

A Coupled OpenFOAM–DEM Framework for Solid–Fluid Multiphase Flow Simulation

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1. Introduction

Solid-fluid multiphase flows are encountered in a wide range of natural and industrial systems, including sediment transport, fluidized beds, and particle processing. In the nuclear field, gas-solid fluidized beds play an important role in nuclear fuel fabrication, particularly in fluidized-bed chemical vapor deposition (FB-CVD) process for coating tristructural-isotropic (TRISO) fuel particles. Stable fluidization and well-distributed particle circulation are important because local variations in gas velocity, particle residence time, and collision-driven mixing can contribute to nonuniform coating growth. CFD-DEM coupling provides an Eulerian-Lagrangian framework that resolves the carrier-fluid motion while tracking individual particles and their collisions, making it well suited to analyze these particle-scale effects and to support operating-window selection for FB-CVD systems [1].

This study presents an unresolved, two-way CFD-DEM framework that connects OpenFOAM to the GPU-parallel SOPHIA DEM solver through a version 2 C application binary interface (C ABI v2). A normalized Gaussian stencil is used consistently for fluid-field interpolation, particle-volume mapping, and reaction force deposition. The present work describes the governing models and coupling procedure and assesses the basic physical consistency of the framework using packed-bed pressure drop behavior relevant to FB-CVD analysis.

2. Numerical method

This section presents the governing equations for the CFD and DEM solvers and describes the interaction between the solid particles and the fluid.

2.1. Governing equations for the fluid phase

The fluid phase is solved in an Eulerian framework on the computational mesh. For an incompressible carrier fluid, the governing equations are the locally averaged Navier-Stokes equations:

$$\frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f \mathbf{u}_f) = 0 \quad (1)$$

$$\begin{aligned} \rho_f \frac{\partial (\alpha_f \mathbf{u}_f)}{\partial t} + \rho_f \nabla \cdot (\alpha_f \mathbf{u}_f \mathbf{u}_f) \\ = -\rho_f \alpha_f \nabla p + \mathbf{R}_{f,p} + \mu \nabla \cdot (\alpha_f \nabla \mathbf{u}_f) \end{aligned} \quad (2)$$

where, α_f is the fluid volume fraction (void fraction), $\mathbf{u}_f$ and ρ_f are the velocity and density of the fluid respectively, p denote the pressure of fluid, μ is the dynamic viscosity. $\mathbf{R}_{f,p}$ is the momentum exchange with particles which is described more detail in section 2.4.

2.2. Govern equations of DEM

The translation and rotational motions of each DEM particle are determined according to Newton's second law:

$$m_a \frac{d\mathbf{v}_a}{dt} = \sum_b \mathbf{F}_{ba} + m_a \mathbf{g} + \mathbf{F}_{f,p} \quad (3)$$

$$I_a \frac{d\boldsymbol{\omega}_a}{dt} = \sum_b (\mathbf{r}_{ac} \times \mathbf{F}_{ba}^t) \quad (4)$$

where m_a and I_a denote the mass and rotational inertia of particle a, respectively, and $\mathbf{r}_{ac}$ is the position vector from the center of particle a toward the contact point c. $\mathbf{F}_{f,p}$ is interaction force between particle and fluid.

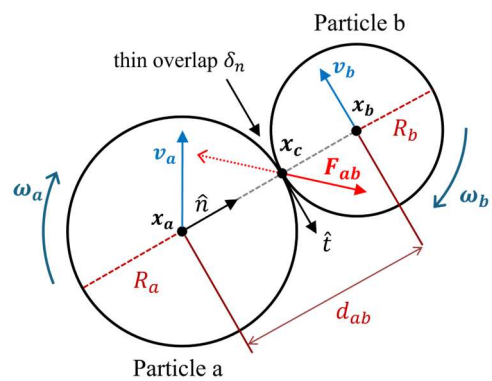


Fig. 1. Scheme of the DEM contact model.

The contact force between two particles is divided into the normal and tangential components, which are further divided into the elastic and damping terms:

$$\begin{aligned} \mathbf{F}_{ab} &= f_{ab}^n \hat{\mathbf{n}} + f_{ab}^t \hat{\mathbf{t}} \\ &= (f_s^n + f_d^n) \hat{\mathbf{n}} + (f_s^t + f_d^t) \hat{\mathbf{t}} \end{aligned} \quad (5)$$

where the unit vector $\hat{n}$ and $\hat{t}$ respectively denote the normal and tangential components between particles a and b. f_{ab}^n and f_{ab}^t represent the magnitude of the normal and tangential components of the contact force, respectively. Subscripts s and d indicate the spring and damper, respectively.

In the Hertz-Mindlin contact model, each term on the RHS of Eq. (5) can be defined as follows:

$$f_s^n = \frac{4}{3} E_{ab}^* \sqrt{R_{ab}^*} \delta_n^{\frac{3}{2}} \quad (6)$$

$$f_d^n = -\sqrt{\frac{10}{3}} \frac{\ln(e)}{\sqrt{\ln(e)^2 + \pi^2}} \sqrt{M_{ab}^* K_n'} v_n \quad (7)$$

$$f_s^t = 8 G_{ab}^* \sqrt{R_{ab}^*} \delta_n \delta_t \quad (8)$$

$$f_d^t = -\sqrt{\frac{10}{3}} \frac{\ln(e)}{\sqrt{\ln(e)^2 + \pi^2}} \sqrt{M_{ab}^* k_t} v_t \quad (9)$$

where e is the restitution coefficient between particles a and b, δ_n and δ_t denote the interparticle overlap in the normal and tangential directions, respectively, and v_n and v_t indicate the relative velocity components in the corresponding directions. M_{ab}^* , R_{ab}^* , E_{ab}^* , and G_{ab}^* represent the equivalent properties for the mass, radius, Young's modulus, and shear modulus, respectively.

2.3. Solid-fluid interaction models

The fluid-to-particle interaction force comprises drag, buoyancy, and pressure gradient contributions:

$$\mathbf{F}_{f,p} = \mathbf{F}_{drag} + \mathbf{F}_{buoyancy} + \mathbf{F}_{pressure} \quad (10)$$

This study uses the Gidaspow drag model [2], which switches between the Wen-Yu correlation [3] and the Ergun correlation [4] according to the fluid volume fraction. The drag forces is written as follows:

$$\mathbf{F}_{drag} = K_p (\mathbf{u}_f - \mathbf{u}_p) \quad (11)$$

$$K_p = \frac{3}{4} C_D Re_p \frac{\mu_f V_p}{d_p^2} \quad (12)$$

where C_D and Re_p are the dimensionless drag coefficient and the particle Reynolds number, respectively. $\mathbf{u}_p$ is the particle velocity, V_p and d_p are the particle volume and diameter, respectively.

The Archimedes buoyancy force and the pressure gradient force are evaluated as follows:

$$\mathbf{F}_{buoyancy} = -\rho_f V_p \mathbf{g} \quad (13)$$

$$\mathbf{F}_{pressure} = -\rho_f V_p \nabla p \quad (14)$$

2.4. Conservative particle-mesh mapping

For a particle p at x_p and a neighboring CFD cell i with centroid x_i and volume V_i , an unnormalized Gaussian weight w_{pi} is first evaluated and then normalized over the stencil S_p . The same normalized weights are used to interpolate a cell-centered fluid quantity q_i to the particle, map the solid volume fraction $\alpha_{s,i}$ and deposit the equal-and-opposite reaction force as the cell source $\mathbf{R}_{f,p,i}$. [5]

$$w_{pi} = \frac{w_{pi}^*}{\sum_{j \in S_p} w_{pj}^*} \quad (15)$$

$$w_{pi}^* = V_i \exp \left[-\frac{|x_i - x_p|^2}{2h^2} \right] \quad (16)$$

$$\mathbf{R}_{f,p,i} = -\frac{1}{V_i} \sum_p w_{pi} \mathbf{F}_{drag,p} \quad (17)$$

Equation (16) defines the single normalized stencil used to interpolate cell-centered fluid quantities to the particle. Equation (17) defines the equal-and-opposite deposition of the selected interphase reaction force. For all packed bed simulations reported here, this reaction consists only of the drag force. The use of the same normalized weights preserves the total deposited drag reaction.

