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A mesh-decoupled height function method for computing interface curvature

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ABSTRACT

In this paper, a mesh-decoupled height function method is proposed and tested. The method is based on computing height functions within columns that are not aligned with the underlying mesh and have variable dimensions. Because they are decoupled from the computational mesh, the columns can be aligned with the interface normal vector, which is found to improve the curvature calculation for under-resolved interfaces where the standard height function method often fails. A computational geometry toolbox is used to compute the heights in the complex geometry that is formed at the intersection of the computational mesh and the columns. The toolbox reduces the complexity of the problem to a series of straightforward geometric operations using simplices. The proposed scheme is shown to compute more accurate curvatures than the standard height function method on coarse meshes. A combined method that uses the standard height function where it is well defined and the proposed scheme in under-resolved regions is tested. This approach achieves accurate and robust curvatures for under-resolved interface features and second-order converging curvatures for well-resolved interfaces.

1. Introduction

Simulations of gas–liquid flows are often significantly influenced by the dynamics at the phase interface. For predictive simulations of relevant engineering flows, an accurate surface tension force is needed to avoid spurious curvature-induced flows near the interface. The surface tension force is directly proportional to the interface curvature, and therefore the problem is reduced to computing an accurate curvature.

The height function method [1–3] is an approach for computing the interface curvature from an approximate representation of the phase interface and is commonly used in the context of volume-of-fluid (VOF) schemes. It has also been used successfully in the context of the accurate conservative level set (ACLS) [4], although this paper will assume that a VOF representation of the interface is available.

The VOF method is a popular technique to capture the location of the phase interface and has been used since the early 1970s when variants of the approach were introduced by DeBar [5], Hirt and Nichols [6], and Noh and Woodward [7]. VOF schemes store the ratio of liquid volume to cell volume, known as the liquid volume fraction α, within each control volume, i.e.,

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$$\alpha = \frac{1}{\mathcal{V}_{\mathrm{CV}}} \int_{\mathrm{CV}} f(\boldsymbol{x}, t)\, \mathrm{d}V, \tag{1}$$

where CV is a control volume (e.g., a computational cell) with volume $\mathcal{V}_{\mathrm{CV}}$ and f is the liquid distribution function, defined as

$$f(\boldsymbol{x}, t) = \begin{cases} 1, & \text{if } \boldsymbol{x} \text{ is in the liquid at time } t, \\ 0, & \text{if } \boldsymbol{x} \text{ is in the gas at time } t. \end{cases} \tag{2}$$

VOF schemes differ in how the liquid volume fraction is transported. Early methods used flux splitting wherein one-dimensional transport steps were used successively [6]. Since then unsplit schemes have been developed, such as the two-dimensional schemes of Pilliod and Puckett [8] and López et al. [9]. The extension of such methods to three dimensions is not straightforward and the development of three-dimensional unsplit schemes has only occurred recently by Hernández et al. [10], Le Chenadec and Pitsch [11], and the fully conservative formulation by Owkes and Desjardins [12].

All VOF methods require calculation of the interface curvature from the liquid volume fraction field. The interface curvature can be computed directly from the α-field by calculating the interface normal as $\boldsymbol{n} = -\nabla\alpha/|\nabla\alpha|$ and the interface curvature as $\kappa = -\nabla \cdot \boldsymbol{n}$. Because the α-field is based on the discontinuous liquid distribution function f, the calculation can be improved by using a smoothed α-field [13]. Note that both approaches often do not converge with mesh refinement [14]. Alternatively, the height function approach has been shown to provide a converging interface curvature.

In its simplest form, the height function method consists in integrating the liquid volume fraction in the pseudo-normal direction in the cell of interest and neighboring cells, creating a collection of heights. The curvature is then calculated using finite difference operators on those heights. The pseudo-normal direction is the Cartesian direction x, y, or z with the largest component of the interface normal vector. Assuming the pseudo-normal direction is x for a computational cell with Cartesian index i, j, k, the heights h are computed using

$$h_{j'k'} = \sum_{i'=i-(N_H-1)/2}^{i+(N_H-1)/2} \alpha_{i'j'k'} \Delta x \quad \text{for} \quad \begin{cases} j' = j-(N_N-1)/2, \ldots, j+(N_N-1)/2, \\ k' = k-(N_N-1)/2, \ldots, k+(N_N-1)/2, \end{cases} \tag{3}$$

where $\alpha_{i'j'k'}$ is the liquid volume fraction within the i', j', k' cell. N_H controls the number of the cells in each column and values of $N_H = 3, 5,$ and 7 have been considered in the literature [15–18]. N_N sets the number of neighboring heights that are computed. For second- and fourth-order methods, $N_N = 3$ and 5, respectively [18]. The curvature is calculated from the heights using finite difference operators such as the second-order operator

$$\kappa = \frac{H_{yy}}{(1+H_y^2)^{3/2}} \tag{4}$$

in two dimensions and

$$\kappa = \frac{H_{yy} + H_{zz} + H_{yy}H_z^2 + H_{zz}H_y^2 - 2H_{yz}H_yH_z}{(1+H_y^2+H_z^2)^{3/2}} \tag{5}$$

in three dimensions, with

$$H_y = \frac{h_{j+1,k} - h_{j-1,k}}{2\Delta y}, \tag{6a}$$

$$H_z = \frac{h_{j,k+1} - h_{j,k-1}}{2\Delta z}, \tag{6b}$$

$$H_{yy} = \frac{h_{j+1,k} - 2h_{j,k} + h_{j-1,k}}{\Delta y^2}, \tag{6c}$$

$$H_{zz} = \frac{h_{j,k+1} - 2h_{j,k} + h_{j,k-1}}{\Delta z^2}, \tag{6d}$$

and

$$H_{yz} = \frac{h_{j+1,k+1} - h_{j+1,k-1} - h_{j-1,k+1} + h_{j-1,k-1}}{2\Delta y\, 2\Delta z}. \tag{6e}$$

Fig. 1 shows a two-dimensional example of the application of the height function method to compute κ_1 with $N_H = 5$. The three heights used to compute κ_1 are shown with solid lines. All of the heights are well defined since each height is computed in a column that contains in a cell that is entirely liquid (i.e., $\alpha = 1$) and cell that is entirely gas (i.e., $\alpha = 0$). With the three heights, Eq. (4) can be used to compute the curvature.

When large interface curvature and under-resolved interface features exist, the number of well-defined heights that are available to compute the curvature can be insufficient. For example, only two well-defined heights are available in