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An Arbitrary Lagrangian Eulerian Formulation with Exact Mass Conservation for the Numerical Simulation of a Rising Bubble in a Viscoelastic Fluid

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Abstract: The arbitrary Lagrangian Eulerian (ALE) framework presented in [Sahin and Guventurk, An Arbitrary Lagrangian-Eulerian framework with exact mass conservation for the numerical simulation of 2D rising bubble problem. International Journal for Numerical Methods in Engineering, 112:2110-2134, (2017)] has been initially extended to three-dimensional multiphase flows. In the present formulation, the governing equations are discretized over the unstructured moving meshes using the divergence-free side-centered finite volume formulation with the exact jump conditions across the interface. Therefore, the pressure field is treated to be discontinuous with the discontinuous treatment of density and viscosity. The surface tension term at the interface is handled as a force tangent to the interface. A special attention is given to the application of the kinematic boundary condition to be compatible with the local and global discrete geometric conservation laws (DGCL) as well as the discrete form of the continuity equation in order to conserve the total mass of both species at machine precision. The mesh deformation is achieved by solving the linear elasticity equations with the modified material properties based on the minimum distance to the interface. Then, the numerical method has been further extended to viscoelastic multiphase flows using the approach in [M. Sahin, A stable unstructured finite volume method for parallel large-scale viscoelastic fluid flow calculations. Journal of non-Newtonian Fluid Mechanics, 166:779-791, (2011)]. The resulting algebraic equations are solved in a fully coupled (monolithic) manner and a one-level restricted additive Schwarz preconditioner with a block-incomplete factorization is utilized within each partitioned sub-domain. The proposed method is initially validated by simulating the classical three-dimensional benchmark problems of a single rising bubble in a Newtonian fluid and then it will be applied to a rising bubble in an Oldroyd-B fluid. The mass of the bubble is conserved and discontinuous pressure field is obtained in order to avoid errors due to the incompressibility condition in the vicinity of the interface.

Keywords: Multiphase Flows, Unstructured Finite Volume, ALE Methods, Geometric Conservation Law, Exact Mass Conservation.

1 Introduction

Numerical simulation of viscous multi-fluid flows with moving boundaries is getting more attention over the past several decades. These flows are frequently encountered in nature and industrial applications such as food processing, targeted drug delivery, drop formation, etc., and the interfacial dynamics has a significant role for output. The complex behavior of multiphase flows still posses significant computational challenges. One of the main difficulties for this type of flows is that the material properties are discontinuous across the interface and the shape and the location of the interface, which are time dependent, are not priori known. In addition, the surface tension should be taken into account, which is a force tangent to the surface and it yields a pressure jump across the interface [1]. However, the pressure jump is not due to the surface tension only but also a consequence of the viscosity jump with nonzero normal derivative of the normal velocity component at the interface [2]. Therefore, across the interface, these jump conditions have to be satisfied accurately. Besides, the numerical algorithm should handle the large distortions at the interface. Furthermore, the mass of the species has to be conserved during the numerical simulation.

The early numerical algorithms to solve multiphase flow problems are mainly based on fixed Cartesian grids [3, 4, 5, 6]. In these algorithms, the density and viscosity jumps, and the surface tension at the interface are smoothed across the interface to avoid numerical instabilities near the interface [7]. Hence, the interface has a finite thickness and is no longer sharp. This assumption yields number of issues. First of all, it smears out the sharp interface due to the used discrete delta function approach and it is only about first-order accurate for general problems [8]. Besides, the smoothing must be over a few grid cells, resulting in a relatively fine mesh or dynamic adaptive mesh refinement. Furthermore, the large variations in the transport properties across the interface lead to relatively stiff algebraic systems [9]. An another approach to solve multiphase flows is to use the Arbitrary Lagrangian-Eulerian (ALE) formulation [10]. The advantage of the technique is that the mesh follows the interface and the governing equations are discretized over unstructured moving meshes. Therefore, the interface is sharply defined. However, the numerical discretization requires that the discrete geometric conservation law (DGCL) [11] should be satisfied at discrete level.

