International Journal of Multiphase Flow 77 (2015) 142–157

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

journal homepage: www.elsevier.com/locate/ijmultiphaseflow

Diffusion-based coarse graining in hybrid continuum–discrete solvers: Theoretical formulation and a priori tests

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ARTICLE INFO

Article history:
Received 5 June 2015
Revised 17 August 2015
Accepted 20 August 2015
Available online 29 August 2015

Keywords:
CFD–DEM
Coarse graining
Multi-scale modeling

ABSTRACT

Coarse graining is an important ingredient in many multi-scale continuum–discrete solvers such as CFD–DEM (computational fluid dynamics–discrete element method) solvers for dense particle-laden flows. Although CFD–DEM solvers have become a mature technique that is widely used in multiphase flow research and industrial flow simulations, a flexible and easy-to-implement coarse graining algorithm that can work with CFD solvers of arbitrary meshes is still lacking. In this work, we proposed a new coarse graining algorithm for continuum–discrete solvers for dense particle-laden flows based on solving a transient diffusion equation. Via theoretical analysis we demonstrated that the proposed method is equivalent to the statistical kernel method with a Gaussian kernel, but the current method is much more straightforward to implement in CFD–DEM solvers. A priori numerical tests were performed to obtain the solid volume fraction fields based on given particle distributions, the results obtained by using the proposed algorithm were compared with those from other coarse graining methods in the literature (e.g., the particle centroid method, the divided particle volume method, and the two-grid formulation). The numerical tests demonstrated that the proposed coarse graining procedure based on solving diffusion equations is theoretically sound, easy to implement and parallelize in general CFD solvers, and has improved mesh-convergence characteristics compared with existing coarse graining methods. The diffusion-based coarse graining method has been implemented into a CFD–DEM solver, the results of which are presented in a separate work.

Introduction

Coarse graining in continuum–discrete modeling

In computational mechanics for solids and fluids, continuum methods based on partial differential equations, e.g., the Navier–Stokes or elasticity equations, are usually discretized by the finite-difference, finite-volume, or finite-element method and used to investigate macroscopic system responses, e.g., structural deformations or fluid flows (Mitchell and Griffiths, 1980; Versteeg and Malalasekera, 2007; Zienkiewicz and Morice, 1971). On the other hand, discrete methods such as molecular dynamics and direct simulation Monte Carlo methods are used to simulate microscopic properties of systems at length- and time-scales that are much smaller than those studies by using continuum methods (Piekos and Breuer, 1996; Belytschko et al., 2002). Continuum and discrete methods are complementary to each other, not only in terms of the length- and time-scales they cover, but also because they are used for different purposes.

Traditionally, continuum and discrete methods have been developed in separate communities without significant interactions. This is partly a reflection of the scale separation in classical continuum mechanics; that is, the scales of the representative volume element (RVE) are many orders of magnitude larger than those of the individual molecules or atoms therein. As a consequence, the phenomena of interests in the macroscopic scales and those in the microscopic scales are dramatically different. However, the past few decades have seen a surge of interests in the development of methods aiming for bridging the continuum and the microscopic scales. These efforts originate from several communities with a diverse physical settings ranging from fracture mechanics (Belytschko and Xiao, 2003; Xiao and Belytschko, 2004) and complex fluids (Donev et al., 2010) to materials sciences (e.g., Delgado-Buscalioni et al., 1833; Eidel, 2009; Müller, 2013; Rottler, 2013; Curtin, 2013). In spite of these efforts, many theoretical and practical challenges exist in these multi-scale models. A particular difficulty that is common among most continuum–discrete solvers is the coupling between the continuum solver and the discrete solver with guaranteed conservation of relevant quantities. This is due to the fact that the

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http://dx.doi.org/10.1016/j.ijmultiphaseflow.2015.08.014
0301-9322/

conservation equations on the two scales are formulated for quantities of vastly different natures, and thus the bridging between the microscopic and macroscopic quantities are critical yet extremely difficult to achieve (Xiao and Belytschko, 2004; Delgado-Buscalioni et al., 1833). In this work we highlight the difficulties of coarse graining in the context of continuum–discrete solvers for dense particle-laden multiphase flows. Subsequently, a strategy that is theoretically meritorious and convenient for numerical implementations is proposed. However, since the difficulties associated with coarse graining are common among many other continuum–discrete methods, it is expected that the strategy developed in this work shall be useful for those methods as well.

Coarse graining in CFD–DEM solvers

Dense particle-laden flows are encountered in a wide range of industrial applications and natural processes including fluidized-bed reactors in chemical engineering (Müller et al., 2008, 2009), pneumatic conveyors in the mineral processing industries (Han et al., 2003), and sediment transport processes in riverine and coastal flows (Drake and Calantoni, 2001; Calantoni et al., 2004). A class of continuum–discrete methods have been proposed and developed in the past two decades, where the fluid (the carrier phase) is modeled with a continuum approach in the Eulerian framework, while the particles (the dispersed phase) are tracked individually in the Lagrangian framework accounting for the inter-particle collisions and fluid–particle interactions. Compared with other alternatives such as the two-fluid model and direct numerical simulations (Kempe and Fröhlich, 2012; Kempe et al., 2014; Esmaeeli and Tryggvason, 1998; 1999), the continuum–discrete approach is able to resolve much of the particle flow physics without requiring excessive computational costs. As such, it has received much attention in multiphase flow research communities and gained increasing popularity in industrial applications as well.

