Journal of Computational Physics 360 (2018) 137–166

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A positivity preserving and conservative variational scheme for phase-field modeling of two-phase flows

Vaibhav Joshi, Rajeev K. Jaiman *

Department of Mechanical Engineering, National University of Singapore, 119077, Singapore

ARTICLE INFO

Article history:
Received 2 June 2017
Received in revised form 24 November 2017
Accepted 17 January 2018
Available online 4 February 2018

Keywords:
Mass conservative
Energy stable
Positivity preserving
Allen–Cahn phase-field
Two-phase flows
Wave-structure interaction

ABSTRACT

We present a positivity preserving variational scheme for the phase-field modeling of incompressible two-phase flows with high density ratio. The variational finite element technique relies on the Allen–Cahn phase-field equation for capturing the phase interface on a fixed Eulerian mesh with mass conservative and energy-stable discretization. The mass conservation is achieved by enforcing a Lagrange multiplier which has both temporal and spatial dependence on the underlying solution of the phase-field equation. To make the scheme energy-stable in a variational sense, we discretize the spatial part of the Lagrange multiplier in the phase-field equation by the mid-point approximation. The proposed variational technique is designed to reduce the spurious and unphysical oscillations in the solution while maintaining the second-order accuracy of both spatial and temporal discretizations. We integrate the Allen–Cahn phase-field equation with the incompressible Navier–Stokes equations for modeling a broad range of two-phase flow and fluid-fluid interface problems. The coupling of the implicit discretizations corresponding to the phase-field and the incompressible flow equations is achieved via nonlinear partitioned iterative procedure. Comparison of results between the standard linear stabilized finite element method and the present variational formulation shows a remarkable reduction of oscillations in the solution while retaining the boundedness of the phase-indicator field. We perform a standalone test to verify the accuracy and stability of the Allen–Cahn two-phase solver. We examine the convergence and accuracy properties of the coupled phase-field solver through the standard benchmarks of the Laplace–Young law and a sloshing tank problem. Two- and three-dimensional dam break problems are simulated to assess the capability of the phase-field solver for complex air-water interfaces involving topological changes on unstructured meshes. Finally, we demonstrate the phase-field solver for a practical offshore engineering application of wave-structure interaction.

1. Introduction

Multiphase flows of two immiscible fluids are encountered in many industrial applications ranging from small-scale droplet interactions [1], phase separation and microstructural evolution in materials [2], bubbly and slug flows in oil and natural gas pipelines to free-surface ocean waves in the marine environment [3,4]. The effects of multiphase flows are crucial from the industrial point of view since they directly impact the design and optimization of engineering structures subjected

* Corresponding author.
E-mail addresses: vaibhav.joshi16@u.nus.edu (V. Joshi), mperkj@nus.edu.sg (R.K. Jaiman).

https://doi.org/10.1016/j.jcp.2018.01.028
0021-9991/

to complex interfacial flow dynamics. Therefore, it is essential to understand these effects through high-fidelity simulations for improved structural designs and safer operational conditions. Of particular interest to the present work is the robust and efficient two-phase modeling of free-surface ocean waves to predict the air-water interface and the hydrodynamic forces on submerged offshore structures.

It is well known that the numerical treatment of two-phase flow involving immiscible fluids poses certain challenges owing to the physical complexity in the representation and the evolution of fluid-fluid interface [5]. The representation of the continuum interface between the two phases can be considered by either interface tracking or interface capturing techniques. For the interface tracking, a boundary between the two fluid sub-domains is explicitly tracked, for example, front tracking [6] and arbitrary Lagrangian–Eulerian [7] methods. While these methods can accurately locate the interface position by tracking the moving boundary or markers on the interface, they may lead to numerical difficulties for relatively larger interface motion and topological changes. During the topological changes, re-meshing can be computationally expensive for interface tracking methods in three dimensions. In the case of interface capturing, no explicit representation of the interface is considered, instead the interface is represented implicitly using a field function throughout the computational domain on an Eulerian grid, such as level-set, volume-of-fluid and phase-field approaches. Through an implicit evolution of the interface field function, topological changes such as merging and breaking of interfaces can be naturally handled by the interface capturing methods. During the evolution of interface, the discontinuous nature of physical quantities such as density, viscosity and pressure can also pose difficulties during the numerical treatment of the interface. In particular, these discontinuities in the properties may lead to unphysical and spurious oscillations in the solution which eventually can result into the unbounded behavior of multiphase flow system. The background fixed mesh has to be sufficiently resolved to capture these discontinuities leading to high computational cost. Furthermore, surface tension effects or capillary forces along the interface need to be accurately modeled. Several models have been discussed in the literature to evaluate the surface tension, one of which is the continuum surface force method [8]. The conservation of mass is another challenge which is crucial for a physically consistent solution of multiphase flow.

