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.

Keywords: immersed boundary, unstructured grid, particulate flow, Fully Resolved Simulations, Non-Newtonian fluid flow, viscoelasticity

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Preprint submitted to Journal of Computational Physics

November 9, 2016

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 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]. DST/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 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, 21, 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, 24, 25, 26, 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 with an immersed boundary based viscoelastic solver for moving bodies in a finite volume setting has not been presented heretofore and this represents the primary highlight of our paper.

The paper is organized as follows. In Section 2, we briefly describe the immersed boundary forcing idea and also present the governing equations. The complete algorithm is described in Section 3. Section 3 also provides details of the interpolation and projection operators used. In Section 4, we present a number of benchmark simulations involving Newtonian and viscoelastic flow around objects in two and in three dimensions and compare results with those reported in the literature to assess the accuracy and correctness of the algorithm. Section 5 summarizes the main conclusions and results from this work.

Figure 1: Domain $\Omega = \Omega_f \cup \Omega_p$ bounded by surface $\mathcal{S}$ containing fluid regions (Ω_f) and particle regions ($\Omega_p = \cup_{i=1}^{N_p} \mathcal{P}_i$). $\mathcal{S}_i$ represent the particle surface

2. Formulation

2.1. Domain Classification

Consider the domain Ω shown in Figure 1 bounded by a surface $\mathcal{S}$, which contains regions occupied by an incompressible viscoelastic fluid (Ω_f) as well as regions occupied by rigid particles (Ω_p). The viscoelastic fluid is composed of polymers additives in a Newtonian solvent. Let N_p denote the total number of rigid particles, $\mathcal{P}_i$ represent the region occupied by particle ‘ i ’ ($1 \leq i \leq N_p$) and $\mathcal{S}_i$ represent the particle surface, so that $\Omega_p = \cup_{i=1}^{N_p} \mathcal{P}_i$ and $\mathcal{S}^p = \cup_{i=1}^{N_p} \mathcal{S}_i$.

The particles may be free to move, or undergo a specified motion in the domain. We are interested in resolving the flow at the scale of the particles and capture the two-way coupling between the particle motion and the surrounding fluid motion.

2.2. Immersed Boundary Forcing

The governing equations for the flow of interest involve mass and momentum conservation for an incompressible fluid in the presence of polymers throughout the domain Ω_f with no-slip boundary conditions on $\mathcal{S}^p$ and appropriate conditions on the outer boundary $\mathcal{S}$ using an immersed boundary formulation. The immersed boundary scheme used is based on the technique proposed by Patankar [31]. The basic idea behind the algorithm is to extend the flow equations over the entire domain Ω , assuming particle regions Ω_p are also filled with fluid that is of density equal to the particle density (ρ_p), resulting in a variable density fluid.

132 Since both fluid and particle are incompressible, the entire system is also incompressible.
 133 Further the motion of the fluid occupying the particle regions is constrained to be a rigid
 134 body motion. This is accomplished by adding an additional volumetric body force term (f_i)
 135 in the momentum conservation equations. This additional source term is referred to as the
 136 immersed boundary(IB) force. The IB force acts only in the vicinity of regions occupied by
 137 the particle and ensures the no slip boundary condition at the particle surface.

138 The governing flow equations over the whole domain Ω in dimensional form are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (1)$$

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}^N}{\partial x_j} + \frac{\partial \tau_{ij}^P}{\partial x_j} + f_i \quad (2)$$

139 In the above equation u_i is the fluid velocity vector, p is pressure, ρ is the density, τ_{ij}^N
 140 is the Newtonian stress tensor, τ_{ij}^P is the additional body stress due to the elasticity of the
 141 polymers and f_i is a volume force term that we will formulate to represent the forcing due
 142 to the immersed boundary on the fluid. Note that ρ is formally a function of space, hence
 143 the divergence of ρu_i is not the same as the divergence of u_i .

144 The Newtonian stress term is given by:

$$\tau_{ij}^N = \mu_s \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (3)$$

145 where μ_s is the viscosity contribution from the solvent. We need a constitutive equation for
 146 the polymer stress in order to close this system of equations. We use three different types of
 147 constitutive equations in this study; Oldroyd-B, FENE-P and single-mode Giesekus[39]. In
 148 these models, an individual member of a dilute concentration of polymers is approximated
 149 as a single dumbbell connected with a nonlinear elastic spring. The polymer stress τ_{ij}^P can
 150 be determined using kinetic theory through the balance of forces acting on the beads of the
 151 dumbbell [39].

152 Oldroyd-B constitutive equation is based on a model for the polymers as microscopic
 153 dumbbells with Hookean springs. The polymer stress τ_{ij}^P is given as [39]:

$$\tau_{ij}^P = \frac{\mu_p}{\lambda} (c_{ij} - \delta_{ij}) \quad (4)$$

where c_{ij} represents the polymer conformation tensor scaled by the equilibrium Hookean spring length and δ_{ij} is the identity tensor. c_{ij} is defined as the pre-averaged dyadic product of the polymer end-to-end vector and is hence a symmetric tensor. The transport equation governing the evolution of c_{ij} can be obtained from kinetic theory by taking the second moment of the distribution function of the dumbbell orientation vector and is given as [39]:

$$\frac{\partial c_{ij}}{\partial t} + u_k \frac{\partial c_{ij}}{\partial x_k} - c_{ik} \frac{\partial u_j}{\partial x_k} - c_{kj} \frac{\partial u_i}{\partial x_k} = -\frac{1}{\lambda} (c_{ij} - \delta_{ij}) \quad (5)$$

where μ_p is the viscosity contribution from the polymer and λ is the characteristic polymer relaxation time scale.

The molecular based FENE-P model assumes that the dumbbell is connected with a finitely extensible nonlinear elastic spring. The FENE-P model is found to be appropriate for fluids which exhibit elasticity while shear thinning modestly. It is also useful for problems with large shear/extension rates since the polymer stresses remain bounded. The polymer stress τ_{ij}^P is given as [39]:

$$\tau_{ij}^P = \frac{\mu_p}{\lambda} \left(\frac{c_{ij}}{\psi} - \delta_{ij} \right) \quad (6)$$

$$\psi = 1 - \frac{c_{kk}}{L^2} \quad (7)$$

where L is the maximum polymer extensibility, non dimensionalized by the equilibrium length of a linear spring $\sqrt{kT/H}$ (where T is the absolute temperature, k is Boltzmanns constant and H is the Hookean spring constant for an entropic spring). The conformation tensor is governed by the following transport equation [39]:

$$\frac{\partial c_{ij}}{\partial t} + u_k \frac{\partial c_{ij}}{\partial x_k} - c_{ik} \frac{\partial u_j}{\partial x_k} - c_{kj} \frac{\partial u_i}{\partial x_k} = -\frac{1}{\lambda} \left(\frac{c_{ij}}{\psi} - \delta_{ij} \right) \quad (8)$$

The mathematical characteristics of Equation 8 is discussed in [40], but we note that if $L \rightarrow \infty$, we recover the Oldroyd-B equation.

172 The third model used is the Giesekus model, which includes an anisotropic drag force on
 173 the dumbbell as a model for dumbbell-dumbbell interactions. The Giesekus model is suitable
 174 for fluids which are elastic and shear thin appreciably. The polymer stress τ_{ij}^P within the
 175 Giesekus model is given as:

$$\tau_{ij}^P = \frac{\mu_p}{\lambda} (c_{ij} - \delta_{ij}) \quad (9)$$

176 The conformation tensor is governed by the following transport equation [39]:

$$\frac{\partial c_{ij}}{\partial t} + u_k \frac{\partial c_{ij}}{\partial x_k} - c_{ik} \frac{\partial u_j}{\partial x_k} - c_{kj} \frac{\partial u_i}{\partial x_k} = -\frac{1}{\lambda} (c_{ij} - \delta_{ij}) - \frac{\zeta}{\lambda} (c_{ik} c_{kj} - 2c_{ij} + \delta_{ij}) \quad (10)$$

177 where ζ is the mobility parameter. Note that, the Oldroyd-B model is a special case of
 178 Giesekus model with the parameter $\zeta = 0$. All three rheological models (Equations 5,8,10)
 179 can be considered as special cases of the following transport equation:

$$\frac{\partial c_{ij}}{\partial t} + u_k \frac{\partial c_{ij}}{\partial x_k} - c_{ik} \frac{\partial u_j}{\partial x_k} - c_{kj} \frac{\partial u_i}{\partial x_k} = -\frac{1}{\lambda} \left(\frac{c_{ij}}{\psi} - \delta_{ij} \right) - \frac{\zeta}{\lambda} (c_{ik} c_{kj} - 2c_{ij} + \delta_{ij}) \quad (11)$$

180 Equations 1, 2 and 11 form a system of 10 coupled partial differential equations, the
 181 solutions of which provide the instantaneous velocity, pressure, polymer conformation and
 182 non-Newtonian stress fields of a fluid with a dilute concentration of polymer additives. We
 183 are given an initial condition on u_i , c_{ij} over the fluid domain Ω_f , and the initial positions
 184 and velocities of all the particles as a part of the problem description, which completely
 185 describes the initial condition of u_i over the whole domain Ω . c_{ij} in the particle regions
 186 Ω_P are set to identity. Suitable boundary conditions for velocity, possibly time dependent,
 187 are also specified at the boundaries $\mathcal{S}$ (inflow/outflow/walls/periodic). c_{ij} also needs to be
 188 specified at inflow boundaries. For outflow boundaries, the convective conditions are used
 189 for c_{ij} as well. There is no need to specify boundary conditions for c_{ij} at the walls, since,
 190 for control volumes on the boundary, there is no flux through the faces coinciding with the
 191 walls and hence c_{ij} at the boundary is completely determined by fluxes through other faces
 192 in the control volume and source term contributions.

