Creating Materials and Energy Solutions

Kinetic Theory Modeling of Turbulent Multiphase Flow

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A Solution Algorithm for Fluid-Particle Flows Across All Flow Regimes

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Outline

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Introduction

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1. Fluid-particle flow are common in many energy applications, such as fluidized bed and risers.
2. Two-Fluid model is the most widely used in simulating this type of flows. However, the hydrodynamic description is inaccurate when particles are dilute.
3. Quadrature-based moment methods (QBMM) can be used to find approximate numerical solutions to the particle kinetic equation, thus model particle motions more accurately. But its explicit nature makes it inefficient when particles are close-packed.
4. Our objective is to develop a solution algorithm that combines the best features of the hydrodynamic and QBMM solvers, which can accurately simulate fluid-particle flows across all flow regimes.

Fluid-Particle Flow Governing Equations

Fluid Continuity:

$$\frac{\partial \rho_g \alpha_g}{\partial t} + \nabla \cdot \rho_g \alpha_g \boldsymbol{U}_g = 0$$

Fluid Momentum:

$$\frac{\partial \rho_g \alpha_g \boldsymbol{U}_g}{\partial t} + \nabla \cdot \rho_g \alpha_g \boldsymbol{U}_g \otimes \boldsymbol{U}_g = \nabla \cdot \rho_g \alpha_g \boldsymbol{\sigma}_g - \nabla p_g + \rho_g \alpha_g \boldsymbol{g} - \rho_p \alpha_p \boldsymbol{M}_{pg}$$

$$\boldsymbol{M}_{pg} = \frac{1}{\tau_p}(\boldsymbol{U}_g - \boldsymbol{U}_p) - \frac{1}{\rho_p}\nabla p_g + \frac{\rho_g}{\rho_p}\nabla \cdot \alpha_g \boldsymbol{\sigma}_g$$

Particle Kinetic:

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

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

Fluid-Particle Flow Governing Equations

Particle Moments Transport:

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot \mathbf{F} - \mathbf{S} \qquad \mathbf{M}^{\gamma}_{ijk} = \int v_1^i v_2^j v_3^j f(\boldsymbol{v})\, d\boldsymbol{v}$$

$$\alpha_p = M^0_{000}, \quad \alpha_p \boldsymbol{U}_p = \begin{bmatrix} M^1_{100} \\ M^1_{010} \\ M^1_{001} \end{bmatrix}, \quad \alpha_p \boldsymbol{U}_p \otimes \boldsymbol{U}_p + \alpha_p \mathbf{P}_p = \begin{bmatrix} M^2_{200} & M^2_{110} & M^2_{101} \\ M^2_{110} & M^2_{020} & M^2_{011} \\ M^2_{101} & M^2_{011} & M^2_{002} \end{bmatrix}.$$

Particle Continuity:

$$\frac{\partial \rho_p \alpha_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \boldsymbol{U}_p = 0$$

Particle Momentum:

$$\frac{\partial \rho_p \alpha_p \boldsymbol{U}_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \left(\boldsymbol{U}_p \otimes \boldsymbol{U}_p + \mathbf{P}_p + \mathbf{G}_p + \mathbf{Z}_p \right) = \rho_p \alpha_p \boldsymbol{g} + \rho_p \alpha_p \boldsymbol{M}_{pg}$$

Particle Particle-Pressure Tensor:

$$\frac{\partial \rho_p \alpha_p \mathbf{P}_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \left(\boldsymbol{U}_p \otimes \mathbf{P}_p + \mathbf{Q}_p + \mathbf{H}_p \right) + \rho_p \alpha_p \left[(\mathbf{P}_p + \mathbf{G}_p) \cdot \nabla \boldsymbol{U}_p + (\nabla \boldsymbol{U}_p)^T \cdot (\mathbf{P}_p + \mathbf{G}_p) \right] = \rho_p \alpha_p \mathbf{E}_{pg} + \rho_p \alpha_p \mathbf{C}_p$$

Particle Kinetic, Collisional and Frictional Flux

Kinetic Flux: $\boldsymbol{U}_p \otimes \boldsymbol{U}_p + \mathbf{P}_p \qquad \mathbf{P}_p = \Theta_p \mathbf{I} - \boldsymbol{\sigma}_p$

$$\boldsymbol{\sigma}_p = 2\nu_{p,k}\boldsymbol{S}_p \qquad \boldsymbol{S}_p = \frac{1}{2}\left[\nabla \boldsymbol{U}_p + (\nabla \boldsymbol{U}_p)^T - \frac{2}{3}(\nabla \cdot \boldsymbol{U}_p)\,\mathbf{I}\right]$$

