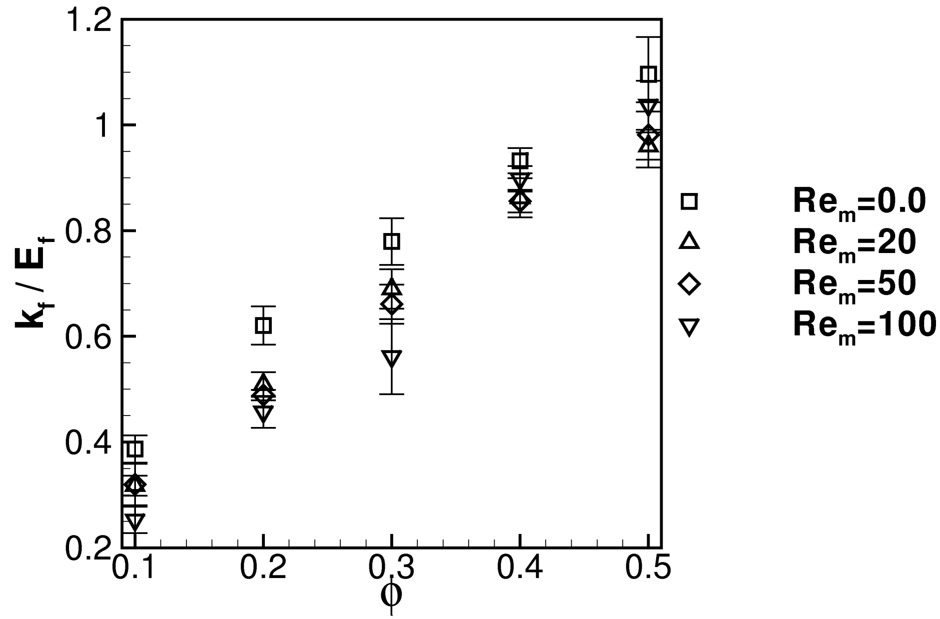
- Gas-phase velocity fluctuations

Gas-phase Velocity Fluctuations





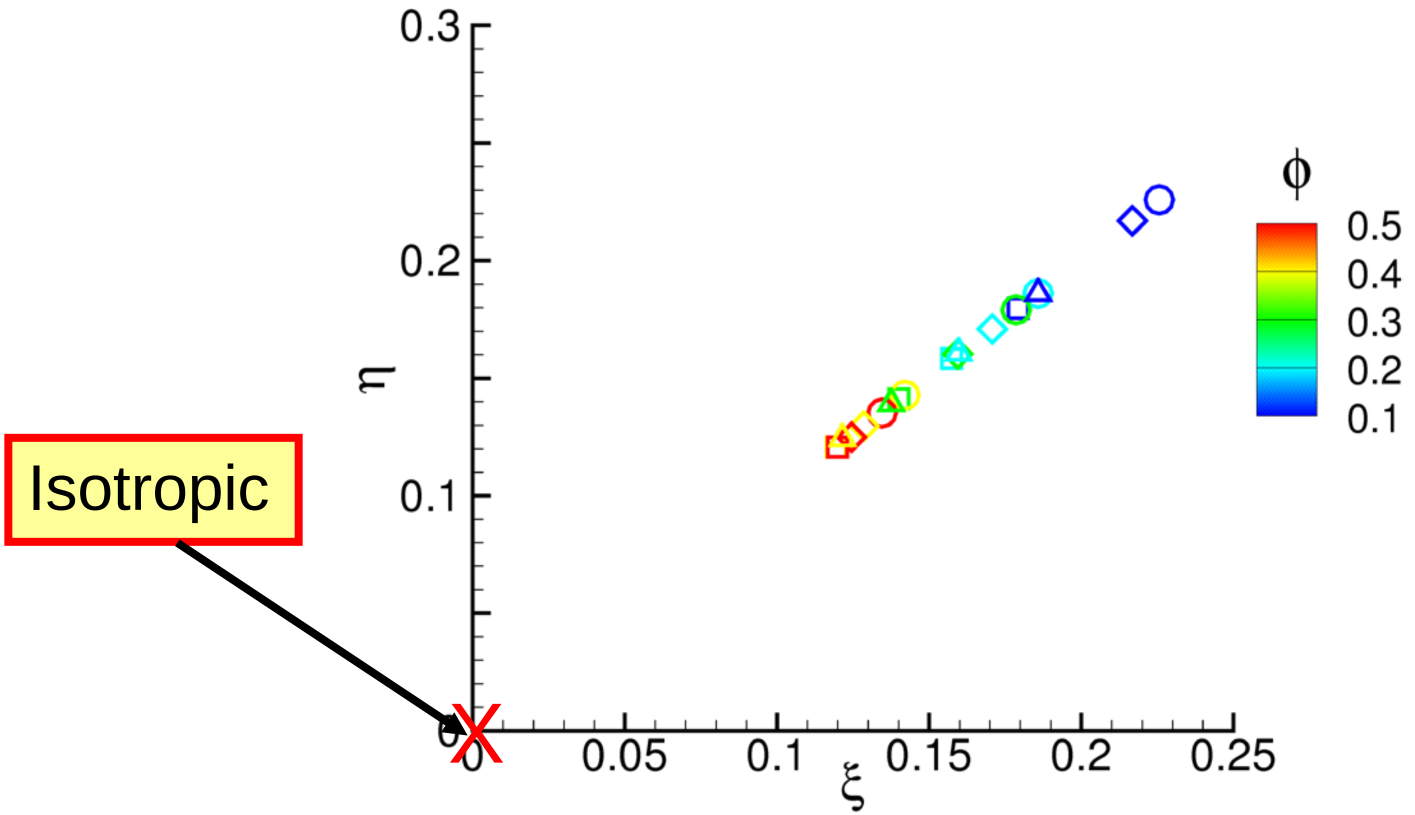
$$k_f = \frac{1}{2}\langle \mathbf{u}''^{(f)} \cdot \mathbf{u}''^{(f)} \rangle$$

