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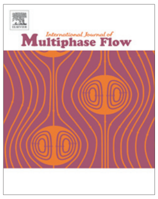

Comparative study of mass-conserving interface capturing frameworks for two-phase flows with surface tension

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ABSTRACT

A variety of frameworks to model two-phase flows with surface tension are available, each with its individual advantages and disadvantages. The understanding of the implications of the different frameworks is essential to conduct accurate and reliable two-phase flow simulations. In the presented study, three mass-conserving interface capturing frameworks are examined and compared. The frameworks can be distinguished by the method to capture and transport the interface, i.e. a compressive VOF method, a VOF-PLIC method and a coupled VOF/level-set method, as well as by the method to evaluate the interface curvature, namely a least-squares fit based on the VOF colour function, a height function technique and finite differencing. The interface frameworks are examined by means of three representative test cases, specifically chosen to assess the accuracy of the curvature evaluation, the prediction of capillary effects and the correct interaction between surface tension, viscous stresses and buoyancy. Most interestingly, the results demonstrate that advanced compressive VOF methods are able to transport evolving interfaces with an accuracy comparable to more complex and computationally expensive interface reconstruction methods, such as the applied VOF-PLIC method, and to predict surface-tension-dominated flows as accurate as coupled VOF/level-set methods. The results also show that, among the tested methods, the height function technique estimates the interface curvature most accurately, although the absolute differences in curvature error and parasitic currents between the methods are small.

1. Introduction

The accurate numerical modelling of interfacial flows is vital for many engineering and scientific applications, such as combustion processes, the cooling of nuclear reactors or metal casting. Notable research efforts have led to a variety of methods, each with its own advantages and disadvantages, and no gold-standard for the simulation of two-phase flows has evolved yet. It is, therefore, essential to understand the implications attached to each individual method. The interface between two fluids is infinitesimally thin with respect to continuum mechanics, which cannot be resolved in a finite volume or finite element framework. The finite resolution of the infinitesimally thin interface leads to three major issues: determination of the interface position, singularity of the molecular force due to surface tension acting at the interface and accurate evaluation of the interface curvature.

Two of the most widely used methods to model interfacial flows are Volume-of-Fluid (VOF) methods (Hirt and Nichols, 1981) and Level-Set (LS) methods (Osher and Sethian, 1988; Sussman et al., 1994). Although not strictly defined, in this manuscript we assume that a VOF method deals with the advection of a possibly discontinuous variable, namely the local volume fraction, and the LS method deals with the advection of a smooth variable, the level-set field. Hence, the VOF method computes the evolution of the volume fraction field which is advected based on the underlying flow. The VOF method inherently conserves mass but generally suffers from the absence of an explicit interface representation and the related inaccuracies of calculating interface curvatures from the available data. On the other hand, LS methods represent the two fluids using a distance function from the closest interface. The *zero* level-set is assigned to the interface and the distance function is advected with the local fluid velocity. LS methods provide accurate results when the interface is advected parallel to one of the coordinate axes but suffer from mass loss if the interface is strongly deformed or in flow fields with considerable vorticity. VOF and LS methods are capable of capturing interface breakup and coalescence without any additional models, although very fine meshes are required.

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The accurate advection of the VOF volume fraction field based on the underlying flow is crucial for the predictive quality of the simulations. Compressive VOF methods calculate the evolution of the VOF volume fraction field by means of a transport equation, discretised using a second-order transient scheme, such as the Crank–Nicolson scheme or the Second-Order Backward Euler scheme (Ubbink and Issa, 1999; Darwish and Moukalled, 2006; Moukalled and Darwish, 2012), and a spatial advection scheme based on a donor–acceptor approach (Lafaurie et al., 1994; Muzaferija et al., 1998; Ubbink and Issa, 1999; Darwish and Moukalled, 2006.) Alternatively, the interface is transported using a geometrical approach, advecting an explicit representation of the interface which is reconstructed from the volume fraction field (Youngs, 1982; Rider and Kothe, 1998; Scardovelli and Zaleski, 1999; van Wachem and Schouten, 2002; Aulisa et al., 2007). The explicit interface is geometrically fitted to the VOF volume fraction field and advected in an Eulerian, Lagrangian or mixed Eulerian–Lagrangian fashion. Using VOF methods, the interface curvature, required to determine the surface force, is evaluated based on the volume fraction field, either calculated directly from the volume fraction field or from a height function which is constructed based on the volume fraction field. When calculating the interface curvature directly from the volume fraction field, the curvature evaluation is adversely affected by aliasing errors (Cummins et al., 2005), since the volume fraction field is abruptly varying in space and the interface curvature is directly related to the second spatial derivative of the volume fraction field. In order to reduce the adverse effects of aliasing errors, the volume fraction field is usually smoothed by means of a convolution function for the purpose of curvature evaluation (Brackbill et al., 1992; Williams et al., 1999; Williams, 2000; Cummins et al., 2005; Francois et al., 2006). Denner and Wachem (2014) developed a technique based on a least-square fit to calculate the interface curvature directly from an unconvoluted or convoluted volume fraction field, providing a higher accuracy and reduced parasitic currents compared to standard finite difference or finite volume methods. A frequently used alternative to evaluate the interface curvature in VOF frameworks are height function (HF) techniques. HF techniques construct fluid heights as a basis for the curvature evaluation by integrating the volume fraction field along the largest interface normal vector component. The curvature is then calculated from the derivatives of the fluid heights. The major drawbacks of HF techniques are inconsistent curvature estimates if the interface is poorly resolved (Cummins et al., 2005; Popinet, 2009), i.e. when the curvature radius approaches the mesh size, and the present limitation to Cartesian meshes.

