Euler-Euler anisotropic Gaussian mesoscale direct numerical simulation of homogeneous cluster-induce gas-particle turbulence

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2015 NETL Workshop on Multiphase Flow Science

Completed Tasks in FY15

MFIX-QBMM

Created collection of gas-particle solvers using quadrature-based moment methods

- Migrated from MFIX-2013 to current MFIX git development repository
- Developed comprehensive post-processing capabilities using Python and VTK package
- Enabled code to run in both DMP and SMP mode
- Developed capability of handling non-uniform grid
- Provided users with a full range of drag models
- Developed realistic wall boundary condition
- Validated code against Euler-Lagrangian simulations
- Developed generalized code structure for multiple MFIX-QBMM solvers
- Developed algorithm to extend QBMM to dense regime

Outline

1. Motivation
2. EE-AG Methods
   - Governing Equations and Moments Method
   - Anisotropic Particle Velocity Distribution
   - Kinetic flux, Forces and Collision Model
3. Homogeneous Gravity-Driven Flow : A Domain Size Study
4. Summery and Future Work
5. Acknowledgements

Motivation

MFIX-QBMM

Validate anisotropic Gaussian particle velocity assumption in EQMOM polydisperse solver in MFIX-QBMM

Gas-particle turbulence model

Disadvantages of Euler-Lagrangian DNS for multiphase turbulence modeling

1. Sophasicated filter techniques has to be used to extract Eulerian particle phase information
2. Computationally expensive when mass loading is high

A novel approach to traditional TFM-KT

The isotropic particle velocity assumption is often not valid, specially for gravity-driven flows

EE-AG Methods : Governing Equations

Gas phase: Continuity and momentum transport equations

$$\frac{\partial}{\partial t}\rho_{\mathrm{g}}\varepsilon_{\mathrm{g}} + \nabla\cdot\rho_{\mathrm{g}}\varepsilon_{\mathrm{g}}\mathbf{U}_{\mathrm{g}} = 0$$

$$\frac{\partial}{\partial t}\rho_{\mathrm{g}}\varepsilon_{\mathrm{g}}\mathbf{U}_{\mathrm{g}} + \nabla\cdot\rho_{\mathrm{g}}\varepsilon_{\mathrm{g}}\mathbf{U}_{\mathrm{g}}\otimes\mathbf{U}_{\mathrm{g}} = \nabla\cdot\varepsilon_{\mathrm{g}}\boldsymbol{\tau}_{\mathrm{g}} - \nabla p + \rho_{\mathrm{g}}\varepsilon_{\mathrm{g}}\mathbf{g} + \mathbf{M}_{\mathrm{lb}}$$

Particle phase: Kinetic equation for velocity NDF $f(\mathbf{v})$

$$\frac{\partial f(\mathbf{v})}{\partial t} + \mathbf{v}\cdot\frac{\partial f(\mathbf{v})}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}}\cdot f(\mathbf{v})\,\mathbf{A} = \mathbb{S}$$

where $\mathbf{A}$ represents acceleration due to forces acting on each particle, $\mathbb{S}$ represents other possible source terms, e.g. particle collisions

EE-AG Methods : Moments Method

Velocity Moments

$$m_{i,j,k} = \int v_x^i v_y^j v_y^k \, f(\mathbf{v}) \, d\mathbf{v}$$

Lower-order moments have particular physical significance:
$m_0 = \varepsilon_\mathrm{p}$, $m_{1,0,0} = \varepsilon_\mathrm{p} U_\mathrm{p}$, $m_{0,1,0} = \varepsilon_\mathrm{p} V_\mathrm{p}$, $m_{0,0,1} = \varepsilon_\mathrm{p} W_\mathrm{p}$

Moments transport equation:

$$\frac{\partial m_{i,j,k}}{\partial t} + \frac{\partial m_{i+1,j,k}}{\partial x} + \frac{\partial m_{i,j+1,k}}{\partial y} + \frac{\partial m_{i,j,k+1}}{\partial z} = F_{i,j,k}$$

$$F_{i,j,k} = \int v_x^i v_y^j v_z^k \left[i v_x^{-1}(A_x) + j v_y^{-1}(A_y) + k v_z^{-1}(A_z) \right] f(\mathbf{v}) \, d\mathbf{v}$$

