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A three-dimensional volume-of-fluid method for reconstructing and advecting three-material interfaces forming contact lines

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A R T I C L E I N F O

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A B S T R A C T

We introduce a piecewise-linear, volume-of-fluid method for reconstructing and advecting three-dimensional interfaces and contact lines formed by three materials. The new method employs a set of geometric constructs that can be used in conjunction with any volume-tracking scheme. In this work, we used the mass-conserving scheme of Youngs to handle two-material cells, perform interface reconstruction in three-material cells, and resolve the contact line. The only information required by the method is the available volume fraction field. Although the proposed method is order dependent and requires *a priori* information on material ordering, it is suitable for typical contact line applications, where the material representing the contact surface is always known. Following the reconstruction of the contact surface, to compute the interface orientation in a three-material cell, the proposed method minimizes an error function that is based on volume fraction distribution around that cell. As an option, the minimization procedure also allows the user to impose a contact angle. Performance of the proposed method is assessed via both static and advection test cases. The tests show that the new method preserves the accuracy and mass-conserving property of the Youngs method in volume-tracking three materials.

1. Introduction

In multi-phase flow simulations, the volume-of-fluid (VOF) method is one of the most commonly used interface capturing techniques due to (a) its mass conserving property, and (b) ease in handling large interfacial deformations. In the VOF method, an indicator function ψ defined as,

$$\psi(\vec{x}) = \begin{cases} 1, & \vec{x} \in \text{Material 1} \\ 0, & \vec{x} \notin \text{Material 1} \end{cases} \tag{1}$$

is used to represent Material 1 shown in Fig. 1. In the discretized form, the VOF function is the fraction of cell volume V occupied by Material 1,

$$\Psi = \frac{1}{V} \int_V \psi \, dV \tag{2}$$

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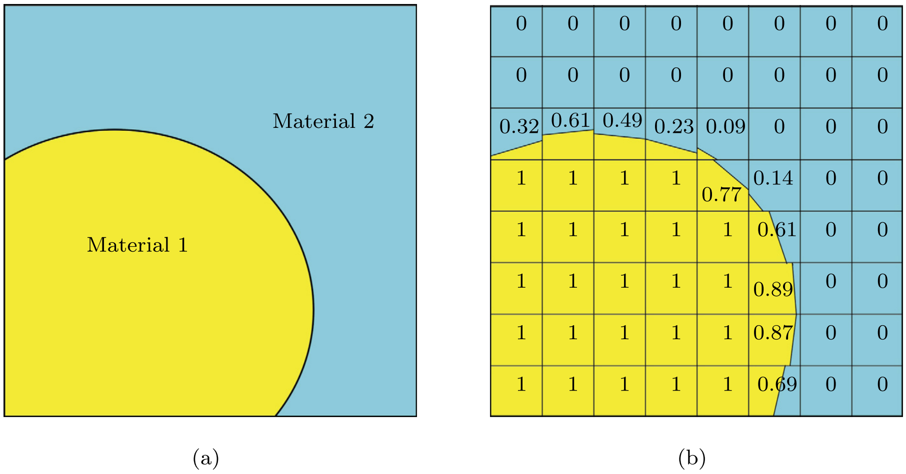

Fig. 1. (a) Interface between two materials. (b) PLIC approximation as linear (planar in 3D) segments of the interface shown in (a).

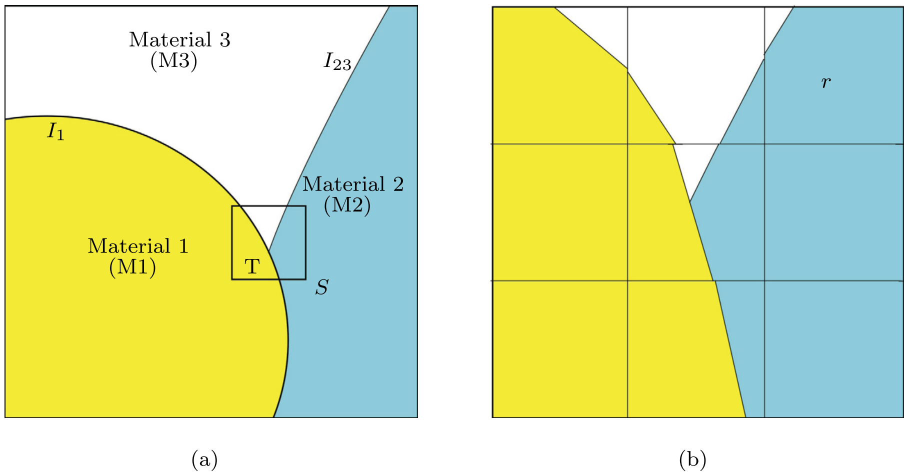

Fig. 2. (a) Three-material configuration where the interface (I_{23}) between materials 2 and 3 is truncated by Material 1 interface (I_1), resulting in a triple point T (contact line in 3D). (b) PLIC representation of interfaces around the triple point bounded by S in (a).

A common approach in the VOF method is to use Piecewise-Linear-Interface-Calculation (PLIC) to reconstruct the material interfaces. Fig. 1 shows the interface approximated as linear (planar in 3D) segments. The numbers shown in Fig. 1(b) correspond to the VOF function F. There exist various volume-tracking methods that rely on PLIC. An example is the Youngs method [1], which has been used in this work. In the Youngs method, to reconstruct the interface, the orientation of each segment is computed by using $\hat{n}_\psi = \frac{\nabla\psi}{|\nabla\psi|}$ [2, p. 37], while its location is determined by matching exactly Material 1's volume fraction.

Now, consider the three-material configuration shown in Fig. 2. We denote by Material 1 (or M1), the material that shares a continuous interface with the other two materials, M2 and M3. For example, in contact line problems, M1 represents the material that forms the contact surface; e.g., a solid surface on which a droplet resides. The interface between materials M2 and M3 intersects with the Material 1 surface resulting in a triple point in 2D and a contact line in 3D (Fig. 2). We have developed a method in the PLIC-VOF context to reconstruct three-material configurations in 3D, capture contact lines and track volumes of three materials. A similar approach based on error minimization was proposed by Choi and Bussmann [3] to resolve three-material cells and the triple point in 2D. The method was later used by Ghasemi et al. [4] to resolve triple points in their study of the interaction between two-phase fluid flows and a moving rigid solid body. Choi and Bussmann [3] noted that their procedure could be extended to 3D conceptually, but was "*significantly more complicated to implement*" owing to "*much more complicated geometry*" [3, p. 1008]. We have presented in this paper a complete set of 3D geometrical constructs needed for the three-material reconstruction method. The proposed geometric constructs, detailed in Appendices and the Supporting Information document, are based on convex 3D polyhedra and are quite general. They are applicable to both structured and unstructured grids. The method presented here is not a direct 3D extension of Choi and