Modeling Particle-Fluid Momentum Transfer in Polydisperse Gas-Solid Flows Through Direct Numerical Simulations Based on the Immersed Boundary Method

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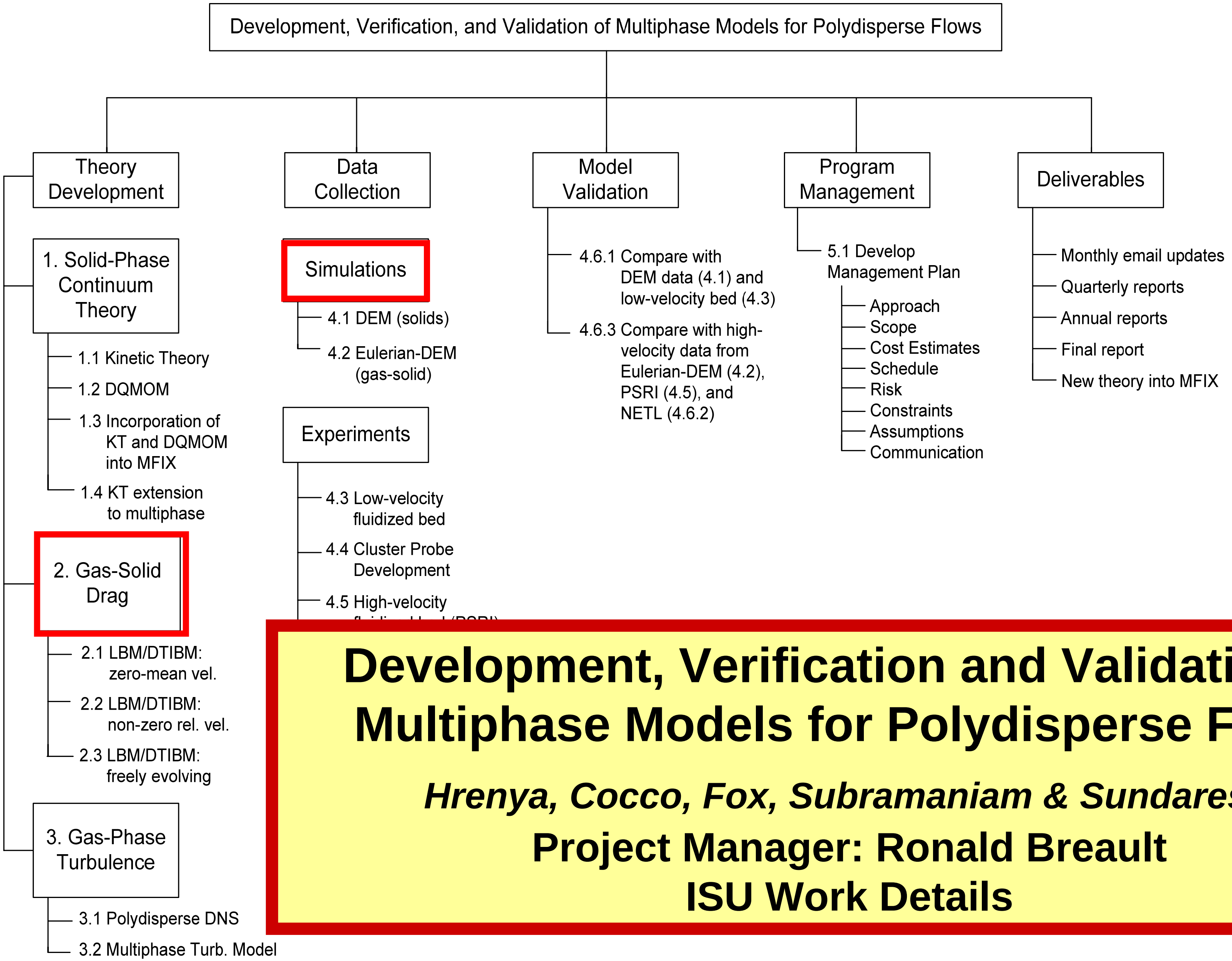
Project scope: Work breakdown structure



Development, Verification and Validation of Multiphase Models for Polydisperse Flows

Hrenya, Cocco, Fox, Subramaniam & Sundaresan

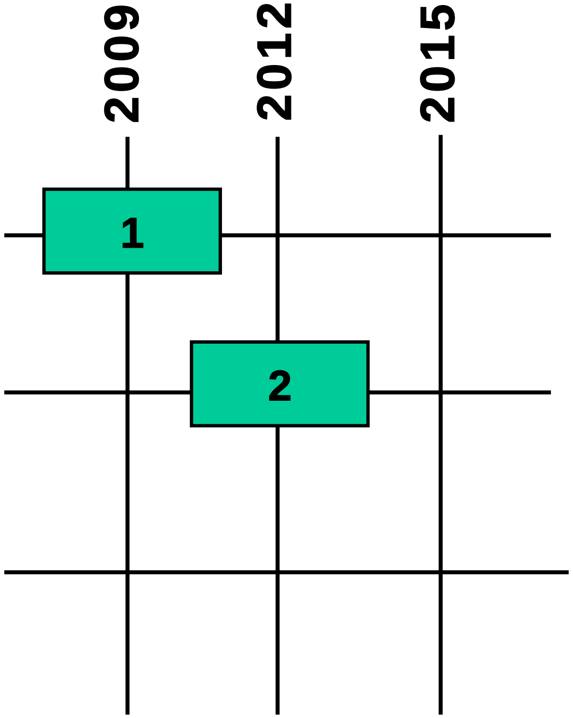
Project Manager: Ronald Breault

ISU Work Details

Connections to Multiphase Flow Roadmap

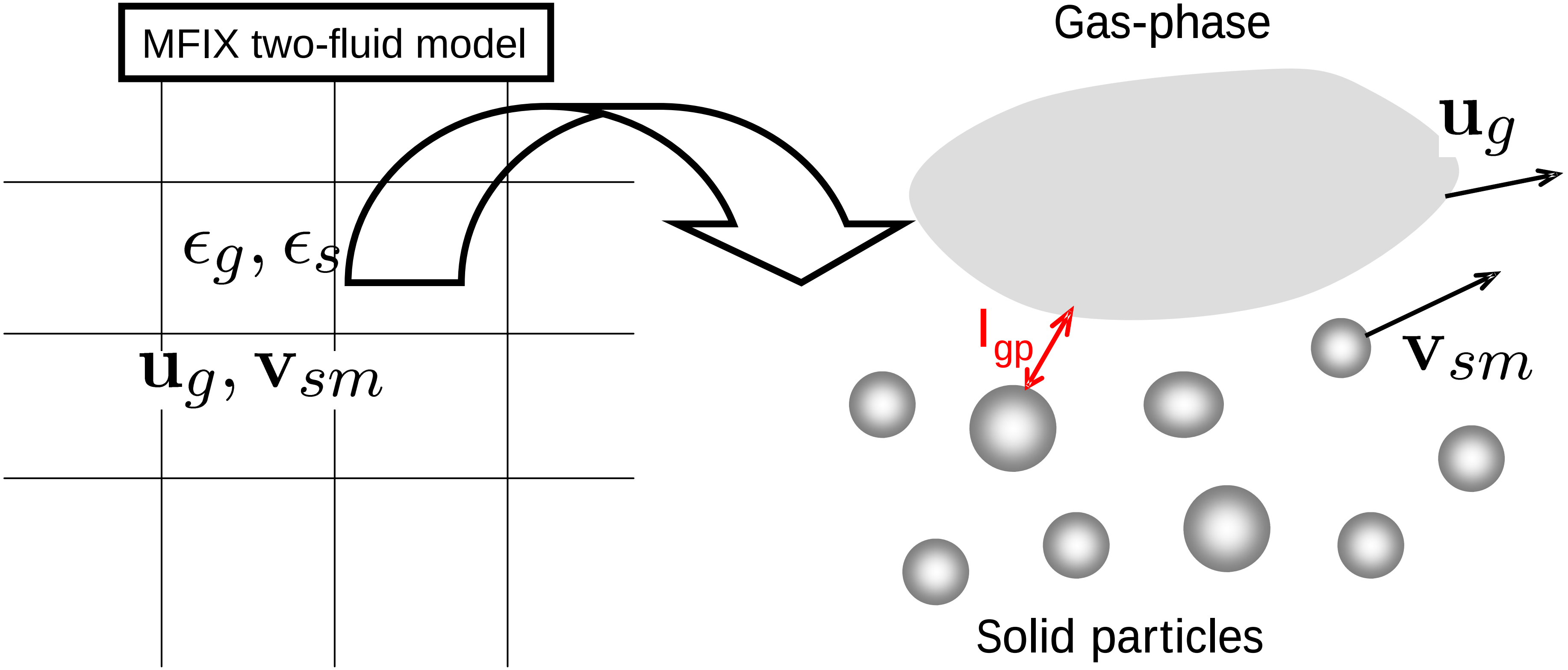
1. Develop drag relations that can handle particle size and density distributions