Among the types of interface capturing methods, the level-set and volume-of-fluid (VOF) are the most popular methods. The VOF method utilizes a volume-of-fluid function to extract the volume fraction of each fluid within every computational cell. While the VOF method conserves mass accurately for incompressible flows, the calculation of interface curvature and normal from volume fractions can be quite complex due to interface reconstruction [9,6,10]. In addition, the smearing of the interface by numerical diffusion causes additional difficulty. On the other hand, the level-set approach can provide a non-smeared interface by constructing a signed-distance function (level-set function) of a discretization point to the interface [11]. The zero-level-set of the distance function provides a sharp interface description and the curvature of the interface can be approximated with high accuracy. However, the level-set method does not conserve mass. The reasons behind the inability of level-set to conserve mass are numerical dissipation introduced due to discretization and re-initialization process to keep the level-set function as a signed distance function [12]. Although methods including high-order discretization scheme [13], improved re-initialization [13–15], coupled particle tracking/level-set [16–18] and coupled level-set/volume-of-fluid [19–21] have been proposed to deal with the mass conservation issue, these hybrid treatments make the overall scheme much more complex and computationally expensive. To improve the mass conservation property, a conservative level-set method was proposed in [22,23] whereby the signed distance function was replaced with a hyperbolic tangent function. However, the re-initialization was necessary to maintain the width of the hyperbolic tangent profile in this case. One of the recent improvements in the level-set approach is the extended finite element method (XFEM) which utilizes the enrichment of shape functions of the elements along the interface region [24]. Both the level-set and the volume-of-fluid techniques utilize some kind of geometric reconstruction for the modeling of fluid-fluid interface, which can be quite tedious to implement in three-dimensions for unstructured grids over complex geometries.

Interface capturing for two-phase flows can be further classified into sharp-interface and diffuse-interface descriptions. For the sharp-interface description, the interface between the two phases is treated as infinitely thin with physical properties such as density and viscosity having a bulk value until the interface discontinuity. In the diffuse-interface description, however, a gradual and smooth variation of physical properties is assumed across the phase interface of a finite thickness. The physical properties are a function of a conserved order parameter which is solved by minimizing a free energy functional based on thermodynamic arguments [25]. Similar to the VOF and level-set methods, the interface location is defined by the contour levels of the phase-field order parameter. Unlike the sharp-interface description, the phase-field formulation does not require to satisfy the jump conditions at the interface and there are rapid but smooth variations of the order parameter and other physical quantities in the thin interfacial region. The diffuse-interface description has been shown to approach the sharp-interface limit asymptotically [26].

The phase-field models originate from the thermodynamically consistent theories of phase transitions via minimization of gradient energy across the diffuse interface. The phases are indicated by an order parameter (ϕ) (e.g., $\phi = 1$ in one phase and $\phi = -1$ in another phase) which is solved over an Eulerian mesh and the interface is evolved. As they fall under the diffuse-interface description, no conditions at the interface between the two phases are required to be satisfied. The surface tension and capillary effects can be modeled as a function of the phase-field order parameter depending on the minimization of the Ginzburg–Landau energy functional. Therefore, these methods do not require any re-initialization or reconstruction at the interface. Furthermore, the mass conservation property can be imparted in a relatively simple manner. The topology changes in the interface can be handled by the phase-field models easily given that the mesh is refined enough to capture these phenomena. Overall, the phase-field models offer attractive physical properties for the modeling