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A Quadratic Spline based Interface (QUASI) reconstruction algorithm for accurate tracking of two-phase flows

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ABSTRACT

A new Quadratic Spline based Interface (QUASI) reconstruction algorithm is presented which provides an accurate and continuous representation of the interface in a multiphase domain and facilitates the direct estimation of local interfacial curvature. The fluid interface in each of the mixed cells is represented by piecewise parabolic curves and an initial discontinuous PLIC approximation of the interface is progressively converted into a smooth quadratic spline made of these parabolic curves. The conversion is achieved by a sequence of predictor–corrector operations enforcing function (C^0) and derivative (C^1) continuity at the cell boundaries using simple analytical expressions for the continuity requirements. The efficacy and accuracy of the current algorithm has been demonstrated using standard test cases involving reconstruction of known static interface shapes and dynamically evolving interfaces in prescribed flow situations. These benchmark studies illustrate that the present algorithm performs excellently as compared to the other interface reconstruction methods available in literature. Quadratic rate of error reduction with respect to grid size has been observed in all the cases with curved interface shapes; only in situations where the interface geometry is primarily flat, the rate of convergence becomes linear with the mesh size. The flow algorithm implemented in the current work is designed to accurately balance the pressure gradients with the surface tension force at any location. As a consequence, it is able to minimize spurious flow currents arising from imperfect normal stress balance at the interface. This has been demonstrated through the standard test problem of an inviscid droplet placed in a quiescent medium. Finally, the direct curvature estimation ability of the current algorithm is illustrated through the coupled multiphase flow problem of a deformable air bubble rising through a column of water.

1. Introduction

Flows with moving interfaces and the associated heat and mass transfer form an integral part of many natural and industrial processes. Most multiphase flows are characterized by the presence of fluid structures over a variety of scales. A common example of this is seen in the disintegration of a liquid jet in air where the characteristic dimension varies from the jet diameter to the size of fine droplets. These diverse flow behaviors are the consequence of interfacial phenomena and related processes, whose understanding is of paramount importance in the design of devices such as injectors. Although numerical modeling offers promising tools in this regard, the added non-linearity of interfacial phenomena makes the modeling of these flows much more challenging.

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Broadly, the available multiphase modeling techniques can be classified as moving-grid and fixed-grid methods based on the relative deformation of the grid with respect to interface dynamics. In a moving-grid method, the computational grid for each fluid sub-domain can be distinctly identified and the grid points located on the interface move along with it to accurately predict the temporal evolution of the interface. However, at large interfacial deformations, the method requires continuous remeshing effort to account for the changes in topology. On the other hand, fixed-grid methods effectively predict the dynamics of the interface using special schemes on a non-deformable grid with less computational effort. The two important classifications of fixed-grid methods are the front-tracking and the front-capturing techniques, which involve explicit and implicit treatment of the interface respectively. The application of a front-tracking technique to represent the interface explicitly by a distribution of marker points connected by spline interpolation was demonstrated by Popinet and Zaleski [1] where the interface dynamics was effectively tracked by Lagrangian advection of these marker points in the flow field. The marker points easily resolve the sub-grid level fluid structures and the use of spline curves helps in the direct estimation of interface attributes like curvature which are required for the evaluation of surface tension forces. In spite of these advantages, difficulties arise with regard to accurate mass conservation and in simulating flows with interface merger and breakup. The front-capturing techniques like volume of fluid (VOF) and level set (LS), on the other hand, effectively resolve macro-fluid structures larger than the grid spacing [2,3]. They use characteristic phase functions for an implicit description of the interface, which automatically handles interface merger and breakup.