193 This model implicitly assumes a uniform polymer concentration throughout the flow

194 domain Ω . The treatment of polymer conformation tensor in the vicinity of particle regions
195 will be discussed as we proceed.

196 2.3. Key non-dimensional quantities

197 Let U be the characteristic velocity and D be the characteristic length scale of the
198 problem. The relevant dimensionless quantities are:

- 199 1. Weissenberg Number(Wi) or Deborah Number(De), which is the ratio of polymer
200 relaxation time(λ) and the characteristic flow time scale(D/U). It describes the degree
201 to which polymers are deformed in a shearing flow of magnitude U/D and therefore is
202 a measure of the elasticity of the solution. i.e $Wi = \frac{\lambda U}{D}$
- 203 2. $\beta = \mu_s/(\mu_s + \mu_p)$, which is the ratio of shear viscosity of the solvent to the zero shear
204 viscosity of the solution. β is a measure of the concentration of the polymer.
- 205 3. Reynolds number, $Re = \rho U D/(\mu_s + \mu_p)$, which is the ratio of inertial forces to viscous
206 forces.

207 2.4. Grid Structure

208 It is assumed that the entire domain Ω and the domain occupied by the particle Ω_p are
209 discretized by an unstructured grid. The fixed grid corresponding to Ω is called the Eulerian
210 grid and the grid corresponding to Ω_p is called the Lagrangian grid. Both Lagrangian
211 and Eulerian grids are volumetric. The unstructured Eulerian grid is defined by a list of
212 coordinates (nodes) at which the field data needs to be solved and a connectivity matrix
213 defining how these nodes are connected to form the underlying volume elements (control
214 volumes). The Lagrangian grid, that represents the rigid particles, are interpreted as a
215 collection of rigid sub-volumes and we do not need any connectivity information. In this
216 paper, we are focusing only on spherical particles discretized by tetrahedral elements and
217 two dimensional circular particles discretized by triangular elements. The choice of using
218 tetrahedral/triangular elements for the Lagrangian grid discretization does not add any
219 additional limitations to the capability of the solver.

220 The particle regions in the Eulerian grid is defined by an indicator function Θ which
 221 has a value of unity inside the particle regions and zero outside the particle regions. As
 222 a consequence of finite resolution, the indicator function is smoothed continuously at the
 223 particle-fluid boundary so that $0 \leq \Theta \leq 1$. The thickness of this "smeared" region is of
 224 the order of the mesh resolution. The construction of the indicator function is discussed in
 225 Section 3.4. The density field can then be written as:

$$\rho = \rho_p \Theta + \rho_f (1 - \Theta) \quad (12)$$

226 As the generality of the current discussion demonstrates, the unstructured finite volume
 227 formulation allows one to apply such a tool to understand the properties of viscoelastic fluid
 228 suspensions in a wide range of complex geometries. In order to illustrate the capability of the
 229 solver, we simulate sedimentation of a dilute suspension of spheres in a Taylor-Couette cell
 230 with shear applied in the direction orthogonal to sedimentation (Section 4.8). The framework
 231 also provides the flexibility to be extended to other rheological models for arbitrary particle
 232 shapes.

233 3. Numerical Algorithm

234 The simulations reported in this paper are performed in CDP, a massively parallel,
 235 unstructured finite-volume-based fluid solver developed at Stanford University's Center for
 236 Turbulence Research [41, 42]. The flow variables (Velocity, density, pressure, and polymer
 237 stress) are collocated in space at the nodes. Each node is associated with a median dual
 238 volume (see Figure 2). The velocity components are temporally staggered with respect to
 239 density and other scalar variables to produce a compact, symmetric discretization of the
 240 continuity equation [43]. The variable density solver uses a fractional step method, which
 241 involves two Poisson solves at each time step to achieve stability without multiple outer
 242 iterations [44]. All the bodyfitted computations reported in this paper are computed using
 243 this basic variable density CDP solver. The immersed boundary approach closely follows
 244 the formulation developed by Apte et al. [33, 34]. The polymer stress term is added as

Figure 2: Control volume associated with a node P , showing sub-edges(plane formed by a cell center, face center and an edge center) and sub-faces (plane formed by a node, face center and edge center).

volumetric source term in the momentum equations and the conformation tensor evolution equation is solved as six coupled scalar transport equations [45, 46]. We have implemented the log-representation of the conformation tensor to ensure positive-definiteness at high Weissenberg numbers [47, 48], where we solve for $A_{ij} = \log(c_{ij}) = R_{ik} \log(D_{kl}) R_{jl}$. Here D_{ij} is the diagonal matrix containing the eigenvalues of c_{ij} and R_{ij} is the orthogonal matrix containing the eigenvectors of c_{ij} . We decompose the velocity gradient transpose such that $\frac{\partial u_j}{\partial x_i} = \Gamma_{ij} + B_{ij} + N_{ik}(c^{-1})_{kj}$, where Γ_{ij} and N_{ij} are antisymmetric and B_{ij} is traceless, symmetric and commutes with c_{ij} . The details of the decomposition can be found in [47, 48]. The evolution equation for c_{ij} (Equation 11) can be transformed to obtain transport equation for A_{ij} :

$$\frac{\partial A_{ij}}{\partial t} + u_k \frac{\partial A_{ij}}{\partial x_k} - (\Gamma_{ik} A_{kj} - A_{ik} \Gamma_{kj}) - 2B_{ij} = -\frac{1}{\lambda} \left(\frac{E_{ij}}{\psi} - \delta_{ij} \right) - \frac{\zeta}{\lambda} E_{ik} (G_{kl} G_{lj} - 2G_{kj} + \delta_{kj}) \quad (13)$$

where $E_{ij} = R_{ik} (D^{-1})_{kl} R_{jl}$ and $G_{ij} = R_{ik} D_{kl} R_{jl}$. A_{ij} is transformed back to c_{ij} to compute the polymer stress.

We present the entire algorithm for the sake of completeness.

3.1. Algorithm

The immersed boundary algorithm proceeds as follows, with superscripts indicating the time level. (Note that variables in Lagrangian grid are capitalized compared to the equivalent variable in the Eulerian grid.)

1. Starting from a divergence free velocity field, advance particle positions explicitly.

$$X_{i,r}^{n+1/2} = X_{i,r}^{n-1/2} + V_{i,r}^n \Delta t \quad (14)$$

$X_{i,r}$ represents the nodal coordinates of Lagrangian grid representing the material volumes of particle ' r ', $V_{i,r}$ represents the center of mass velocity of particle ' r ' and Δt is the time step.

2. Predict velocity components, mass flux(q) and conformation tensor values at the next time level using Adams-Bashforth extrapolation

$$\widehat{u}_i^{n+1} = 2u_i^n - u_i^{n-1} \quad (15)$$

$$(\widehat{q})^{n+1} = 2(q)^n - (q)^{n-1} \quad (16)$$

$$\widehat{A}_{ij}^{n+3/2} = 2A_{ij}^{n+1/2} - A_{ij}^{n-1/2} \quad (17)$$

The mass flux $q = \rho u_i n_i$, where n_i is the local normal.

