Applied Mathematical Modelling 37 (2013) 570–585

Contents lists available at SciVerse ScienceDirect

Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

A novel algorithm based on parameterization method for calculation of curvature of the free surface flows

H. Saghi [a], M.J. Ketabdari [b,*], M. Zamirian [c]

[a] Department of Civil Engineering, Ferdowsi University, Mashhad, Iran
[b] Faculty of Marine Technology, Amirkabir University of Technology, Tehran, Iran
[c] Department of Mathematics, Azad University of Bojnourd, Bojnourd, Iran

ARTICLE INFO

Article history:
Received 22 May 2011
Received in revised form 17 February 2012
Accepted 29 February 2012
Available online 9 March 2012

Keywords:
Parameterization method
Curvature
Free surface flows
Surface tension
Volume of fluid

ABSTRACT

In this paper, a new approach based on parameterization method is presented for calculation of curvature on the free surface flows. In some phenomena such as droplet and bubble, surface tension is prominent. Therefore in these cases, accurate estimation of the curvature is vital. Volume of fluid (VOF) is a surface capturing method for free surface modeling. In this method, free surface curvature is calculated based on gradient of scalar transport parameter which is regarded as original method in this paper. However, calculation of curvature for a circle and other known geometries based on this method is not accurate. For instance, in practice curvature of a circle in interface cells is constant, while this method predicts different curvatures for it. In this research a novel algorithm based on parameterization method for improvement of the curvature calculation is presented. To show the application of parameterization method, two methods are employed. In the first approach denoted by, three line method, a curve is fitted to the free surface so that the distance between curve and linear interface approximation is minimized. In the second approach namely four point method, a curve is fitted to intersect points with grid lines for central and two neighboring cells. These approaches are treated as calculus of variation problems. Then, using the parameterization method, these cases are converted into the sequences of time-varying nonlinear programming problems. With some treatments a conventional equivalent model is obtained. It is finally proved that the solution of these sequences in the models tends to the solution of the calculus of variation problems. For verification of the presented methods, curvature of some geometrical shapes such as circle, elliptic and sinusoidal profile is calculated and compared with original method used in VOF process and analytical solutions. Finally, as a more practical problem, spurious currents are studied. The results showed that more accurate curve prediction is obtained by these approaches than the original method in VOF approach.

1. Introduction

Motion of fluids with a free surface such as droplet splashing and bubble, are important phenomena in many fields of fluid mechanics. Therefore, some researches have been focused on solving this problem using different numerical techniques. Since the location of the free surface is driven by the gross motions of the fluid, accurate simulation of such phenomena is very cumbersome. To simulate this problem, precise modeling of surface tension is vital. In these problems, interface

* Corresponding author. Address: 424 Hafez Avenue, P.O. Box 15875-4413, Tehran, Iran.
E-mail address: Ketabdar@aut.ac.ir (M.J. Ketabdari).

0307-904X/$ - see front matter © 2012 Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.apm.2012.02.043

normal vectors and curvatures, are required to model surface tension. Volume of fluid method is one the surface capturing techniques for interface modeling of two phase flows. There are different methods for modeling of curvature. The most widely used technique is calculation of the spatial derivatives of the scalar function based on VOF at any instant. In this method, the gradient of the scalar function [1] is normal to the interface. Then, by taking the divergence of this interface vector, the second derivative of the scalar function, i.e. the interface curvature is obtained. The methods of discretization of the surface tension are associated with the interface curvature. They are the main source of error in surface tension simulation [2]. To reduce this error, various researches have been performed [2–5]. For example, Francois et al. [2] impose an exact balance between the surface tension and pressure forces to model surface tension into a volume-of-fluid (VOF) method and so, no spurious currents are induced in a flow provided. Some researchers employed the VOF-based height-function method [2,6,7] to obtain the curvatures with second-order accuracy. In this method, the interface curvature is obtained from the derivatives of the height function. However, it leads to poor results, if an interface is not adequately resolved [8]. Poo and Ashgriz [9] utilized a second-order polynomial to calculate the curvature. In a method known as PROST [10], the data is fitted iteratively with a 2D or 3D parabola.

Surface tension along with an interface arises from forces between molecules in a fluid. Surface tension is important when Webber number (We) is much greater than unity ($We \gg 1$) in high Reynolds numbers ($\mathrm{Re} \gg 1$) or when Capillary number (Ca) is much lower that unity ($Ca \ll 1$) for small Reynolds numbers ($\mathrm{Re} \ll 1$). These parameters are defined as:

$$We = \frac{\rho L U^2}{\sigma}, \tag{1}$$

$$Ca = \frac{\mu U}{\sigma}, \tag{2}$$

$$\mathrm{Re} = \frac{\rho U L}{\mu}, \tag{3}$$

where σ is the surface tension, ρ is the fluid density, U is the velocity scale, L is the length scale and μ is the fluid dynamic viscosity. The focus of this paper is calculation of curvature based on the parameterization method (PM). To illustrate this new approach, the volume-of-fluid method is used to represent the interface. Then intersection points of interface and grid lines are determined. Calculus of variation problems (CVP) is achieved using three line method (TLM) and four point method (FPM) approaches. The solutions of these CVPs are the Optimal Curve (OC) in the form of $f(\cdot)$. In fact $f(\cdot)$ is the approximation of surface flow. Substituting the sequence of polynomials, $p_n(\cdot)$, $n = 1,2,\ldots$, instead of $f(\cdot)$ in the CVPs (PM), the sequence of Time-varying Nonlinear Programming Problems (TNLPP) is achieved. It should be noted that variables of TNLPPs are the constant coefficients of polynomials. Sequence of TNLPPs can be converted to the sequence of Nonlinear Programming Problems (NLPP) with some calculations. It is proved that the NLPPs solution tends to the solution of CVP. Finally, NLPPs solution leads to two polynomials as the OCs of the FPM and TLM. The accuracy and performance of the new method are demonstrated via numerical test cases with known curvatures.

2. Curvature simulation

In this section, the interface cell curvature was modeled with original (VOF) and PM methods.

2.1. Original (VOF) method

The successful approaches for handling free surface problems can be categorized as surface tracking and surface capturing methods. Surface tracking methods try to solve the flow in the fluid region while the free surface is treated as a moving boundary of the computational domain. This usually satisfies the kinematic boundary conditions. In this technique, free surface locations can be determined precisely. Surface capturing methods simulate both fluid regions on a fixed grid system. In these methods, the free surface can be identified using a marker function such as the marker particles in the marker and cell (MAC) method [11] or the volume fraction in VOF method [12–14]. To determine the volume fraction of each phase (e.g. air and water) in VOF method, a scalar transport equation which is colour function (F) is solved in all computational cells as [15]:

$$\frac{\partial F}{\partial t} + \vec{\nabla} \cdot (F\vec{U}) = 0. \tag{4}$$

So that:

$$\begin{cases} F = 1 \quad \textit{for cells inside fluid } 1, \\ F = 0 \quad \textit{for cells inside fluid } 2, \\ 0 < F < 1 \quad \textit{for free surface cells}. \end{cases} \tag{5}$$

The interface unit normal vector and curvature of free surface can be calculated from the gradient of F as: