Discrete and Chimera Particle Simulation:

Novel Lagrangian Extensions and Applications

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Abstract

Particle based assays are rapidly gaining momentum in clinical diagnosis, food/airborne toxin detection and drug therapy and many other areas. Accurate characterization of interactions between bulk and Partcile-surface necessitates the fundamental understanding of coupled fluid and bead motion (Fluid-Solid Momentum Transfer). We have developed the models that fully integrate Lagrangian transport of the beads, convective-diffusive transport of species and bio-molecular surface binding reactions on the micro and macro particles.

Key Words

Bead, Micro-sphere, Macro-particle

Introduction

Two-phase modeling strategies can be broadly classified as follows [1]:

1. **Two-Fluid (Eulerian fluid – Eulerian solid) -** In this method, the dispersed phase is regarded as a continuum and the mixture is treated as the flow of two immiscible fluids within an Eulerian framework [1]. While the two-fluid approach provides for a robust formulation of particle-fluid interactions, there are substantial difficulties associated with prescribing continuum properties for the particle phase, boundary conditions and numerical diffusion effects. These difficulties essentially restrict the applicability of these models to a maximum loading factor of 20% of particles by volume.
2. **Trajectory (Eulerian fluid – Lagrangian solid) –** In this approach, the particle motion is computed in a Lagrangian framework. Multiple, polydisperse beads, binding heterogeneity, etc., are readily accounted for.

   For the accurate characterization of the interaction between fluid and solid, two development paths are recommended:

   2.1. Discrete Particle Simulation (DPS) blends the strengths of the Eulerian & Lagrangian techniques presented. This uses an enhanced Lagrangian technique with resolved collisions along with a two-fluid formulation for the fluid phase that accounts for volume exclusion by solids [2, 3]. For low bead concentrations, this simplifies to the Trajectory approach. Figure 1 shows the schematic illustrating the Discrete Particle Simulations Method.

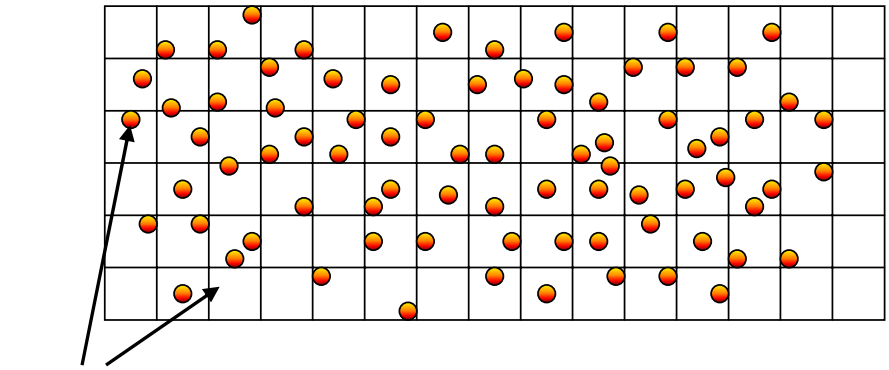

Figure 1: Schematic Illustrating Discrete Particle Simulation

2.2 Chimera Particle Simulation (CPS): This is a high-fidelity approach, based on chimera or overset methodology, to explicitly simulate moving beads, fully resolving the associated boundary layers. Immersed boundary techniques from the D.D. Joseph group at Minnesota can also resolve flow around finite sized particles [4, 5]. However, their algorithm uses a single grid, is constrained to use unstructured grids and requires expensive re-meshing for every time step.

Table 1.1 gives the comparison of features of DPS and CPS methods.

	Discrete Particle Simulation	**Chimera Particle Simulation**
Model Usage	Small beads	Large beads
Bead Model	Isolated Point Particle	Arbitrary, finite-sized
Fluid Model	Navier-Stokes with adequate source terms for the coupling between both phases	Navier-Stokes equations, no need for modeled source terms
Flow Particle Coupling	Volumetric source/sink terms using drag law	Velocity no-slip on bead surface, full hydrodynamics
Bead Mass Transfer	Ranz-Marshall Type Correlation	Exact Boundary Layer Transport Solution
Bead Coverage	Homogeneous, point value	Surface binding inhomogeneties tracked
Computational Speed/Cost	Fast & less expensive (can handle thousands of beads)	Slow & more expensive (restricted to hundreds of beads)

Table 1.1: Comparison between Discrete & Chimera Particle Simulations

The choice between Discrete and Chimera Particle Simulations is mainly based on the need to resolve the particle details such as surface structure and particle deformation. The particle size compared to device/channel dimensions is related to the required computational effort..