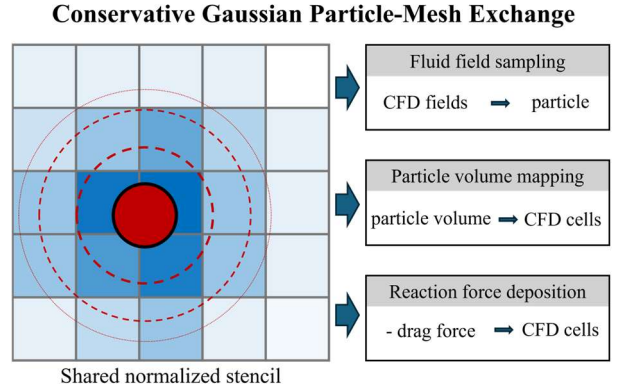


Fig. 2. Shared normalized gaussian stencil for conservative particle-mesh exchange.

3. Code implementation

OpenFOAM is used for the fluid phase, while the in-house SOPHIA solver evaluates particle contacts and time integration in parallel on a GPU. The coupling is implemented through a solver-independent OpenFOAM fvOption and C ABI v2, which exchanges compact particle and force buffers between the CPU-based CFD calculation and the GPU-based DEM calculation. This separation keeps the CFD solver interface independent of the internal DEM implementation and permits DEM subcycling within each CFD time step.

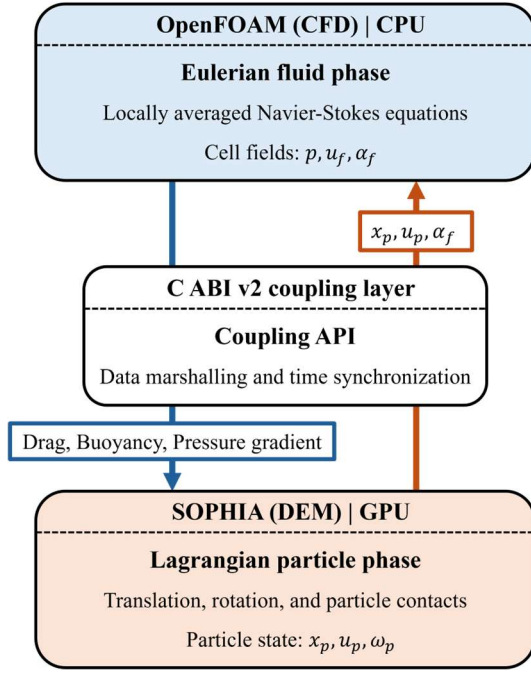


Fig. 3. Coupling architecture of the OpenFOAM-SOPHIA(DEM) framework through the C ABI v2 interface.

At each coupling exchange, SOPHIA supplies particle positions and translational and angular velocities. OpenFOAM locates the particles, constructs the normalized Gaussian stencils, maps the particle volume to obtain α_f , and samples the local fluid fields. The interaction models then evaluate the particle forces. Their equal-and-opposite reactions are deposited on the CFD mesh before the pressure-velocity system is advanced. The updated forces are transferred through C ABI v2, after which SOPHIA performs the required GPU-parallel DEM substeps. The sequence is summarized in Fig. 4.