$$E_f = \frac{1}{2}\langle \mathbf{W} \rangle \cdot \langle \mathbf{W} \rangle$$

Non-turbulent kinetic energy decreases with Reynolds number and reaches an asymptote

Non-turbulent kinetic energy increases with volume fraction

State of Anisotropy of Reynolds Stress



Reynolds stress tensor is anisotropic in the bed

Flow becomes isotropic with increasing volume fraction

Summary

- ❑ Drag laws for mono- and bi-disperse suspensions
- ❑ Particle velocity fluctuations
- ❑ Gas-phase velocity fluctuations

➢ Non-turbulent velocity fluctuations contain a significant fraction of the flow energy in gas-solid flows

➢ The Reynolds stress tensor is highly anisotropic with higher stresses in the flow direction than in the cross-stream directions

➢ Energy budget analysis of Reynolds stress tensor shows this behavior is associated with the anisotropy of dissipation and interphase TKE transfer tensors*

*Xu, Y., Subramaniam, S., 2010. *Effect of particle clusters on carrier flow turbulence: a direct numerical simulation study*. (In review)

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PUReIBM Monodisperse Drag law

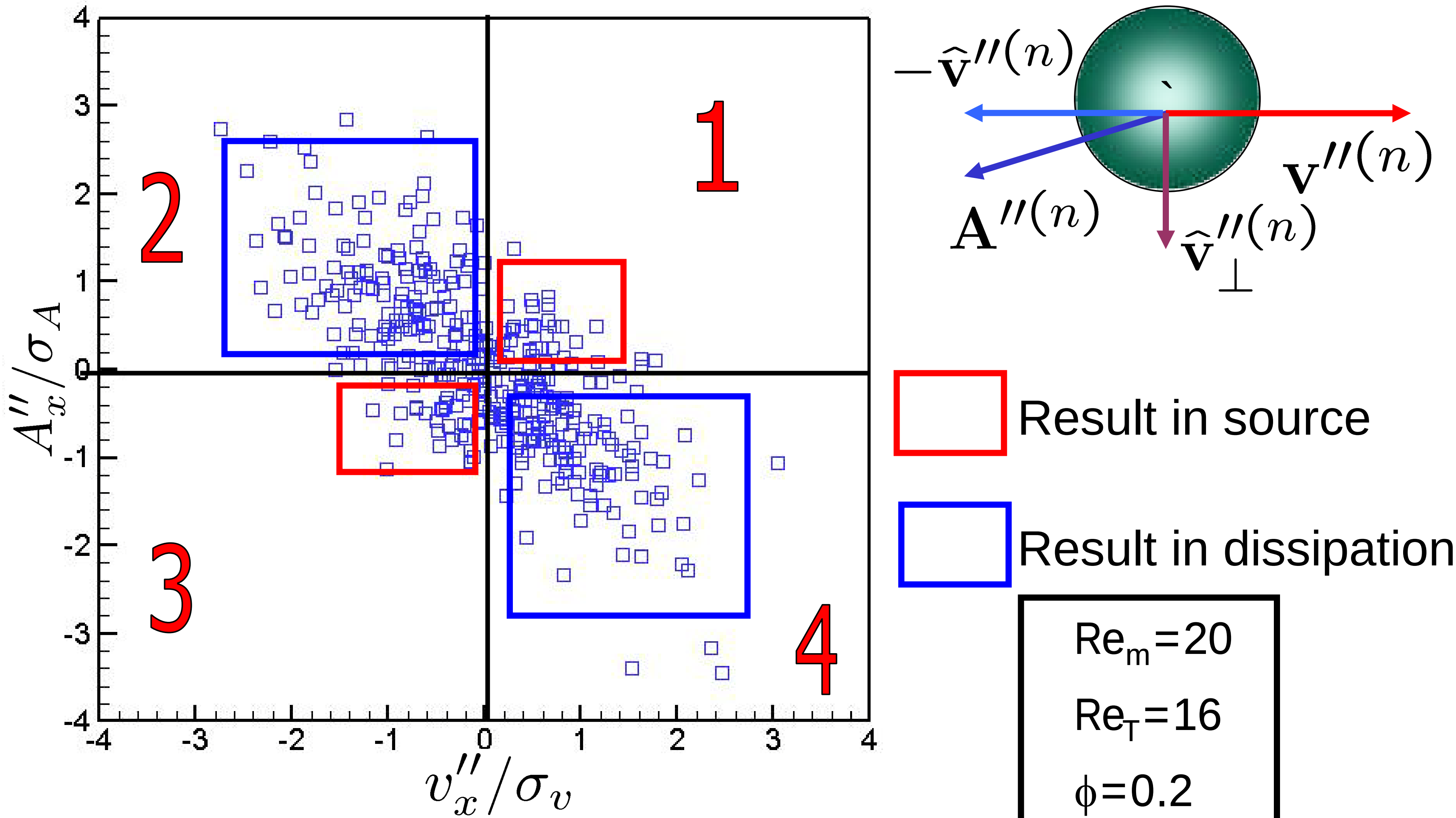
$$F(\phi, \mathrm{Re}_m) = \frac{F_{\mathrm{Isol}}(\mathrm{Re}_m)}{(1-\phi)^3} + F_\phi(\phi) + F_\phi^{\mathrm{Re}_m}(\phi, \mathrm{Re}_m)$$

$$F_{\mathrm{Isol}}(\mathrm{Re}_m) = 1 + 0.15\mathrm{Re}_m^{0.687}$$

$$F_\phi(\phi) = \frac{5.81\phi}{(1-\phi)^3} + 0.48\frac{\phi^{1/3}}{(1-\phi)^4}$$

$$F_\phi^{\mathrm{Re}_m}(\phi, \mathrm{Re}_m) = \phi^3 \mathrm{Re}_m \left(0.95 + \frac{0.61\phi^3}{(1-\phi)^2}\right)$$