Collisional Flux: $\mathbf{G}_p = [2(1+e)\alpha_p g_0 \Theta_p - \nu_{p,b} \nabla \cdot \boldsymbol{U}_p]\mathbf{I} - 2\nu_{p,c}\boldsymbol{S}_p$

Frictional Flux: $\mathbf{Z}_p = \frac{Fr}{\rho_p \alpha_p} \frac{(\alpha_p - \alpha_{p,fr,min})^r}{(\alpha_{p,max} - \alpha_p)^s} \left(\mathbf{I} - \frac{2\sin\phi}{\|\boldsymbol{S}_p\|}\boldsymbol{S}_p\right)$

Granular Pressure: $p_p = p_{p,k} + p_{p,c} + p_{p,f}$

Particle Viscosity: $\nu_p = \nu_{p,k} + \nu_{p,c} + \nu_{p,f}$

Kinetic and Collisional Heat Flux: $\mathbf{Q}_p + \mathbf{H}_p = -\frac{2}{3} k_\Theta \nabla \otimes \mathbf{P}_p$

Operator-splitting scheme for all flow regimes

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot h_1 \mathbf{F} + \nabla \cdot (h_2 \mathbf{F} + \mathbf{G} + \mathbf{Z}) = \mathbf{S}$$

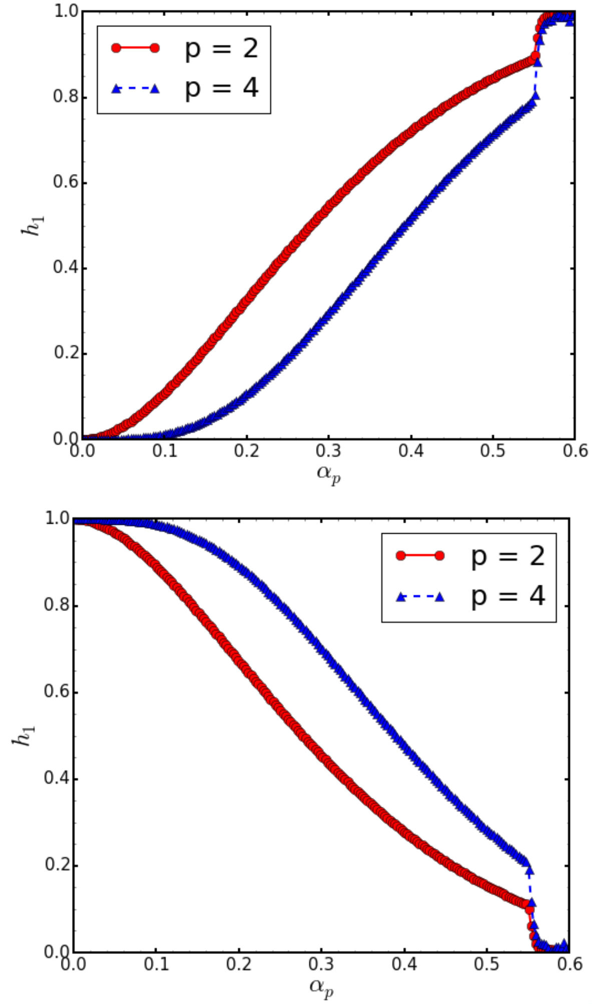
$$h_1 = 1 - h_2$$

$$h_2 = \left(\frac{p^*_{p,c} + p_{p,f}}{p_{p,k} + p^*_{p,c} + p_{p,f} + \varepsilon} \right)^p$$

$$p^*_{p,c} = 2(1+e)\rho_p \alpha_p^2 g_0 \Theta_p$$

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot h_1 \mathbf{F} = \mathbf{0}$$

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot (h_2 \mathbf{F} + \mathbf{G} + \mathbf{Z}) = \mathbf{S}$$



h2

h1

Hydrodynamic solver: $$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot (h_2 \mathbf{F} + \mathbf{G} + \mathbf{Z}) = \mathbf{S}$$

Particle Volume Fraction:

$$\frac{\partial \alpha_p}{\partial t} + \nabla \cdot h_2 \alpha_p \boldsymbol{U}_p = 0$$