3. Immersed boundary force predictor. The IB force predictor $\hat{f}_i^{n+1}$ is evaluated from the velocity field predictor following steps 9 to 12 using $\widehat{u}_i^{n+1}$ in place of u_i^{n+1} . From the new position of the particle, the indicator function Θ can be reevaluated at the nodes in the Eulerian grid. The construction of Θ is discussed in Section 3.4. The density can then be calculated as

$$\rho^{n+3/2} = \rho_p \Theta^{n+3/2} + \rho_f (1 - \Theta^{n+3/2}) \quad (18)$$

4. First Poisson solve: The predicted values of mass flux components are corrected in this step such that they satisfy the continuity equation discretely. The correction is expressed in terms of a temporary scalar field ϕ :

$$(q)^{n+1} = (\widehat{q})^{n+1} + \frac{\delta\phi}{\delta x_i} n_i \quad (19)$$

Equation 19 can be substituted in the discrete continuity equation (20) to obtain the first constant coefficient Poisson system, that can be solved to obtain the scalar field ϕ .

$$\Delta_V \frac{\rho^{n+3/2} - \rho^{n+1/2}}{\Delta t} + \sum_{se, sf} (\rho u_i n_i)^{n+1} \Delta_A = 0 \quad (20)$$

Here se, sf refers to sub-edges and sub-faces respectively (Figure 2). Δ_V is the local volume and Δ_A is the local area.

5. Solve for the polymer conformation tensor components. The six scalar equations for A_{ij} (Equation 13) are solved using the following discretization, with the value of ψ obtained from the last time step (See step 14). Due to the hyperbolic nature of the tensor evolution equation, we can expect sharp gradients of polymer stress and hence the convection terms are discretized using a quadratic upwind interpolation for convective kinematics (QUICK) scheme.

$$\begin{aligned} \Delta_V \frac{A_{ij}^{n+3/2} - A_{ij}^{n+1/2}}{\Delta t} + \sum_{se, sf} (u_i n_i)^{n+1} \overline{A_{ij}^{n+1}} \Delta_A &= \Delta_V \Gamma_{ik}^{n+1} A_{kj}^{n+1} - \Delta_V A_{ik}^{n+1} \Gamma_{kj}^{n+1} \\ &+ 2\Delta_V B_{ij}^{n+1} + \frac{\Delta_V}{\lambda} \left(\frac{E_{ij}^{n+1/2}}{\psi^n} - \delta_{ij} \right) - \Delta_V \frac{\zeta}{\lambda} E_{ik}^{n+1/2} (G_{kl}^{n+1/2} G_{lj}^{n+1/2} - 2G_{kj}^{n+1} + \delta_{kj}) \end{aligned} \quad (21)$$

where $\mathcal{G}_i$ is the discrete gradient operator and overbar $\overline{(\)}$ is the spatial averaging operator [42].

6. Transform $A_{ij}^{n+3/2}$ to obtain $c_{ij}^{n+3/2}$ and correct polymer conformation tensor components. Polymers do not stretch when undergoing rigid body motion. Hence the conformation tensor c_{ij} should be identity (δ_{ij}) inside the particle regions. At this point however c_{ij} does not satisfy this constraint because the velocity field does not correspond to rigid body motion. This could result in unphysical stretching of polymers

inside the particle regions which would lead to numerical instability. To prevent this, we correct the conformation tensor components here by explicitly setting them to δ_{ij} in the regions occupied by the particle in the Eulerian grid

$$c_{ij}^{n+3/2} = \delta_{ij}, \forall \theta = 1 \quad (22)$$

7. Solve momentum equation.

$$\begin{aligned} \Delta_V \frac{\rho^{n+1} \hat{u}_i^{n+1} - \rho^n u_i^n}{\Delta t} + \sum_{se, sf} (\rho u_i n_i)^{n+1} \bar{u}_i^{n+1/2} \Delta_A = -\Delta_V \mathcal{G}_i p^{n-1/2} + \\ \Delta_V \mathcal{G}_j (\tau_{ij}^P)^{n+3/2} + \frac{\mu_s}{2} \sum_{se, sf} (S + S^T)(\hat{u}_i^{n+1} + u_i^n) + \mathcal{F}_i \Delta_V + \hat{f}_i^{n+1} \Delta_V \end{aligned} \quad (23)$$

where S is the normal derivative times the area operator and S^T is its transpose as discussed in [42]. $\mathcal{F}_i$ represents the external body force acting on the fluid.

8. Second Poisson solve.

The velocity field does not satisfy the continuity equation at this point. The next step is to solve for the new pressure and correct the velocity field so that the continuity equation is satisfied.

$$\Delta_V \frac{\rho^{n+1} u_i^* - \rho^{n+1} \hat{u}_i^{n+1}}{\Delta t} = \Delta_V \mathcal{G}_i p^{n-1/2} \quad (24)$$

$$\frac{(\rho u_i n_i)^{n+1} - (\rho u_i n_i)^*}{\Delta t} = -\frac{\delta p^{n+1/2}}{\delta x_i} n_i \quad (25)$$

Equation 25 can be substituted in the discrete continuity equation (20) to obtain the second constant coefficient Poisson system, that can be solved to obtain the new pressure field $p^{n+1/2}$. The velocity correction can then be applied as :

$$\frac{\rho^{n+1} u_i^{n+1} - \rho^{n+1} \hat{u}_i^{n+1}}{\Delta t} = -\mathcal{G}_i p^{n+1/2} \quad (26)$$

9. Interpolate velocity from Eulerian grid to Lagrangian grid. The nodal velocity field u_i^{n+1} is interpolated to the rigid body material volume using the scheme discussed in Section 3.3. The interpolated velocity field in the Lagrangian grid is denoted by $U_{i,r}$ for the particle r' .

310 10. Estimate the linear velocity ($V_{i,r}$) and angular velocity ($\omega_{i,r}$) of the particle from $U_{i,r}$

$$\mathcal{M}_r V_{i,r}^{n+1} = \sum_{\mathcal{P}_r} \rho_P \Delta_{V,L} U_{i,r} \quad (27)$$

$$\mathcal{I}_r \omega_{i,r}^{n+1} = \sum_{\mathcal{P}_r} \rho_P \Delta_{V,L} (\epsilon_{ijk} R_j U_{k,r}) \quad (28)$$

311 where $\mathcal{M}$ is the total mass of the particle, $\mathcal{I}$ is the moment of inertia of the particle,
 312 $\Delta_{V,L}$ is the local volume in the Lagrangian grid, R_i is the position vector of a point
 313 with respect to the particle centroid. The summation is over all the particle volumes
 314 in the region $\mathcal{P}_r$.

315 11. Evaluate the rigid body motion $(^{RBM}V)_{i,r}$ from $V_{i,r}$ and $\omega_{i,r}$

$$(^{RBM}V)_{i,r} = V_{i,r}^{n+1} + \epsilon_{ijk} \omega_{j,r}^{n+1} R_k \quad (29)$$

316 12. Compute the rigid body constraint force $(^{RBM}F_{i,r})$ in the Lagrangian grid.

$$(^{RBM}F)_{i,r} = -\frac{U_{i,r} - (^{RBM}V)_{i,r}}{\Delta t} \quad (30)$$

317 The immersed boundary force (f_i) is obtained by projecting $(^{RBM}F)_{i,r}$ to the Eulerian
 318 grid, details of which are given in Section 3.4. The nodal velocity field in Eulerian grid
 319 is then modified as

$$u_i^{n+1} = u_i^{n+1} + \Delta t f_i \quad (31)$$

320 Without any additional treatment, this simulates a force and torque free particle. The
 321 two-way coupling is captured through the evaluation of rigid body motion (Step 9-11)
 322 and the modification of fluid velocity field due to the IB forcing term f_i . The particle
 323 regions in the Eulerian grid is convected as well, since it is treated as a fluid.

324 13. Check for convergence in the immersed boundary forcing term (f_i), return to Step 4
 325 if inner iterations are required

14. This step is required only if we are using the FENE-P fluid. Equation for conformation tensor trace c_{kk} is advanced and a value for ψ^{n+1} is obtained in a way that ensures polymer conformation (and hence stress) boundedness. The evolution equation for c_{kk} can be obtained by contracting Equation 8

$$\frac{\partial c_{kk}}{\partial t} = R_{kk} - \frac{1}{\lambda} \left(\frac{c_{kk}}{\psi} - 3 \right) \quad (32)$$

where R_{kk} represents the contributions from the advection term and the upper convected derivative terms, viz.

$$R_{kk} = -u_j \frac{\partial c_{kk}}{\partial x_j} + c_{kj} \frac{\partial u_k}{\partial x_j} + c_{jk} \frac{\partial u_k}{\partial x_j} \quad (33)$$

Equation 32 can be discretized using Crank-Nicholson for the term c_{kk}/ψ and treating all other terms explicitly to give a quadratic equation for ψ^{n+1}

$$(\psi^{n+1})^2 - \left(\psi^n - \frac{\Delta t}{L^2} R_{kk}^n + \frac{\Delta t}{2\lambda} \frac{1 - 2\psi^n}{\psi^n} - \frac{3\Delta t}{\lambda L^2} \right) \psi^{n+1} - \frac{\Delta t}{2\lambda} = 0 \quad (34)$$

The roots of equation 34 are non-zero, real and opposite in sign. By choosing the positive root, we can guarantee that the polymer stress remains upper bounded.[45]

3.2. Search in unstructured meshes

In the IB scheme discussed above, a set of unstructured grids are free to move inside an underlying domain Ω which is also discretized by an unstructured grid. The Eulerian grid is partitioned among the processors. Since the algorithm requires transfer of data between two grids, one of the key components is the identification of the finite volume in Ω within which the interpolating points in Ω_P lie. This is a potentially expensive search that could affect the parallel scaling of the solver.