Source and Dissipation of temperature from DNS

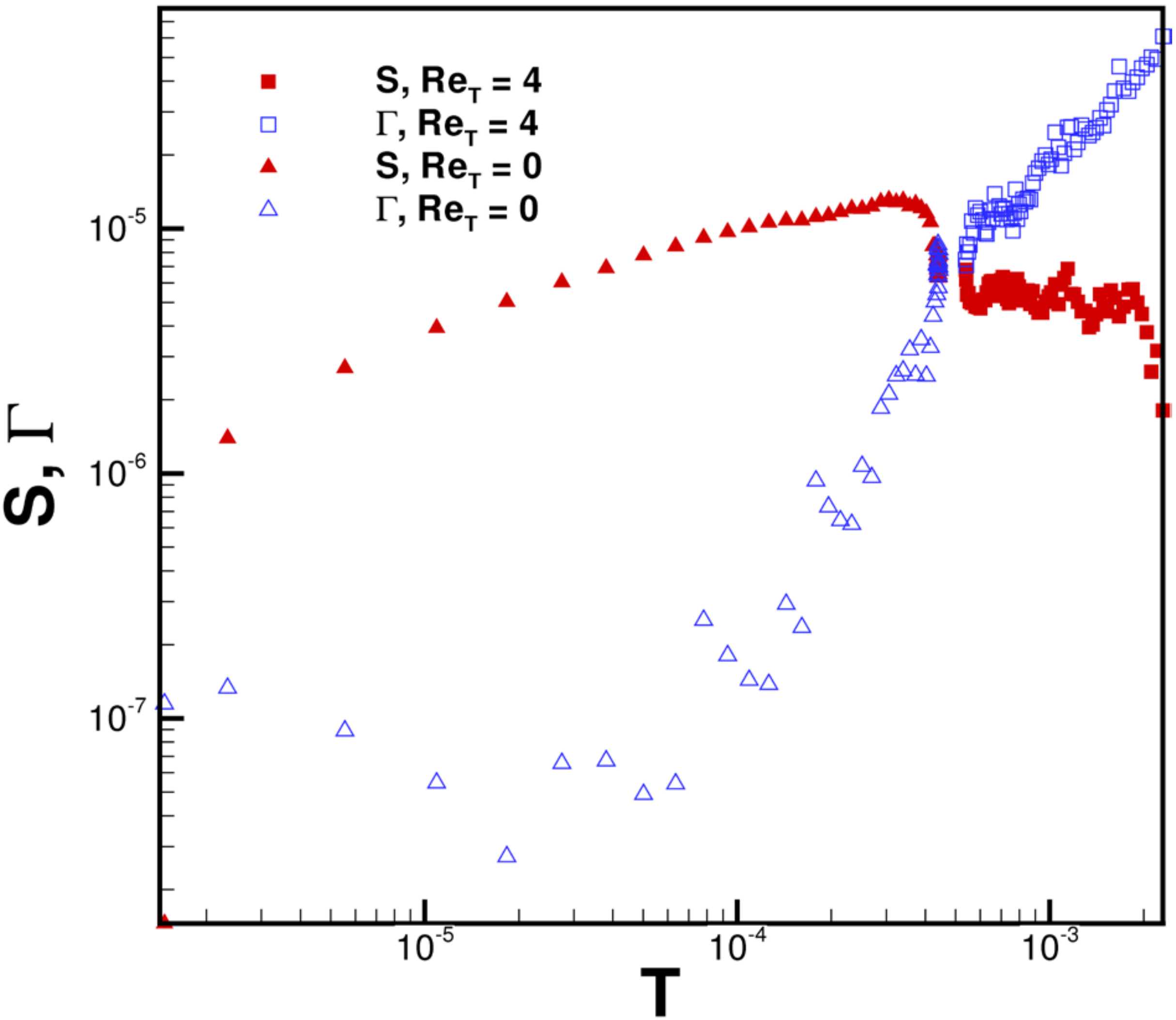


$Re_m=20$

$Re_T=16$

$\phi=0.2$

Source and Dissipation: Freely Evolving Suspension



$Re_m = 20$

$St = 111$

$\phi = 0.2$

- Phase space plots for two different initial conditions
- Steady state is a stable attractor
- Both configurations reach the same steady temperature, source and dissipation

Particle Acceleration Model – Langevin Form

- Simple extensions of mean particle acceleration models lead to only a sink term in granular temperature evolution