2. Development of constitutive relations for continuum models from high fidelity simulations

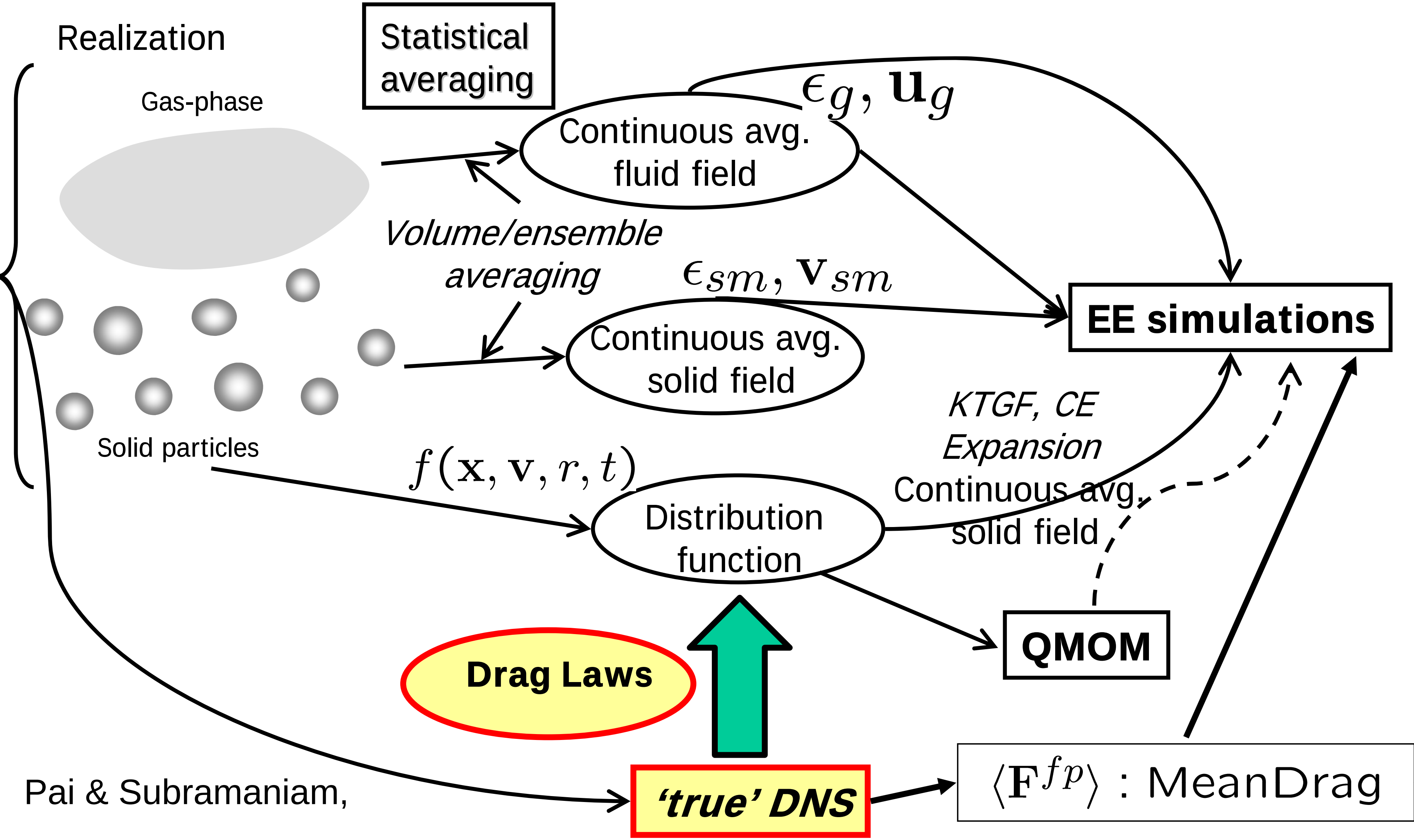


Shankar Subramaniam, Iowa State U.

MFIX Two-Fluid Model



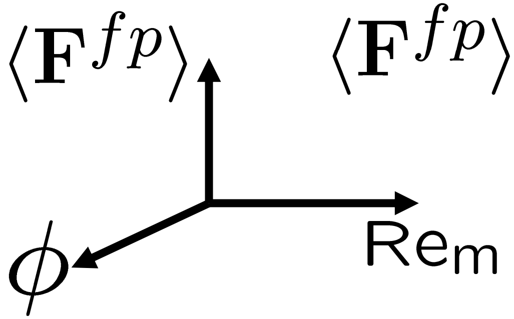
Gas-particle interaction ⇒ Drag Laws: Correlations for ***average*** force on particles



Pai & Subramaniam,

JFM (2009) (to appear)

Drag Laws (Computational)

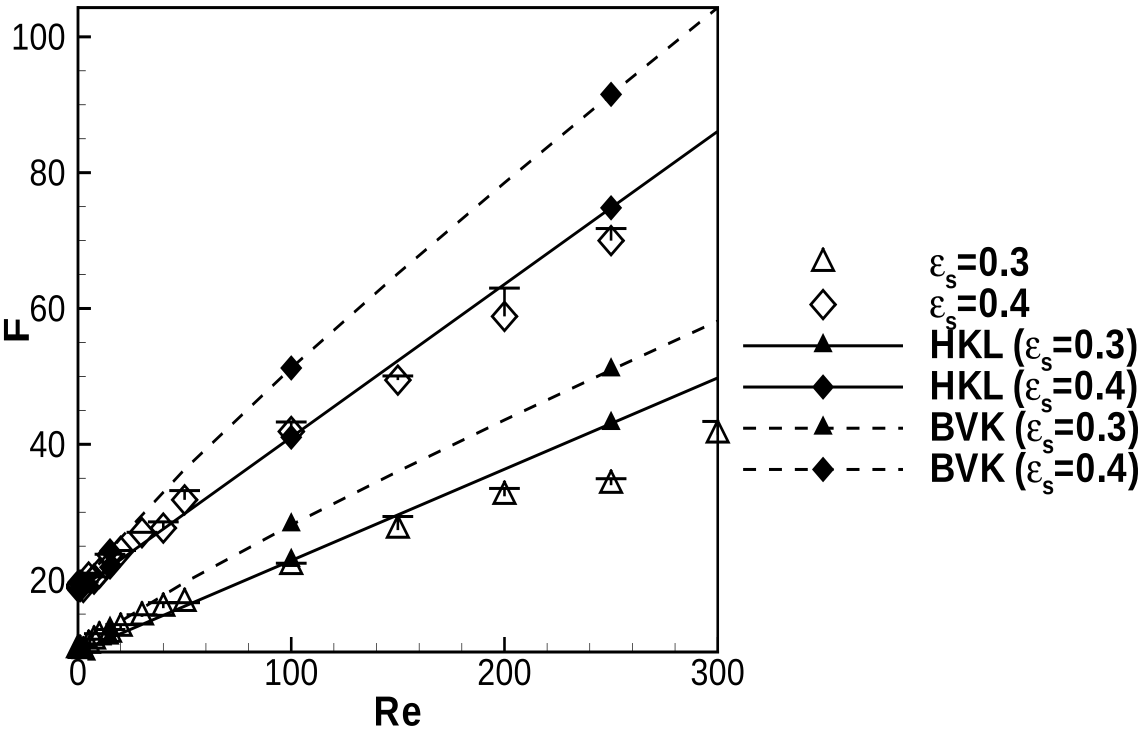


$$\langle \mathbf{F}^{fp} \rangle = \langle \mathbf{F}^{fp} \rangle (\phi, \mathrm{Re_m})$$

Monodisperse drag laws

- ➢ Hill et al (JFM 2001)
- ➢Beetstra et al (AiChE, 2007)

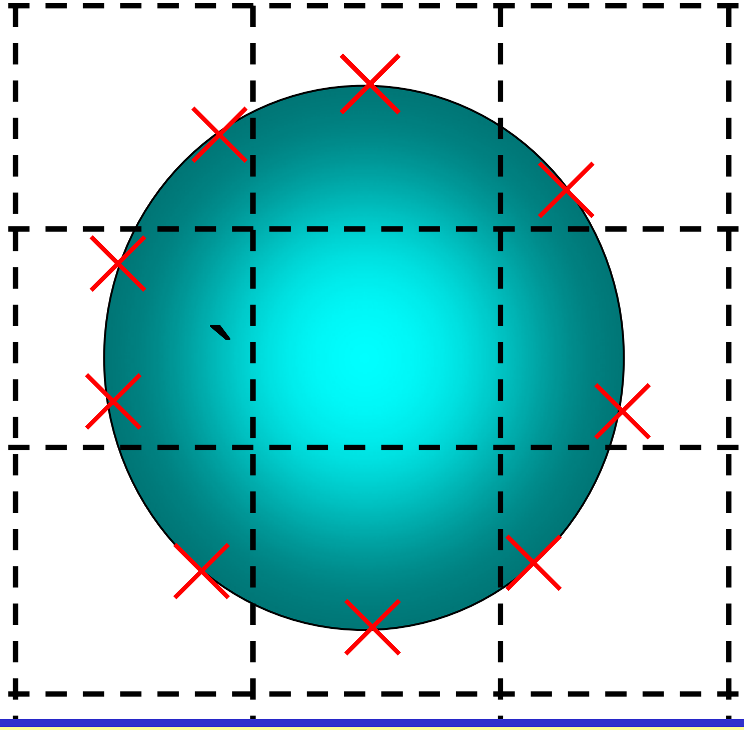
Using Lattice Boltzmann Method (LBM)

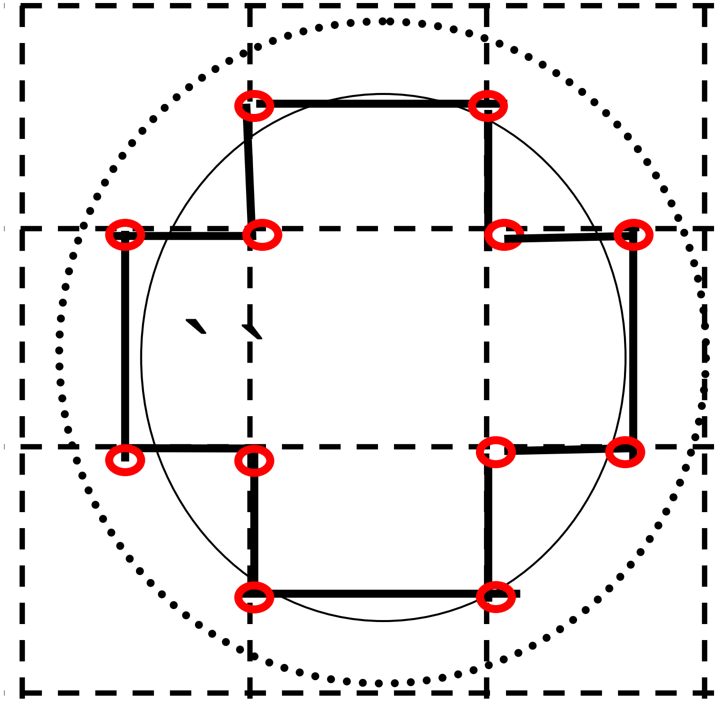


Present Approach: Immersed Boundary Method (IBM)