In the current work, the Arbitrary Lagrangian Eulerian (ALE) approach [12] has been initially extended to three-dimensions to solve incompressible multiphase fluid flow problems while satisfying the exact mass conservation for each species at machine precision. The pressure field is treated to be discontinuous across the interface with the discontinuous treatment of density and viscosity. The discontinuous treatment of pressure field helps us to avoid errors due to the incompressibility condition in the vicinity of the interface. The surface tension term at the interface is treated as a force tangent to the interface and computed using the straight line integral of tangent vectors at the interface. The jump conditions are exactly satisfied across the fluid-fluid interface. The parasitic currents are found to be very sensitive to the numerical calculation of normal vectors. Several different normal vector calculation methods have been investigated in order to reduce the parasitic currents to machine precision in three-dimensions. The nonlinearities related due to the unknown interface location and the convection terms are treated using several Newtons's sub-iterations. The resulting algebraic equations are solved in a fully coupled (monolithic) manner and a one-level restricted additive Schwarz preconditioner with a block-incomplete factorization (ILU) within each partitioned sub-domains is utilized for the resulting fully coupled system. The multiphase algorithm has also been further extended to isothermal viscoelastic non-Newtonian fluids by solving the Oldroyd-B fluid equations using an approach similar to that of [13].

2 Problem Statement

The governing equations for the incompressible multiphase Oldroyd-B fluid flow in the Cartesian coordinate system can be written as follows: the continuity equation

$$-\oint_{\partial\Omega_e} \mathbf{n}\cdot\mathbf{u}\, dS = 0 \tag{1}$$

the Oldroyd-B equation

$$\lambda \int_{\Omega_d} \left[\frac{\partial \mathbf{T}}{\partial t} dV + (\nabla \mathbf{u})^\top \cdot \mathbf{T} - \mathbf{T}\cdot\nabla\mathbf{u}\right] dV + \lambda \oint_{\partial\Omega_d} [\mathbf{n}\cdot(\mathbf{u}-\dot{\mathbf{x}})]\,\mathbf{T} dS = \mu_p \oint_{\partial\Omega_d} \mathbf{n}\cdot(\nabla\mathbf{u}+\nabla\mathbf{u}^\top) dS + \int_{\Omega_d} \mathbf{T} dV \tag{2}$$

the momentum equations

$$\rho \int_{\Omega_d} \frac{\partial \mathbf{u}}{\partial t} dV + \rho \oint_{\partial\Omega_d} [\mathbf{n}\cdot(\mathbf{u}-\dot{\mathbf{x}})]\,\mathbf{u} dS + \oint_{\partial\Omega_d} \mathbf{n} p dS = \mu_s \oint_{\partial\Omega_d} \mathbf{n}\cdot(\nabla\mathbf{u}+\nabla\mathbf{u}^\top) dS + \oint_{\partial\Omega_d} \mathbf{n}\cdot\mathbf{T} dS + \rho \int_{\Omega_d} \mathbf{g} dV \tag{3}$$

Across the fluid-fluid interface the following jump condition must be satisfied:

$$[\![\mu_s(\nabla\mathbf{u}+\nabla\mathbf{u}^\top) + \mathbf{T} - p\mathbf{I}]\!]\cdot\mathbf{n} = -\sigma\kappa\mathbf{n} \tag{4}$$

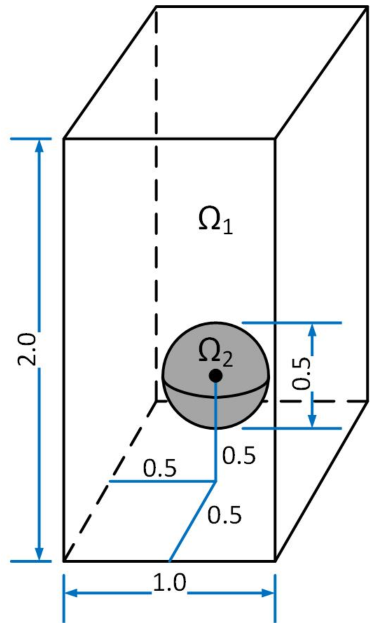

Figure 1: Illustration of a rising bubble problem.

In these equations, V is the control volume, S is the control volume surface area, $\mathbf{n}$ represents the outward normal vector, $\mathbf{u}$ represents the local fluid velocity vector, $\dot{\mathbf{x}}$ represents the grid velocity, p is the pressure, $\mathbf{T}$ is the viscoelastic extra stress tensor, ρ represents the fluid density, μ_s and μ_p represent the solvent and polymer dynamic viscosities, respectively, λ is the relaxation time, $\mathbf{g}$ represents the gravity vector, σ represents the surface tension coefficient and κ represents the curvature at fluid-fluid interface.

3 Numerical Results

In order to assess the accuracy of the present ALE algorithm, the benchmark problem of a single rising bubble $\Omega_2 = \Omega_2(t) \subset \Omega$ in a Newtonian fluid in three-dimensions [14] is initially presented for a cuboid tank $\Omega = [0,1] \times [0,2] \times [0,1]$. The computational domain is illustrated in Figure 1. The bubble is lighter than the surrounding fluid $\Omega_1 = \Omega \setminus \Omega_2(t)$. Therefore, the bubble will rise and change its shape due to the buoyancy effects. The material properties of the both fluids are provided in [14] and presented in Table 1. The physical boundary conditions on the walls are set to no-slip boundary condition.