The evolution for the level-set field is governed by a combination of two equations: a scalar linear convection equation for the level-set field and a reinitialisation algorithm that ensures the level-set field remains a signed *distance* function. The latter is essential, because the level-set value is used to evaluate the material properties of the fluid near the interface from a convoluted Heavyside function (when continuity is enforced on these properties). The reinitialisation can be achieved through direct computation of the distance to the interface or through solution of an additional partial differential equation to enforce the length of the gradient to become unity. Alternative approaches avoid reinitialisation through modification of the velocity field for convection of the level-set field away from the interface, see e.g. (Sethian, 1999; Osher and Fedkiw, 2003). The interface normal vector and the interface curvature can be computed directly from the level-set field, because of the smoothness of the function in the vicinity of a smooth interface, using standard finite difference or finite volume methods. Because the level-set field is locally Lipshitz (Sussman et al., 1994), its derivatives can be approximated with the same order of accuracy as the field itself, contrary to common misconception.

In recent years, the coupling of VOF methods and level-set methods (Sussman, 2000; Sussman et al., 2007; Son, 2003; van der Pijl et al., 2005; Gerlach et al., 2006; Park et al., 2009; Sun and Tao, 2010; Wang and Tong, 2010; Lv et al., 2010; Kees et al., 2011), often called VOF-LS or CLSVOF methods, has experienced considerable attention. The basic idea behind combining VOF methods and LS methods is to exploit the advantages and mask the disadvantages of the two approaches. A VOF method is used to ensure mass conservation and a level-set method is used to accurately compute the interface normal vector and the interface curvature, since the level-set function is smooth and continuous, applying standard finite difference or finite volume methods. The LS distance function is either reconstructed based on the advected VOF colour function (Park et al., 2009; Sun and Tao, 2010; Wang et al., 2012) or the LS distance function is advected separately and coupled with the VOF method subsequently (Sussman, 2000; van der Pijl et al., 2005; Sussman et al., 2007; Son, 2003; Gerlach et al., 2006; Wang and Tong, 2010). Results presented in a number of studies, e.g. in Sun and Tao (2010), Sussman (2000), and Lv et al. (2010), show a reduction of error in curvature using VOF-LS methods compared to traditional VOF methods and improved mass conservation properties compared to standard LS methods.

Given the number of available methods to model two-phase flows as well as the number of numerical problems associated with two-phase flow modelling, a comprehensive understanding of the capabilities of the available methods is pivotal for a successful application to complex two-phase flow problems. In this paper we assess the strength and weaknesses of three mass-conserving interface capturing frameworks: a compressive VOF framework, a VOF-PLIC framework and a coupled VOF/level-set framework. The frameworks are compared by means of three representative test cases specifically chosen because of their particular informative value for the assessment of interface capturing/tracking methods for surface-tension-dominated flows. The analysis of the results and comparison of the considered methods focuses on the accurate evaluation of the interface curvature, the prediction of capillary stability, and the correct interaction of viscous stresses, surface tension effects and buoyancy. The presented results highlight specific differences concerning the capabilities of the three methods and reveal interesting similarities in the predictive quality of the methods. The presented findings are of lasting interest to the two-phase flow community as it can serve as a benchmark for future model development and can help choosing the best suited method for a given problem.

In Section 2 the governing equations and the numerical methods are outlined. Section 3 presents the test cases and elaborates on their significance for the validation of interface capturing/tracking methods. The results are presented and discussed in Section 4 and the article is concluded in Section 5.

2. Numerical methods

In a fluid system containing two immiscible and incompressible Newtonian fluids, the continuity and momentum equations are defined as

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_j u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{\mu}{\rho}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + g_i + \frac{f_{s,i}}{\rho}, \tag{2}$$

where subscript i denotes the coordinate axis, u_i is the velocity of the flow field, p represents the pressure, g_i is the gravitational acceleration and $f_{s,i}$ is the surface force per unit volume.