"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 (in review)

IBM- LBM Comparison





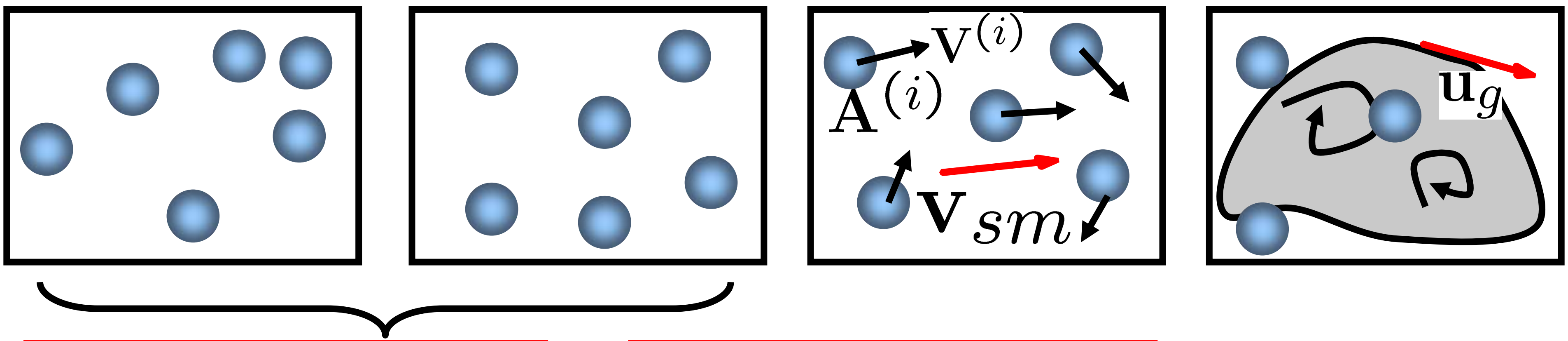
- IBM : Continuum Navier-Stokes Solver
- Incompressible flow solution: elliptic pressure solve
- Sphere: impose BC on boundary
- Drag : integrating stress tensor at sphere boundary (crosses)

- LBM : Discretized distribution function of fluid molecules
- Parallel local operations, always compressible; Ma = Kn Re
- Sphere : Stair-step function
- Drag: reported for hydrodynamic radius (dotted circle)

Mean Drag

Drag Laws: Correlations for ***average*** force on particles

⇒ What is the averaging performed over?



Particle Configurations

Particle velocity distribution

Particle acceleration distribution: from DNS

Fluid velocity fluctuations (not necessarily turbulence)

Modeling approach ⇒ $f(\mathbf{x}, \mathbf{v}, r, t)$

One-particle distribution function

Drag Law Model

$$f(\mathbf{x}, \mathbf{v}, r, t)$$

- One-particle distribution function (Mean number density)

Modified KTGF (Hrenya)

QMOM (Fox)

Accounts for:

- dependence on particle size
- dependence on particle velocity

Does not explicitly account for:

- neighbouring particle effects
- effect of fluid

⇒ Need to be modeled

Mean Drag

Conditional average of acceleration (drag)

$$\langle \mathbf{F}^{fp} \rangle (\mathbf{x}, t) = \int_{[\mathbf{v}, r]} m(r) \langle \mathbf{A} \mid \ldots, \mathbf{x}, \mathbf{v}, r; t \rangle f(\mathbf{x}, \mathbf{v}, r, t)\, d\mathbf{v}\, dr$$

Instantaneous Particle Acceleration Models

Drag Law: Mean Acceleration

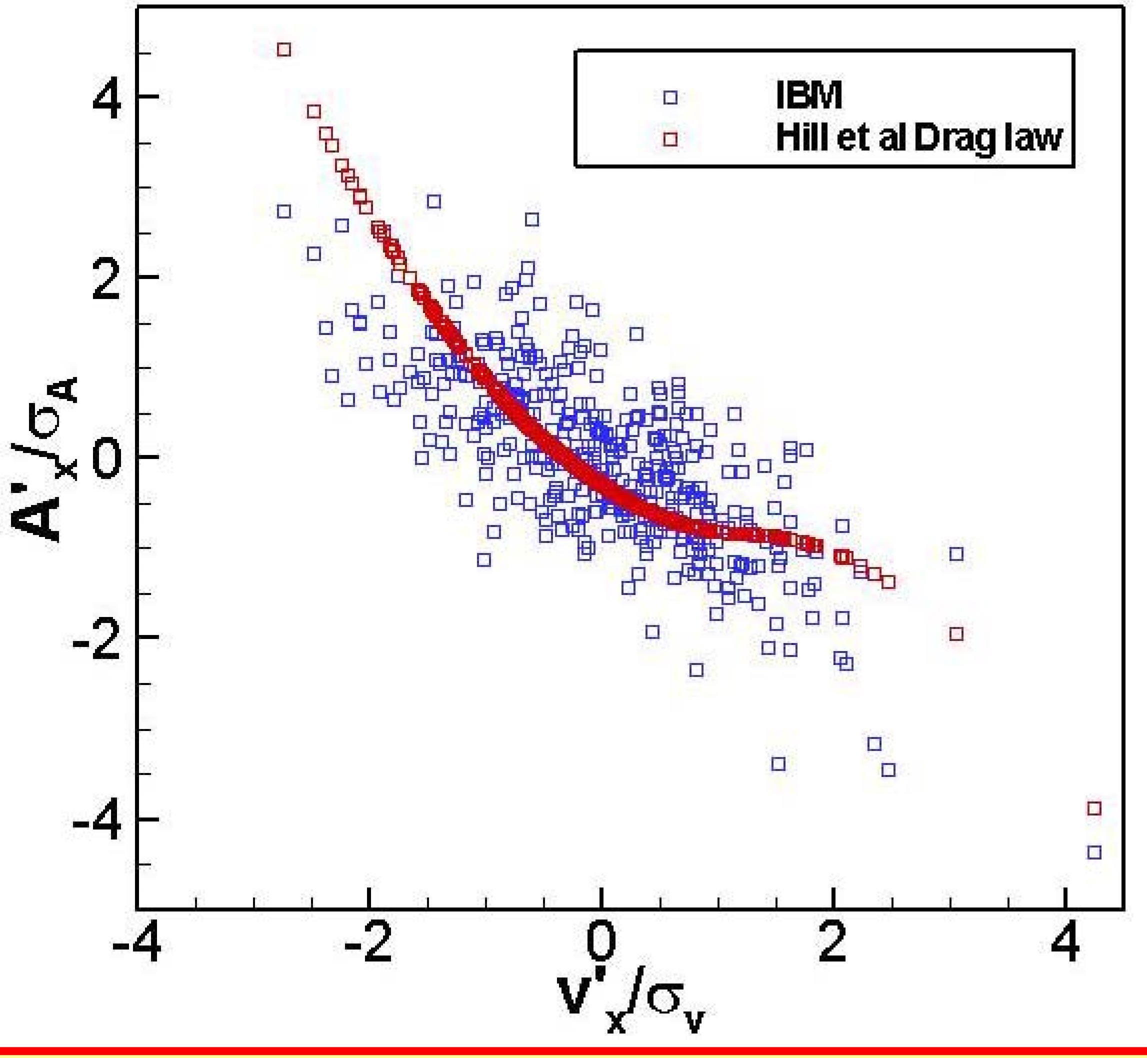
$$\langle A_i \rangle = \beta \left(\langle v_i \rangle - \left\langle u_i^{(f)} \right\rangle \right)$$

Simple extension of mean acceleration model to instantaneous particle acceleration

$$A_i = -\beta W_i$$

$$W_i = v_i - \left\langle u_i^{(f)} \right\rangle$$

Fluctuating Particle Acceleration-velocity Scatter



$Re_m=20$

$Re_T=16$

$\phi=0.2$

$$A_i = -\beta W_i$$

β: Hill et al.
(JFM 2001)

Drag law applied to velocity distribution does not recover the acceleration distribution

Role of Particle Acceleration Fluctuations

Continuum model (MFIX-EE)

Mean particle acceleration

Affect granular temperature equation

Fluctuations in particle acceleration:

$\langle A_i'' v_j'' \rangle$

- correlate with fluctuations in particle velocity

$S + \Gamma_{vis}$

Koch (Phys. Fluids 1990)

Fluctuations in particle acceleration:

- generate a hierarchy of moments

Need a model for:

$$\langle \mathbf{A} \mid \ldots, \mathbf{x}, \mathbf{v}, r; t \rangle$$

provide closures for ***ALL*** moments

To account for effect of fluid phase, neighbour particle interactions etc

Instantaneous Particle Acceleration Model

$$dv_i = A_i^{(d)} dt + B_{ij} d\mathcal{W}_j$$

→ Langevin Model

Drift term

$$dv_i = -\beta_{(i)} \langle W_i \rangle dt - \gamma_{ij} v_j'' dt + \Sigma_{ij} d\mathcal{W}_j$$

Mean slip

Velocity fluctuations (particle velocity distribution)

Wiener process

(effect of neighbouring particle + fluid phase fluctuations)