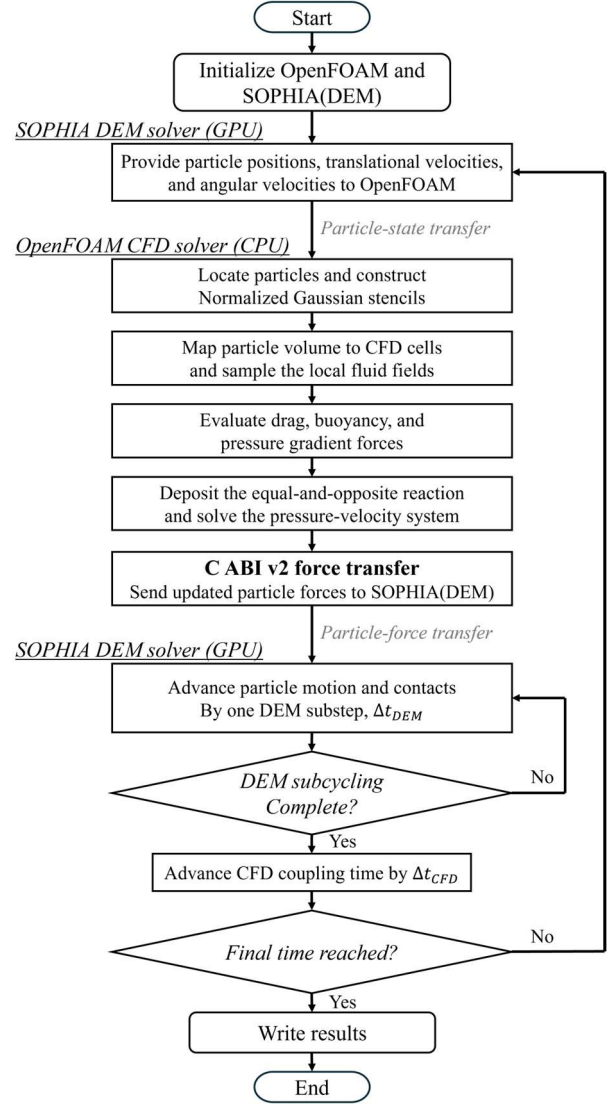


Fig. 4. Computational flowchart of the OpenFOAM-SOPHIA(DEM) CFD-DEM coupling algorithm.

4. Validation

A packed-bed benchmark was first used to assess the momentum exchange implemented in the coupled solver (Fig. 5, Table I).

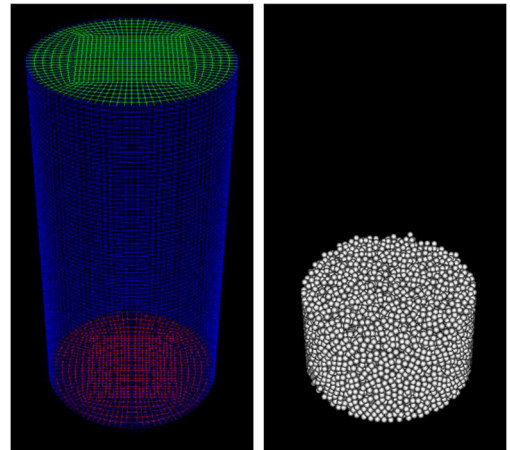


Fig. 5. CFD mesh (left), DEM domain (right).

Table I. Conditions used for the packed-bed to fluidized-bed transition simulations.

Parameter	Value
Pipe geometry	• $R = 0.040$ m • $L = 0.160$ m
CFD mesh	• 92,160 hexahedra • 28,800-cell packed-bed zone
Fluid	• $\rho_f = 1.2$ kg/m ³ • $\mu_f = 1.8\text{e-}5$ Pa · s
Particles	• $N = 10,000$ • $d_p = 0.003$ m • $\rho_p = 600$ kg/m ³
Initial bed	• $H_0 = 0.0497$ m • $\varepsilon_0 = 0.434$
Time steps	• CFD: $5.0\text{e-}5$ s • DEM: $2.5\text{e-}5$ s

As shown in Fig. 6, the simulated pressure drop differed from the Ergun correlation prediction [4] by approximately 3% over the fixed-bed range. This agreement supports the basic physical consistency of the drag force evaluation and equal-and-opposite reaction force deposition in the coupled implementation.

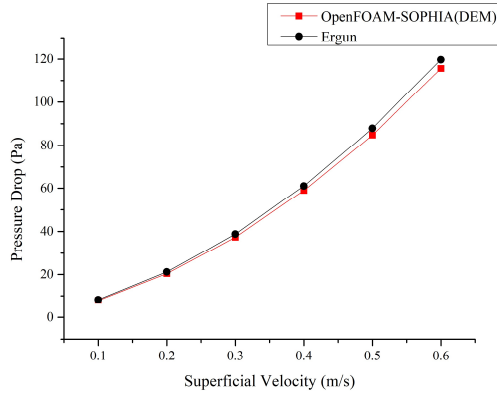


Fig. 6. Comparison of packed-bed pressure drop obtained with the coupled OpenFOAM-SOPHIA(DEM) solver and the Ergun correlation [4].