Particle Velocity :

$$\frac{\partial \alpha_p \boldsymbol{U}_p}{\partial t} - \nabla \cdot \left(h_2 \alpha_p \boldsymbol{U}_p \otimes \boldsymbol{U}_p - \frac{p_p^*}{\rho_p} \boldsymbol{I} - 2\alpha_p \nu_p^* \boldsymbol{S}_p \right) = \alpha_p \boldsymbol{g} - \frac{\alpha_p}{\tau_p} (\boldsymbol{U}_g - \boldsymbol{U}_p) - \frac{\alpha_p}{\rho_p} \nabla p_g - \alpha_p \rho_g \nabla \cdot \alpha_g \boldsymbol{\sigma}_g.$$

$$p_p^* = h_2 p_{p,k} + p_{p,c} + p_{p,f} \qquad \nu_p^* = h_2 \nu_{p,k} + \nu_{p,c} + \nu_{p,f}$$

Particle Granular Temperature :

$$\frac{3}{2} \left(\frac{\partial \alpha_p \Theta_p}{\partial t} - \nabla \cdot h_2 \alpha_p \Theta_p \boldsymbol{U}_p \right) = \nabla \cdot (\alpha_p k_\Theta^\dagger \nabla \Theta_p) - \left(\frac{p_p^\dagger}{\rho_p} \mathbf{I} - 2\alpha_p \nu_p^\dagger \mathbf{S}_p \right) : \nabla \boldsymbol{U}_p - 3 \left(\frac{1 - e^2}{2\tau_c} - \frac{1}{\tau_p} \right) \alpha_p \Theta_p$$

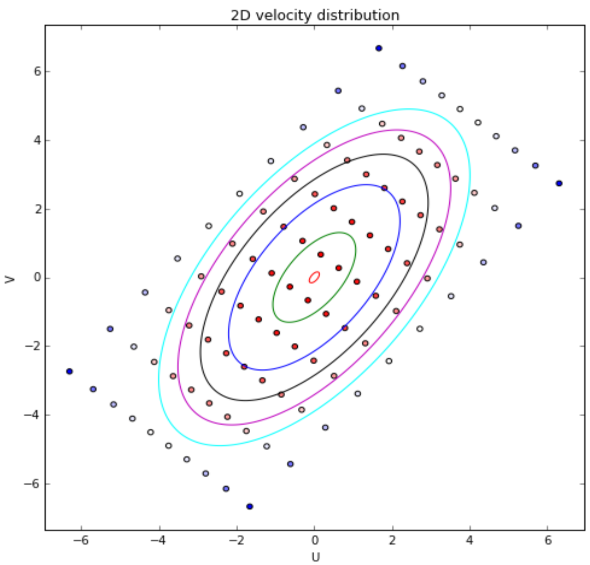
$$p_p^\dagger = h_2 p_{p,k} + p_{p,c} \qquad \nu_p^\dagger = h_2 \nu_{p,k} + \nu_{p,c} \qquad k_\Theta^\dagger = h_2 k_{\Theta,k} + k_{\Theta,c}$$

Free transport solver: $\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot h_1 \mathbf{F} = \mathbf{0}$

Anisotropic Gaussian Velocity Distribution:

$$f(\boldsymbol{v}) = \frac{\alpha_p}{(2\pi|\mathbf{P}_p|)^{3/2}} \exp\left[-\frac{1}{2}(\boldsymbol{v} - \boldsymbol{U}_p) \cdot \mathbf{P}_p^{-1} \cdot (\boldsymbol{v} - \boldsymbol{U}_p)\right]$$

3D Gauss-Hermite Quadrature



Granular Stress Tensor Transport

$$\frac{\partial \rho_p \alpha_p \boldsymbol{\sigma}_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \left(h_2 \boldsymbol{U}_p \otimes \boldsymbol{\sigma}_p - \frac{2}{3} k_\Theta^* \nabla \otimes \boldsymbol{\sigma}_p \right) = \rho_p \alpha_p \left(\boldsymbol{S}_{2,flux} - \boldsymbol{S}_2 \right)$$

$$\boldsymbol{S}_{2,flux} = \frac{2p_p^\dagger}{\rho_p \alpha_p} \boldsymbol{S}_p - 2\nu_p^\dagger \left[\boldsymbol{S}_p \cdot \nabla \boldsymbol{U}_p + (\nabla \boldsymbol{U}_p)^T \cdot \boldsymbol{S}_p - \frac{2}{3}(\boldsymbol{S}_p : \nabla \boldsymbol{U}_p)\mathbf{I} \right]$$

$$\boldsymbol{S}_2 = \left[\frac{2}{\tau_p} + \frac{(3-e)(1+e)}{2\tau_c} \right] \boldsymbol{\sigma}_p$$