γ_{ij}

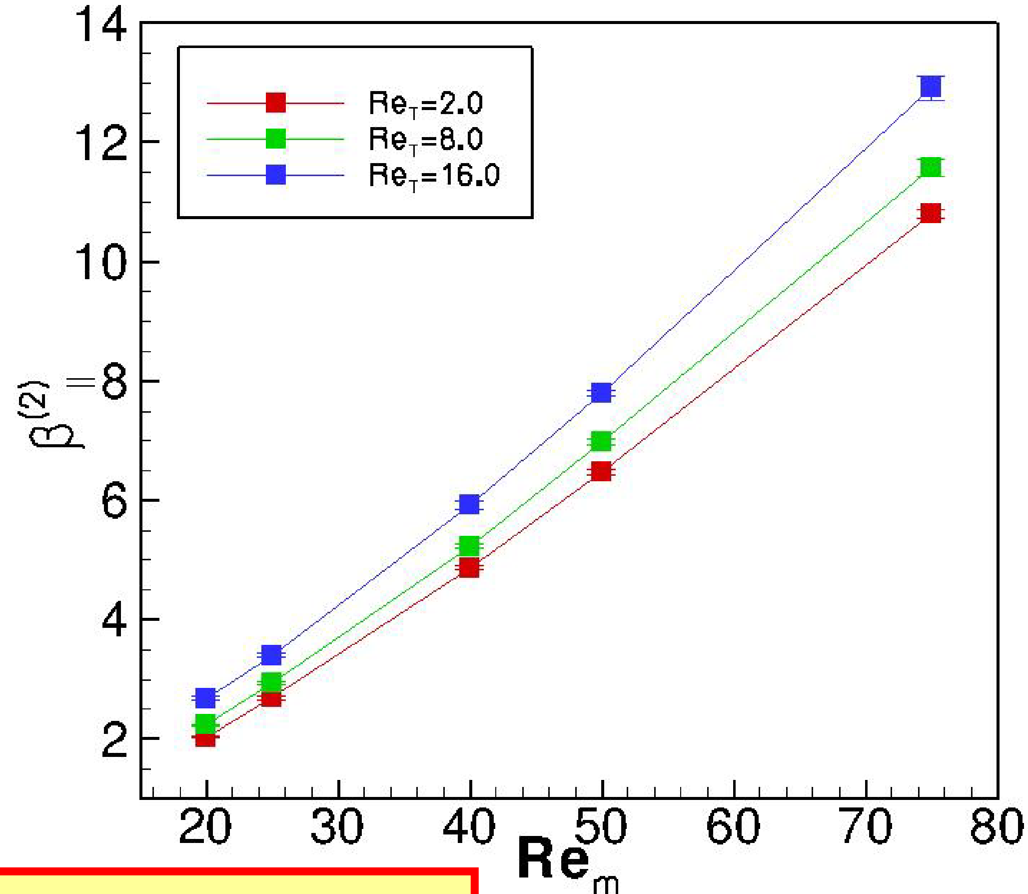
- inverse of Lagrangian particle velocity autocorrelation time
- how long particle retains memory of initial velocity
- function of Stokes number

Langevin Model: Coefficients

$$\beta_{(i)} = \beta_{(i)}\left(\phi, \mathrm{Re_m}, \mathrm{Re_T}\right)$$

- Depends on volume fraction
- Reynolds number based on mean slip velocity
- Reynolds number based on particle granular temperature

Volume fraction = 0.2



γ, Σ → Freely evolving suspensions

Langevin Model: Coefficients

$$dv_i'' = -\gamma v_i'' dt + \Sigma d\mathcal{W}_j$$

Use Lagrangian structure function

$$D_L(s) = \left\langle \left[v_i''(t+s) - v_i''(t) \right]^2 \right\rangle$$

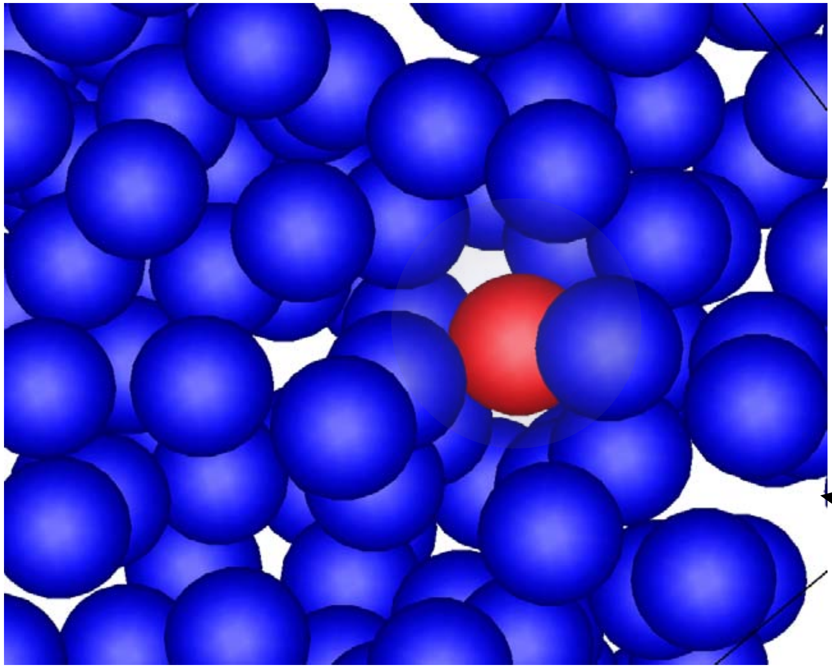
Lagrangian structure function for Langevin model

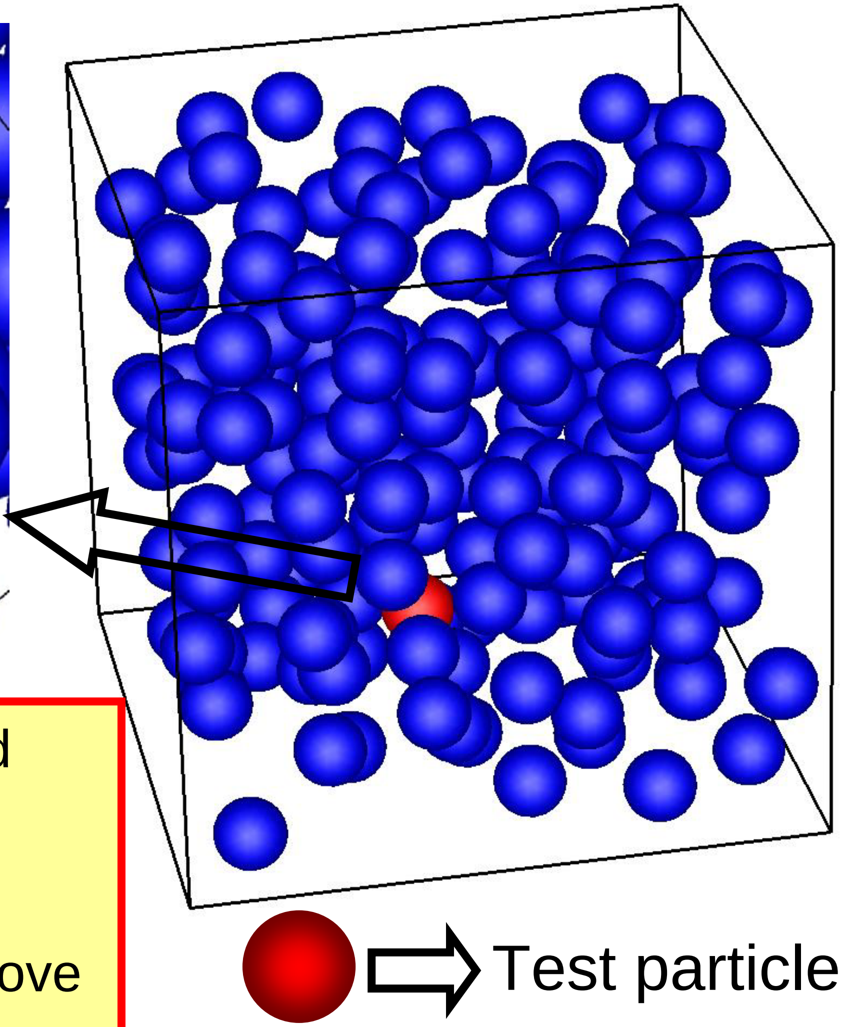
$$D_L^*(s) = \Sigma^2 s$$

$$\frac{\Sigma^2}{2\gamma} = \frac{1}{3} T$$

Extract the structure function from the DNS of freely evolving suspensions (particles feel the fluid force)

Test Particle in a Homogeneous Assembly

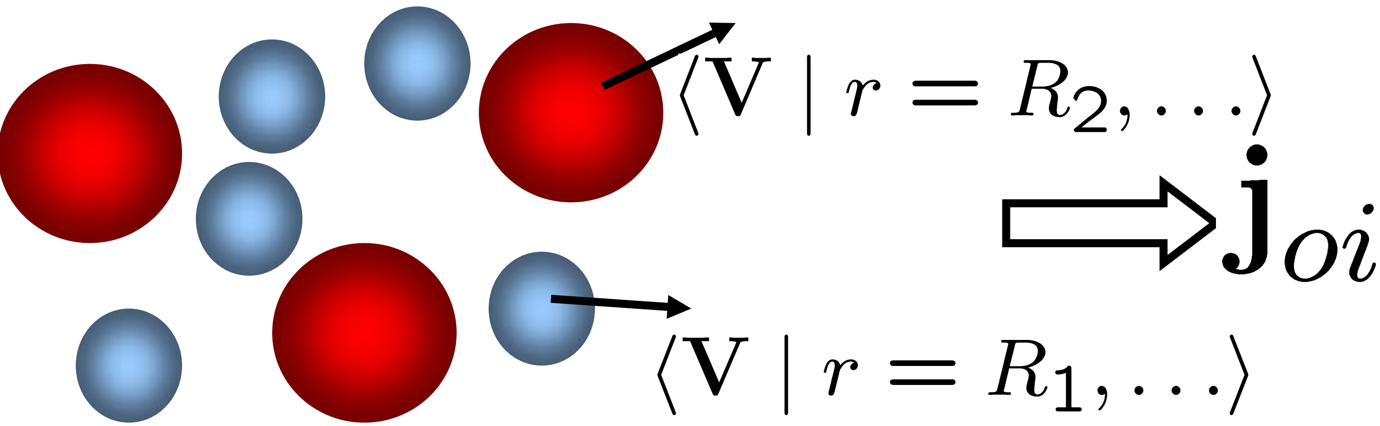




- Assembly of fixed particles: initialized with a velocity distribution
- Particles within radius of influence of moving test particle are allowed to move
- Velocity autocorrelation and Lagrangian structure function will be extracted to determine coefficients