Quadrature-Based Moment Methods (QBMM) are introduced to attain closure of higher-order moments (spatial fluxes) and $F_{i,j,k}$

EE-AG Methods : Anisotropic Particle Velocity Distribution

Distribution function:

$$g(\mathbf{u}-\underline{\mu},\underline{\underline{\Sigma}}) = \frac{1}{(2\pi)^{3/2}\sqrt{|\underline{\underline{\Sigma}}|}}\exp\left[-\frac{(\mathbf{u}-\underline{\mu})^T(\mathbf{u}-\underline{\mu})}{2\underline{\underline{\Sigma}}}\right]$$

where $\underline{\mu}$ is the mean, $\underline{\underline{\Sigma}}$ is the velocity covariance tensor.

Ten velocity moments:

$$M_0,\quad \underline{M_1} = \begin{bmatrix} M_{1,0,0} \\ M_{0,1,0} \\ M_{0,0,1} \end{bmatrix},\quad \underline{\underline{M_2}} = \begin{bmatrix} M_{2,0,0} & M_{1,1,0} & M_{1,0,1} \\ M_{1,1,0} & M_{0,2,0} & M_{0,1,1} \\ M_{1,0,1} & M_{0,1,1} & M_{0,0,2} \end{bmatrix}$$

Moment inversion:

$$\varepsilon_{\mathrm{p}} = M_0,\quad \underline{\mu} = \frac{\underline{\underline{M_1}}}{M_0},\quad \underline{\underline{\Sigma}} = \frac{\underline{\underline{\underline{M_2}}}}{M_0} - \underline{\mu}\otimes\underline{\mu},\quad \Theta = \frac{1}{3}tr(\underline{\underline{\Sigma}})$$

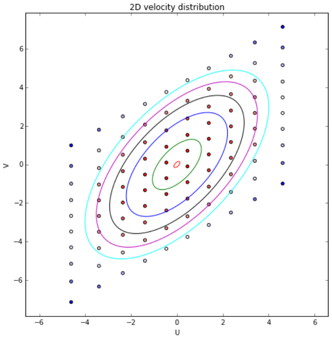
EE-AG Methods : 3-D Gauss-Hermite Quadrature

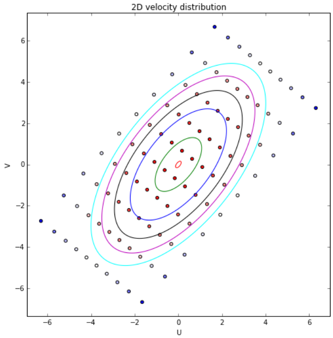
$$g(\underline{u}-\underline{\mu},\underline{\underline{\Sigma}}) = \sum_{i=1}^{N_{hq}}\sum_{j=1}^{N_{hq}}\sum_{k=1}^{N_{hq}} \tilde{\rho}_i\tilde{\rho}_j\tilde{\rho}_k \delta(\underline{u}, \underline{\underline{A}} \cdot \begin{bmatrix} \tilde{u}_i \\ \tilde{u}_j \\ \tilde{u}_k \end{bmatrix} + \underline{\mu}) = \sum_{\alpha=1}^{N_{hq}^3} \tilde{\rho}_\alpha \delta(\underline{u}, \underline{\tilde{u}}_\alpha)$$

A 2-D example : $\underline{\mu} = [0;0]$, $\Theta = 1.0$, $\underline{\underline{\Sigma}} = [0.9, 0.6; 0.6, 1.1]$

Cholesky : $\underline{\underline{A}} \cdot \underline{\underline{A}}^T = \underline{\underline{\Sigma}}$

Spectral : $\underline{\underline{S}} \cdot \underline{\underline{\Lambda}} \cdot \underline{\underline{S}}^T = \underline{\underline{\Sigma}}$, $\underline{\underline{A}} = \underline{\underline{S}} \cdot \sqrt{\underline{\underline{\Lambda}}}$,