Wall boundary conditions

Hydrodynamic solver:

$$\nu_p^* \frac{\partial \boldsymbol{U}_{p,t}}{\partial x_w} = -h_{2,w} \phi_s \mathcal{V}_w \boldsymbol{U}_{p,t} - \frac{p_{p,f} \tan \phi_w}{\rho_p \alpha_p} \frac{\boldsymbol{U}_{p,t}}{|\boldsymbol{U}_{p,t}|} \qquad \mathcal{V}_w = (\pi/6)\sqrt{3\Theta_p}$$

$$k_\Theta^\dagger \frac{\partial \Theta_p}{\partial \boldsymbol{x}_w} = h_{2,w} \left[\phi_s \mathcal{V}_w |\boldsymbol{U}_{p,t}|^2 - \frac{3}{2}\left(1 - e_w^2\right) \mathcal{V}_w \Theta_p \right]$$

Free transport solver:

$$\mathbf{F}_w = h_{1,w}(\alpha_p) \int_{\boldsymbol{v}\cdot\boldsymbol{n}_w > 0} \mathbf{G}_r(\boldsymbol{v}) \left(\boldsymbol{v} \cdot \boldsymbol{n}_w\right) d\mathcal{S}_w$$

$$f_r(\boldsymbol{v}) = \phi_s f_{r,d}(\boldsymbol{v}) + (1 - \phi_s) f_{r,s}(\boldsymbol{v})$$

$$f_{r,s}(\boldsymbol{v}) = f_i \left(\boldsymbol{v} - (1 + e_w)(\boldsymbol{v} \cdot \boldsymbol{n}_w)\boldsymbol{n}_w\right)$$

Example kinetic theory coefficients in hydrodynamic model for particle phase

$$\tau_p = \frac{4\rho_p d_p^2}{3\rho_g \nu_g C_D Re_p}$$

$$Re_p = \frac{\alpha_g d_p |\boldsymbol{U}_g - \boldsymbol{U}_p|}{\nu_g}$$

$$C_D = \max\left[\frac{24}{Re_p}\left(1 + Re_p^{0.687}\right), 0.44\right]\alpha_g^{-2.65}$$

$$\eta = \frac{1}{2}(1+e)$$

$$g_0 = \frac{1 - \frac{1}{2}\alpha_p}{(1-\alpha_p)^3}$$

$$\tau_c = \frac{d_p}{6\alpha_p g_0 \sqrt{\Theta_p/\pi}}$$

$$\Delta^* = \eta^2 \Theta_p \mathbf{I} + (1-\eta)^2 \mathbf{P}_p$$

$$\nu_{p,b} = \frac{8\eta\alpha_p g_0 d_p \sqrt{\Theta_p}}{3\sqrt{\pi}}$$

$$p_{p,k} = \rho_p \alpha_p \Theta_p$$

$$p_{p,c} = 4\rho_p \eta \alpha_p^2 g_0 \Theta_p - \rho_p \alpha_p \nu_{p,b} \nabla \cdot \boldsymbol{U}_p$$

$$p_{p,f} = Fr \frac{\left(\alpha_p - \alpha_{p,fr,min}\right)^r}{\left(\alpha_{p,max} - \alpha_p\right)^s}$$

$$\nu_{p,k} = \frac{1}{2}\Theta_p \left[\frac{1}{\tau_p} + \frac{\eta(2-\eta)}{\tau_c}\right]^{-1} \left[1 + \frac{8}{5}\eta(3\eta - 2)\alpha_p g_0\right]$$

