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Importance of curvature evaluation scale for predictive simulations of dynamic gas–liquid interfaces

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ABSTRACT

The effect of the scale used to compute the interfacial curvature on the prediction of dynamic gas–liquid interfaces is investigated. A new interface curvature calculation methodology referred to herein as the Adjustable Curvature Evaluation Scale (ACES) is proposed. ACES leverages a weighted least squares regression to fit a polynomial through points computed on the volume-of-fluid representation of the gas–liquid interface. The interface curvature is evaluated from this polynomial. Varying the least squares weight with distance from the location where the curvature is being computed, adjusts the scale the curvature is evaluated on. ACES is verified using canonical static test cases and compared against second- and fourth-order height function methods.

Simulations of dynamic interfaces, including a standing wave and oscillating droplet, are performed to assess the impact of the curvature evaluation scale for predicting interface motions. ACES and the height function methods are combined with two different unsplit geometric volume-of-fluid (VoF) schemes that define the interface on meshes with different levels of refinement. We find that the results depend significantly on curvature evaluation scale. Particularly, the ACES scheme with a properly chosen weight function is accurate, but fails when the scale is too small or large. Surprisingly, the second-order height function method is more accurate than the fourth-order variant for the dynamic tests even though the fourth-order method performs better for static interfaces. Comparing the curvature evaluation scale of the second- and fourth-order height function methods, we find the second-order method is closer to the optimum scale identified with ACES. This result suggests that the curvature scale is driving the accuracy of the dynamics. This work highlights the importance of studying numerical methods with realistic (dynamic) test cases and that the interactions of the various discretizations is as important as the accuracy of one part of the discretization.

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1. Introduction

Many gas–liquid flows are controlled by the dynamics at the phase interface, particularly the surface tension force. For example, in the atomization of a liquid fuel into droplets, the surface tension force controls the growth of interfacial instabilities that break apart the liquid core, forming ligaments and droplets that may again break apart if the flow inertia

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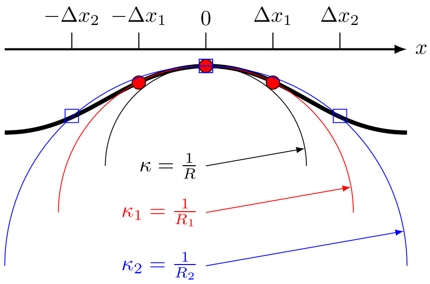

Fig. 1. Gas–liquid interface shown with thick line. Exact curvature shown with κ. Discrete curvatures κ_1 and κ_2 are computed on small and large scales, respectively.

is larger than the surface tension force. For predictive simulations, of this and other gas–liquid flows, the surface tension force needs to be accurate and should converge with mesh refinement.

The surface tension force $\boldsymbol{f}_\sigma = \sigma\kappa\boldsymbol{n}$ depends on the surface tension coefficient σ (assumed constant), curvature of the gas–liquid interface κ, and the interface normal vector $\boldsymbol{n}$ [1]. In this work we focus on the problem of computing an accurate interfacial curvature. Many methods have been developed to compute curvatures and the approach depends on the underlying methodology used to track or capture the phase interface. A variety of interface tracking methods exist such as deforming meshes [2] and Lagrangian marker particle [3]. Interface capturing schemes use an implicit representation of the interface and include level set [3] and volume-of-fluid schemes [4]. Of all these methods that provide the interface location, the volume-of-fluid (VoF) method is very common. The VoF approach captures the interface by storing the ratio of liquid volume to cell volume, a quantity known as the liquid volume fraction. This work on assessing the curvature evaluation scale and the proposed ACES method use geometric VoF schemes as the interface capturing method, although the result may be applicable to other methodologies.

Computing curvatures from VoF methods can be challenging since VoF methods only store the liquid volume fraction and computing derivatives of this discontinuous quantity leads to large discretization errors [1]. As a result, more advanced numerical methods have been developed, such as smoothing the discontinuous liquid volume fraction function [5]. However, even with smoothing, the methods fail to converge [6]. An alternative and popular approach is the height function method [7–9]. This method integrates the liquid volume fraction along columns aligned with the computational mesh to remove the discontinuity and allows for standard finite difference operators to be used to compute the curvature. The method has been shown to converge under mesh refinement for test cases with exact liquid volume fraction fields [10].

While the height function method is simple in principle, the columns used to define the heights often need to be modified in realistic engineering flows, and several modifications have been proposed including: 1) changing the number of cells used in the columns [11–13,10], 2) using a combination of heights and widths for interfaces with high curvatures [14], 3) decoupling the columns from the computational mesh [15], and even applying the approach to level sets [16]. ACES avoids many of these challenges since the least squares regression provides more flexibility than the height function method.

The curvature evaluation scale refers to the size of the computational stencil used by the discretization to compute the curvature. Fig. 1 provides an example of a continuous function representing an interface and two numerical discretizations of the function and their associated curvatures. The two discretizations use three function values with different spacing ($\Delta x_1 < \Delta x_2$) and thus scales. It is clear that the curvature evaluation scales can drastically impact the computed curvature. Curvature evaluation scales are limited when using the height function method. Stencil size can be varied leading to second- and fourth-order formulations [10]. The fourth-order scheme has a larger curvature evaluation scale, but the schemes are limited to these scales, unless more development occurs.

The proposed ACES method provides an alternative to the height function method and allows for the curvature scale to be easily adjusted. ACES computes the interface curvature by fitting a polynomial to interfacial points computed from the VoF interface representation. The fit is performed with a weighted least squares regression. The ACES method is similar to techniques used in interface tracking schemes [17–19] as ACES fits the interface represented by interfacial points. The weighting of interfacial points in the weighted least squares fit is similar to the kernel used in convolution methods that smooth the liquid volume fraction by weighting the volume fractions by their distance from the location the curvature is being computed [20]. Applying the polynomial fit to interfacial points computed from a VoF implementation is a novel contribution of this work. Details of the ACES methodology are provided in Section 2. ACES and our implementations of the height function method (Section 3) are verified with static interfaces and results are provided in Section 4.

There has been a lot of work on developing and testing interface curvature schemes [9,11–15]. However, the authors are not aware of any work that studies the effect of the curvature evaluation scale on dynamic interfaces. Some notable studies compare the second- and fourth-order height function methods [21,22,10]. Sussman and Ohta [21] compare the second- and fourth-order height function methods using the parasitic currents test case, which tests the coupling of the curvature calculation with a Navier–Stokes solver, but only for very small interface perturbations. Zhang and Fogelson [23] compute the curvature of a transported interface and vary the scale the curvature is computed on, but the transport is not coupled with a Navier–Stokes solver. In this work, we perform dynamic simulations with different curvature scales and show that

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