EE-AG Methods: Kinetics-Based Moment Fluxes

Spatial moment fluxes are decomposed into two contributions corresponding to positive and negative velocity in each spatial direction:

$$F^x_{i,j,k} = Q^{x,+}_{i,j,k} + Q^{x,-}_{i,j,k}$$

$$Q^{x,+}_{i,j,k} = \int_0^\infty u^{i+1} v^j w^k f\left(\underline{u}\right) d\underline{u} = \sum_{\alpha=1}^{N_{hq}^3} \mathbf{max}(\tilde{u}_\alpha, 0) \tilde{\rho}_\alpha \tilde{u}^i_\alpha \tilde{v}^j_\alpha \tilde{w}^k_\alpha$$

$$Q^{x,-}_{i,j,k} = \int_{-\infty}^0 u^{i+1} v^j w^k f\left(\underline{u}\right) d\underline{u} = \sum_{\alpha=1}^{N_{hq}^3} \mathbf{min}(\tilde{u}_\alpha, 0) \tilde{\rho}_\alpha \tilde{u}^i_\alpha \tilde{v}^j_\alpha \tilde{w}^k_\alpha$$

Realizablity condition: $$\Delta t = CFL \min_\alpha \left(\frac{\Delta x}{|\tilde{u}_\alpha|}, \frac{\Delta y}{|\tilde{v}_\alpha|}, \frac{\Delta z}{|\tilde{w}_\alpha|} \right)$$

EE-AG Methods: Drag and Gravity

Contributions to evolution of moments due to drag force acting on each particle are directly computed, operating on Hermite quadrature velocities $\underline{\tilde{u}}$ by solving an ODE:

$$\frac{d\underline{\tilde{u}}_{\mathrm{p}}}{dt} = \underline{A}_d + \underline{g} = K_D \left(\underline{u}_g - \underline{\tilde{u}}_{\mathrm{p}}\right) + \underline{g}$$

$$\underline{\tilde{u}}'_{\mathrm{p}} = \underline{\tilde{u}}_{\mathrm{p}} e^{-K_D \Delta t} + \left(1 - e^{-K_D \Delta t}\right) \left(\underline{u}_g + \frac{\underline{g}}{K_D}\right) = \underline{\tilde{u}}_{\mathrm{p}} e^{-K_D \Delta t} + \underline{u}_t$$

If a constant Stokes drag model is used, which K_D is independent of $\underline{u}_{\mathrm{p}}$, then,

$$\underline{\mu}' = \underline{\mu}_{\mathrm{p}} e^{-K_D \Delta t} + \underline{u}_t$$

$$\underline{\underline{\Sigma}}' = \underline{\underline{\Sigma}} e^{-2K_D \Delta t} + 2e^{-K_D \Delta t} \underline{\mu}_{\mathrm{p}} \otimes \underline{u}_t + \underline{u}_t \otimes \underline{u}_t$$

And momentum exchange to gas phase can be calculated as following,

$$\underline{F}_{D,pg} = \frac{\rho_p \pi d_{\mathrm{p}}^3}{6} \varepsilon_{\mathrm{p}} \underline{\mu}_{\mathrm{p}}$$

EE-AG Methods: Particle Collisions

Collision source term: BGK model

$$\mathbb{C} = \frac{1}{\tau_\mathrm{p}} \left(f^* - f \right)$$

$$\underline{\underline{\Sigma}}' = \frac{12 g_0 \varepsilon_\mathrm{p} \sqrt{\Theta}}{\sqrt{\pi} d_\mathrm{p}} \left(\underline{\underline{\Lambda}} - \underline{\underline{\Sigma}} \right),$$

$$\underline{\underline{\Lambda}} = \omega^2 \Theta_\mathrm{p} \underline{\underline{I}} + (\omega^2 - 2\omega + 1) \underline{\underline{\Sigma}}, \qquad \omega = \frac{1+e}{2}$$

