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A Coupled Immersed Interface and Level Set Method for Three-Dimensional Interfacial Flows with Insoluble Surfactant

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Abstract. In this paper, a numerical method is presented for simulating the 3D interfacial flows with insoluble surfactant. The numerical scheme consists of a 3D immersed interface method (IIM) for solving Stokes equations with jumps across the interface and a 3D level-set method for solving the surfactant convection-diffusion equation along a moving and deforming interface. The 3D IIM Poisson solver modifies the one in the literature by assuming that the jump conditions of the solution and the flux are implicitly given at the grid points in a small neighborhood of the interface. This assumption is convenient in conjunction with the level-set techniques. It allows standard Lagrangian interpolation for quantities at the projection points on the interface. The interface jump relations are re-derived accordingly. A novel rotational procedure is given to generate smooth local coordinate systems and make effective interpolation. Numerical examples demonstrate that the IIM Poisson solver and the Stokes solver achieve second-order accuracy. A 3D drop with insoluble surfactant under shear flow is investigated numerically by studying the influences of different physical parameters on the drop deformation.

AMS subject classifications: 76D07, 65M06

Key words: 3D immersed interface method, level-set method, insoluble surfactant, Stokes interfacial flow, drop deformation.

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1 Introduction

Surfactant is an organic amphiphilic compound which consists of a hydrophilic head and a hydrophobic tail. It tends to adhere to the fluid interface and reduces the surface tension. Surfactant plays an important role in many applications in the industries of food, cosmetics, oil, etc. Due to many important applications and the associated computational challenges for surfactant dynamics, several new numerical methods have been proposed recently based on different interface tracking/capturing techniques, including the arbitrary Lagrangian-Eulerian method [5, 32], the front-tracking or immersed boundary method [10,12–14,19], the volume of fluid (VOF) method [8], the level-set method [28,31], and the diffusive interface method [27], just to name a few.

The traditional (still popular) approach to deal with the jump conditions of flow variables and fluxes across the interface is the continuum surface force (CSF) approach. In the CSF approach, a smooth discrete δ function is used to regularize the Navier-Stokes/Stokes equations by distributing the singular forces into a small neighborhood of the interface. The CSF approach is based on Peskin's immersed boundary (IB) method, see e.g., [23]. The IB method was originally developed in [22] for computing the blood flow in humans' heart. Most of the previously mentioned methods belong to the CSF approach. In this approach, however, the physical jumps of the pressure, and the gradient of the velocity are smeared out in the numerical solution. Generally the CSF type methods can only achieve first order accuracy.

Motivated by improving the accuracy of the IB method, LeVeque and Li [15] proposed the immersed interface method (IIM), in which the numerical schemes at the grid points adjacent to the interface are redesigned to incorporate the jump conditions. Consequently the IIM captures the jumps in a sharp fashion. Numerical evidence and theoretical analysis have shown that the IIM can achieve second order accuracy, see e.g., [2, 4, 6, 17].

As for interfacial flows with surfactant, an approach was proposed in [28], which coupled the IIM as the flow solver and an Eulerian level-set method as the surfactant solver. This approach was applied to the simulation of surface phase separations in [18], and the surfactant-laden drop-drop interactions in [29]. All these works were in 2D.

Despite many works of 2D IIM in the literature(see e.g., [17]), there have been few works of 3D. In [4] a 3D solver of IIM for elliptic interface problems was developed. The formulation of [4] assumes that the jumps for the solution and the flux are explicitly given on the interface, though the interface is implicitly represented by a level-set function. This explicit jump assumption may be inconvenient when in conjunction with the level-set techniques. Some local interface reconstruction is needed when a non-standard surface least square interpolation is used to calculating the surface derivatives of the jumps. In [4] this 3D solver was applied to an inverse problem of shape identification, however, it has not been utilized to simulate a moving and deforming interface in a complex fluid yet.

Geared toward fully 3D simulation of two-phase flows with surfactant, a different version of the 3D IIM Poisson solver is presented in this paper. In this solver we assume that the jumps of the solution are implicitly given by functions defined at the grid points