- The proposed particle acceleration model of the Langevin equation form for the increment in particle velocity is given by

$$dv_i = -\beta_{ij}\langle W_j \rangle dt - \gamma_{ij} v''_j dt + B_{ij} dW_j$$

Mean slip velocity

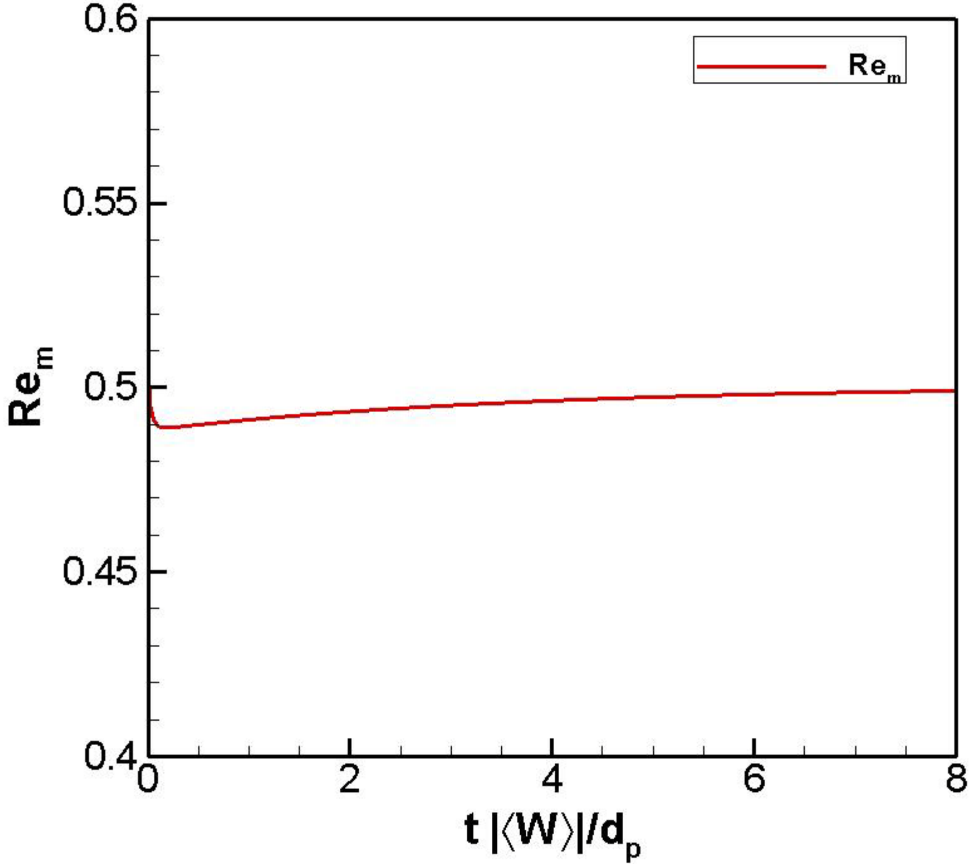
Particle velocity fluctuations

Hydrodynamic effects of neighboring particles

- Using a simplified form of the Langevin equation for the velocity fluctuation, the evolution of granular temperature *T* is derived for dilute suspension case with elastic particles in Stokes flow (velocity distribution is Maxwellian(Koch, 1990)

$$dv''_i = -\gamma v''_i dt + B dW_i \quad \Longrightarrow \quad \frac{dT}{dt} = -2\gamma T + B^2$$

