A sharp VOF method for modeling 2D contact line moving on complex geometrical boundary by using an embedded boundary approach

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Abstract:

A geometrical volume-of-fluid method is proposed to study the 2D contact line moving on complex geometries, which are modeled using an embedded boundary approach. We introduce a novel VOF advection scheme that exactly conserves the volume fraction when an embedded boundary is present in the same interfacial cell. Additionally, a modified height function method is implemented to accurately enforce the contact angle condition at the embedded boundary. Building on these contributions, we achieve, for the first time within the sharp VOF method framework, accurate simulation of contact line dynamics on complex solid substrates.

Keywords: Volume-of-fluid, embedded boundary, geometrical advection, height function, contact line dynamics.

Introduction:

Contact line problems are ubiquitous in both nature and industry, representing multiphase scenarios where immiscible fluids interact with solid boundaries. The main challenge lies in the motion of the liquid/gas interface near the boundary, particularly for Cartesian grids cut by the embedded boundary. This situation presents two problems: conserving VOF advection in cells cut by the embedded boundary and accurately implementing the contact angle condition at the embedded boundary. Various studies have used VOF-type methods [1], but these two problems remain unsolved due to the presence of two sharp interfaces (the liquid/gas interface and the embedded boundary) within the same discretized cell. These challenges motivate us to propose a novel methodology for simulating contact line dynamics in more general situations involving irregular solid substrates.

Numerical Methods:

To address these problems, we first implement a "flood algorithm" [2] to reconstruct the liquid/gas interface when the embedded boundary is present in the same discretized cell. We find that the traditional geometrical VOF advection method, designed for regular fluid domains, fails to conserve local fluid mass in the presence of irregular embedded boundaries, which is primarily because the embedded solid leads to over- or under- estimation of the volume flux through the cell faces. To solve this problem, a method that ensures local volume conservation by adjusting the geometrical width of the advection area to compensate for the flux error is proposed. The second part involves developing a height function (HF) method to accurately implement the contact angle condition at the embedded boundary. We design a novel HF method to estimate the height interface containing the contact line. A parabola fitting method is implemented to obtain the ghost values of the HF in solid cells fully immersed in the embedded solid. Based on this expanded stencil template, the contact angle condition can be precisely enforced at the embedded boundary.

Results and discusison:

Fig. 1(a) shows the first example: a liquid ring rotating around a cylinder. Using our method, the error in local volume conservation is about 10^{-14}, while global volume conservation is maintained at the order of 10^{-15}. The second example involves droplet spreading on a flat plate inclined at $45°$ and on a cylinder of the same size

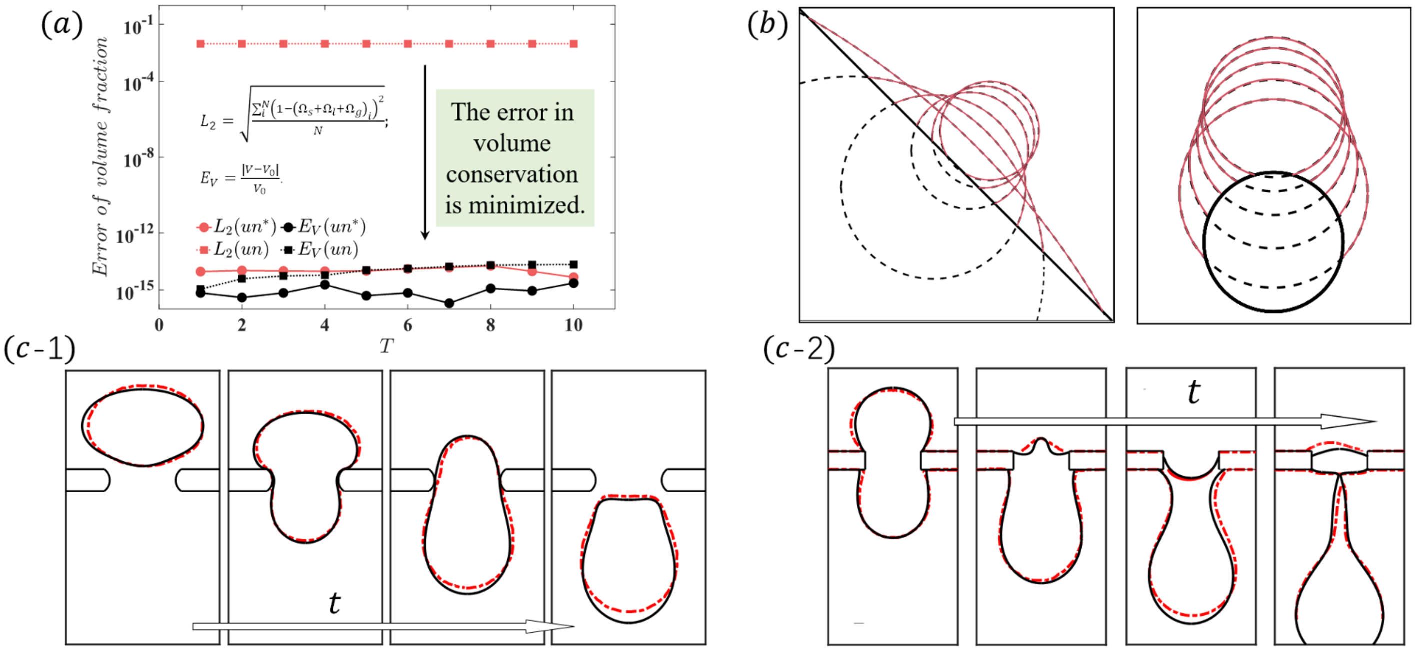

Figure 1: (a) Error of volume conservation. (b) Shapes of droplet driven by surface tension at equilibrium. (c) Droplet impacts plate with a round (c-1) or sharp (c-2) orifice.

as the droplet. The shapes at equilibrium are indicated by the red solid line in Fig. 1(b), while the black dashed lines represent the theoretical outlines. The last example involves a droplet impacting a plate with a round or sharp orifice, compared with the experiment in [3] represented by the black lines in Fig. 1(c). The red lines show the shapes from our simulation.

Conclusion:

We propose a novel hybrid volume-of-fluid (VOF) and embedded boundary method for numerically simulating contact line dynamics on complex geometries. Numerical results demonstrate that this method ensures both local and global mass conservation. Additionally, the contact angle condition can be precisely enforced at the embedded boundary. In future work, we will focus on extending this method to 3D simulations.

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