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Algorithms in a Robust Hybrid CFD-DEM Solver for Particle-Laden Flows

Heng Xiao[1,*] and Jin Sun[2]

[1] *Institute of Fluid Dynamics, ETH Zürich, 8092 Zürich, Switzerland.*
[2] *Institute for Infrastructure and Environment, The University of Edinburgh, Edinburgh EH9 3JL, United Kingdom.*

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Abstract. A robust and efficient solver coupling computational fluid dynamics (CFD) with discrete element method (DEM) is developed to simulate particle-laden flows in various physical settings. An interpolation algorithm suitable for unstructured meshes is proposed to translate between mesh-based Eulerian fields and particle-based Lagrangian quantities. The interpolation scheme reduces the mesh-dependence of the averaging and interpolation procedures. In addition, the fluid-particle interaction terms are treated semi-implicitly in this algorithm to improve stability and to maintain accuracy. Finally, it is demonstrated that sub-stepping is desirable for fluid-particle systems with small Stokes numbers. A momentum-conserving sub-stepping technique is introduced into the fluid-particle coupling procedure, so that problems with a wide range of time scales can be solved without resorting to excessively small time steps in the CFD solver. Several numerical examples are presented to demonstrate the capabilities of the solver and the merits of the algorithm.

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Key words: Fluid-particle interaction, particle-laden flow, discrete element method, computational fluid dynamics, hybrid model.

1 Introduction

Particle-laden flows occur in many industrial and natural settings. For example, fluidized bed reactors are widely used in chemical and petroleum industries to carry out multiphase chemical reactions, where gas with high velocity is injected to beds of solid particles to achieve effective heat transfer, mass mixing, and accelerated reactions. In coastal engineering, waves mobilize and suspend sediments from beaches and transport sand

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[*] Corresponding author. *Email addresses:* `xiaoh@ethz.ch` (H. Xiao), `j.sun@ed.ac.uk` (J. Sun)

particles with the flow. In these examples, the fluid-particle and particle-particle interactions play important roles. Fluid-particle interactions are also found in blood flows [1], sand dune evolution [2], and other geological flows.

In the systems described above, the fluids are often modeled in the Eulerian frame with Navier Stokes equations or their variants. The particles can also be modeled in the Eulerian frame, where particle volume fraction and particle flow field velocities are described and solved, and the individual particle motions are not tracked. This approach is referred to as two-fluid model [3,4], since the particle phase is also treated as a fluid. Another approach is to track the movement of each individual particle based on the forces exerted on the particle by the fluid and by other particles, which is referred to as the hybrid computational fluid dynamics-discrete element method (CFD-DEM) model. In both approaches, depending on the treatment of the fluid-particle and particle-particle interactions, the numerical methods can be categorized as one-way coupling (fluid-to-particle action only), two-way force coupling (fluid-particle mutual interactions), and four-way coupling (fluid-particle interactions and particle-particle collisions) [5]. For dilute flows with small solid volume fractions, one-way or two-way coupling are sufficient. For dense flows, which are common in fluidized-bed reactors and geological processes such as sediment transport, the solid volume fraction could be very high (above 60% in certain regions), and fluid-particle interactions and particle-particle collisions are both important. Another feature of geological flows and many other particle-laden flows is the wide range of particle sizes. We aim to model the dense flows occurring in industrial and natural processes with wide ranges of particle-size distributions, and thus the CFD-DEM approach with four-way coupling is necessary. The mathematical models and the numerical methods for these problems are the focuses of this paper.

Cundall and Strack [6] first used DEM to model granular flows without interstitial fluids in geotechnical engineering back in the 1970s. The hybrid CFD-DEM approach to model particle-laden flows was attempted later to solve industrial fluid-particle flows [7] and gained popularity in the past two decades. This approach has been used by many researchers to simulate multiphase flows in chemical engineering processes [8, 9] and other applications [10]. Wachem et al. [11] compared various formulations and closure models in the simulation of dense gas-solid systems. Kafui et al. [12] clarified the equations used in the literature for CFD-DEM modeling. On the numerical aspect, Sundaram and Collins [13] presented an efficient algorithm for their numerical model simulating dilute suspensions with fluid-particle and particle-particle interactions. However, there are still several difficulties associated with fluid-particle interactions in the dense flows that have not been addressed in previous studies. Specifically, the following challenges were encountered in our attempts to model dense particle-laden flows:

1. There is still a lack of proper schemes to translate between Eulerian fields based on unstructured meshes and Lagrangian particle quantities,

2. The fluid-particle interaction terms in the fluid momentum equation, if treated explicitly, often cause convergence difficulty in flows with high volume faction of particles.