

A FULLY IMPLICIT ALE FORMULATION INCLUDING SURFACE TENSION FOR MULTIPHASE FLOWS

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Abstract. A fully implicit (monolithic) arbitrary Lagrangian-Eulerian (ALE) approach has been developed to solve incompressible multiphase flow problems in three-dimensions. The numerical algorithm is based on the div-stable face-centered unstructured finite volume method. The mass of each species is conserved exactly at the machine precision by giving a special attention to satisfy the discrete geometric conservation law (DGCL) and the continuity equation. To avoid errors due to the incompressibility condition in the vicinity of the interface, the pressure field is treated to be discontinuous across the interface with the discontinuous treatment of density and viscosity. The surface tension term at the fluid-fluid interface is treated as a force tangent to the interface. The resulting large system of algebraic equations are solved in a fully coupled manner in order to improve the time step restrictions due to the Courant-Friedrichs-Lewy (CFL) and capillary waves. The implementation of the preconditioned Krylov subspace algorithm, matrix-matrix multiplication, restricted additive Schwarz preconditioner, and the access to HYPRE library are carried out using the PETSc software package developed at the Argonne National Laboratories.

1 INTRODUCTION

The numerical simulations of multiphase flows poses a major research challenge from both theoretical and computational points of view. Some difficulties emerge due to the complex behavior of the multiphase flows, which are mainly discontinuous material properties across the interface such as density and viscosity, and the evolving interface is a priori unknown. In addition, the surface tension, which is a force tangent to the interface [1] that yields a jump across the interface has to be taken into account. Surface tension alone is not the only source for pressure jump across the interface, but together with the

viscosity jump with nonzero normal derivative of the normal component of the velocity at the interface [2]. Therefore, across the interface, these jump conditions have to be satisfied accurately. Another challenge for the simulation of multiphase flows is to conserve the mass of the each species, which is important to obtain an accurate solution and especially critical for the accuracy of the long-term simulations. Furthermore, the propagation of the capillary waves on the interface between two fluids imposes a restriction on the numerical time step in addition to the Courant-Friedrichs-Lewy (CFL) restriction. Therefore, the numerical simulation of multiphase flows is rather demanding in terms of the required computer power.

2 MATHEMATICAL FORMULATION

The Arbitrary Lagrangian and Eulerian (ALE) approach [4] has been extended to three-dimensions to solve incompressible multiphase flows in a fully implicit manner. The incompressible Navier-Stokes equations are discretized using the div-stable face-centered unstructured finite volume method [5] based on the Arbitrary Lagrangian and Eulerian formulation. The continuity equation is satisfied within each element and the summation of the continuity equations can be exactly reduced to the domain boundary, which is important for the mass conservation. The mass of each species is conserved exactly at the machine precision by giving a special attention to satisfy the geometric conservation law (DGCL) at machine precision. To avoid errors due to the incompressibility condition in the vicinity of the interface, the pressure field is treated to be discontinuous across the interface with the discontinuous treatment of density and viscosity. 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 fluid-fluid interface. The jump conditions are also exactly satisfied. It is observed that the parasitic currents are found to be very sensitive to the numerical calculation of normal vectors, and therefore several different normal vector calculation methods have been investigated in order to reduce the parasitic currents. The resulting algebraic equations are solved in a fully coupled (monolithic) manner since the mesh deformation algorithm may lead to inadmissible small elements, which require an extremely small time step due to the Courant-Friedrichs-Lewy (CFL). Furthermore, the propagation of the capillary waves also impose a the time-step restriction. Two different approaches are used for the preconditioning of the algebraic linear system: The first one is based the multiplication of the original system with an upper triangular preconditioner, which results in a scaled discrete Laplacian instead of a zero block in the original system due to the divergence-free constraint. The second one is based on the block factorization similar to that of the projection method and the parallel algebraic multigrid solver BoomerAMG is used for the scaled discrete Laplacian provided by the HYPRE library [7]. The implementation of the preconditioned Krylov subspace algorithm [6], matrix-matrix multiplication, the restricted additive Schwarz preconditioner and access to the HYPRE library [7] are carried out using the PETSc [8] software package developed at the Argonne National Laboratories in order to improve the parallel performance. The computational domain is decomposed into a set of partitions using the METIS library [9].

3 PROBLEM STATEMENT

3.1 The Rising Bubble Problem

In this problem, the simulation of a bubble $\Omega_2 = \Omega_2(t) \subset \Omega$ within a cuboid tank $\Omega = [0, 1] \times [0, 2] \times [0, 1]$ is performed as it is presented in [10]. 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 are provided by [10] and presented in Table 1. The deformation and rise of the bubble are illustrated in Figure 1. The physical quantities such as center of mass, rise velocity, mass conservation are investigated and the results are compared with the results available in the literature.

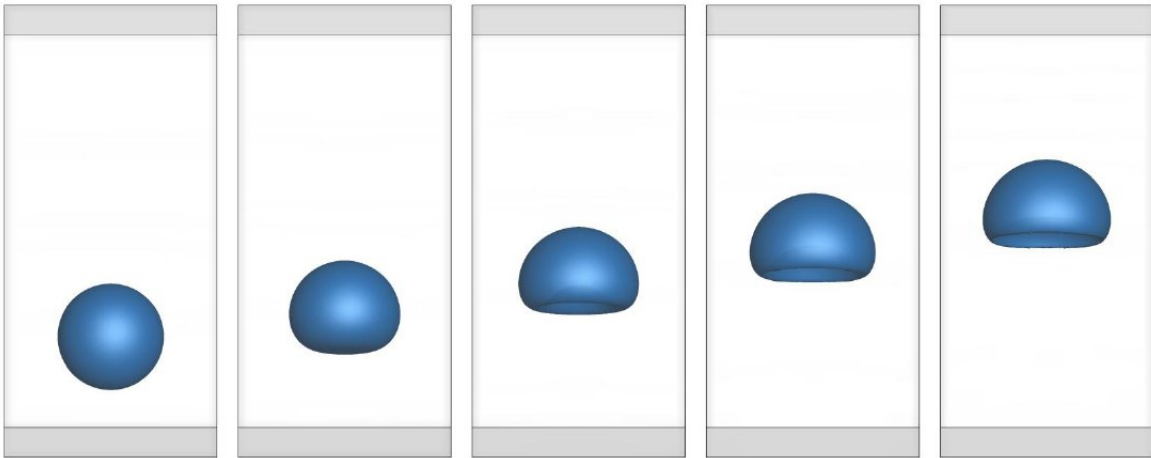


Figure 1: Deformation and rise of the bubble for the rising bubble problem.

Table 1: Physical parameters and dimensionless numbers for rising bubble problem.

ρ_1	ρ_2	μ_1	μ_2	g	σ	Re	Eo	ρ_1/ρ_2	μ_1/μ_2
1000	1	10	0.1	0.98	1.96	35	125	1000	100

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