To examine whether this fixed-bed agreement was retained through incipient fluidization, the velocity range was subsequently extended using the same geometry, material properties, and coupling models.

At incipient fluidization, the Ergun pressure gradient was balanced against the buoyancy-corrected particle weight. Using the independently determined initial geometric void fraction ($\varepsilon_0 = 0.434$) gave $u_{mf,Ergun} = 0.717$ m/s. The CFD-DEM value was estimated from the intersection of a least-squares fit to the non-fluidized points ($u_s = 0.68 - 0.70$ m/s) and the post-onset pressure plateau, giving $u_{mf,sim} = 0.704$ m/s. The relative difference was 1.9%.

Particle motion remained negligible through $u_s = 0.70$ m/s, for which the terminal RMS vertical particle speed was $6.1\text{e-}5$ m/s, but increased to $4.1\text{e-}3$ m/s at $u_s = 0.71$ m/s. The completed post-onset pressure drops at $u_s = 0.71$ m/s, 0.72 m/s, 0.74 m/s, 0.76 m/s, 0.78 m/s, and 0.80 m/s were yielding a plateau of 161.5 ± 0.8 Pa (sample standard deviation). This value was within

2.3% of the buoyancy-corrected bed weight pre cross-sectional area (165.2 Pa), as shown in Fig. 7.

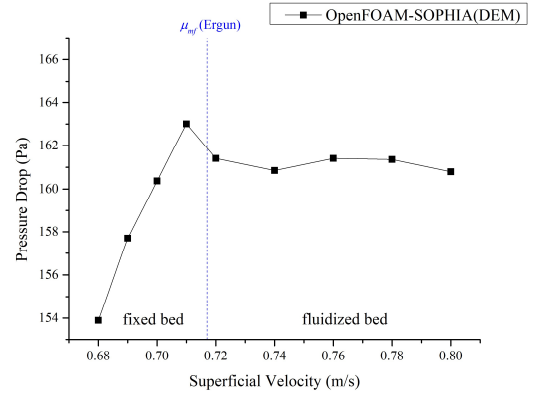


Fig. 7. Pressure drop across the packed-bed to fluidized-bed transition.

The present comparison is not an exhaustive validation: Gaussian kernel width sensitivity, direct comparison with FB-CVD experiments were outside the scope of this study. These items should be addressed before the framework is used for quantitative coating-process prediction.

5. Conclusion

A two-way OpneFOAM-SOPHIA(DEM) framework was developed for unresolved solid-fluid multiphase flow simulation. The C ABI v2 interface and normalized Gaussian exchange operator provide a consistent route for fluid interpolation, particle-volume mapping, and reaction force deposition. The fixed-bed benchmark reproduced the Ergun pressure drop within 3%, while the completed velocity sweep predicted the minimum fluidization velocity within 1.9% of Ergun estimate based on the initial geometric void fraction. Above incipient fluidization, the six post-onset cases produced a pressure plateau of 161.5 ± 0.8 Pa, close to the buoyancy-corrected bed weight, while pressure and void fraction formed statistically stationary late-time plateaus at fixed velocity. These capabilities provide a foundation for analyzing particle circulation and gas-solid interaction in nuclear FB-CVD process. Extension of the framework to an energy-conserving compressible-flow solver, together with coupling of a multicomponent species-transport model, is currently in progress to enable thermochemical FB-CVD simulations. The GPU-parallel SOPHIA backend is intended to reduce the DEM cost associated with contact detection and particle time integration in large-particle simulations; however, wall-clock speedup was not measured here, so CPU-GPU performance and multi-GPU scaling should be quantified in future work. Further mesh, time-step, kernel width, and experiment-based validation is also required before predictive FB-CVD application.

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