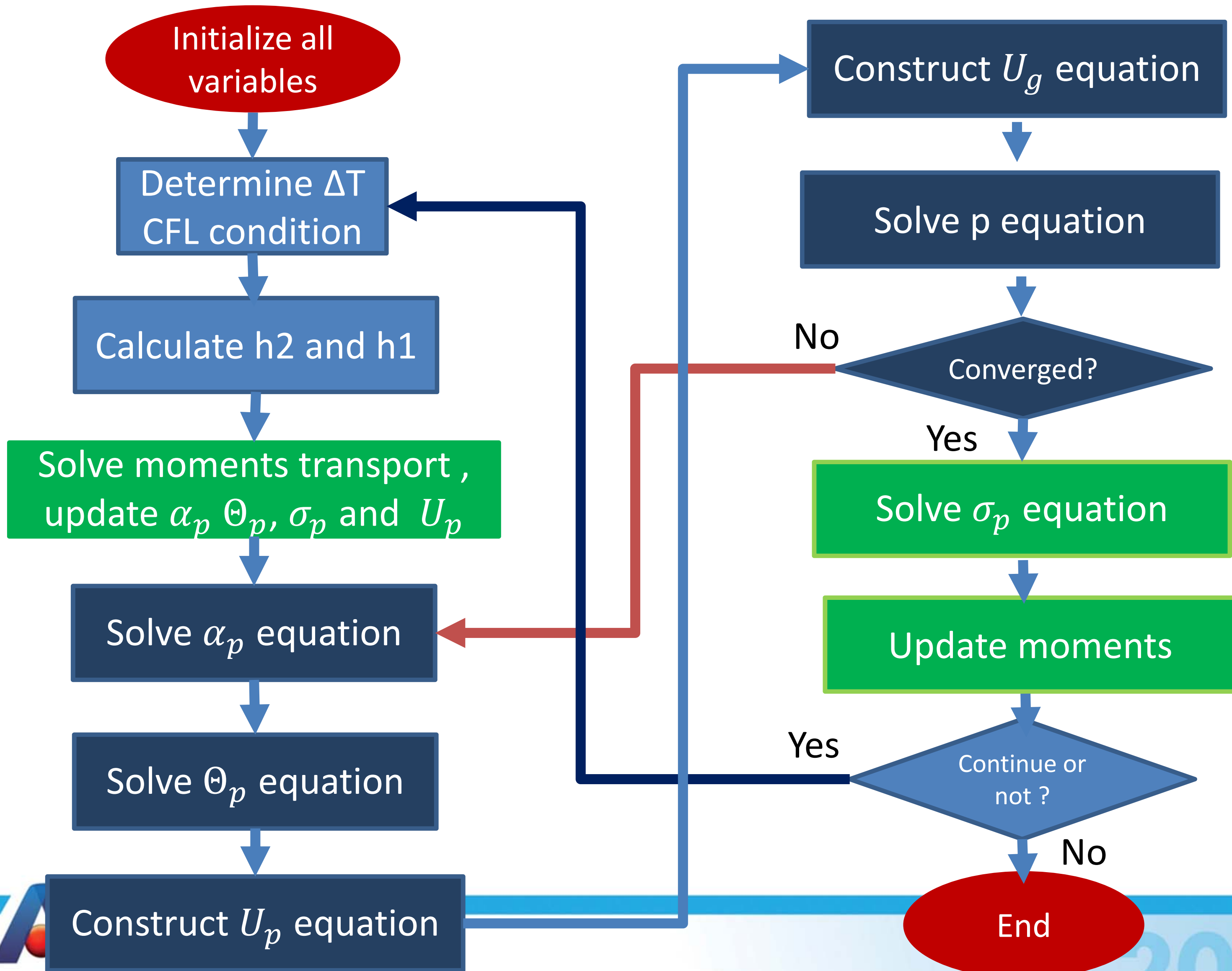
$$\nu_{p,c} = \frac{8\eta\alpha_p g_0}{5}\nu_{p,k} + \frac{3}{5}\nu_{p,b}$$

$$\nu_{p,f} = \frac{p_{p,f}}{\rho_p \alpha_p \|\boldsymbol{S}_p\|}\sin\phi$$

$$k_{\Theta,k} = \frac{5}{2}\Theta_p \left[\frac{3}{\tau_p} + \frac{4\eta(41-33\eta)}{\tau_c}\right]^{-1} \left[1 + \frac{12}{5}\eta^2(4\eta - 3)\alpha_p g_0\right]$$

$$k_{\Theta,c} = \frac{12\eta\alpha_p g_0}{5} k_{\Theta,k} + \frac{3}{2}\nu_{p,b}$$

