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A sharp-interface Cartesian grid method for viscoelastic fluid flow in complex geometry

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ABSTRACT

Computational methods based on Cartesian mesh are popular in simulating fluid flow with moving boundaries of complex geometry. In this paper, a sharp-interface Cartesian grid method is proposed for simulating viscoelastic fluid flow. We implement a finite volume numerical scheme with an improved Rhie-Chow interpolation on the open-source toolbox OpenFOAM. In the benchmark test of flow past a stationary cylinder, the velocity for Newtonian fluid flow is found to be second-order accurate with linear/bi-linear fitting functions for local reconstruction and third-order accurate with quadratic fitting functions. Only first-order accuracy is achieved with current solver for the Oldroyd-B fluid flows due to the difficulty in handling the extra stress near the boundary. However, our sharp-interface Cartesian grid method has been verified to correctly predict the extra stress on the surface of the cylinder. Simulation results of confined Oldroyd-B fluid flow past a pair of cylinders are also reported. A comparison between the proposed sharp-interface Cartesian grid method and a smoothed-interface immersed boundary method is carried out with respect to accuracy and efficiency.

1. Introduction

Developing numerical methods for simulating viscoelastic fluid flow with stationary or moving boundaries of complex geometry is critical for the study of many particulate flow problems. Interesting topics previously studied include: behavior of a single particle in a micro-channel flow of complex fluid with rotation [1,2] and cross-flow migration [3–8], flow-induced evolution of microstructure in a non-Newtonian suspension matrix [9–16] and self-propulsion of micro-swimmers in a bio-fluid [17–19].

Previous simulations of particulate flows focused on approximating the flow with potential flow, Stokes flow, or point-type-particle flow. Important features, such as viscosity, inertia or the particle orientation were neglected. In direct simulation of particulate flow with fully resolved hydrodynamics, either a body-fitted mesh that conforms to the solid-fluid interface, or a Cartesian mesh with extra handling at the interface is employed. The body-fitted mesh can resolve the boundary field accurately but with high expense in re-meshing. The Cartesian mesh requires less math operations in the discretisation of differential equations, and its regularity is more promising for the optimization of load-balancing on parallel machines.

Early direct numerical simulation of particulate flow with a viscoelastic medium used a finite element method on a body-fitted mesh, with fluid motion described by the Navier-Stokes equations and solid motion described by the Newton–Euler equations. At each time iteration, the simulation includes three steps: an automatic re-meshing step according to new positions of particles, a projection step mapping the flow field from the old mesh to the new mesh, and the solving of governing equations on the new mesh [20]. Huang and Feng first used this method for simulating a viscoelastic fluid flow around a stationary cylinder [21]. Later on, Feng et al. reported a study of moving boundary case using the same method [22]. Huang et al. improved the numerical scheme by introducing the ALE moving mesh technique for calculating the motion of particles [23,24]. The ALE method allows the mesh inside the computational domain to move arbitrarily, allowing precise tracking of interfaces in a fluid-structure system. D'Avino et al. used an ALE-based finite element method to study cross-flow migration of particles subjected to a Giesekus fluid shear flow in 2D [4]. They reduced the re-meshing cost by constricting the re-

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meshing region to a narrow channel. Code verification was done by a comparison with the result using a fictitious domain method. The fictitious domain method was found to require a calculation time about 10 times higher than the ALE method, in which a body-fitted mesh was used to resolve the boundary flow. Such body-fitted mesh was more efficient than the uniform Cartesian mesh used in the fictitious domain method. However, it is worth to notice while simulating a system of multiple particles, the Cartesian mesh would be much more efficient. D'Avino et al. later presented a 3D simulation of the dynamics of a particle suspended in a Giesekus fluid under confined shear using the same method [3]. To reduce the cost in re-meshing, they avoided updating the particle position in the main flow direction by assigning the grid with a corresponding velocity instead. The same method had been adopted for a series of studies on the dynamics of a spherical particle with ignorable inertial effects in confined viscoelastic fluid flow including i) the formation of a separatrix that distinguishes the cross-stream migration direction [6], ii)the design rule of viscoelasticity induced single-line focusing equipment [25], iii)the effect of shear-thinning and the effect of secondary flow on the cross-stream migration [7]. The re-meshing step becomes the bottleneck of performance in large scale simulations thereafter, as it introduces a substantial computational complexity.

In a Cartesian grid method, there are several grid cells that are partly covered by the immersed object. They should be interpreted as in a two-phase state. These Eulerian cells are not physically well-defined, when the surface of the immersed object is rigid. The volume-of-fluid (VOF) method [26] introduces a new parameter “volume fraction of fluid” to the computational model, so that the solid can be treated as a general fluid with extremely high viscosity. The VOF method is commonly adopted in solving multiphase flow with fluid-fluid interface or free surface [27].