Test Case – MFIX-DEM: Mean Slip Velocity Evolution



- Mean slip velocity is recovered exactly

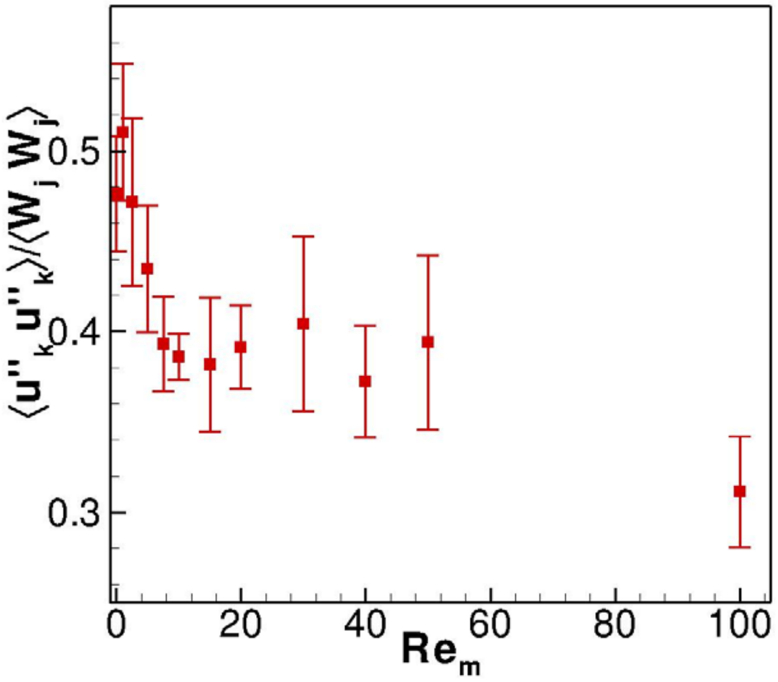
Gas Phase Instability in gas-solid flows

Velocity fluctuations in gas-phase

- Non-turbulent due to existence of particles
- Turbulent due to instabilities in the upstream flow

High level of non-turbulent velocity fluctuations due to dispersed phase $(k_f = 0)$

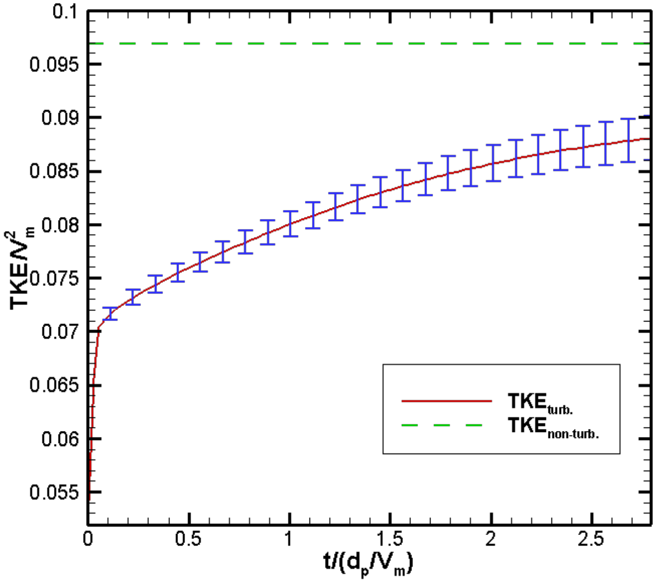
Non-turbulent velocity fluctuations are comparable to turbulent fluctuations, and are significant in gas-solid flows.



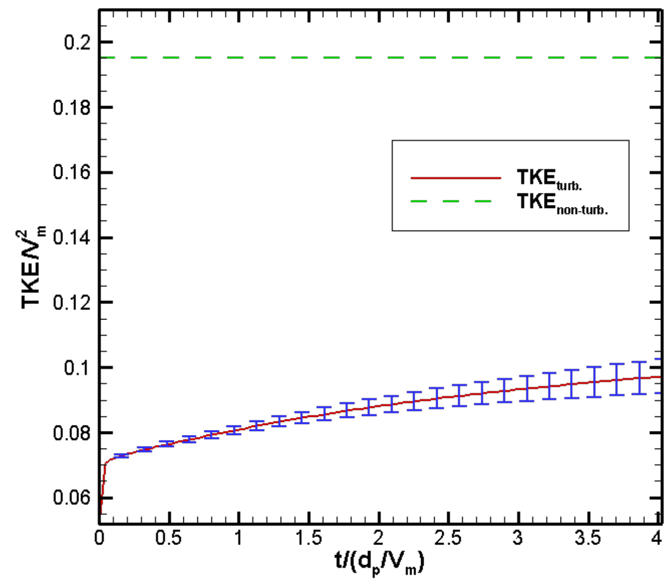
Comparison of turbulent and non-turbulent cases