Solution algorithm

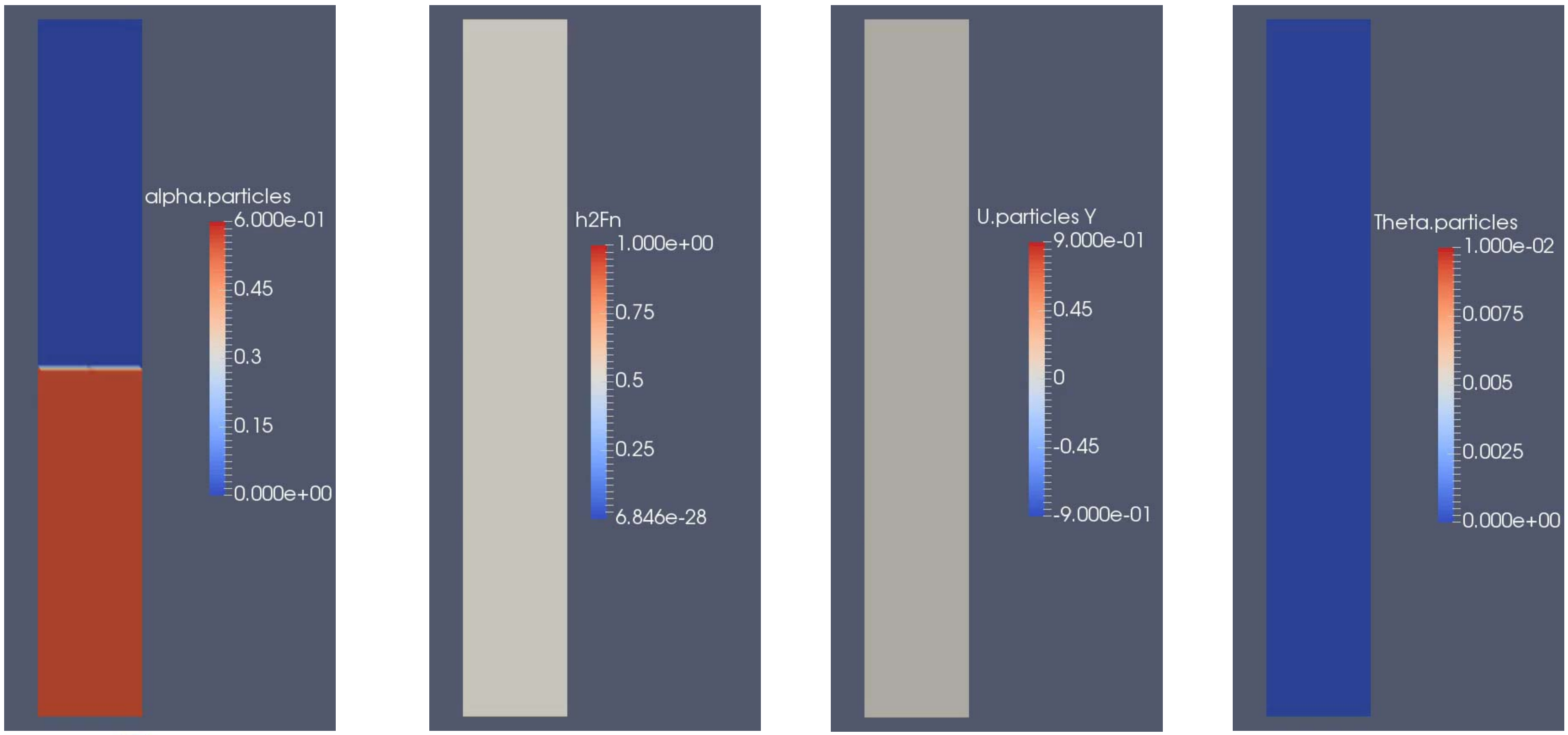


Example results, test case 1: fluidized bed

$D_p = 300\mu m$ $\rho_p = 2500Kg/m^3$ $\rho_g = 1.2Kg/m^3$ $\nu_g = 1.8 \times 10^{-5}m^2/s$