The search step involves finding a set of two numbers (i_{proc}, i_{cv}) for each node in the Lagrangian grid, where i_{proc} denotes the processor rank that contains the control volume inside which the point lies and i_{cv} is the global index (unique identifier over the entire computational grid) of the control volume. Since the partitioning in CDP is common-node

based, each processor has a unique set of control volumes and hence the search generally returns a unique result. In the unlikely scenario of the point lying exactly on the boundary of a control volume, it is assigned to the processor with lowest rank. We use alternating digital tree (ADT) [49] to perform the search, which is an extension of the digital tree search technique. Digital trees are recursive data structures constructed by defining a root, and assigning an element to one of two branches based upon whether the bounding box of that element satisfies some geometric condition. The setup time and tree storage requirements for digital trees are roughly proportional to the number of elements making them particularly suited for unstructured meshes.

3.3. Interpolation and Spreading

There are two steps in the algorithm that require inter-phase transfer of data. In Step 9 of the algorithm we need to interpolate velocity from the Eulerian grid to the Lagrangian grid. The interpolation involves the following steps:

1. Searching : Locating the material point in the Eulerian grid (i_{proc}, i_{cv}) as discussed in Section 3.2.
2. Building a stencil : Once the point is located, we build a stencil, which is a set of nodes in the vicinity of the control volume i_{cv}
3. Weighted Sum : Assign weights to the nodes of the stencil and perform a weighted sum of the quantity of interest to obtain the interpolated value.

In Step 12 of the algorithm, we need to spread force from the Lagrangian grid back to the Eulerian grid. Spreading involves partitioning the force acting on the Lagrangian point into the nodes of the stencil. These operations are discussed below.

Typically IB methods are Cartesian grid based [22, 24, 26, 23], and it is common to use a class of regularized delta functions [22] as kernels in transfer between Lagrangian and Eulerian locations. These kernels utilize the structure and simplicity of a Cartesian grid to provide a compact operator. However, such kernels are not suitable in an unstructured grid setting because of the inherent lack of ordering among the neighboring locations. In this paper, we use two strategies for interpolation and spreading as discussed below.

375 The first strategy is using Shepherd's method[50], which is an inverse distance(ID) inter-
 376 polation approach. Once the control volume containing the Lagrangian point is identified,
 377 we use the nodes that make up the control volume (denoted by $nodes(i_{cv})$) as the stencil. Let
 378 $Q^{(i)}$ denote the quantity we are trying to interpolate in the Lagrangian grid at the location
 379 $X_k^{(i)}$ and $q^{(j)}$ be the corresponding quantity in the Eulerian grid at location $x_k^{(j)}$, then

$$Q^{(i)} = \sum_{j \in nodes(i_{cv})} w^{(i,j)} q^{(j)} \quad (35)$$

$$w^{(i,j)} = \frac{1/(d^{(i,j)})^2}{\sum_{k \in nodes(i_{cv})} 1/(d^{(i,k)})^2} \quad (36)$$

$$d^{(i,j)} = \| X_k^{(i)} - x_k^{(j)} \|_2 \quad (37)$$

380 where superscripts denote the node number, $x^{(j)}$ are the nodal coordinates in the Eulerian
 381 grid, $w^{(i,j)}$ are the weights of interpolation, $d^{(i,j)}$ denotes the distance between node j in the
 382 Eulerian grid and the Lagrangian point, $\| \cdot \|_2$ is the L^2 norm operator.

383 The second interpolation strategy is the Moving Least Squares (MLS), following the
 384 approach proposed by Vanella et al [51]. Once the control volume containing the Lagrangian
 385 point is identified, we find the node (i_{no}) closest to the Lagrangian point in the control
 386 volume. The stencil is then constructed as the set of neighbors of the closest nodes (denoted
 387 by $nb(i_{no})$). Neighbors of a node are the set of nodes that share at least one control volume
 388 with the given node including itself (This would result in 27 neighbors for an internal node
 389 in a Cartesian grid). Let $P(X_k)$ denote the linear basis function :

$$P^T(X_k) = \begin{bmatrix} 1 & X_1 & X_2 & X_3 \end{bmatrix} \quad (38)$$

390 Then using the MLS method $Q^{(i)}$ can be approximated as :

$$Q^{(i)} = P^T(X_k^{(i)})Z \quad (39)$$

391 where Z is the vector of unknown coefficients of size 4×1 . Z can be obtained by
 392 minimizing the following weighted L^2 norm :

$$J = \sum_{j \in nb(i_{no})} W(X_k^{(i)} - x_k^{(j)}) [P^T(x_k^{(j)})Z - q^{(j)}] \quad (40)$$

393 Minimizing J w.r.t Z results in

$$AZ = BY \quad (41)$$

$$A = \sum_{j \in nb(i_{no})} W(X_k^{(i)} - x_k^{(j)}) P(x_k^{(j)}) P^T(x_k^{(j)}) \quad (42)$$

$$B = \left[W(X_k^{(i)} - x_k^{(j_1)}) P(x_k^{(j_1)}) \dots W(X_k^{(i)} - x_k^{(j_{nnb})}) P(x_k^{(j_{nnb})}) \right] \quad (43)$$

$$Y^T = \left[q^{(j_1)} \dots q^{(j_{nnb})} \right] \quad (44)$$

394 In the above equations $\{j_1, j_2, \dots, j_{nnb}\}$ are the indices of neighboring nodes of i_{no} and nnb
 395 is the number of neighbors. We can express $Q^{(i)}$ as

$$Q^{(i)} = \Psi^T(X_k^{(i)})Y \quad (45)$$

$$\Psi^T(X_k^{(i)}) = P^T(X_k^{(i)})A^{-1}B \quad (46)$$

396 Here Ψ denotes the weights at each point in the stencil similar to $w^{(i,j)}$ in the ID inter-
 397 polation. The weight function used here is a simple cubic spline:

$$W(x_k) = \begin{cases} 2/3 - 4r + 4r^3 & \text{if } r^{(i)} \leq 0.5 \\ 4/3 - 4r + 4r^2 - 4/3r^3 & \text{if } 0.5 \leq r^{(i)} \leq 1 \\ 0 & \text{if } r > 1.0 \end{cases} \quad (47)$$

398 where $r = \|x_k\|_2 / h$, with h being the local mesh resolution, computed as the maximum
 399 distance from a node to its neighbors.

400 The second inter-phase transfer of data occurs in Step 12 of the algorithm where the
 401 rigid body constraint force is spread from the Lagrangian grid to the Eulerian grid. The
 402 spreading operation is performed using the same stencil as that of interpolation, the only
 403 difference being that we use the weights of interpolation to partition force among the nodes
 404 of the stencil. We also need to scale the interpolation weights by a factor so that we ensure
 405 force conservation in the spreading step. The constant factor c can be obtained as :

$$c = \frac{\Delta_{V,L}^{(i)}}{\sum_{j \in stencil} w^{(i,j)} \Delta_V^{(j)}} \quad (48)$$

406 where $\Delta_{V,L}^{(i)}$ is the volume at the location $X_k^{(i)}$ in the Lagrangian grid and $\Delta_V^{(j)}$ is the
 407 volume at location $x_k^{(j)}$ in the Eulerian grid.

408 Compared to ID interpolation, MLS is linearly exact and typically less dependent on the
 409 exact location of the stencil points, however MLS requires the determination of the inverse
 410 of an ill-conditioned matrix.