- Simulating two random configurations for turbulent non-turbulent cases
- The first case is uniformly distributed particles configuration
- The second case is clustered-particle configuration
- The simulation is performed for four multiple independent simulations
- Reynolds number based on mean-slip velocity is 50 for all cases
- Turbulent cases are initialized by Re_λ=12

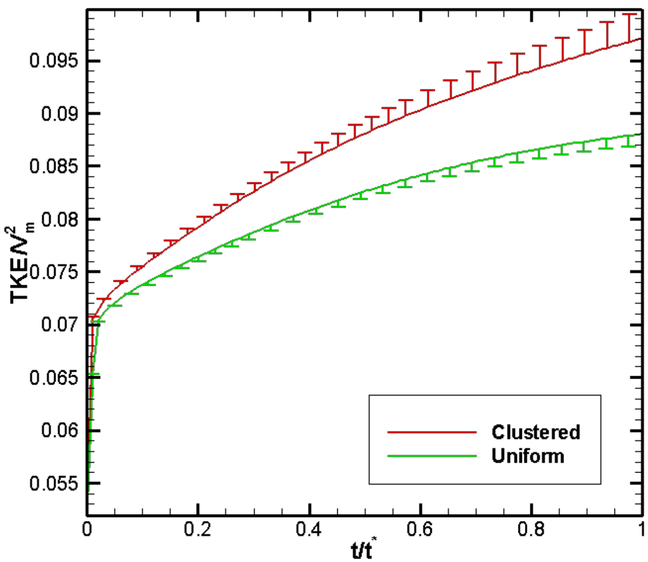
Comparison of turbulent and non-turbulent cases



