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A general, mass-preserving Navier–Stokes projection method

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ABSTRACT

The conservation of mass is a common issue with multiphase fluid simulations. In this work a novel projection method is presented which conserves mass both locally and globally. The fluid pressure is augmented with a time-varying component which accounts for any global mass change. The resulting system of equations is solved using an efficient Schur-complement method. Using the proposed method four numerical examples are performed: the evolution of a static bubble, the rise of a bubble, the breakup of a thin fluid thread, and the extension of a droplet in shear flow. The method is capable of conserving the mass even in situations with morphological changes such as droplet breakup.

1. Introduction

A wide variety of techniques have been proposed to model multiphase fluid systems with incompressible, immiscible fluids. These include explicit front-tracking techniques [1,2], the volume-of-fluid method [3,4], the phase-field method [5–7], and the level set method [8,9]. A constant challenge in each of these techniques is the conservation of mass during the course of the simulation. Each of these methods handles this challenge differently. For example, the volume-of-fluid methods have excellent mass conservation properties [10] at the expense of requiring complex heuristic interface reconstructions techniques to calculate geometric quantities such as curvature [11–13].

Unfortunately, there are many physical systems where high accuracy of geometric quantities is required. One example is models of liposome vesicles where interfacial forces depend on high order derivatives of the interface's curvature [14–16]. Unlike volume-of-fluid techniques, front tracking, phase-field, and level-set methods are able to provide higher geometric accuracy. This accuracy is obtained at the expense of natural volume conservation and thus special care must be taken to ensure that mass does not change over the course of a simulation.

There have been numerous attempts to improve the mass conservation of such methods. For example, level set methods have been adjusted by Lagrangian particles which are used to correct the level set function [17,18] or level sets have been combined with volume of fluid methods [19]. Other simply shift the interface function to match the volume constraint [20].

The major issue with these types of corrections is that the interface becomes decoupled from the underlying flow field. As an example consider an interface on a uniform Cartesian grid, Fig. 1. The interface begins on the left side and the underlying fluid flow-field dictates that it should move to the right one grid spacing. After this time step it is determined that errors in the simulation resulted in a mass gain. A simple and often-used correction is to simply move the interface to obtain mass conservation. In this case the effect is the interface will not move the full amount that the underlying flow field dictates. The movement of the interface and the underlying flow field have become decoupled. Any externally applied correction for front-tracking, phase-field or level set methods will demonstrate similar behavior.

In this manuscript a different approach is taken. Instead of adjusting the interface to achieve mass conservation a novel Navier–Stokes projection method is developed which ensures mass conservation. Unlike the previous method, here the interface is simply advected with the underlying flow-field; it is the flow-field itself which explicitly takes into account any possible mass loss. As will become apparent later in the manuscript, it is useful to think of this method as modifying the pressure so that it can handle not only local incompressibility but also global mass conservation. Note that while this manuscript will focus on a particular Navier–Stokes numerical implementation, the concept presented here extends to any type of multiphase fluid simulation that uses a projection method.

The remainder of the manuscript is as follows. In Section 2 the single-fluid formulation of multiphase fluid flow is briefly described. The novel mass-preserving Navier–Stokes projection

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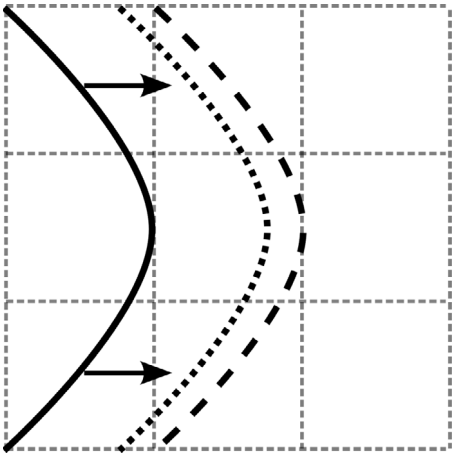

Fig. 1. Schematic of velocity-interface decoupling. The interface begins on the left (solid line). The underlying flow field dictates that the interface moves to the right and should end as the dash-line after a single time step. Due to an externally applied correction the interface instead ends the time step at the dotted line.

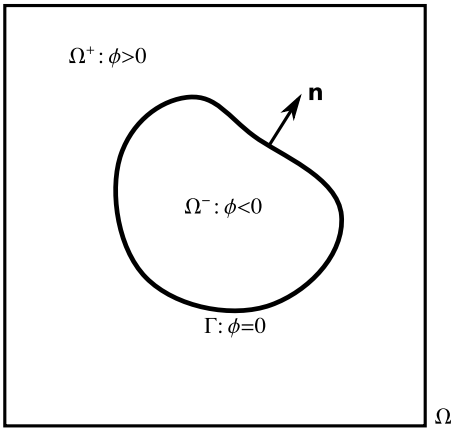

Fig. 2. The level-set description of a multiphase fluid system. The outward facing normal is shown for clarity.

method is described in Section 3. The numerical implementation is given in Section 4, which is followed by numerical experiments in Section 5. A short conclusion is presented in Section 6.