The cutting-cell method uses an embedded body-fitted mesh near the immersed boundary based on a Cartesian mesh for resolving the boundary flow [28–30]. The cutting cell method calculates the intersections between the Lagrangian grid which represents the moving boundary and the stationary Cartesian grid. These intersections in conjunction with the original vertexes in the fluid part form new irregular units. The boundary conditions therefore can be exactly enforced on the boundary. The difficulties in applying the method lie in a) the complexity of computing the intersections, especially in 3D; b) the possible generation of computational units with small volume, where cell combination is necessary to avoid instability.

The immersed boundary method [31] tracks moving boundaries with a moving Lagrangian grid but solves the fluid flow on a stationary Eulerian grid. The exchange of information between the Lagrangian grid and the Eulerian grid is accomplished by interpolation operations with a smoothed-delta function. This method can be quickly implemented based on any existing numerical solvers and then extended to simulate viscoelastic fluid flow. Goyal and Derksen demonstrated its capability through the simulation of spherical particles sedimenting in a FENE-CR fluid flow [32]. The smoothed delta function would result in a smooth transition of velocity across the sharp solid-fluid interface thus the stress on the interface becomes much less accurate than a body-fitted mesh method, even non-physical. In addition, an empirical hydrodynamic radius was suggested to make a better prediction of drag force because the original method gave a over-predicted drag [32,33].

The fictitious domain method is a popular method for simulating particulate flow on the structured mesh. A common feature of this method and the immersed boundary method is the involvement of the solid part in solving the fluid flow. The solid-fluid motion is handled implicitly and there are no explicit steps to calculate the force and torque on the particles. Glowinski et al. proposed a distributed Lagrange multiplier/fictitious domain method with a finite element scheme [34]. The motion of the entire computational domain was described by a combined equation [34–36]. The rigid body motion constraint in the solid part was particularly enforced by adding an appropriate distributed Lagrangian multiplier term into that equation. Singh et al. developed the viscoelastic version of the method for the simulation of particle sedimentation in a 2D Oldroyd-B fluid flow [37]. Yu et al. investigated the sedimentation of 102 circular particles in a shear-thinning fluid in 2D [38] and the sedimentation of a single spherical particle in a Bingham fluid [39].

However, both the immersed boundary method and the fictitious domain method are difficult to resolve the flow field at the solid-fluid interface, where high shear rate or extensional rate might result in a high viscoelastic stress in viscoelastic fluid flows. In this study, we proposed a sharp-interface Cartesian grid method for simulating viscoelastic fluid flow based on the methods reported in [40,41]. The flow field in the vicinity of the solid-fluid interface is reconstructed using a polynomial fitting function, with which the Dirichlet or the Neumann boundary conditions can be well-imposed. Our numerical scheme is distinguished from previous studies in [40,41] in the following aspects: a) our implementation considers an improved Rhie-Chow interpolation [42,43], which is introduced to avoid the chequer-board effect associated with co-located grid; b) the solver is capable of resolving the viscoelastic stress at the solid-fluid interface accurately in a viscoelastic fluid flow; c) the code developed is fully compatible for parallel simulation on MPI-based clusters. New aspects of this study also include: a) a new study of Oldroyd-B fluid flow past a pair of cylinders with a blockage of 50%; b) a comparison of the proposed sharp-interface Cartesian grid method with the smoothed-interface immersed boundary method in terms of accuracy and parallel efficiency.

The rest of this paper is organized as follows, Section 2 presents the detail of numerical scheme in solving the governing equations. Section 3 evaluates the order of accuracy in space and verifies the correctness of the implementation for simulating Newtonian fluid flow. Section 4 evaluates the order of accuracy in space and verifies the capability of the method for simulating a confined Oldroyd-B fluid flow past a stationary cylinder with a blockage of 50%. To highlight the advantage of the sharp-interface Cartesian grid method, Section 4 also describes the simulation of flow past two closely positioned cylinders. Section 5 compares the proposed sharp-interface Cartesian method with a smoothed-interface immersed boundary method. Section 6 concludes the paper.

2. Numerical method

2.1. Governing equations

The incompressible fluid flow is governed by the Navier–Stokes equations composed of a momentum equation and a continuity equation.

$$\partial_t \underline{u} + \underline{u} \cdot \nabla \underline{u} = -\nabla p + \frac{\nabla \cdot \underline{\underline{\sigma}}}{\rho_f} + \underline{\nabla p_0} \tag{1}$$

$$\nabla \cdot \underline{u} = 0 \tag{2}$$

where $\underline{\underline{\sigma}}$ is the total stress, ρ_f is the density of the fluid, ∂_t indicates a partial derivative with respect to time, $\underline{\nabla p_0}$ has a constant component in the streamwise direction, which represents a constant pressure gradient used for driving the flow, p is the corrected kinematic pressure. $\underline{\underline{\sigma}}$ has the solvent viscous part $\underline{\underline{\sigma}}_s$ and the viscoelastic part $\underline{\underline{\sigma}}_p$, and is given by $\underline{\underline{\sigma}} = \underline{\underline{\sigma}}_s + \underline{\underline{\sigma}}_p$. The viscous part is dependent on the strain rate tensor, $\underline{\underline{\sigma}}_s = \eta_s(\nabla \underline{u} + \nabla \underline{u}^T)$, where η_s