Uniform case



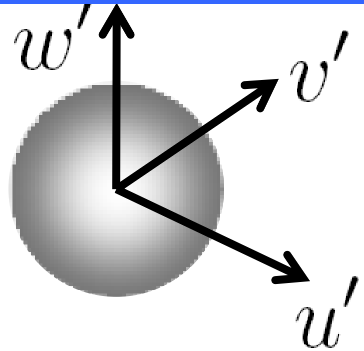
Cluster case

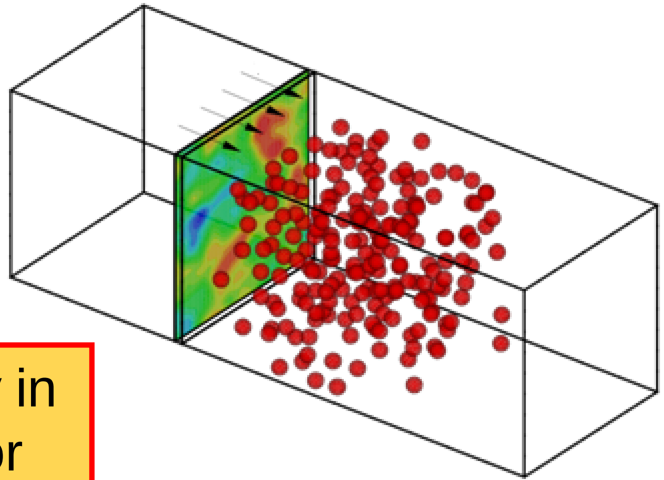


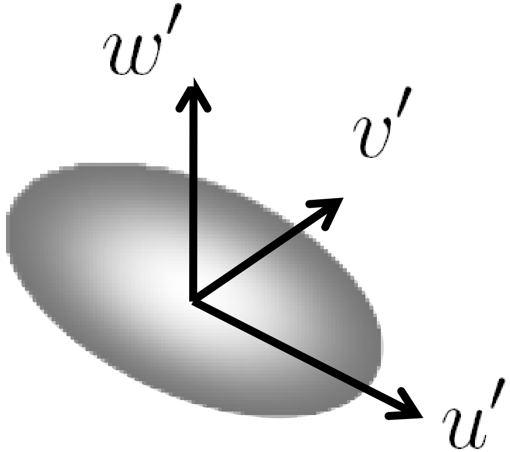
Comparison of two cases

Enhancement of fluctuating velocities energy due to clustering of particles

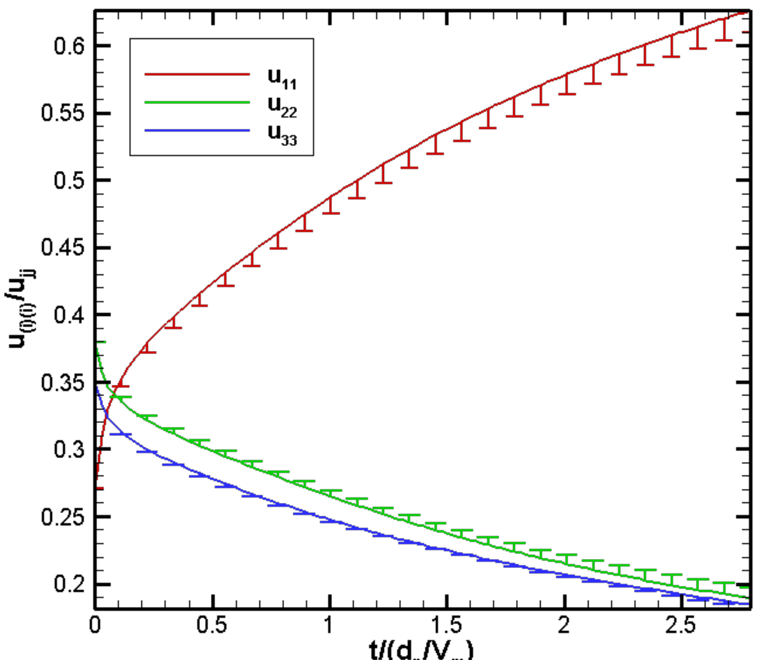
Effect of particles on velocity fluctuations



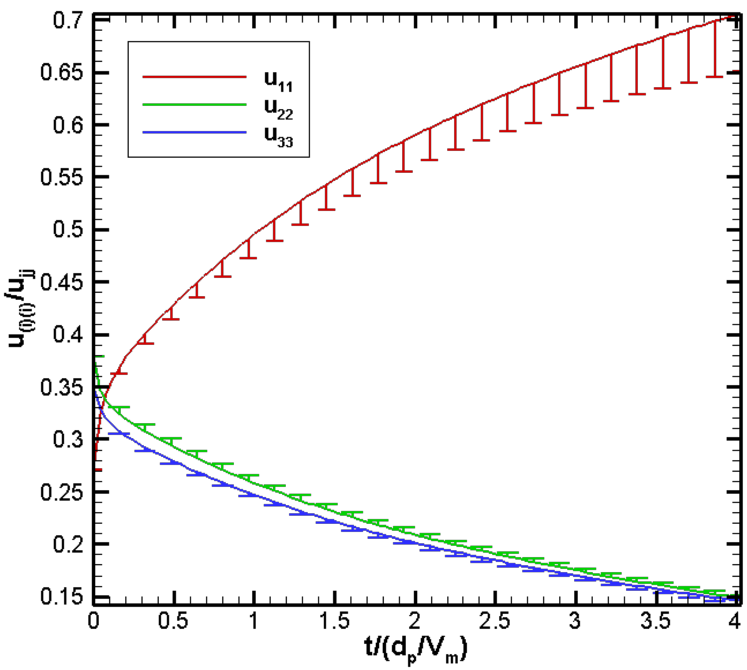




High level of anisotropy in Reynolds stress tensor



Uniform configuration



Cluster configuration

Summary

- Non-turbulent velocity fluctuations are as significant as turbulent velocity fluctuations in gas-solid flows.
- The Reynolds stress tensor is highly anisotropic in stream-wise direction. The normal stress in flow direction increases, while the other two normal stresses decrease.
- The energy budget analysis of Reynolds stress tensor shows this behavior is associated with the anisotropy of dissipation and interphase TKE transfer tensors[1].
- The level of TKE and anisotropy increase as the flow passes over clusters of particles, compared to uniformly distributed particles.

[1] Xu, Y., Subramaniam, S., 2010. Effect of particle clusters on carrier flow turbulence: a direct numerical simulation study. (Submitted to *Flow, Turbulence and Combustion*, in review)