Collisional flux term: collisional pressure tensor

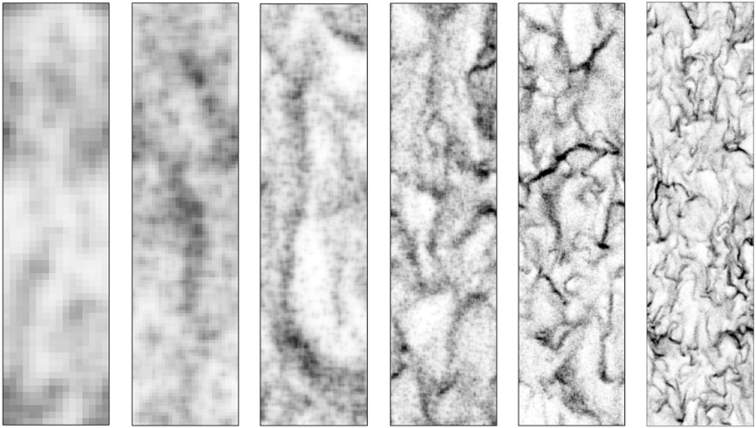
$$\underline{\underline{P}}_{coll} = \frac{4}{5} \omega \varepsilon_\mathrm{p}^2 g_0 \left(3 \Theta_\mathrm{p} \underline{\underline{I}} + 2 \underline{\underline{\Sigma}} \right)$$

$$\frac{d\underline{M}_1}{dt} = \nabla \cdot \underline{\underline{P}}_{coll}$$

Homogeneous Gravity-Driven Flow: A Domain Size Study

Influence of domain size on CIT statistics

In gravity-driven gas solids flows, slip velocity between clusters and gas drive turbulence, referred to as cluster-induced turbulence (CIT)

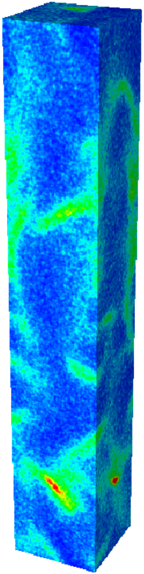


(a) Case 1 (b) Case 2 (c) Case 3 (d) Case 4 (e) Case 5 (f) Case 6

Euler-Lagrange Mesoscale DNS

NGA[2]

- Eulerian fluid solver
  - Arbitrarily high-order DNS/LES code
  - Conservation of mass, momentum, kinetic energy
  - Lagrangian dynamic LES model of Elie et al.(2005)
  - Effective viscosity of Gibilaro et al.(2007) : $\nu_{\mathrm{g}}^{*} = \nu_{\mathrm{g}} \left[\left(1 - \varepsilon_{\mathrm{p}}\right)^{-2.8} - 1.0 \right]$
- Lagrangian particle tracking
  - 2^{nd}-order Runge-Kutta for particle ODEs
  - Soft-sphere collision model
  - Linear drag : $\underline{A} = \left(\underline{u}_{\mathrm{g}} - \underline{u}_{\mathrm{p}}\right) / \tau_D$
- Interphase exchange
  - Filter based on the convolution of mollification and diffusion
  - Fully conservative, implicit treatment



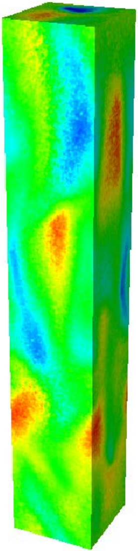
Simulation Configuration

- 3D triply-periodic domain
- Gas mass flow rate forced : $\langle \varepsilon_g u_g \rangle = 0$
- Constant Stokes drag model : $\tau_D = \rho_p d_p^2/(18\mu_g)$

$$\mathrm{Re} = \frac{\rho_g \tau_D g d_p}{\mu_g} = 0.5, \quad \phi = \frac{\rho_p \varepsilon_p}{\rho_g \varepsilon_g} = 10.1, \quad e = 0.9$$