The quantities such as center of mass, rise velocity and mass conservation are investigated and the results are compared with the other results available in the literature [14]. For the numerical simulations, 2 different meshes M1 and M2 are used which are presented together with the meshes provided in [14] in Table 2. The center of mass can be computed as

$$\mathbf{X}_c(t) = (x_c, y_c, z_c) = \frac{\int_{\Omega_2(t)} \mathbf{x} dxdydz}{\int_{\Omega_2(t)} dxdydz}. \tag{5}$$

and the rise velocity is given by

$$\mathbf{U}_c(t) = (u_c, v_c, w_c) = \frac{d\mathbf{X}_c}{dt} = \frac{\int_{\Omega_2(t)} \frac{\partial \mathbf{x}}{\partial t} dxdydz + \oint_{\partial\Omega_2(t)} \mathbf{x}(\mathbf{n} \cdot \frac{d\mathbf{x}}{dt}) dA}{\int_{\Omega_2(t)} dxdydz} = \frac{\oint_{\partial\Omega_2(t)} \mathbf{x}(\mathbf{n} \cdot \mathbf{u}) dA}{\int_{\Omega_2(t)} dxdydz}. \tag{6}$$

As it may be seen from Figure 2 and Figure 3-[a], the solution shows a relatively good agreement with the results of NaSt3D. Nevertheless, it is necessary to have a closer look to the curves. A detailed picture of the results indicates that the mesh M2 gives a relatively more accurate result. However, the results of the mesh

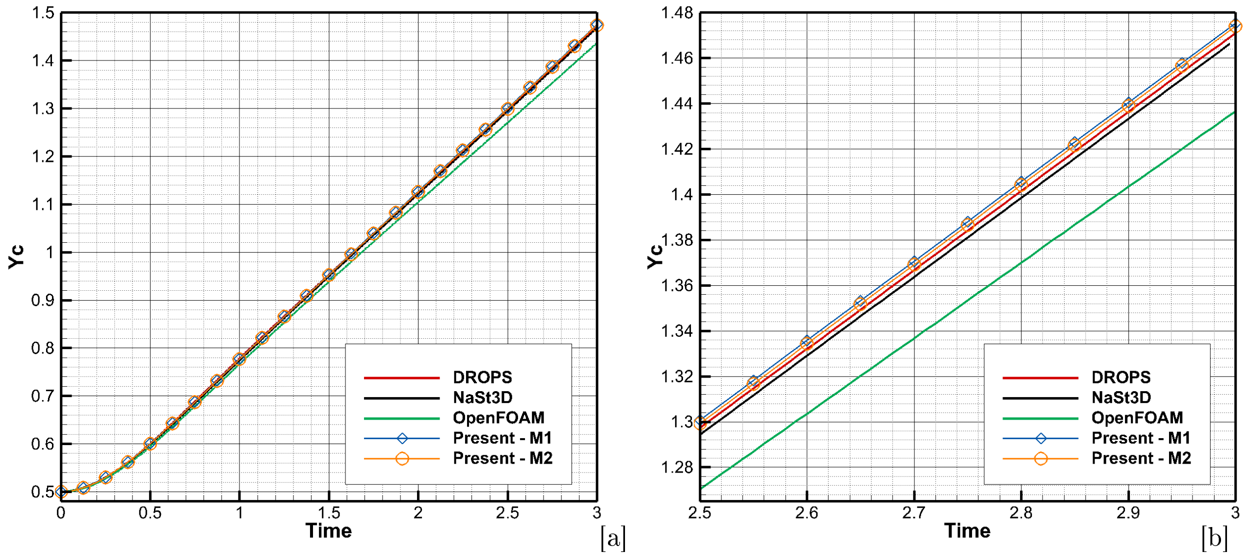

Figure 2: Time variation of bubble mass center on meshes M1 and M2 and their comparison with the result of [14] [a] and close-up view [b].

M1 show slight deviation from that of the results from NaSt3D. On the other hand, there is a difference with the rise velocity results of DROPS for both meshes M1 and M2. In addition, the results of OpenFOAM differ from all the results and the oscillations can be seen in the rise velocity. The present ALE algorithm conserves the mass of the both species at the machine precision since it employs the compatible kinematic boundary condition [12], which is in accord with the local and global geometric conservation laws [11]. The volume of the bubble can be computed as

$$\text{Volume} = \int_{\Omega_2(t)} dxdydz = \sum_{e=1}^{ne} V_e. \tag{7}$$

and its variation with time is provided in Figure 3-[b]. The results show that the total mass of the bubble is conserved at machine precision irrespective of the employed mesh resolution. However, since the bubble surface is presented by quadrilateral elements with straight edges, the initial bubble volume values differ slightly.