411 3.4. Evaluation of the indicator function

412 As discussed in Section 2.4, the particle regions in the Eulerian grid are defined by an
 413 indicator function Θ which has a value of unity inside the particle regions and zero outside
 414 the particle regions. The indicator function can be thought of as a projection of unity from
 415 the Lagrangian grid to the Eulerian grid and we could use the spreading operators defined in
 416 Section 3.3 to perform this projection. However, this does not guarantee that Θ be exactly
 417 unity inside the particle regions, nor does it ensure that $0 \leq \Theta \leq 1$ because of the nature of
 418 the interpolation. Hence we use a different strategy for the construction of Θ . For simplicity,
 419 assume that there is only one particle. Let R be the radius of the particle and $r^{(i)}$ be the
 420 distance of point $x_k^{(i)}$ in the Eulerian grid from the center of the sphere. The following
 421 criteria is used to define Θ :

$$\Theta^{(i)} = \begin{cases} 1 & \text{if } r^{(i)} \leq R_{min} \\ 0 & \text{if } r^{(i)} \geq R_{max} \\ g(\epsilon^{(i)}) & \text{otherwise} \end{cases} \quad (49)$$

where $R_{min} = R - s$, $R_{max} = R + s$, $\epsilon^{(i)} = (r^{(i)} - R_{min})/(R_{max} - R_{min})$ and s is the thickness of the smeared region.

The function $g(\epsilon)$ is assumed to be a fourth order polynomial

$$g(\epsilon) = c_0 + c_1\epsilon + c_2\epsilon^2 + c_3\epsilon^3 + c_4\epsilon^4 \quad (50)$$

satisfying the following conditions :

1. $g(0) = 1$
2. $g(1) = 0$
3. $\frac{dg}{d\epsilon} = 0$ at $\epsilon = 0$
4. $\frac{dg}{d\epsilon} = 0$ at $\epsilon = 1$
5. $\sum_i \Theta^{(i)} v^{(i)} = \frac{4}{3}\pi R^3$. The summation is completed over the Eulerian grid.

The smearing length s needs to be chosen in terms of the characteristic mesh resolution h , defined as the maximum distance between a node and its neighbor in the Eulerian grid. Note that h can be computed in the beginning of the simulation using brute force. If s is chosen much smaller than h , then there could be sub-grid scale displacements of the particle, which will not alter the indicator function in the Eulerian grid. Moreover, the resulting steep density gradients could result in numerical instability. In this regard, it can be argued that s needs to be chosen close to the mesh resolution h . At the same time with a large value of s , the density gradients will be smoother near the interface, making the system numerically less stiff, at the cost of having a less sharp solid-fluid interface in the Eulerian grid.

Hence we need to choose a value of s , which is small enough to retain a sharp interface, but large enough to ensure numerical stability. We perform a simple numerical experiment by simulating a confined two-dimensional cylinder of radius a moving at a specified uniform velocity ($Re = 1$). The density ratio ρ_p/ρ_f was chosen to be 10, which is less than the maximum density ratio used in the paper. This problem is chosen because the velocity and pressure field is independent of the density ratio and this helps in isolating the errors introduced by the choice of smearing length s . We report the maximum error in the velocity

(a) Error in velocity

(b) Error in pressure

Figure 3: Maximum error in velocity(U) and pressure(P) fields between body-fitted (BF) and immersed boundary (BF) calculations as a function of smearing length s for two grid resolutions. The density ratio, $\rho_p/\rho_f = 10$

and pressure field in Figure 3 compared to the body-fitted computations, as a function of the smearing length (s) for two different mesh resolutions. Firstly, we are able to achieve stable computations at this density ratio for $s = h$. Also the error in velocity and pressure fields increase with smearing length as expected. Hence for the rest of the paper we have chosen the characteristic mesh resolution as the smearing length ($s = h$).

4. Validation

4.1. Taylor Green Vortex

Taylor-Green vortices are a two-dimensional, stationary array of decaying vortices in a Newtonian fluid with the following analytical solution for the velocity and pressure fields:

$$u(x, y, t) = \sin(k_x x) \cos(k_y y) e^{-(k_x^2 + k_y^2) \nu t} \quad (51)$$

$$v(x, y, t) = -\frac{k_x}{k_y} \sin(k_y y) \cos(k_x x) e^{-(k_x^2 + k_y^2) \nu t} \quad (52)$$

$$p(x, y, t) = \frac{1}{2}(\cos^2(k_y y) \frac{k_x^2}{k_y^2} - \sin^2(k_x x)) e^{-2(k_x^2 + k_y^2) \nu t} \quad (53)$$

In order to test the order of accuracy of the interpolation and spreading operators, we simulate this flow in a three-dimensional periodic cubical domain, with an immersed spherical body at the center of the domain. The wavenumbers in both directions ($k_x = k_y = k$) are set to 2π . The relevant length scale in this problem is the wavelength $\lambda = \frac{2\pi}{k}$. The viscosity ($\mu = \mu_s$) is set to 0.1 kg/(ms) and the density is set to $\rho_f = 1.0 \text{ kg/m}^3$, so that the Reynolds number ($Re = \frac{\rho_f U \lambda}{\mu}$) at time $t = 0$ is 10. The computational domain size is $2\lambda \times 2\lambda \times 2\lambda$ and the radius of the sphere is 0.5λ . The immersed sphere is treated as a stationary placeholder with a known (analytical) velocity field in this simulation, not as a rigid particle and hence this is a one-way coupled problem. The analytical solutions provide the initial condition as well as the desired velocity in the immersed particle grid at all times.

We performed grid convergence study for this test case by systematically refining both the Eulerian and the Lagrangian grid, with the Lagrangian grid being about twice as fine as the Eulerian grid. Figure 4 shows the maximum error in velocity for different grid sizes for the plain flow solver (without IB coupling) and the coupled IB flow solver. First we find that second order convergence of the base solver is retained. However, the error increases in the presence of the immersed object. The error is an order of magnitude higher with the inverse distance(ID) interpolation scheme. A similar behavior is reported by Apte et al. [33]. However, the error is smaller in the case of Moving Least Square(MLS) interpolation scheme. Note that MLS uses a wider stencil for interpolation compared to ID. Hence the interface is sharper in the case of ID interpolation.

4.2. Newtonian flow over a circular cylinder

In this section, we simulate steady flow past a circular cylinder of diameter d placed at the center of a rectangular domain of dimensions $40d \times 40d$. The freestream velocity U is imposed at the inlet, a convective outflow condition is imposed at the outlet and slip boundary conditions are imposed on the lateral boundaries. Simulations are carried out at Reynolds numbers ($Re = \frac{\rho U d}{\mu}$) 10, 20 and 40 in a uniform Cartesian grid with a resolution

Figure 4: Maximum error in velocity in case of Taylor-green vortices in a Cartesian grid illustrating second order convergence for both ID (inverse-distance) and MLS (moving least squares) interpolation schemes.

of $d/15$. This is a one-way coupled problem as the cylinder velocity (equals zero), is known at all times. Hence step 10 and 11 in the algorithm are skipped and the known velocity is used as the $(^{RBM}V)_i$ while computing the IB forcing term. The total drag experienced by the cylinder is the volumetric sum of the IB force f_i .

Table 1 compares the drag coefficients obtained by our immersed boundary (IB) solver and the body-fitted (BF) solver with other numerical simulations [52, 53, 54] and experiments [55], showing that the IB solver is able to predict the drag very well at this coarse resolution.

Table 1: Comparison of drag coefficients for Newtonian flow past a circular cylinder

Re	IB	BF	Park et al. [52]	Sucker et al [53]	Tritton et al[55]	Silva et al [54]
10	2.82	2.83	2.78	2.67		2.81
20	2.07	2.03	2.01	2.08	2.22	2.04
40	1.58	1.51	1.51	1.73	1.48	1.54

Figure 5 compares IB and BF results in detail at $Re = 10$. The fields are compared along

two curves s and s_+ . The curve s follows the surface of the cylinder and the curve s_+ is offset from the surface such that it follows the edge of the smeared region. We use the curve s_+ for making comparison of velocity derivatives because the calculation of derivatives along this curve does not involve the values at the grid points inside the particle. It is clear that the IB solver is able to accurately capture velocity as well as its derivatives with a relatively coarse resolution.

4.3. Viscoelastic flow past cylinder

In this section we consider the two-dimensional viscoelastic flow of Oldroyd-B fluid past a cylinder of radius a that is placed in the center of a plane channel (see Figure 6). The ratio of channel height H to cylinder radius a is 4. The cylinder radius a is used as the characteristic length scale and the mean inlet velocity U is used as the characteristic velocity scale so that the Reynolds number $Re = \rho U a / \mu_0$ and Deborah number $De = \lambda U / a$. The simulations are carried out at $Re = 0.05$.