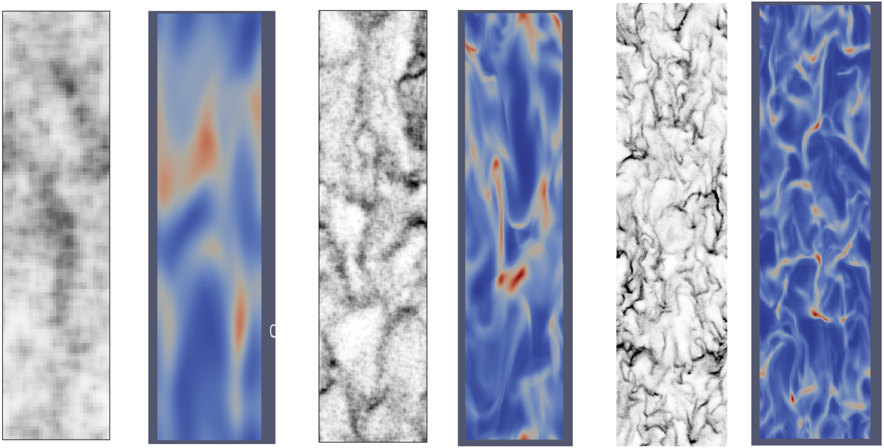
$$\mathcal{V} = \tau_p g = 0.1 m/s, \quad \mathcal{L} = \tau_p^2 g = 2.5 mm$$

Domain size	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
$L_1/\mathcal{L}$	4.03	8.06	16.13	32.26	64.51	129.01
$L_2/\mathcal{L}$	1.01	2.02	4.03	8.06	16.13	32.25
$L_3/\mathcal{L}$	1.01	2.02	4.03	8.06	16.13	32.25
N_1	64	128	256	512	1024	2048
N_2	16	32	64	128	256	512
N_3	16	32	64	128	256	512
N_p	1,678	13,417	107,329	858,629	6,869,032	54,952,240



Instantaneous particle volume fraction field

Case2 Case 4 Case 6

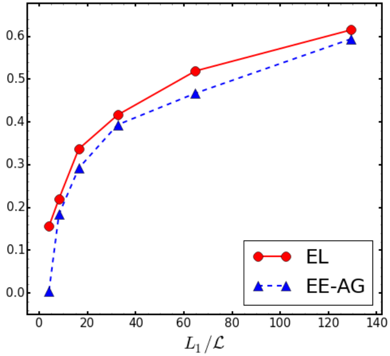


EL EE-AG EL EE-AG EL EE-AG

Comparison between EL and EE-AG simulation results

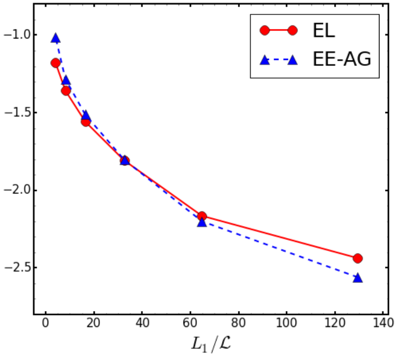
Particle phase-averaged settling velocity,

$$\left\langle u_{p,1} \right\rangle_p / \mathcal{V}, \quad \mathcal{V} = \tau_D g$$



Deviation of volume fraction fluctuations

$$D = \left(\left\langle {\alpha'_p}^2 \right\rangle^{1/2} - \sigma_p \right) / \left\langle \alpha_p \right\rangle$$

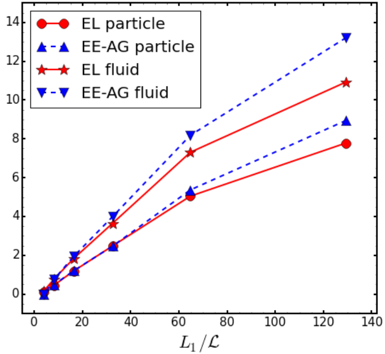


Comparison between EL and EE-AG simulation results

Total fluctuation energy

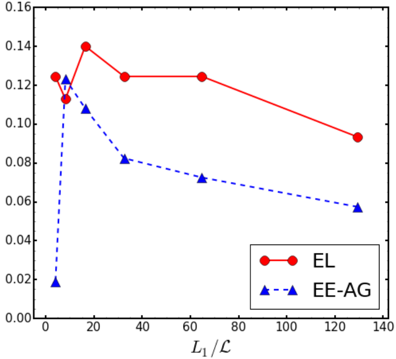
$$\kappa_\mathrm{p}/\mathcal{V}^2, \kappa_\mathrm{p} = \left\langle \underline{u}_\mathrm{p}'' \cdot \underline{u}_\mathrm{p}'' \right\rangle_\mathrm{p} + 3/2\Theta_\mathrm{p}$$

$$k_\mathrm{g}/\mathcal{V}^2, k_\mathrm{g} = \left\langle \underline{u}_\mathrm{g}''' \cdot \underline{u}_\mathrm{g}''' \right\rangle_\mathrm{g}$$