Table 1: Physical parameters and dimensionless numbers.

ρ_1	ρ_2	μ_1	μ_2	g	σ	Re	Eo	ρ_1/ρ_2	μ_1/μ_2
1000	100	10	1	0.98	24.5	35	10	10	10

Table 2: Computational meshes and time step used for the simulation of the rising bubble problem.

Mesh	h_{max}	h_{min}	Δt
Present - M1	$1/16$	$1/32$	$2.5 \cdot 10^{-3}$
Present - M2	$1/32$	$1/64$	$2.5 \cdot 10^{-3}$
DROPS	$1/4$	$1/32$	$2.5 \cdot 10^{-4}$
NaSt3D	$1/121$	$1/121$	$\mathcal{O}\left(10^{-4}\right)$
OpenFOAM	$1/256$	$1/256$	$1.0 \cdot 10^{-4}$

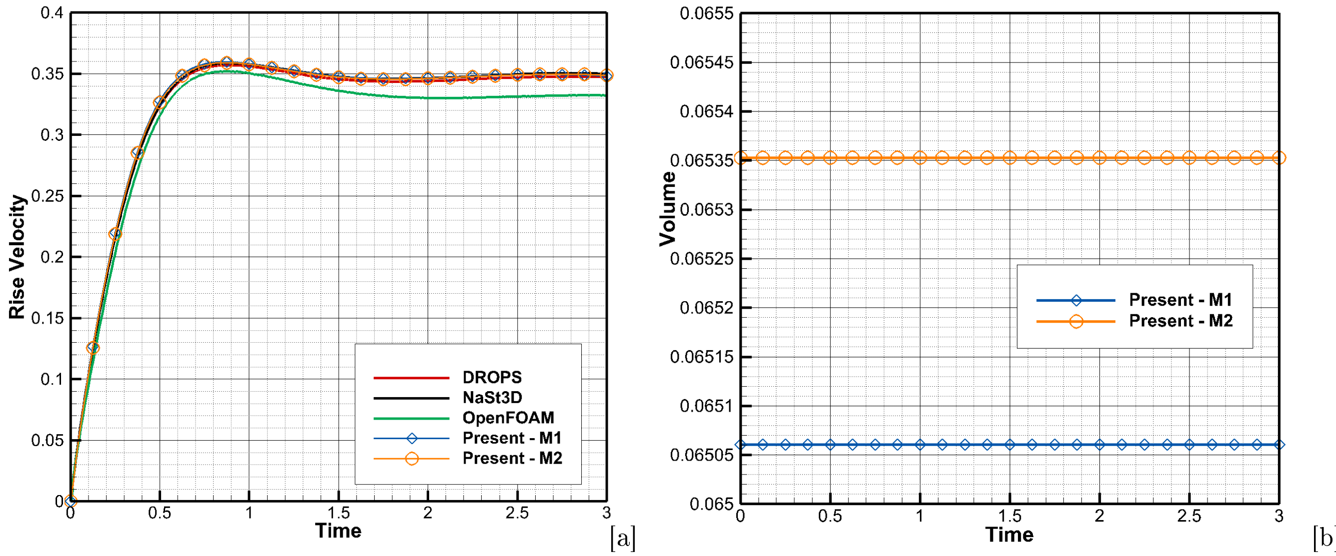

Figure 3: Time variation of bubble rise velocity on meshes M1 and M2 and their comparison with the result of [14] [a] and bubble volume variation with time on meshes M1 and M2.

4 Conclusion and Future Work

A parallel fully coupled unstructured ALE algorithm has been implemented for three-dimensional multiphase flow problems. The jump conditions across the fluid-fluid interface are exactly satisfied and the mass of both species is conserved at machine precision. The nonlinearities related due to the unknown interface location and the convection terms are treated using several Newtons's sub-iterations. The resulting algebraic equations are solved in a fully coupled (monolithic) manner and a one-level restricted additive Schwarz preconditioner with a block-incomplete factorization (ILU) within each partitioned sub-domains is utilized. The present algorithm has been successfully tested for the classical benchmark problem of a rising bubble in a Newtonian fluid. The numerical simulations with the Oldroyd-B fluid will be presented during the ICCFD10 conference. In the future, we will consider to use the conservative interpolation method described in [15] with a octree-based mesh generation algorithm in order to allow remeshing for more complex multiphase flow problems.

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