2. Single-fluid Navier–Stokes equations

In this section a brief introduction to the single-fluid formulation of multiphase fluid flow is presented. In a multiphase fluid system the interface between two immiscible fluids evolves over time. In this work a level-set description of the interface is used. Let the evolving interface be given as the set of points where the level-set function is zero, $\Gamma(t) = \{\boldsymbol{x} : \phi(\boldsymbol{x}, t) = 0\}$. The evolution of the level set function $\phi(\boldsymbol{x}, t)$ over time will implicitly determine the location of the interface. Following convention the interior fluid, Ω^-, is given by $\phi < 0$ while the outer fluid, Ω^+, is given by $\phi > 0$, Fig. 2. The entire domain is given as $\Omega = \Omega^+ \cup \Omega^-$. Using the level-set description it is possible to obtain geometric information of the interface easily. For example, the outward facing normal is simply $\boldsymbol{n} = \nabla\phi/\|\nabla\phi\|$ while the total curvature can be calculated as $\kappa = \nabla \cdot \boldsymbol{n}$.

In each domain the Navier–Stokes equations hold,

$$\rho^{\pm}\frac{D\boldsymbol{u}^{\pm}}{Dt} = -\nabla p^{\pm} + \nabla \cdot \left(\mu^{\pm}\left(\nabla\boldsymbol{u}^{\pm} + \nabla^T\boldsymbol{u}^{\pm}\right)\right) + \boldsymbol{b}^{\pm}, \tag{1}$$

$$\nabla \cdot \boldsymbol{u}^{\pm} = 0, \tag{2}$$

where ρ is the fluid density, μ is the fluid viscosity and $\boldsymbol{b}$ is any body force term, such as gravity. The fluid equations are coupled by a jump in the stress at the interface,

$$\left[-p\boldsymbol{n} + \mu\left(\nabla\boldsymbol{u} + \nabla^T\boldsymbol{u}\right)\right] \cdot \boldsymbol{n} = \boldsymbol{f}, \tag{3}$$

where $[\ ]$ indicates the jump of a quantity (outside minus inside) across the interface and $\boldsymbol{f}$ are any forces, such as tension, which act on the interface.

A difficulty in multiphase fluid simulations is the solution of this set of coupled but discontinuous differential equations. Some techniques, such as the Immersed Interface Method [21], augment the discretization of the differential equations to take into account the jumps across the interface. Another technique, which is explained here, is to model the domain as a "single" fluid with spatially varying properties [9,22]. The interface condition, Eq. (3), is accounted for by converting the singular force contribution at the interface into a body-force term localized around the interface.

Define the smooth Heaviside, $H_\varepsilon(\phi)$, function as

$$H_\varepsilon(\phi) = \begin{cases} 0 & \phi < -\varepsilon \\ \frac{1}{2}\left[1 + \frac{\phi}{\varepsilon} + \frac{1}{\pi}\sin\left(\frac{\pi\phi}{\varepsilon}\right)\right] & |\phi| \leq \varepsilon \\ 1 & \phi > \varepsilon \end{cases} \tag{4}$$

where ε is proportional to the grid spacing. From the definition of the Heaviside function define the smoothed Dirac-Delta function as $\delta_\varepsilon(\phi) = \partial H_\varepsilon(\phi)/\partial\phi$,

$$\delta_\varepsilon(\phi) = \begin{cases} 0 & |\phi| > \varepsilon \\ \frac{1}{2\varepsilon}\left[1 + \cos\left(\frac{\pi\phi}{\varepsilon}\right)\right] & |\phi| \leq \varepsilon. \end{cases} \tag{5}$$

The use of the Heaviside and Dirac functions allows for the calculation of the volume enclosed by a given level set as well as the surface area as integrals over the domain,

$$V(\phi) = \int_\Omega (1 - H_\varepsilon(\phi))\,\|\nabla\phi\| dV, \tag{6}$$

$$A(\phi) = \int_\Omega \delta_\varepsilon(\phi)\|\nabla\phi\|\, dV, \tag{7}$$

where $\|\nabla\phi\|$ accounts for situations where ϕ is not a signed distance function [23]. Depending on the form of $H_\varepsilon(\phi)$ and $\delta_\varepsilon(\phi)$, the $\|\nabla\phi\|$ term might not be needed.

Using the Heaviside function the density and viscosity are given by $\rho_\varepsilon(\phi) = \rho^- + \left(\rho^+ - \rho^-\right)H_\varepsilon(\phi)$ and $\mu_\varepsilon(\phi) = \mu^- + \left(\mu^+ - \mu^-\right)H_\varepsilon(\phi)$. These functions also allow for the transformation of singular interface forces into localized body force terms. For example, let the only singular interfacial force be from a uniform surface tension, $\boldsymbol{f} = \sigma\kappa\boldsymbol{n}$, where σ is the coefficient of surface tension. In conjunction with the smoothed density and viscosity definitions this results in a single Navier–Stokes equation valid in the entire domain,

$$\rho_\varepsilon(\phi)\frac{D\boldsymbol{u}}{Dt} = -\nabla p + \nabla \cdot \left(\mu_\varepsilon(\phi)\left(\nabla\boldsymbol{u} + \nabla^T\boldsymbol{u}\right)\right) - \sigma\delta_\varepsilon(\phi)\kappa\nabla\phi + \boldsymbol{b}_\varepsilon(\phi), \tag{8}$$

$$\nabla \cdot \boldsymbol{u} = 0, \tag{9}$$

where the body force term has been written as a smooth function of the level-set and the velocity is assumed to be continuous across the interface. This type of single-fluid formulation for multiphase flow has been used to model bubbles and droplets [24,25] and vesicles [15,26].

The results below focus on bubbles and droplets under the influence of surface tension and gravity. Therefore, the interface and body force are restricted to this particular case. The dimensionless form of the single-fluid Navier–Stokes equations can be obtained by defining a characteristic length l_0, and velocity u_0, from which a characteristic time can be obtained, $t_0 = l_0/u_0$.