Discrete element method (DEM) is introduced by Cundall and Strack (1979) and is widely used in the modeling of dry granular flows where the fluid flow is not dynamically important (except for cohesion and lubrication forces). Readers are referred to a recent review by Guo and Curtis (2015) on this subject. Proposed in the 1990s by Tsuji et al. (1993), the CFD (computational fluid dynamics)–DEM approach is the earliest developed continuum–discrete method for dense particle-laden flows. Other variants such as LES (large eddy simulation)–DEM and SPH (smooth particle hydrodynamics)–DEM have been developed recently (e.g., Zhou et al., 2004; Potapov et al., 2001; Sun et al., 2013). However, since the coarse graining procedure is common among this type of the continuum–discrete methods, in this work we describe the coarse graining method with CFD–DEM applications in mind. The proposed method is, however, applicable to other similar methods as well.

In CFD–DEM, the fluid is described by the volume-averaged Navier–Stokes equations (Anderson and Jackson, 1967). The effects of the particle-to-fluid interactions are accounted for in the fluid continuity and momentum equations mainly through the presence of the following three terms: solid volume fraction ε_s, and solid phase velocities $\mathbf{U}_s$, fluid–particle forces $\mathbf{F}_{fp}$ (primarily consisting of drag force $\mathbf{F}_d$ and buoyancy). These are field quantities based on the CFD mesh, and are obtained from the locations, the sizes, and the velocities of each individual particles as well as the fluid forces acting on them. The mapping from particle-scale quantities to macroscopic quantities is also referred to as coarse graining, averaging, or aggregation in the literature (Xiao and Sun, 2011; Zhu and Yu, 2002). We will use "coarse graining" and "averaging" interchangeably in this work.[1] This seemingly simple operation involves several challenges when performed in practical CFD–DEM solvers. First, theoretically the procedure is not unique (Zhu and Yu, 2002), but the coarse grained fields can have profound influences on the CFD–DEM simulation results. Second, there are several constraints on the procedure, e.g., it must conserve the relevant physical quantities such as particle mass and momentum, both for the interior particles and for those near the domain boundaries (e.g., walls). Satisfying these constraints simultaneously is challenging. Moreover, since industrial CFD simulations often involve complex geometries and necessitate using meshes of poor quality, the procedure should be able to accommodate these meshes without negatively impacting the CFD–DEM simulation results. Finally, it should be easy to implement and amiable to parallelization, a technology that is ubiquitously used in modern CFD codes. Numerous averaging techniques have been proposed and used in the literature (Wu et al., 2009a, 2009b; Zhu and Yu, 2002; Xiao and Sun, 2011). To the authors' knowledge, however, a method satisfying all the criteria above is still lacking. The objective of this work is to develop an averaging strategy that is theoretically sound, easy to implement in industrial CFD solvers, and capable of handling generic meshes used in these CFD solvers. Due to space considerations, the current paper focuses primarily on the theoretical analysis and a priori evaluations of the proposed method without actually testing it in a CFD–DEM solver. Its implementation in CFD–DEM solvers and the evaluation of the performances are deferred to a separate, companion paper of the present work (Sun and Xiao, 2015).

The rest of the paper is organized as follows. In Section "Review of existing coarse graining methods" the desirable features of averaging methods are discussed in detail, and existing algorithms in the literature are reviewed, compared, and evaluated against the properties in this list. Section "Diffusion-based coarse graining algorithm" presents the proposed averaging algorithm, demonstrates its theoretical equivalence to the statistical kernel method, and examines its characteristics based on the theoretical analysis. In Section "A priori numerical tests", a priori averaging tests are conducted to examine the performance of the proposed method and to compare with the results obtained with other averaging methods. Implementation details and computational costs considerations are discussed in Section "Discussion". The paper is summarized in Section "Conclusion".

Review of existing coarse graining methods

Some of the commonly used and recently developed coarse graining methods in the CFD–DEM literature include the particle centroid method (PCM), the divided particle volume method (DPVM), the statistical kernel method, and the recently proposed two-grid formulation. These methods will be critically reviewed below with their advantages and shortcomings examined. The discussion here is constrained to particle-resolving simulations where particle–fluid interfaces are not resolved. The continuum–discrete solvers where particle interfaces are explicitly resolved, e.g., with immersed boundary method (Kempe et al., 2014) or lattice-Boltzmann method (Chen et al., 1991; Yin and Koch, 2008; Yin and Sundaresan, 2009), are beyond the scope of the present work, since the averaging algorithms discussed in this paper are not directly applicable to those methods. The methods where particles are represented as porous bodies are omitted from the discussion here as well.

Desirable properties of coarse graining procedure in CFD–DEM solvers

In the context of implementation in CFD–DEM solvers for particle-laden flows, we first outline below a few desirable properties that a coarse graining method should have. This "wish list" will serve as the

[1] The terminology "coarse graining" here should not be confused with its usage in other contexts. In DEM (and in molecular dynamics) simulations, "coarse-graining" is also used to denote the process of representing a large number of real particles with a small number of "super-particles" to reduce computational costs while retaining essential dynamics of the system.