The fully developed parabolic velocity profile is specified at the inlet along with the conformation tensor c_{ij} associated with this velocity profile[56]. A convective outflow condition for velocity is imposed at the outlet and no-slip conditions are imposed at the channel walls. This benchmark problem is considered as a stringent test of the numerical algorithm because of the presence of upstream and downstream stagnation points, which leads to steep stress boundary layers on the surface of the cylinder and in the wake.[57]

4.3.1. Dilute Solution

Two-dimensional viscoelastic flow past a cylinder has been extensively studied in the literature, both experimentally[58] and numerically [59, 60, 61] [62]. Recently Goyal et al. [36] have used immersed boundary method coupled with a Lattice-Boltzmann framework to study this problem. We compare our results to those reported in [59, 36]. The computational domain used is $L = 80a$, with a length of $L_d = 39a$ downstream of the rear stagnation point of the cylinder (see Figure 6) and the fluid considered here is a dilute Oldroyd-B fluid with $\beta = 0.59$ consistent with the one used by Alves et al. [59]. The Eulerian domain is discretized by a uniform Cartesian grid of resolution h .

(a) $C_P = P/(\frac{1}{2}\rho U_\infty^2)$

(b) u/U_∞

(c) $\frac{\partial u_x}{\partial x}$

(d) $\frac{\partial u_x}{\partial y}$

(e) $\frac{\partial u_y}{\partial x}$

(f) $\frac{\partial u_y}{\partial y}$

Figure 5: Comparison of pressure, velocity and velocity gradients between immersed boundary (IB) and body-fitted (BF) calculations for the flow of Newtonian fluid past cylinder at $Re = 10$.

Figure 6: Geometry for flow past cylinder computations. The cylinder is centered at origin.

Figure 7: Comparison of drag coefficient (C_d) for flow past cylinder in an Oldroyd-B fluid.[59, 36]. The grid resolution is $h = a/30$ for the IB simulations

Table 2: Comparison of drag coefficient for flow past cylinder in an Oldroyd-B fluid ($\beta = 0.59$) [59]. The resolution reported for the simulation results from Alves et al.[59] is the smallest cell size around the cylinder surface

De	IB($h = a/15$)	IB($h = a/30$)	IB($h = a/60$)	Alves et al($h \approx a/420$)
0	139.15	135.37		132.35
0.1	136.39	133.58		130.36
0.2	132.29	129.66		126.63
0.3	128.49	126.01		123.31
0.4	125.56	122.97		120.61
0.5	123.49	121.23		118.83
0.6	122.16	120.04	118.61	117.79
0.7	121.41	119.43		117.32
0.8	121.13	119.18		117.36
0.9	121.21	119.47	118.23	117.85
1.0	121.58	119.88		118.52

Table 2 compares the drag coefficient with Alves et al. [59] for different grid resolutions $a/15, a/30, a/60$. Our simulations capture the decay in drag coefficient until $De = 0.7$ (Figure 7), followed by a marginal increase. The drag coefficients computed using IB method are consistently about 2% higher than those reported by Alves et al[59] for the grid resolution $a/30$.

Figure 8 shows the streamwise velocity profiles along the centerline downstream of the cylinder for $De = 0, 0.6, 0.9$ ($h = a/30$). The velocity profiles are in good agreement with the data reported by Alves et al[59]. The Newtonian velocity profile is fore-aft symmetric at this Reynolds number ($Re = 0.05$). In case of $De = 0.6, 0.9$, the velocity decays over a longer distance compared to the Newtonian case. This 'extended wake' behavior is also observed in the case of spheres sedimenting in a viscoelastic fluid [63, 64]. The velocity profile upstream of the cylinder is identical for the Newtonian and viscoelastic cases.

Figure 8: Stream-wise velocity along the centerline of the channel for flow past cylinder in an Oldroyd-B fluid.[59]. (The mesh resolution is $h = a/30$ for IB computations)

Figure 9: Polymer stress (τ^P_{xx}) along the downstream centerline of the channel for flow past cylinder in an Oldroyd-B fluid.[59](The mesh resolution is $h = a/30$ for IB computations)

Figure 10: Grid convergence of polymer stress (τ_{xx}^P) along the downstream centerline of the channel for flow past cylinder in an Oldroyd-B fluid [59]

Figure 9 shows the elastic stress component τ_{xx} along the centerline, in the downstream of the cylinder ($h = a/30$). The elastic stresses grow with Deborah number and resolving this high stress gradient in the wake requires high spatial resolution [59]. The required resolution is particularly high for Oldroyd-B fluids as shown in [57]. It is clear that we lack the spatial resolution beyond $De = 0.6$, to resolve the elastic stress accurately. Although the elastic stresses are not well captured at this resolution for higher Deborah numbers, the drag force is predicted well. The same behavior was reported in [36]. Figure 10 shows the grid convergence of polymer stress along the centerline for $De = 0.6, 0.9$. The stresses are resolved better with increasing resolution. For $De = 0.6$, we achieve convergence at a resolution of about $a/30$, whereas for $De = 0.9$, we achieve convergence at a resolution of about $a/120$.

4.3.2. Ultradilute solution

Bajaj et al. [57] studied the viscoelastic flow around a confined cylinder for an ultradilute Oldroyd-B fluid and FENE-P fluid using Finite Element(FEM) computations. They showed

Figure 11: Streamwise velocity (u_x) and velocity gradient ($\kappa_{xx} = \frac{\partial u_x}{\partial x}$) for an ultradilute solution along the centerline in the wake of the cylinder [57]

that when $De \approx 1$, the polymers flowing along the centerline downstream of the cylinder undergo a coil-stretch transition resulting in the breakdown of Finite Element computations in the case of the Oldroyd-B fluid. The computational difficulty arises from the existence of large polymer stress and stress gradients within narrow regions of the flow, which becomes harder to resolve with higher De . In the case of FENE-P fluids, the coil-stretch transition leads to polymer molecules extending close to their fully-extended length, with the maximum stress remaining bounded with increasing De . We carried out these computations using the IB solver in a domain of length $L = 120a$, $L_d = 59a$ (see Figure 6) similar to the one used by Bajaj et al. [57]. The Eulerian domain is discretized by a uniform Cartesian grid and we present mesh converged results in this section. Since the fluid is ultradilute, the parameter β is set to 1. Hence the velocity field is identical to that of a Newtonian fluid (independent of De) and the elastic stresses $\tau_{ij}^P = 0$

Figure 11 shows that the streamwise velocity (u_x) and velocity gradient ($\kappa_{xx} = \frac{\partial u_x}{\partial x}$) profiles along the centerline, downstream of the cylinder are in close agreement with Bajaj et al [57].

Figure 12: Comparison of c_{xx} component of conformation tensor computed using our IB solver with those reported by Bajaj et al. [57].

First we present the results for an Oldroyd-B fluid. Our finite volume computations break down beyond $De = 0.8$, whereas Bajaj et al. [57] had reported that their FEM computations break down beyond $De \approx 1$. We are unable to achieve convergence in polymer conformation tensor components at $De = 1$. At the highest Deborah number $De = 0.8$ for which we obtained convergence, our simulations capture the variation of c_{xx} with good accuracy, as shown in Figure 12. c_{xx} has a value close to 1 near the rear stagnation point and ultimately return to the value of 1 far downstream in the region of fully developed flow. Since the velocity gradient is positive in the downstream centerline (Figure 11), this means that c_{xx} attains a maxima at some point in the wake $x = x^*$. At the maxima, the value of c_{xx} is [57]:

$$c_{xx}|_{x=x^*} = \frac{1}{1 - 2\lambda\kappa_{xx}|_{x=x^*}} \quad (54)$$

Computational difficulties arise when the value of $\lambda\kappa_{xx}|_{x=x^*}$ approaches 0.5, due to the inability to resolve the very large stress. At $De = 1.0$, where our computations fail, the value of $\lambda\kappa_{xx}|_{x=x^*} \approx 0.4977$ [57].

Figure 13a shows the dependence of the location of the maxima (x^*) with De . The

(a)

(b)

Figure 13: Variation of location of the maxima(x^*) of c_{xx} in the downstream centerline and the velocity gradient at the maxima ($\lambda\kappa_{xx}|_{x=x^*}$) as a function of De [57]

Figure 14: Dependence of non-dimensional strain rate $\lambda\kappa_{xx}|_{x=x^*}$ with De [57]

Figure 15: Coil-stretch transition in the cylinder wake for an ultradilute solution of Oldroyd-B fluid [57]

simulations predict that location of the maxima (x^*) moves away from the stagnation point with increasing De for the Oldroyd-B fluid, consistent with the findings of Bajaj et al. [57]. It follows from Figure 11 that the velocity gradient at the maxima $\kappa_{xx}|_{x=x^*}$ continuously decreases (Figure 13b). The steep increase in $c_{xx}|_{x=x^*}$ as $\lambda\kappa_{xx}|_{x=x^*}$ approaches 0.5 is shown in Figure 15. This behavior is due to the well-known coil-stretch transition in extensional flows of an Oldroyd-B fluid, leading to an unbounded stress [39]. The reason for coil-stretch transition in this case is the extended period of time a polymer molecule spend in the vicinity of the stagnation point, which leads to a significant accumulation of strain[57]. As a consequence of the coil-stretch transition in the wake of the cylinder, the resolution required to accurately capture this high stress exponentially increase with De [57].