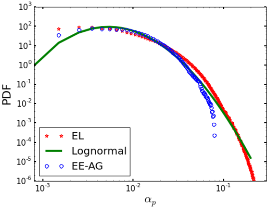
Granular energy contribution to total particle fluctuating energy

$$\frac{3\Theta_\mathrm{p}}{2\kappa_\mathrm{p}}$$

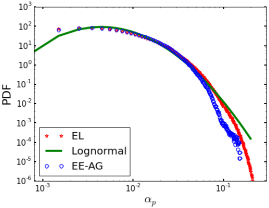


Paricle Volume Fraction Distribution

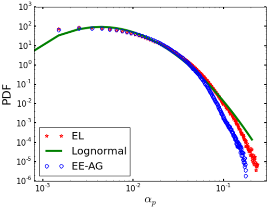
Case 4



Case 5



Case 6



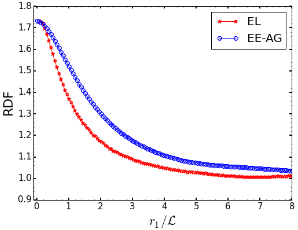
Case 6	$\langle \alpha_p'^2 \rangle / \langle \alpha_p \rangle^2$	$\langle \alpha_p'^3 \rangle / \langle \alpha_p'^2 \rangle^{3/2}$	$\langle \alpha_p'^4 \rangle / \langle \alpha_p'^2 \rangle^2$
EL	0.8373	2.3672	12.1904
EE-AG	0.7438	2.0864	9.9130

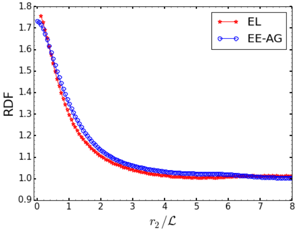
Radial Distribution Function : Case 5, 6

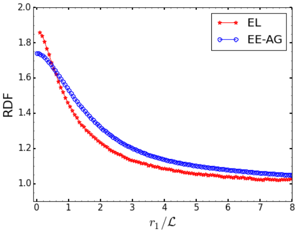
$$g_0(r) = \frac{\langle \alpha_p(x,t)\, \alpha_p(x+r,t)\rangle}{\langle \alpha_p(x,t)\rangle \langle \alpha_p(x+r,t)\rangle}$$

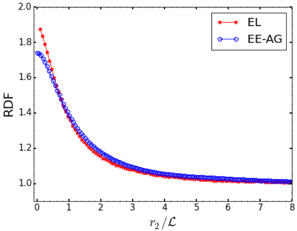
Streamwise direction

Spanwise direction





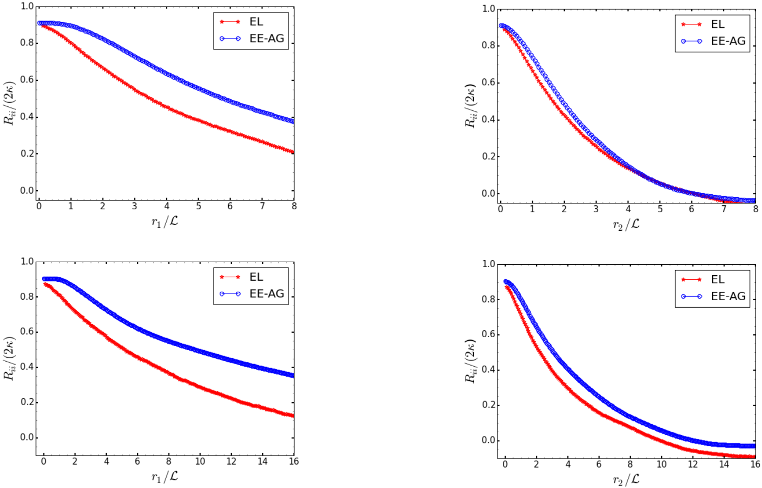




Particle Phase Velocity Cross-correlations : Case 5, 6

$$R^p_{i,j}(r) = \frac{\langle \alpha_p(x,t)\,\alpha_p(x+r,t)\rangle\, u''_{p,i}(x,t)\, u''_{p,j}(x+r,t)}{\langle \alpha_p(x,t)\,\alpha_p(x+r,t)\rangle}$$

