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A 3D front-tracking approach for simulation of a two-phase fluid with insoluble surfactant

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Resumo

Surface active agents play a significant role on interfacial dynamics in multiphase systems. While the understanding of their behavior is crucial to many important practical applications, realistic mathematical modeling and computer simulation represent an extraordinary task. By employing a front-tracking method with Eulerian adaptive mesh refinement capabilities in concert with a finite volume scheme for solving an advection-diffusion equation constrained to a moving and deforming interface, the numerical challenges posed by the full three-dimensional computer simulation of transient, incompressible two-phase flows with an insoluble surfactant are efficiently and accurately tackled in the present work. The individual numerical components forming the resulting methodology are here combined and applied for the first time. Verification tests to check the accuracy and the simulation of the deformation of a droplet in simple shear flow in the presence of an insoluble surfactant are performed, the results being compared to laboratory experiments as well as to other numerical data. In all the cases considered, the methodology presents excellent conservation properties for the total surfactant mass (even to machine precision under certain circumstances).