Drag laws: Effect of Particle Size Distribution

Bidisperse Example



Flux of size-class relative to mean solids flux (Hrenya)

Segregation due to drag manifests as flux of size-class relative to mean solids flux

$$\langle \mathbf{A} \mid r = R_\alpha, \ldots \rangle - \langle \mathbf{A} \mid \ldots \rangle$$

Driving force is drag conditional on size

Instantaneous Particle Acceleration Model

Extension to bidisperse case $\langle W_i \mid r = R_\alpha \rangle = \langle v_i \mid r = R_\alpha \rangle - \left\langle u_i^{(f)} \right\rangle$

$$m^\alpha dv_i^\alpha = -\beta_{(i)}^{\alpha\eta} \langle W_i \mid r = R_\eta \rangle \, dt - \gamma_{ij}^{\alpha\eta} v''^{(\eta)}_j \, dt + \Sigma_{ij}^{\alpha\eta} d\mathcal{W}_j^{\eta}$$

$$\begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \end{pmatrix} \qquad \begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \end{pmatrix} \qquad \begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \end{pmatrix}$$

Effect of species diffusion velocity on mean drag of a size class

Effect of particle velocity distribution in a size-class

Effect of neighbor particles

All terms include effect of the presence of other size-class

Mean drag: Bidisperse (Equal Velocities)

$$m^\alpha dv_i^\alpha = -\beta_{(i)}^{\alpha\eta} \langle W_i \mid r = R_\eta \rangle dt - \gamma_{ij}^{\alpha\eta} v''^{(\eta)}_j dt + \Sigma_{ij}^{\alpha\eta} d\mathcal{W}_j^\eta$$

no relative velocity between size classes

$$F^*_{D-\alpha} = \frac{\left| \langle \mathbf{F} \rangle_{D-\alpha} \right|}{3\pi\mu D_\alpha (1-\phi) \left| \langle \mathbf{W} \right| r = R_\alpha ; t \rangle |}$$

Average drag force per particle

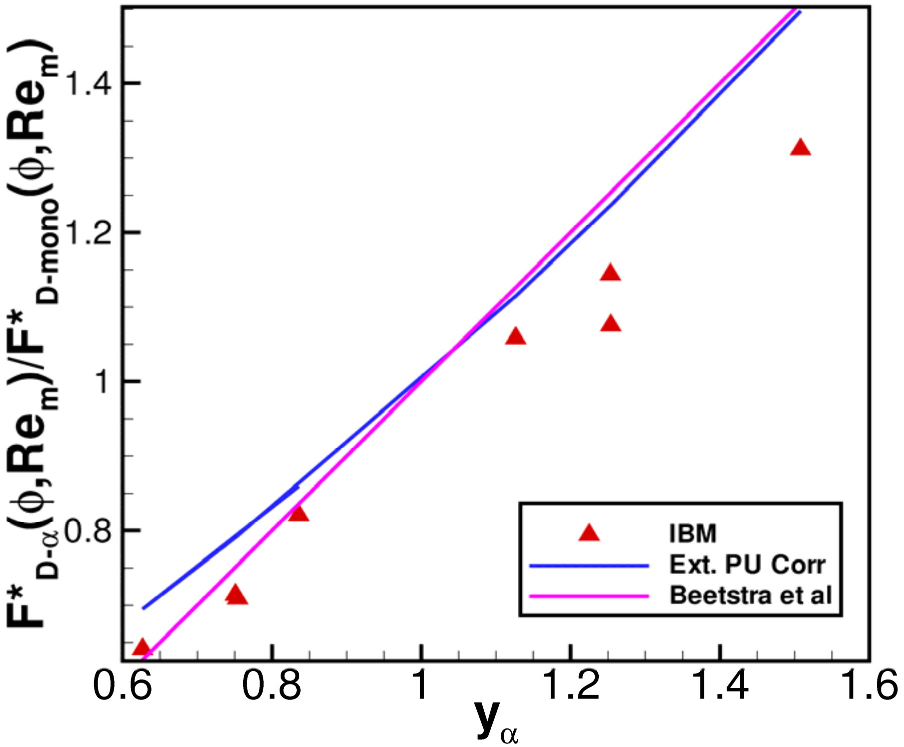
Express the mean drag in terms of an equivalent monodisperse suspension (Sauter mean diameter)

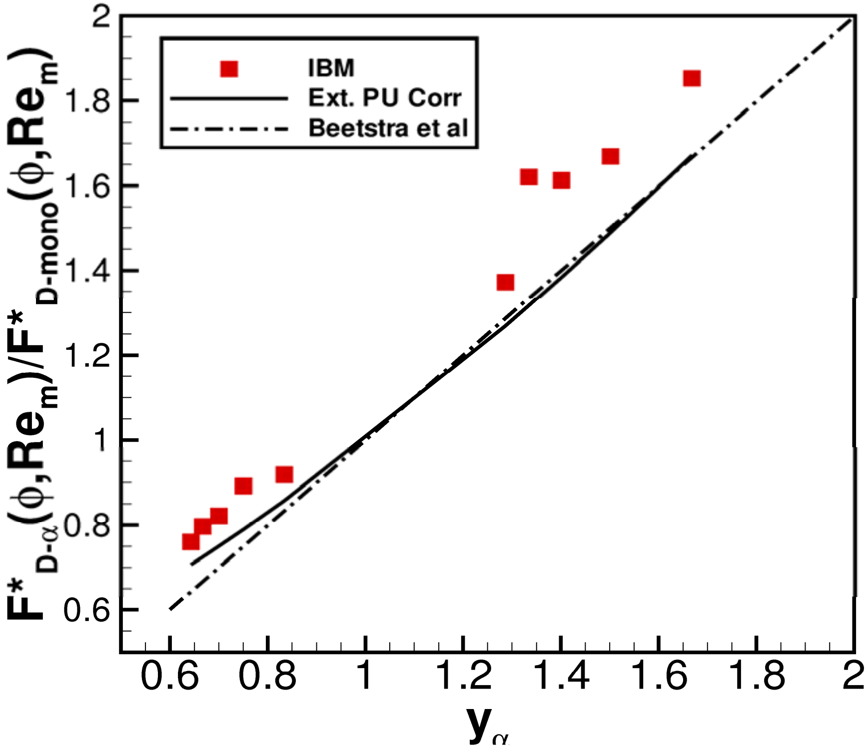
$$y_\alpha = \frac{D_\alpha}{\langle D \rangle}$$

$$\frac{F^*_{D-\alpha}(\phi, \mathrm{Re}_m)}{F^*_{D-\mathrm{mono}}(\phi, \mathrm{Re}_m)} = y_\alpha$$

No dependence on Reynolds number (Beetstra et al. AiChE J. 2007)

IBM Bi-disperse Simulations : Normalized force





Vol. fraction = 0.2

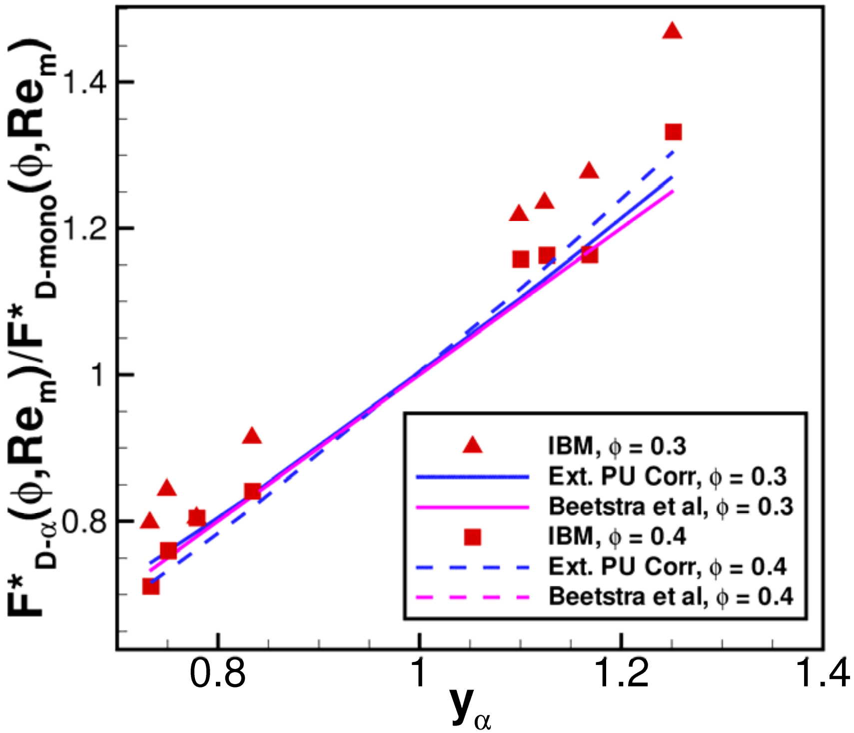
- **Re_m = 20**
- **D_2/D_1 = 1.5, 2**
- **ϕ_2/ϕ_1 = 1, 2, 3, 4**