Streamwise direction | Spanwise direction

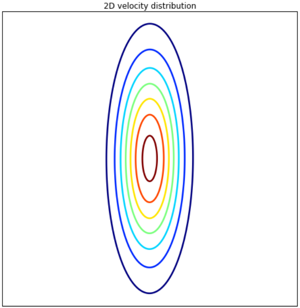


Particle Velocity Anisotropy : Case 6

	$\frac{\left\langle u''^2_{p,1} \right\rangle_\mathrm{p}}{(2k_\mathrm{p})}$	$\frac{\left\langle u''^2_{p,2} \right\rangle_\mathrm{p}}{(2k_\mathrm{p})}$	$\frac{\left\langle u''^2_{p,1} \right\rangle_\mathrm{p}}{\left\langle u''^2_{p,2} \right\rangle_\mathrm{p}}$
EL	0.7878	0.1061	7.4251
EE-AG	0.8453	0.07735	10.9282

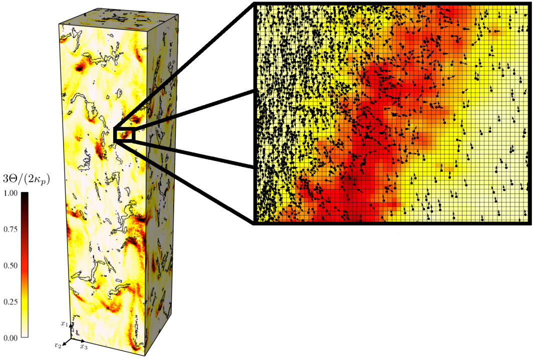
	$\frac{\langle \Sigma_{11} \rangle_\mathrm{p}}{(3\langle \Theta_\mathrm{p} \rangle)}$	$\frac{\langle \Sigma_{22} \rangle_\mathrm{p}}{(3\langle \Theta_\mathrm{p} \rangle)}$	$\frac{\langle \Sigma_{11} \rangle_\mathrm{p}}{\langle \Sigma_{22} \rangle_\mathrm{p}}$
EL	0.5284	0.2358	2.2409
EE-AG	0.6095	0.1952	3.1224

Particle velocity distribution in XY plane

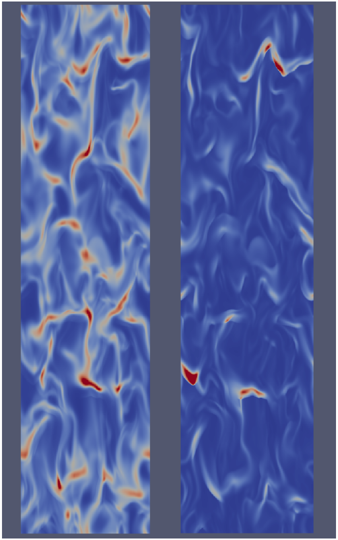


Particle Compressive Heating

EL



EE-AG : α_{p}, Θ_{p}



Summary and Future Work

Conclusions

- Novel approach to model gas-particle flows with quadrature-based moment methods using Anisotropic Gaussian particle velocity assumption
- Comparison between EL and EE-AG methods has demonstrated assumption for particle velocity is valid and this novel method can be used to perform mesoscale DNS for gas-particle flows

Plans for future work

- **Extend QBMM models to dense regime**
- Perform mesoscale DNS of wall-bounded channel flow to study gas-particle turbulence, such as effect of size distribution on cluster size
- Detailed validation of EQMOM based polydisperse solver with EL simulation data for polydisperse gas-particle flows, to study particle size effect on clustering
- Implement a new multiphase turbulence model, and validate against EL simulations

Acknowledgment

Financial support from DOE - National Energy Technology Laboratory (Contract Number: DE-AC02-07CH11358)

Tasks completed in FY15

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- Developed comprehensive post-processing capabilities using Python and VTK
- Prepared documentation and tutorials for code
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