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Fully resolved viscoelastic particulate simulations using unstructured grids

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ABSTRACT

Viscoelastic particulate suspensions play a key role in many energy applications. Our goal is to develop a simulation-based tool for engineering such suspensions. This study is concerned with fully resolved simulations, wherein all flow scales associated with the particle motion are resolved. The present effort is based on Immersed Boundary (IB) methods, in which the domain grids do not conform to the particle geometry. The particles are defined on a separate Lagrangian mesh that is free to move over an underlying Eulerian grid. An immersed boundary forcing technique for moving bodies within an unstructured-mesh, non-Newtonian viscoelastic flow solver is thus developed and described. This method is implemented in a massively parallel, finite-volume-based incompressible fluid solver. A number of flows, simulated using this method are presented to assess the accuracy and correctness of the algorithm.

1. Introduction

Suspensions of rigid particles dispersed in a fluid are common in many engineering applications. A few examples include fluidized bed, sediment transport, blood flow, coal-based combustion chambers, biomass gasifiers, oil sands mining, foods, pharmaceuticals and personal care products. In many of these cases, the fluid in which particles are dispersed are often viscoelastic in nature.

The numerical study of such particulate flows provides a very important source of insight into the physical processes that govern the interaction between particles and fluids. Often we need to resolve flow at the scale of the particle in order to gain a comprehensive understanding of the underlying physics. This paper is concerned with fully resolved simulations (FRS) of rigid particles suspended in complex fluids using a Finite-Volume approach. In FRS, all scales associated with the fluid flow and the hydrodynamic forces on the particle are directly evaluated, unlike in point-particle approaches where drag and lift correlations are used to estimate forces on the particles.

Conventionally, one solves fluid flow problems with rigid particles computationally, by generating a grid that conforms to the body of the particle (termed a 'body-fitted' grid). One then discretizes the governing equations on this body-fitted grid and applies no-slip boundary conditions at the particle surface. There are several numerical techniques which use such body-conforming grid formulations to solve flows with moving boundaries including Arbitrary Lagrangian–Eulerian (ALE) [1], Deforming-Spatial-Domain/Stabilized-Space–Time (DSD/SST) [2]. ALE uses a moving mesh scheme to handle the time

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dependent fluid domain, which typically involves solving the mesh motion through a partial differential equation using the known boundary displacements [3,4] or interpolation schemes (like Radial basis functions (RBF) [5], Inverse Distance Weighting (IDW) [6]). ALE based finite element method has been used to simulate rigid particles in viscoelastic fluids to study particle migration [7] and alignment [8,9]. DSD/SST formulations uses the concept of simultaneous discretization in space and time via finite elements together with least-squares-type stabilization to solve problems in deforming domains [10,11].

The primary disadvantage of such methods is the grid generation process that accounts for the complexity of the rigid boundaries. This is a bigger concern if the particles are free to move, in which case the generated mesh needs to be stretched and translated in order to retain a body-fitted grid. In the case of large displacements, one might need to generate a completely new mesh, which could be very time consuming, particularly in complex geometries. One also requires a method of projecting the solution onto the new mesh. Recent studies have used the extended finite element method (XFEM) in order to alleviate these problems [12]. XFEM was originally developed to study the propagation of cracks in structures [13], later extended to flow problems [14]. In this method, the finite element shape functions are locally enriched by using additional degrees of freedom in order to handle discontinuities [12]. Choi et al. [15,9] used XFEM in combination with ALE to study viscoelastic particulate flows.

Our effort is based on the class of Immersed Boundary (IB) methods. We use the term IB method as a generic term for methods that simulate flows with embedded boundaries on grids that do not conform to the shape of these boundaries [16]. There are various alternative terms used in literature such as Fictitious domain [17], Cartesian Grid methods [18] and Embedded boundary methods [19] to identify such techniques.

The IB method was first used by Peskin [20] to study flow patterns around heart valves and has since evolved as a powerful tool for studying fluid–structure interaction problems. The key idea behind this method is to use a fixed Eulerian mesh for the computation and represent the immersed object using a Lagrangian mesh, which is free to move inside the Eulerian mesh. Since the Eulerian mesh is fixed, a clear advantage of IB over body-fitted grid techniques is that frequent re-meshing of the domain as well as a procedure to project the solution onto the new grid is not required as the particles move. Both steps have negative impacts on the simplicity, accuracy, robustness, and computational cost of the solution procedure, especially in cases involving large motions. However, implementing the no-slip boundary condition is not straightforward in IB methods since the grid does not conform to the solid boundary. Peskin [20–22] used the idea that an IB exerts a singular force on the fluid, and hence the no-slip boundary condition would appear as a source-term in the momentum equations. A variety of models have been proposed to calculate this force field [23–27].

Goldstein et al. [28] used concepts of feedback control based on the difference between the velocity solution and the boundary velocity to compute the force on the rigid immersed surface (termed 'Virtual Boundary Formulation'). This model can be thought of as a system of virtual springs and dampers attached to the boundary points. This technique introduces additional free parameters (stiffness and damping constants) and resolving the characteristic time scales of oscillation of the spring-damper systems leads to a severe restriction in the time step [29]. Fadlun et al. [30] proposed a direct formulation of the forcing term to overcome the time step restrictions and limitations of the virtual boundary formulation. This method relies on the modification of the entries of the matrix of the discretized momentum equations such that the solution leads to the correct velocity at the boundary points. However, this method leads to oscillations in the IB forcing term in case of moving boundaries. Ye et al. [18] proposed a method (termed the 'Cartesian Grid Method') for simulating two dimensional unsteady, viscous, incompressible flows over complex geometries in which a control volume near the immersed boundary is reshaped into a body-fitted trapezoidal shape and using a second order interpolation scheme near the immersed boundary. Uhlmann [23] used IB methodology with the direct and explicit forcing for the simulation of particulate flows. In this method, the forcing term is evaluated at the Lagrangian markers based on the desired rigid-body motion and a preliminary velocity obtained explicitly without using the forcing term. Thereafter the forcing is spread into the Eulerian grid using regularized delta functions.

The present effort is based on the approach proposed by Patankar et al. [31] as well as Sharma et al. [32], and further developed by Apte et al. [27,33,34]. Patankar et al. [31] introduced a fast Lagrange multiplier technique to compute the IB forcing that eliminated the need of an iterative procedure. Apte et al. [34] developed this approach for a finite volume solver in colocated grids with improved spatial and temporal accuracy. It was assumed in this development that the particle regions are fluids with density equal to the particle density.

There have been a limited number of IB studies in viscoelastic fluid. Singh et al. [35] used a distributed Lagrange multiplier (DLM) method for simulating the motion of rigid particles suspended in an Oldroyd-B fluid. Goyal et al. [36] coupled lattice-Boltzmann methods and an immersed boundary method for studying particles sedimenting in a viscoelastic fluid. Recently De et al. [37] studied viscoelastic flow through an ideal porous structure (represented by a periodic arrangement of cylinders) using a finite volume based immersed boundary method in a staggered Cartesian grid. The positions of the particles were held fixed in this study.

One recurring theme among the aforementioned finite volume based IB methods is the use of Cartesian grids for discretizing the Eulerian domain. This choice stems from the fact that the method does not require body-fitted meshes. However, Cartesian grids are only effective in representing a simple domain, i.e. a box filled with a fluid in which a complex body is immersed. Hence our focus is on developing IB methods which can be applied even in an unstructured grid setting. Recently Hu et al. [38] had used an immersed boundary method using unstructured anisotropic mesh adaptation and penalization techniques for solving Newtonian flow past fixed objects. The combination of using an unstructured mesh