$L_x = 0.15m$ $L_y = 1m$ $N_x = 30$ $N_y = 200$

α_p h_2 $U_{p,y}$ Θ_p

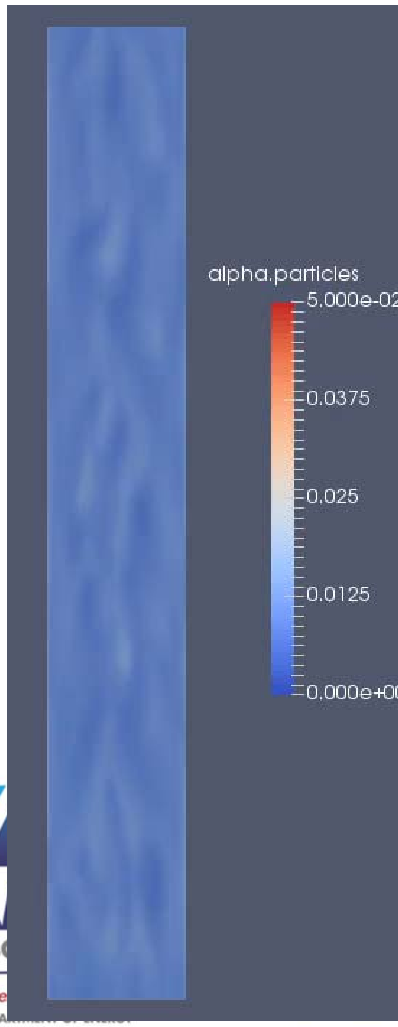


Example results, test case 2 : vertical channel riser

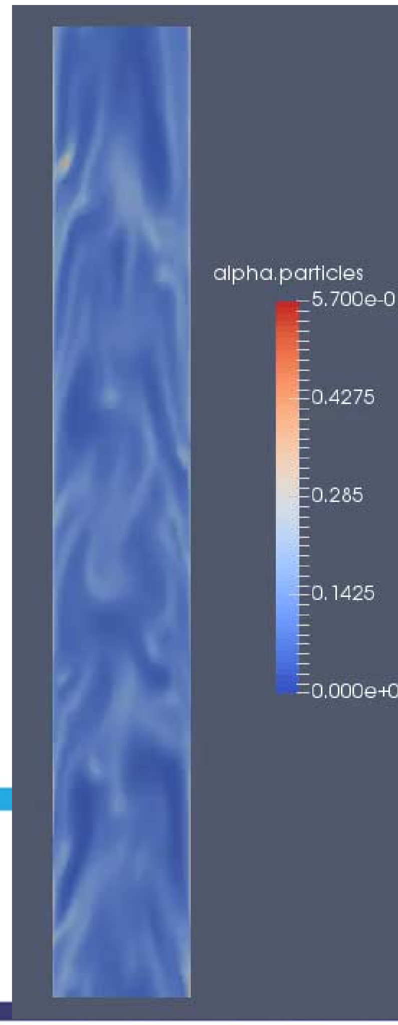
$D_p = 100\mu m$ $\rho_p = 1000Kg/m^3$ $\rho_g = 1Kg/m^3$ $\nu_g = 1.8 \times 10^{-5} m^2/s$