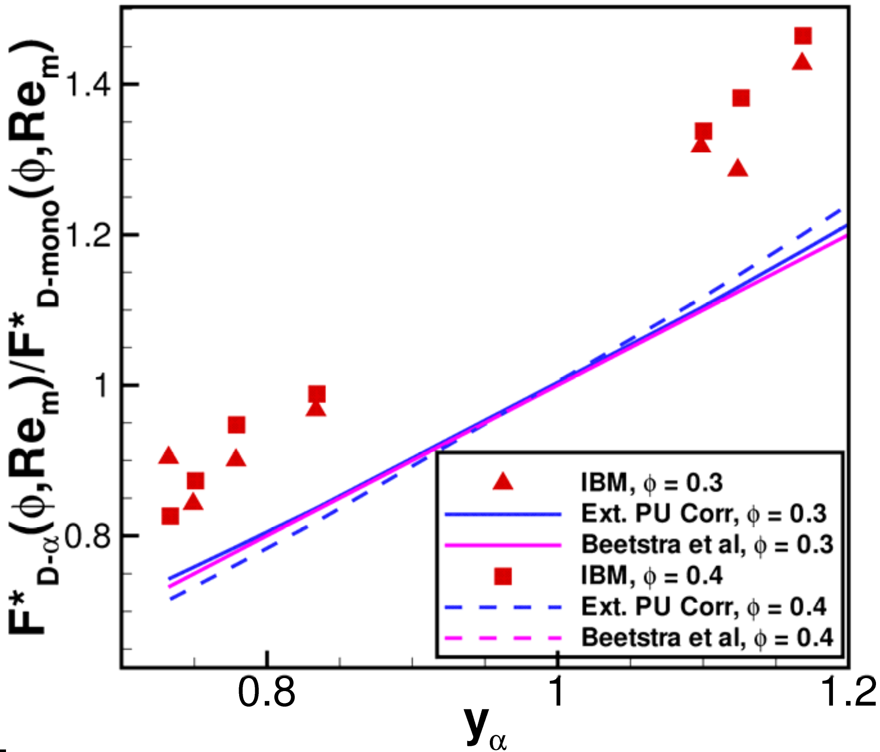
$D_1/\Delta x$: 20
L/D_2 : 6
MIS : 4

- **Re_m = 50**
- **D_2/D_1 = 1.5**
- **ϕ_2/ϕ_1 = 0.5, 1, 2, 3, 4**

IBM simulations indicate a dependence on Reynolds number

IBM Bi-disperse Simulations : Normalized force





- $Re_m = 50$
- $D_2/D_1 = 1.5$
- $\phi_2/\phi_1 = 1, 2, 3, 4$

Vol. fraction = 0.3, 0.4

$D_1/\Delta x$: 30
L/D_2 : 4
MIS : 4

- $Re_m = 65$
- $D_2/D_1 = 1.5$
- $\phi_2/\phi_1 = 1, 2, 3, 4$

Magnitude of drag also is different at higher Reynolds numbers

Current Efforts

1. Development of test particle simulations to extract coefficients of the Langevin model
2. Propose a new bi-disperse drag law at moderate Reynolds numbers
3. Data-driven exploration of the parameter space for DNS of polydisperse systems
4. Publication in preparation

   "Effect of hydrodynamic forces on particle velocity fluctuations in suspensions at moderate Reynolds numbers". S. Tenneti, R. Garg, S. Subramaniam, R.O. Fox, C.M. Hrenya. *In preparation, to be submitted to NETL special issue journal (2009)*

Acknowledgements

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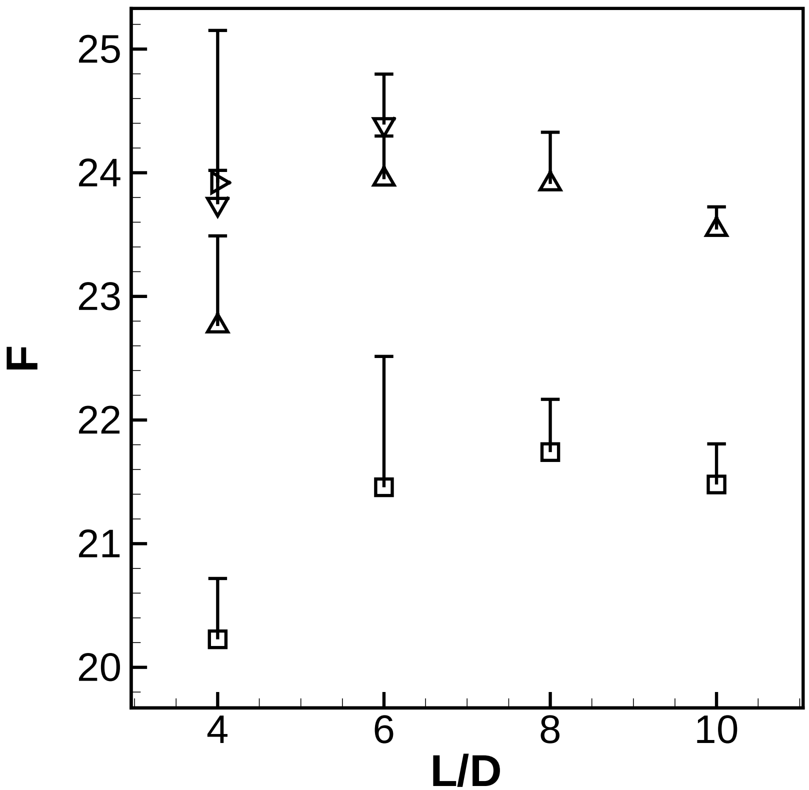
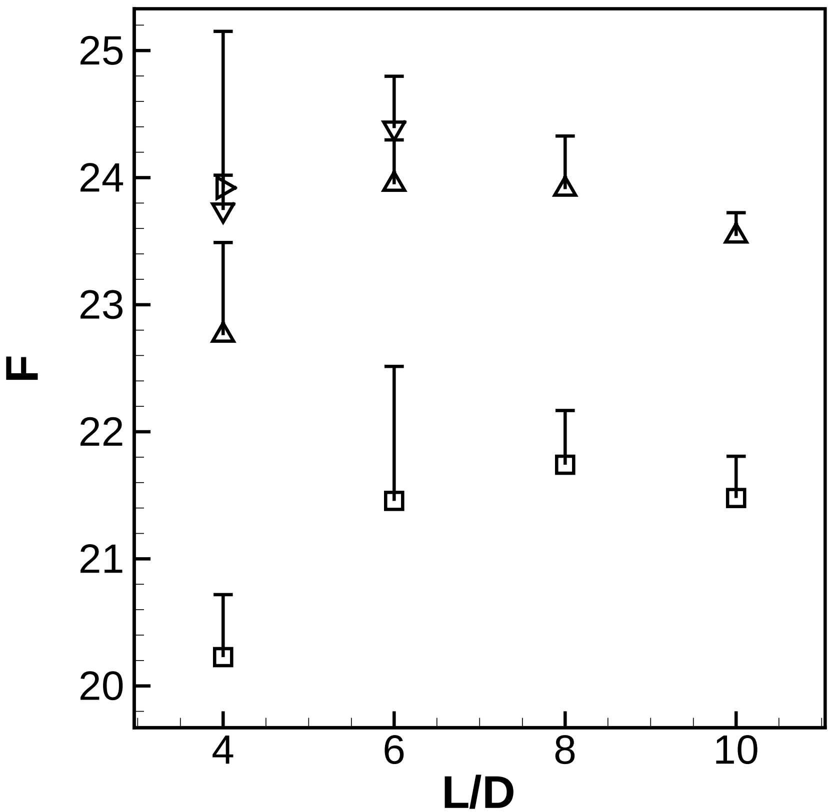
- Rahul Garg, Iowa State University

