On a relation between the sharp and diffusive interface models

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Introduction

The experiments reveal the macroscopic gas/liquid interface is a region of a finite thickness $\epsilon_h \sim \sqrt{k_B T/\sigma}$, where k_B is the Boltzmann constant, T is absolute temperature and σ surface tension coefficient; $\epsilon_h \sim 5\text{Å}$ due to stochastic motion caused by thermal capillary waves [1]. As the interface thickness is negligible when compared with the characteristic flow length scale, the interface is often approximated with help of the three dimensional Heaviside function $H(\psi)$. This leads to the sharp interface model represented in the VOF or SLS methods by the level-sets of the Heaviside $H(\psi = 0) = 1/2$ and/or signed-distance $\psi(H = 1/2) = 0$ functions, see [2, 3] respectively. The mathematical relation between these two sharp interface representations in the limit of $\epsilon_h \to 0$ has been introduced in [4], therein, the consistent solution of the re-initialization equation for the conservative $\alpha(\psi)$ and signed-distance $\psi(\alpha)$ level-set functions is proposed. In the present paper we postulate a physical interpretation of the model equations derived in [4]. It is demonstrated, these equations can be obtained in terms of the ensemble averaging of sharp interface disturbed by the field of stochastic forces and the conservative closure of correlation between the velocity fluctuations in the direction normal to the interface and the instantaneous interface position given by the Dirac's delta function: $\langle \mathbf{w}' \cdot \mathbf{n}_\Gamma \delta(\psi) \rangle$. As a result, a new interpretation of the regularized Heaviside function $\alpha(\psi)$ and the signed distance function $\psi(\alpha)$ is postulated. We argue, the probability of finding one of the two phases sharing the regularized, non-flat interface in the phase equilibrium state is given by $\alpha(\psi) = [1 + \tanh(\psi(\alpha)/2\epsilon_h)]/2$, i.e., the cumulative function in the logistic distribution, where the signed distance function $\psi(\alpha) = \epsilon_h ln\{\alpha(\psi)/[1-\alpha(\psi)]\}$ is its first quantile and $\epsilon_h = d\sqrt{3}/\pi$ where d denotes the standard deviation. The relation between $\alpha(\psi)$–$\psi(\alpha)$ allows mapping between different representations of the regularized $\epsilon_h \neq 0$ or sharp $\epsilon_h = 0$ interface [4, 5, 6]. Furthermore, this work discusses the relation between the sharp interface model and the diffusive Allen-Cahn [5] interface model assuming a continuous change of density across the interface with regard to the order parameter $\alpha(\psi)$. We argue that $\alpha(\psi)$ interpreted as probability of finding the expected position of the regularized interface is a conserved quantity and the order parameter of the new phase field model. This is in contrast to works in the extant literature based on results from [5]. Moreover, we demonstrate solution of the re-initialization equation in the statistical interface model is equivalent to finding the minimum of Helmholtz free energy at the non-flat interface. The functional derivative of the term used to modify the original Ginzburg -Landau functional can be related to the capillary force added to the momentum equation in the one fluid model of the two-phase flows separated by the immiscible interfaces.

Numerical results

The mathematical form of the equations of the statistical interface model permits an introduction of a new Lagrangian scheme for the advection of the level-set functions. This scheme allows convergence of the re-initialization equation on gradually refined grids independent from the number of re-initialization steps, moreover, the convergence rate order of the interface shape and curvature is the same as theoretical order of the numerical schemes used for discretization of the advection and re-initialization equations. Namely, the second-order approximation allows complete, second-order convergence of the interface shape and curvature during advection of the circular interface in the divergence free velocity field without deformation. Results obtained with the second-order accurate MUSCL TVD Eulerian scheme (E) and new Lagrangian scheme (L) are presented in Figure. 1.

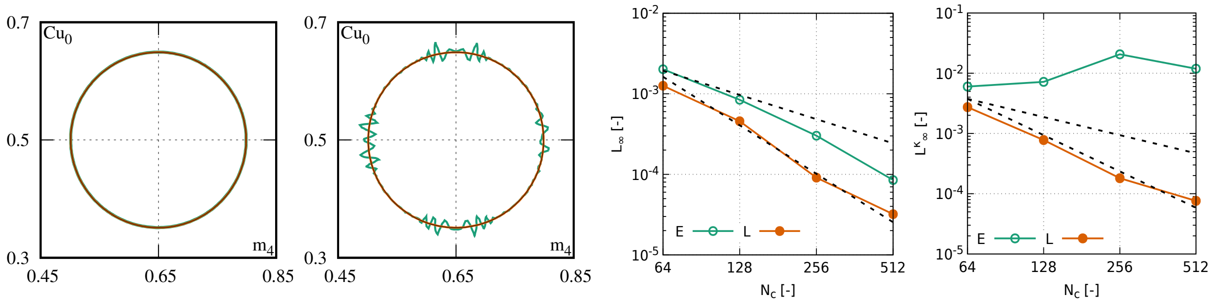

Figure 1: The interface shape (left) and curvature (right) obtained using the Eulerian (green solid lines) and Lagrangian (orange solid lines) schemes after one revolution of the circular interface in the divergence free velocity field without deformation, and their convergence rates on gradually refined grids illustrated using L_∞ norm. The black solid line depicts analytical solution. Only the new Lagrangian scheme derived using the advection equation of the statistical interface model achieves the complete second-order convergence rate depicted with stepper of the two black-dashed lines.

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