$L_x = 0.05m$ $L_y = 0.35m$ $N_x = 56$ $N_y = 280$

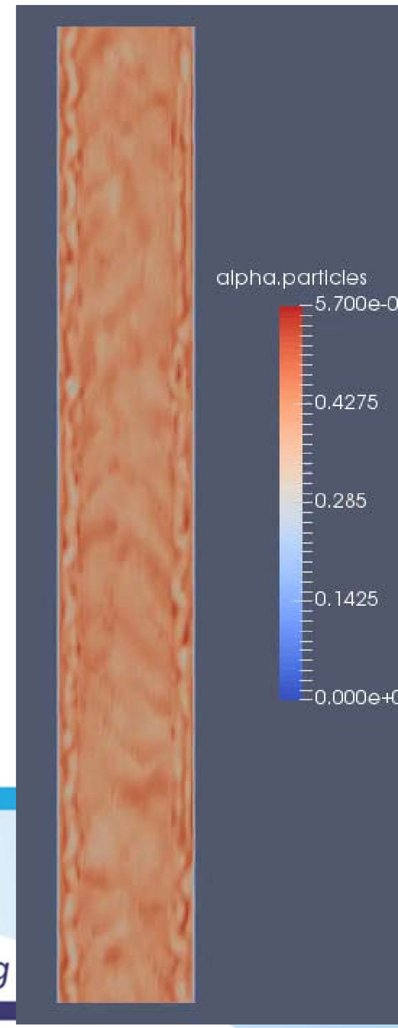
$< \alpha_p >= 0.01$



$< \alpha_p >= 0.1$



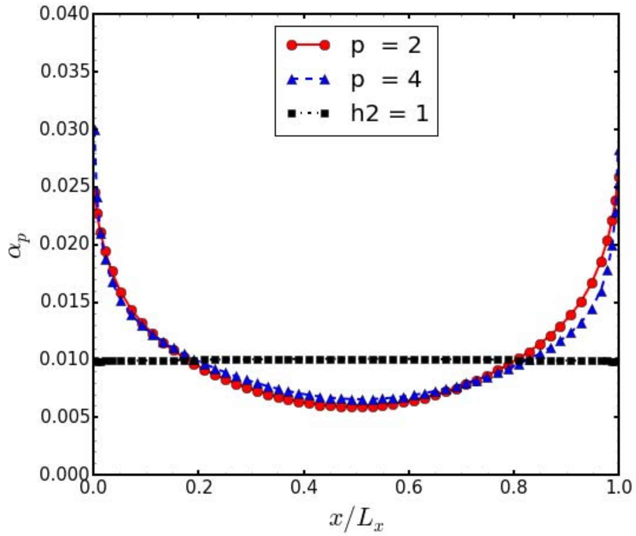
$< \alpha_p >= 0.4$



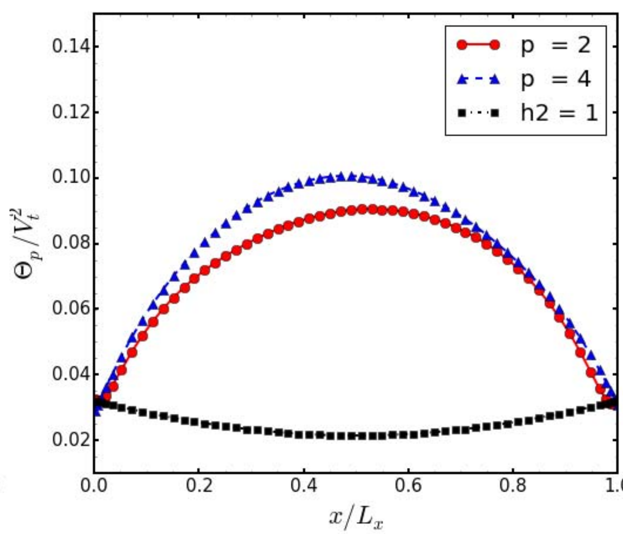
Example results, test case 2 : vertical channel riser

$$< \alpha_p >= 0.01$$

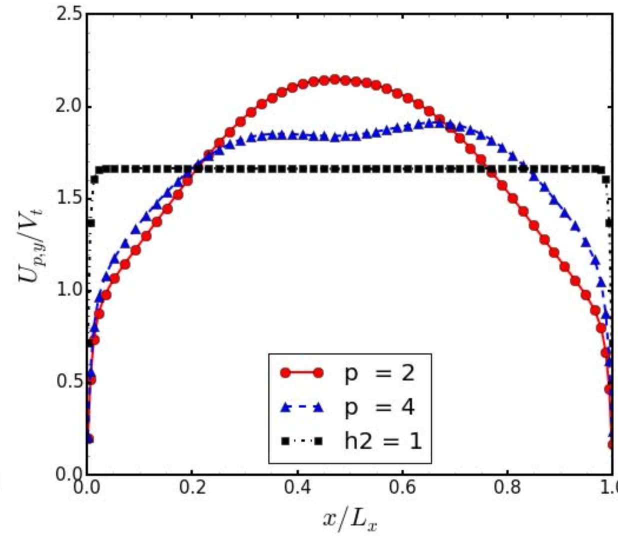
α_p



Θ_p



U_p



Conclusions

1. A solution algorithm is proposed to accurately treat all fluid-particle regimes occurring simultaneously.
2. This algorithm is based on splitting the free-transport flux solver dynamically and locally in the flow. In close-packed to moderately dense regions, a hydrodynamic solver is employed, while in dilute to very dilute regions a kinetic-based finite-volume solver is used in conjunction with quadrature-based moment methods.
3. To illustrate the accuracy and robustness of the proposed solution algorithm, it is implemented for particle velocity moments up to second order, and applied to simulate gravity-driven, gas-particle flows exhibiting cluster-induced turbulence.
4. By varying the average particle volume fraction in the flow domain, it is demonstrated that the flow solver can handle seamlessly all flow regimes present in fluid-particle flows.

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Questions ?

Semi-discretized equations

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