BACKUP

IBM Numerical convergence





- Re_m = 20
- ϕ = 0.3

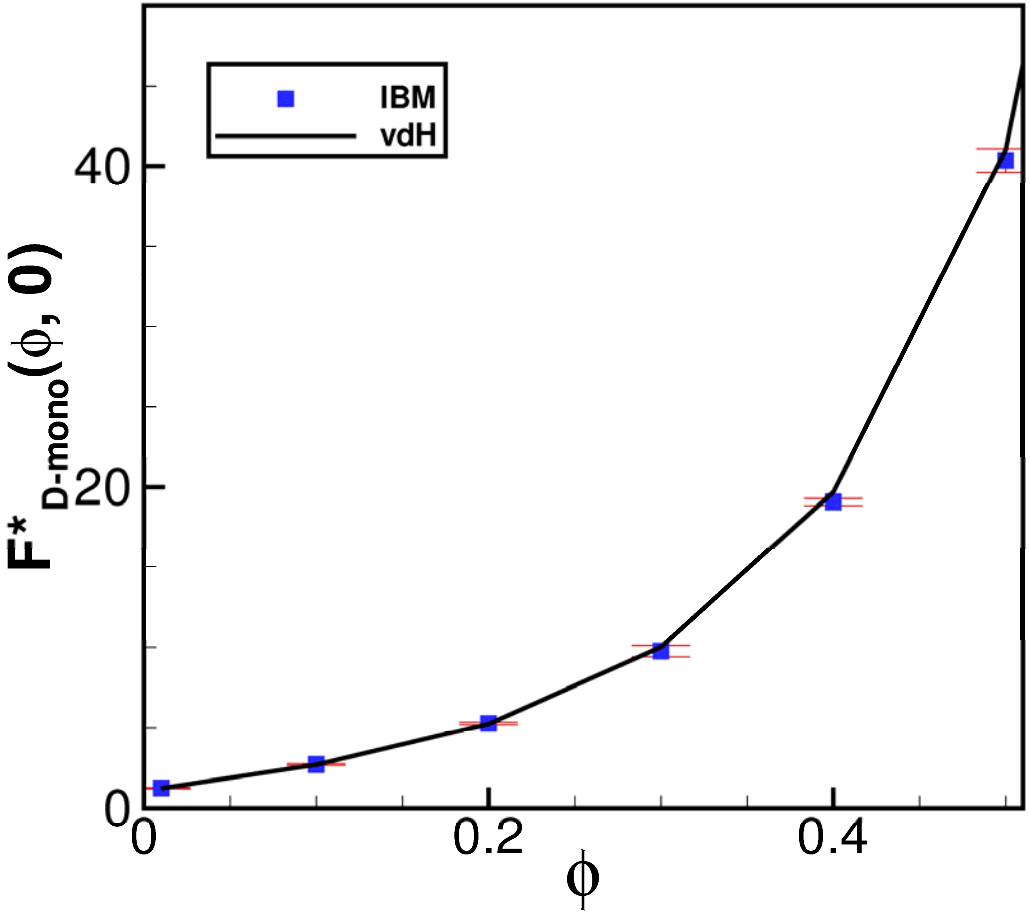
- Re_m = 20
- ϕ = 0.4

D /Δx : 10, 20, 30

MIS : 5

IBM : Monodisperse Stokes Flow Regime

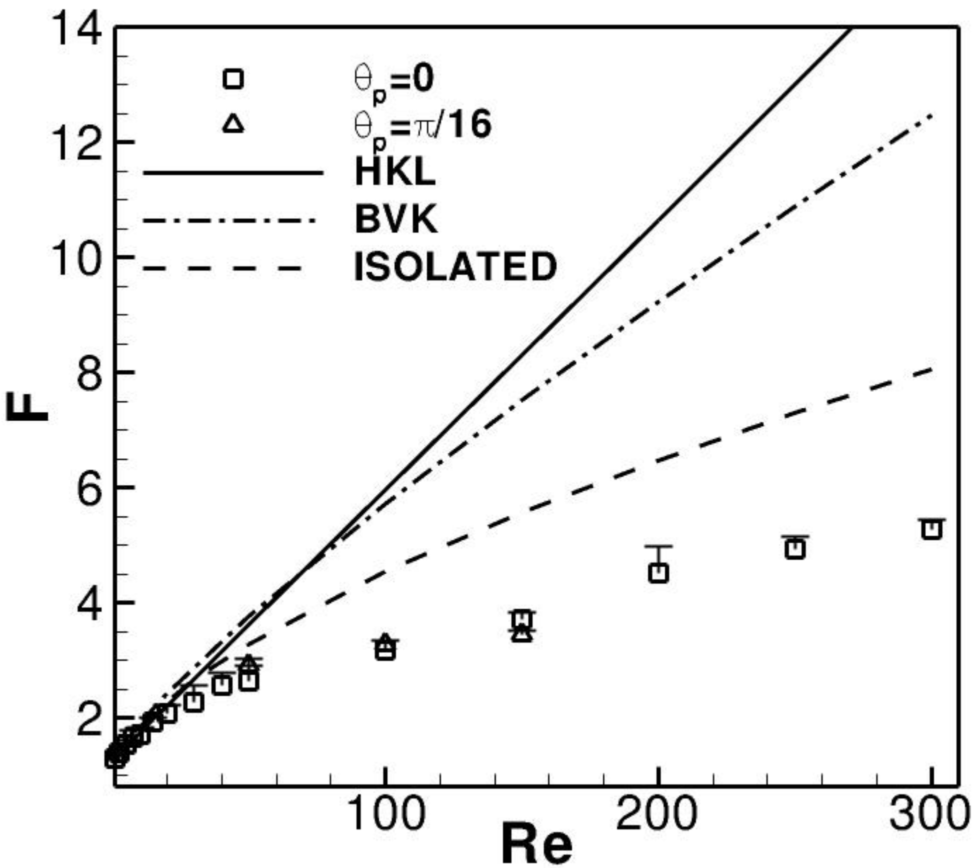
$$F^*_{D-\mathrm{mono}}(\phi,0) = \frac{10\phi}{(1-\phi)^2} + (1-\phi)^2\left(1+1.5\sqrt{\phi}\right)$$



Random arrays
Re=0.01
D/Δx :10-40
L/D : 4-15
MIS : 5

Excellent agreement of IBM with LBM drag law in Stokes regime

IBM : Monodisperse Dilute Arrays

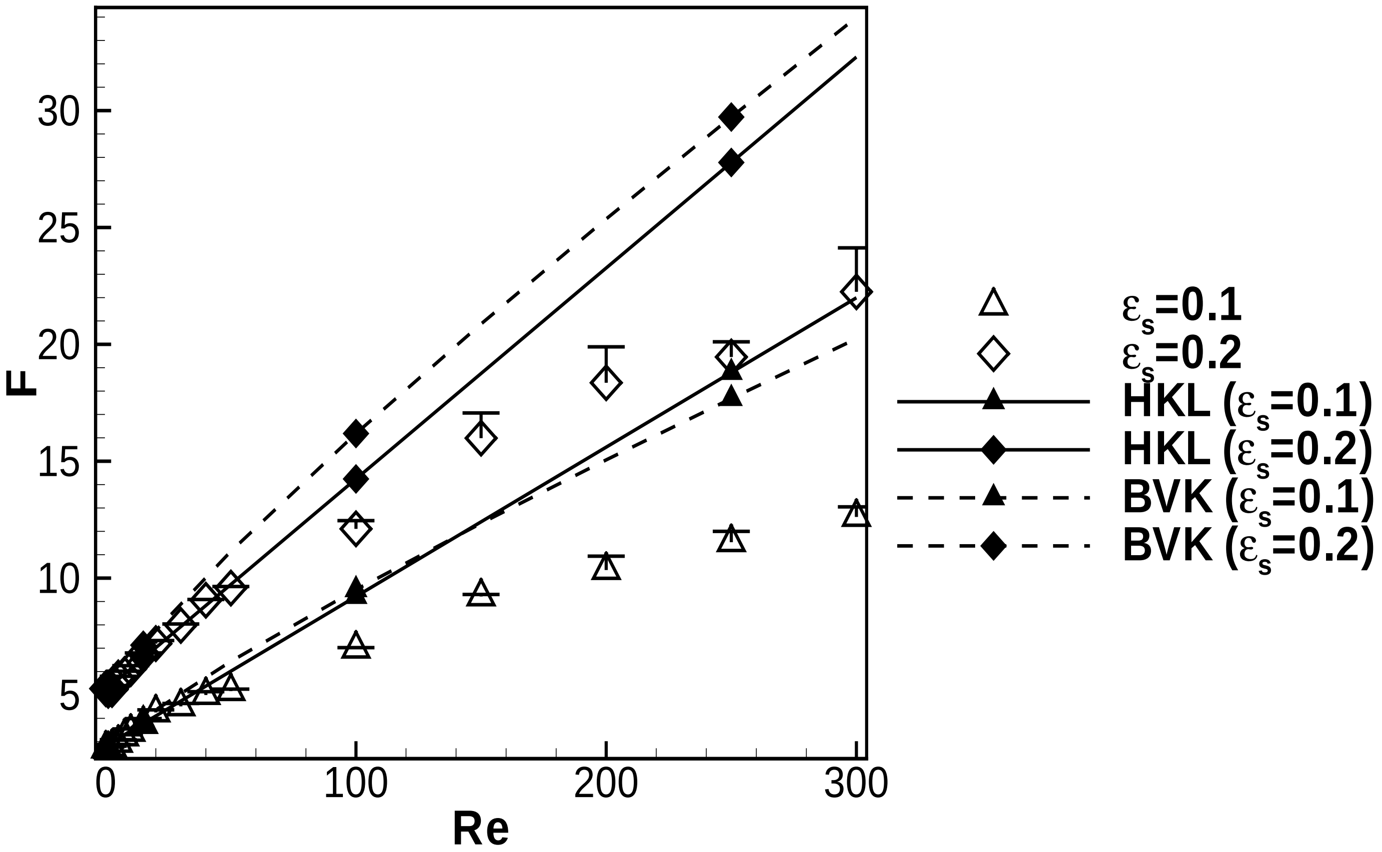


Volume Fraction = 0.01

D /Δx = 10

L/D = 15

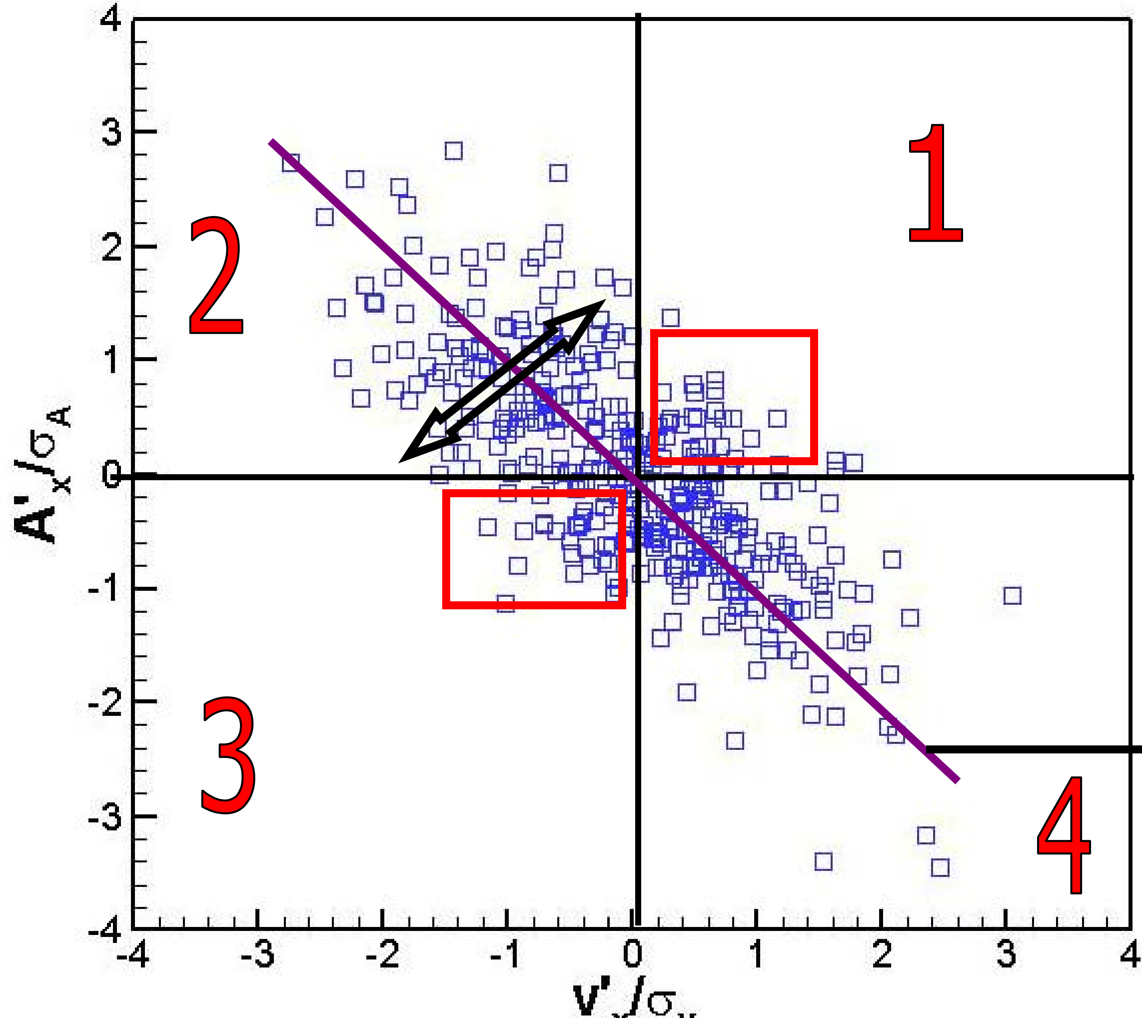
IBM : Monodisperse Moderately Dense Arrays