The level set method uses the signed distance (ϕ) of grid points from the interface for an implicit representation. The advection of the distance function 'ϕ' and its subsequent re-initialization leads to the transient evolution of the interface. Even though the level set method is attractive due to the differentiable properties of distance function, a complete conservation of mass in the domain using level set is still a challenging issue. On the contrary, the VOF method enforces strict volume conservation of various constituent phases and uses a discrete volume fraction distribution (F) to represent the interface. The cells are assigned with F value between 0 and 1, based on the volume fraction of the primary fluid (in the case of a binary system) in the cell. The discontinuous nature of the volume fraction 'F' necessitates two geometric procedures, namely: interface reconstruction and fluid advection, to track the fluid volumes. The interface reconstruction procedure involves estimation of the approximate orientation and position of the interface within the cell and the advection process geometrically evaluates the material volume flux through the cell faces based on the reconstructed interface.

Issues in VOF method primarily arise due to the non-uniqueness of interface reconstruction procedure. Earlier reconstruction methods like DeBar's piecewise linear approximation [4], the stair-step approximation of Hirt and Nichols [2] and SLIC (Simple Line Interface Calculation) reconstruction of Noh and Woodward [5] resulted in unphysical 'flotsam' and 'jetsam' even for simple flow configurations. Notable improvement in the reconstruction procedure was brought in by the Youngs' PLIC [6] algorithm (Piecewise Linear Interface Calculation) which allowed the interfaces to be represented by straight line segments normal to the gradient of volume fraction (F). The precise location of these line segments within each cell is then obtained based on the volume of primary fluid in the cell. In spite of its simplicity and robustness, the sensitivity of the PLIC reconstruction on the algorithm used to calculate the volume fraction gradients, renders it non-unique. Also, the PLIC representation suffers from discontinuity of interface shape across the cell boundaries and the linear approximation of the interface is insufficient to allow for the direct estimation of attributes like the local interfacial curvature. These factors have given rise to the widespread use of special curvature calculation methods based on the volume fraction distribution. The convolution (CV) technique of Williams et al. [7] uses a mollified volume fraction distribution obtained from the application of various smoothing kernels. Other accurate methods include Height Function (HF) technique of Cummins et al. [8] where the discrete sums of volume fractions are used to obtain the curvature information.

Alternatively, direct estimation of curvature using higher order approximations of the interface within mixed cells have been considered by a few researchers. The Piecewise Parabolic Interface (PPIC) reconstruction was first presented by Price et al. [9], where a second order equation was used to represent the interface. The method involves an iterative non-linear optimization scheme to obtain the coefficients of quadratic expression. A similar generalized three-dimensional approach was presented by Renardy and Renardy [10] and a direct estimate of curvature was used to calculate the surface tension force in the interfacial cell. Although these methods possess higher interface reconstruction accuracy and lower magnitudes of spurious currents (which are generally caused by error in the curvature estimation and the imbalance between pressure gradients and surface tension force), the iterative error minimization procedure employed in these methods renders them computationally intensive. Moreover, the parabolic interfaces obtained from these methods still suffer from discontinuities at the cell boundaries. The other class of higher order methods proposed by Ginzburg and Wittum [11] and Lo'pez et al. [12] involve cubic spline based interface reconstruction. In [11], an initial spline passing through the midpoints of the PLIC interface is evolved into a cubic spline which conserves mass exactly in each of the mixed cells. The computations involve the simultaneous solution of '$3n$' equations (n – number of mixed cells forming the spline) subjected to volume constraint in each cell. The cubic spline aids in the direct estimation of curvature using a continuous form of interface representation in the whole domain; however, it tends to produce wavy interfaces in some cases due to the non-locality of errors.

In the current work, a new two-dimensional Quadratic Spline based Interface (QUASI) reconstruction algorithm is presented, where piecewise quadratic curves are used to represent the interface within each cell. A continuous quadratic spline across the mixed cells ($0 < F < 1$) is then evolved from a sequence of predictor–corrector operations, where the end points of an initial PLIC interface approximation are corrected to enforce function and derivative (C^0 and C^1) continuities at the cell boundaries. Simple analytical expressions have been derived for all the steps involved which effectively minimize the computational effort required for the current algorithm. The use of higher order curves with constraints results in unique and