In the case of the FENE-P model, we are able to achieve convergence in the polymer stress at higher De . Figure 12 compares our FENE-P predictions of the component c_{xx} along the downstream centerline at $De = 1.5, 2.0$ with Bajaj et al [57]. As seen in Figure 13a, the location of maxima (x^*) of c_{xx} moves away from the stagnation point for small values of De , while at higher De the maxima shifts closer to the stagnation point eventually attaining a roughly constant value. The value of $\lambda\kappa_{xx}|_{x=x^*} = 0.5$ is not relevant for FENE-P fluids.

588 $\lambda\kappa_{xx}|_{x=x^*}$ exceeds 0.5 with increasing De (Figure 14). Figure 15 shows that c_{xx} remain
589 bounded at high $\lambda\kappa_{xx}|_{x=x^*}$ and our simulations capture this curve well.

590 4.4. Flow Past Sphere

591 In this section, we investigate the accuracy of the immersed boundary scheme in predict-
592 ing the drag coefficient for uniform flow past a fixed sphere. This is also a one-way coupled
593 problem as the sphere velocity ($U = 0$), is known at all times. Hence step 10 and 11 in the
594 algorithm are skipped and the known velocity is used as the $(^{RBM}V)_i$ while computing the
595 IB forcing term. The total drag experienced by the sphere is the volumetric sum of the IB
596 force f_i . In both cases the interpolation scheme used is the inverse distance scheme.

597 4.4.1. Newtonian

598 The test case used here is same as that in Apte et al. [27], where a sphere of radius a
599 is placed at $(5a, 0, 0)$ in a square domain of range $(0, -10a, -10a)$ to $(20a, 10a, 10a)$. except
600 that the grids used here are tetrahedral unstructured. The Lagrangian grid is about twice
601 finer relative to the Eulerian grid resolution. There are about 12 Eulerian cells across the
602 particle domain. Table 3 compares the drag coefficient obtained numerically with those
603 obtained from experimental correlations [65]. The drag coefficients are predicted well again
604 for a reasonably coarse resolution.

Table 3: Comparison of drag coefficient for flow past sphere in a Newtonian fluid [65]

Re	IB	Correlation [65]
10	4.32	4.24
20	2.66	2.69
40	1.79	1.82
100	1.15	1.18

4.4.2. Viscoelastic

In this section, we study the flow past sphere in a FENE-P fluid and compare relevant results with the simulation results from Yang et al. [66] and Padhy et al. [67]. The sphere is confined in a tube such that the sphere-to-tube radius ratio, a/R is 0.243. The relevant FENE-P fluid parameters are $\mu_T = \mu_s + \mu_p = 13.76Pas$, $\lambda = 0.7925s$, $L = 30$, $\beta = 0.59$ [63]. A cylindrical tube of length $30a$ is discretized into 2.3 million tetrahedral elements with smaller elements near the sphere. A fixed immersed sphere is kept at a distance of $5a$ from the inflow boundary. The relevant velocity scale in this problem is the inlet flow velocity (U_∞) and the relevant length scale is the radius of the sphere (a). The Reynolds number is set at $Re = 0.05$. The flow Weissenberg is given by $Wi = \lambda U_\infty / a$.

Figure 16 plots the normalized drag coefficient (the ratio of viscoelastic drag(K_V) to Newtonian drag(K_N)) as a function of flow Weissenberg number. There is good agreement between our IB simulation results and those obtained by the finite element code by Yang and Khomami [66]. Our results also compare well with Padhy et al [67], who used the bodyfitted version of the same finite volume code CDP. The simulations capture the initial reduction in drag coefficient before the coefficient increases with Wi .

We now make detailed comparison between bodyfitted(BF) and immersed boundary (IB) simulations at $Wi = 5$. Both BF and IB simulations are carried out at identical resolutions. We compare the fields in the $x - y$ plane along the curves s and s_+ as shown in Figure 17a. The curve s starts at the upstream centerline, follows the sphere surface and continues downstream. The curve is defined such that the upstream stagnation point is the origin. On the other hand, the curve s_+ is slightly offset from the sphere surface, such that it passes through the boundary of the "smeared region". We use the curve s_+ for the comparison of conformation tensor components, because the "smeared" region is computationally treated as a fluid-solid mixture and interpolation of values to this curve does not involve effects from the interior of the solid where c_{ij} is explicitly set to identity.

Figure 17b and 17c shows that we capture the velocity and pressure along the curve s with good accuracy. We also see that viscoelasticity results in an "extended" wake[64]. The conformation tensor components are compared in Figure 18. We see that c_{ij} is captured

Figure 16: Comparison of normalized drag coefficient for flow past sphere in a FENE-P fluid. [66] [63] [67]

634 accurately in the downstream and upstream directions, with good accuracy along the curved
 635 path. We also qualitatively compare the polymer conformation tensor trace (c_{kk}) profile in
 636 the $x - y$ plane (Figure 18), which shows that the errors are primarily concentrated in the
 637 thin boundary layer over the surface of the sphere (in the vicinity of curve s_+).

638 4.5. Sedimentation of a circular cylinder

639 In this section, we simulate the sedimentation of an infinitely long rigid circular cylinder
 640 of diameter d , in a bounded cavity of dimensions $[0, 8d] \times [0, 24d]$. This is a two-way coupled
 641 problem as the particle is free to move under the action of gravity. This test case is same as
 642 the one presented in Glowinski et al [17]. The initial position of the cylinder is $(4d, 16d)$ and
 643 the gravity(g) is along the y-axis. The cylinder and the fluid are initially at rest. The particle
 644 density ($\rho_p = 1.25\rho_f$) and the viscosity μ correspond to a maximal cylinder Reynolds number
 645 of about $Re = \frac{\rho_f U d}{\mu} = 17.3$, where U is the settling velocity. The simulations are carried out
 646 in a Cartesian grid of resolution $d/50$ for different time steps $\Delta t = 10^{-3}, 7.5 \times 10^{-4}$.

647 Figure 19 shows the time evolution of settling velocity. The cylinder reaches a uniform
 648 velocity quickly and the results are in good agreement with Glowinski et al [17]. The

(a) Definition of Curves s and s_+

(b) $P/(\frac{1}{2}\rho U_\infty^2)$

(c) u/U_∞

Figure 17: Comparison of velocity and pressure along the curve s between immersed boundary(IB) and body-fitted(BF) calculations for the flow of FENE-P fluid past sphere at $Re = 0.05$ and $Wi = 5$. The curves s and s_+ are defined in subfigure (a)

(a) Body-fitted Simulation

(b) Immersed Boundary Simulation

(c) C_{11}

(d) C_{22}

(e) C_{12}

(f) C_{kk}/L^2

Figure 18: Comparison between immersed boundary (IB) and body-fitted (BF) calculations for the flow of FENE-P fluid past sphere at $Re = 0.05$ and $Wi = 5$. (a)-(b) Normalized polymer conformation tensor trace (c_{kk}/L^2) profile in the $x - y$ plane. (c)-(f) Conformation tensor components along the curve s_+

Figure 19: Time evolution of settling velocity of a circular cylinder falling under gravity in a Newtonian fluid [17]

simulation results did not change appreciably by reducing the time step, showing the time step convergence.

4.6. Sphere sedimenting in a FENE-P fluid

In this section, we study the dynamics of a sphere of radius a falling under gravity in a circular channel of radius $4.32a$ filled with a FENE-P fluid ($\beta = 0.35, L^2 = 250$). The sphere and the fluid are at rest initially and we are interested in the transient as well as steady state settling velocity of the particle. The simulations are carried out in unstructured tetrahedral grids of three different grid resolutions ($a/4, a/8, a/16$). At steady state, the Reynolds number $Re = \frac{\rho_f U_\infty a}{\mu_0} = 0.01$ and Weissenberg number $Wi = \frac{\lambda U_\infty}{a} = 2.7$

Figure 20 shows the time evolution of the velocity of the sphere. Unlike the case of a Newtonian fluid, there is a velocity overshoot and subsequent damping before achieving the steady state settling velocity. The existence of this overshoot in viscoelastic fluids is well documented in literature [68] [69] [70]. It is evident that the dynamics (i.e settling velocity) of the particle is consistently predicted at different grid resolutions. However, similar to

Figure 20: Time evolution of velocity magnitude for the simulation of a freely falling sphere under gravity in a FENE-P fluid. ($Re = 0.01, Wi = 2.7$)

the case of flow past cylinder (Section 4.3.1), the polymer conformation tensor is under-predicted at the more coarse grid resolutions. This is qualitatively shown in Figure 21. It is clear that in case of a moving particle, we need higher resolution to capture the polymer stresses accurately. This is because in addition to the solid-fluid interface being smeared, the interface moves as well.

4.7. Rotation of sphere in viscoelastic shear flow

Snijkers et al. [71] studied the effect of viscoelasticity of the suspending liquid on the rotation rate of a freely suspended, torque free, inertialess, density matched, rigid, non-Brownian sphere in an externally imposed shear flow by means of three-dimensional finite element simulations. They used single mode Giesekus model for obtaining the simulation results with the parameters obtained by fitting the rheological data. We used the same parameters for our IB simulations ($\zeta = 3.2 \times 10^{-4}$, $\beta = 0.611$, $\lambda = 6.18s$). The shear Weissenberg number is given by $Wi = \lambda\gamma$, with γ being the shear rate. The IB simulations are carried out in a domain of size $20a \times 20a \times 70a$, with x being the vorticity direction, y

Figure 21: Grid convergence of the trace of polymer conformation tensor (c_{kk}/L^2) for a freely falling sphere under gravity in a FENE-P fluid ($Re = 0.01, Wi = 2.7$)

Figure 22: Comparison of rotation rates of a sphere in viscoelastic shear flow with Snijkers et al. [71]

being the flow gradient direction and z being the flow direction is a uniform grid of resolution $a/8$, where a is the radius of the sphere. We enforce periodic boundary conditions among x and z directions and walls imposing a shear flow in the y direction. The comparison between IB simulations and the simulations by Snijkers et al. [71] is shown in Figure 22 for Wi in the range 0 to 5, showing good agreement. The simulations capture the reduction in rotation speed, relative to the Newtonian case (shown in dashed line in Figure 22), which is consistent with experiments [72].

4.8. Sedimentation under orthogonal shear

In this section, we study the sedimentation of suspension of spheres in viscoelastic fluids under imposed shear perpendicular to the direction of sedimentation. This problem is relevant in the hydraulic fracturing process used during the drilling of oil and gas wells [73] and serves as an example to demonstrate the capability of the solver. Experiments [74, 75] have shown that the settling velocity of particles is reduced (or the drag force is increased) in Boger fluids subject to orthogonal shear. Padhy et al. [67] investigated sedimentation of a single particle in elastic Boger fluids under orthogonal shear using numerical simulations

and found a decrease in settling velocity consistent with the experiments. The results of the single sphere experiments [74], in comparison with concentrated suspension experiments [75] indicate that the particle concentration is very important in determining the settling rates.

Here we study the effect of suspension concentration on settling rate of a suspension of spheres in a FENE-P fluid ($\lambda = 0.9s$, $\beta = 0.34$, $L^2 = 250$, $\mu_s = 0.3298Pas$, $\rho_f = 1302.6kg/m^3$). The schematic of the simulation is shown in Figure 23. The inner cylinder is at rest, while the outer cylinder is rotating at a constant angular velocity of ω_o . We use periodic boundary conditions in the sedimentation direction under the assumption that the bottom wall of the Taylor-Couette cell is very far away. The problem details are listed below:

- Inner cylinder radius, $R_i = 7.55cm$
- Outer cylinder radius, $R_o = 8.55cm$
- Cylinder gap, $h = R_o - R_i = 1cm$
- Cylinder height $H = 4.8cm$
- Sphere diameter $d = 4.8mm$
- Sphere density $\rho_p = 2790kg/m^3$

The domain is discretized using hexahedral elements with about 20 Eulerian cells across the particle diameter resulting in a total of 19 million elements. For multiple particles, we need to model inter-particle collision to prevent unphysical overlap. For this simulation, we use the repulsive potential collision model proposed by Glowinski et al. [17]. The particle concentrations(ϕ) considered here are 1% to 5%, resulting in 42 to 210 particles in the domain.

The non-dimensional parameters of interest are the shear Weissenberg number ($Wi = \frac{\lambda\omega_o R_o}{h}$) and the flow Weissenberg number ($\theta = \frac{\lambda U}{d}$), where U is the settling velocity. Figure 24a shows the variation of relative drag for a single particle settling in the Taylor-Couette cell as a function of shear Weissenberg number. In this figure, U_0 is the settling velocity in the absence of shear ($Wi = 0$), U is the settling velocity at the given Wi and the results

Figure 23: Schematic for orthogonal shear simulations. R_i is the inner cylinder radius, R_o is the outer cylinder radius, H is the height of the cylinder, $\vec{g}$ is the gravity. The inner cylinder is at rest and outer cylinder is rotating at an angular velocity ω_o .

are presented in terms of U_0/U . The flow Weissenberg number at zero shear $\theta_0 = \frac{\lambda U_0}{d}$ is 1.93. We see a reduction in settling velocity with increasing Wi similar to the observations in [67].

Next, we look at how the settling velocity is affected as a function of particle concentration ϕ in Figure 24b at a fixed $Wi = 1.07$. The results are presented in terms of $U_{single}/\bar{U}$, where U_{single} is the settling velocity of a single sphere and $\bar{U}$ is the mean settling velocity of the suspension at the given concentration ϕ . It is clear that the settling velocity is significantly reduced with increasing concentration. At 1% concentration, there is a drag increase by a factor of 1.1 relative to a single sphere and the factor goes up to 1.4 at 5% concentration. We look at the wake structure of polymers in Figure 25, where iso-surfaces of the trace of conformation tensor (c_{kk}) are plotted in order to understand the nature of particle-particle interactions. For $Wi = 0$ (Figure 25a), the polymer stretch in the wake is essentially similar to those corresponding to simple sedimentation (Figure 21). At $Wi = 1$, the applied shear, tends to extend the polymer stretching in the shear direction as seen in Figure 25b. The

Figure 24: Relative reduction in settling velocity for (a) single particle as a function of shear Weissenberg number and (b) suspension of spheres as a function of concentration (ϕ) between 1% and 5% at a fixed $Wi \approx 1$

length of polymer wake is also reduced as the flow Weissenberg number reduces. In case of a suspension, we see that particle interactions modify the wake structure. In Figure 25c, which is a 2% suspension, we can clearly see some of the polymer wake being "split" by trailing spheres, while there are also locally isolated particles which have retained the wake structure corresponding to a single particle. The particle-wake interactions become more complex in the case of 5% suspension. This discussion shows that even a concentration of 1% cannot be considered dilute enough for such polymeric fluids and single particle simulations will not be able to capture this complex interaction, which further underlines the usefulness of the computational tool developed.

5. Conclusion

A numerical formulation for fully resolved simulation of particles moving in viscoelastic fluid is presented based on the Immersed Boundary (IB) technique. The governing equations are extended over the whole domain including the particle regions, which are assumed to be

(a) $Wi = 0$, Single particle

(b) $Wi \approx 1$, Single particle

(c) $Wi \approx 1$, $\phi \approx 0.02$

(d) $Wi \approx 1$, $\phi \approx 0.05$

Figure 25: Iso-surface of the trace of the conformation tensor (c_{kk}) at 10% of the maximum stretching showing wake interaction in suspensions

745 filled with fluid that is of density equal to the particle density and a rigidity constraint force is
 746 applied in the particle regions that enforce rigid body motion. The inter phase interpolations
 747 are performed using either Shepherd’s method or Moving least squares. We simulated several
 748 benchmark flows in order to validate the algorithm. The second order accuracy of the
 749 solver was retained as shown in the Taylor Green vortex simulations. Simulation of flow
 750 past cylinder in an ultradilute Oldroyd-B fluid revealed the coil stretch transition that
 751 resulted in the breakdown of computation beyond $De \approx 1$. It was shown that coarse
 752 grids under-predict the polymer stretch. We also demonstrated the capability of the solver
 753 in predicting the dynamics of a freely suspended particle by performing simulations of a
 754 sedimenting cylinder in a Newtonian fluid, a sedimenting sphere in a FENE-P fluid and
 755 a sphere subjected to shear flow in a Giesekus fluid. Finally, we solve the problem of a
 756 suspension of spheres sedimentating under orthogonal shear in a viscoelastic fluid and show
 757 that particle concentrations as small as 1% cannot be considered dilute.

758 Acknowledgments

759 The authors acknowledge support from the U.S. Army High Performance Computing
 760 Research Center (AHPCRC) Grant# W911NF07200271, and support from Stanford Uni-
 761 versitys Certainty computer cluster, which is funded by the American Recovery and Rein-
 762 vestment Act (ARRA) of 2009 (grant number: W911NF07200271). In addition, this work
 763 was supported by the National Science Foundation under Grant No. CBET-1337051.

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