$D / \Delta x = 30$

$L/D = 5$

Fluctuating particle acceleration-velocity scatter



Re$_m$=20

Re$_T$=16

ϕ=0.2

$$\mathrm{Re_m} = \frac{\rho_f (1-\phi)|\langle \mathbf{W} \rangle D}{\mu_f}$$

$$\mathrm{Re_T} = \frac{D T^{1/2}}{\nu_f}$$

Dilute Stokes flow

Note: some positive velocity fluctuations (less slip) result in *positive* acceleration fluctuations (more drag)

Drag law forms: Bi-disperse (Equal Velocities)

van der Hoef et al

$$F^*_{D-\alpha}(\phi,0) = y_\alpha F^*_{D-\mathrm{mono}}(\phi,0)$$

$$y_\alpha = \frac{D_\alpha}{\langle D \rangle} \qquad \langle D \rangle = \frac{\sum_{\alpha=1}^{2} N_\alpha D_\alpha^3}{\sum_{\alpha=1}^{2} N_\alpha D_\alpha^2}$$

Yin et al

$$F^*_{D-\alpha}(\phi,0) = \frac{1}{1-\phi} + \left(F^*_{D-\mathrm{mono}}(\phi,0) - \frac{1}{1-\phi}\right)\left[a y_\alpha + (1-a) y_\alpha^2\right].$$

Drag law forms: Bi-disperse (Equal Velocities)

$$F^*_{D-\alpha} = F^*_{D-\alpha}\left(\phi, \mathrm{Re}_m\right)$$

Mixture Reynolds number

$$\mathrm{Re_m} = \frac{\rho_f (1-\phi) |\langle \widetilde{\mathbf{V}} \rangle - \langle \mathbf{u}^{(f)} \rangle| \langle D \rangle}{\mu_f}$$

Mass-weighted mean particle velocity

$$\left\langle \widetilde{\mathbf{V}} \right\rangle = \frac{\sum_{\alpha=1}^{2} \rho_\alpha \phi_\alpha \left\langle \mathbf{v} \right| r = R_\alpha; t \rangle}{\sum_{\alpha=1}^{2} \phi_\alpha \rho_\alpha}$$

Beetstra et al

$$F^*_{D-\alpha}(\phi, \mathrm{Re}_m) = y_\alpha F^*_{D-\mathrm{mono}}\left(\phi, \mathrm{Re}_m\right)$$

Drag law forms: Bi-disperse (Equal Velocities)

$$F^*_{D-\alpha} = F^*_{D-\alpha}\left(\phi, \mathrm{Re}_m\right)$$

Mixture Reynolds number

$$\mathrm{Re_m} = \frac{\rho_f (1-\phi)|\langle\widetilde{\mathbf{V}}\rangle - \langle\mathbf{u}^{(f)}\rangle||\langle D\rangle}{\mu_f}$$

Mass-weighted mean particle velocity

$$\left\langle \widetilde{\mathbf{V}} \right\rangle = \frac{\sum_{\alpha=1}^{2} \rho_\alpha \phi_\alpha \left\langle \mathbf{v} \right| r = R_\alpha; t\rangle}{\sum_{\alpha=1}^{2} \phi_\alpha \rho_\alpha}$$

Extension of Yin et al's drag law

$$F^*_{D-\alpha}\left(\phi, \mathrm{Re}_m\right) = F^*_{D-\alpha}\left(\phi, 0\right)\left[1 + \alpha'(\phi, \mathrm{Re}_m)\mathrm{Re}_m\right]$$

Beetstra et al: Monodisperse drag law

Instantaneous particle acceleration model

$$dv_i = A_i^{(d)} dt + B_{ij} d\mathcal{W}_j$$

Langevin Model

$$dv_i = -\beta_{(i)} \langle W_i \rangle dt - \gamma_{ij} v_j'' dt + \Sigma_{ij} d\mathcal{W}_j$$

Second moment of particle velocity

$$\frac{d}{dt}\langle v_i'' v_j'' \rangle = \Sigma_{ik}\Sigma_{jk} - \gamma_{il}\langle v_j'' v_l'' \rangle - \gamma_{jk}\langle v_i'' v_k'' \rangle$$

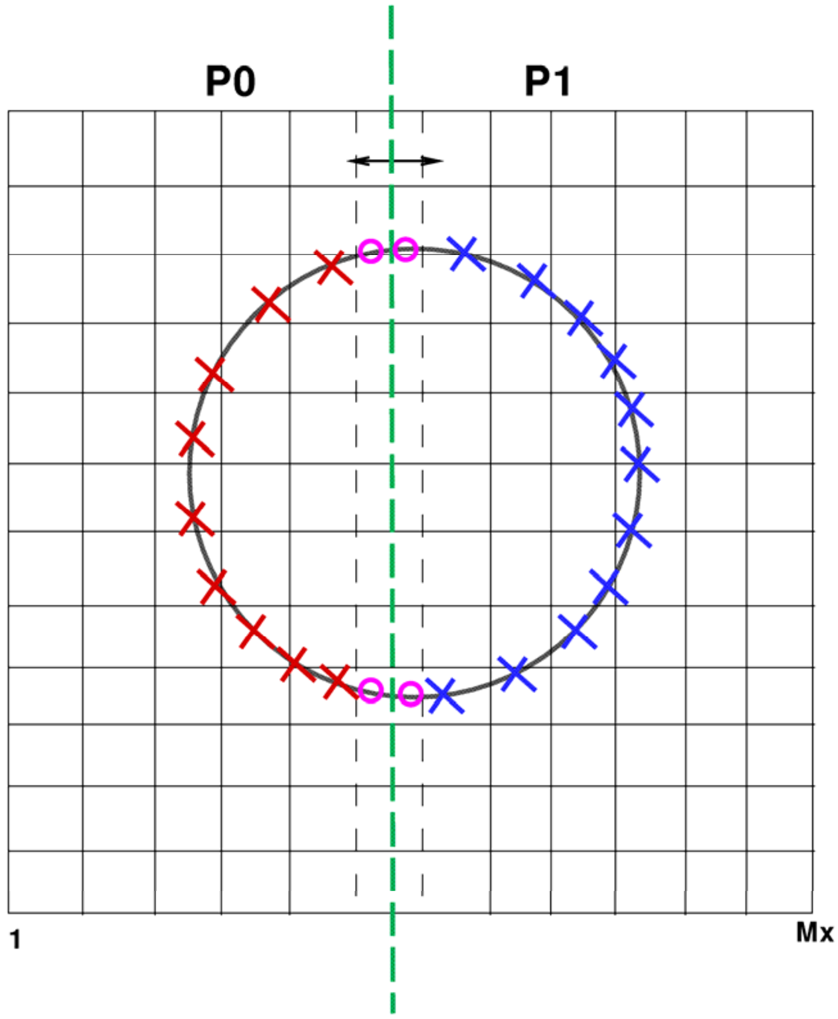
$$m\frac{d}{dt}\langle v_i'' v_j'' \rangle = S_{ij,h} - \Gamma_{ij,h}$$

Sangani & Koch (1999)

Bidisperse Simulations: Resolution Rquirements

- Smaller particles must be well resolved
  - Vol. fraction = 0.2, Re = 100, $D/\Delta x = 30$
- Box length should be large compared to larger diameter
  - $L/D_2 = 6$
- Number of larger paritcles must be large enough

Required box size: 360^3: Need for parallel IBM



Schematic of domain decomposition

Parallel IBM: Details

- Cyclic tridiagonal system of equations
- Previously used Gauss-Siedel : iterative solver
  - Bad for parallelization (Need to communicate in every iteration)
- Implemented direct solver based on Sherman-Morrison formula
  - Results in solving two tridiagonal systems
- Parallelized tridiagonal solver
  - Parallel partition algorithm (LANL)

Parallel IBM: Validation Study

$$\epsilon_l = \frac{1}{M_x M_y M_z} \sum_{i=1}^{M_x} \sum_{j=1}^{M_y} \sum_{k=1}^{M_z} \left| Q_l^{(p)}(i,j,k) - Q_l^{(s)}(i,j,k) \right|$$

Configuration	$\frac{D}{\Delta x}$	ϵ_1	ϵ_2	ϵ_3	ϵ_4
Simple	46.4	0.63271616E-14	0.86949156E-16	0.88190940E-16	0.41440159E-14
FCC	29.24	0.23248653E-14	0.62514764E-15	0.62624656E-15	0.13055491E-14
Monodisperse	20	0.12112644E-11	0.79061513E-12	0.86040804E-12	0.57968924E-12
Bi–disperse	15	0.30301074E-15	0.89068307E-16	0.11269121E-15	0.65079639E-16

Validity of parallel IBM established: good for production runs