A conservative diffuse-interface method for compressible two-phase flows

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Abstract

In this article, we propose a novel conservative diffuse-interface method for the simulation of compressible two-phase flows. The proposed method discretely conserves the mass of each phase, momentum and total energy of the system. We use the baseline five-equation model and propose interface-regularization (diffusion-sharpening) terms in such a way that the resulting model (a) maintains the conservative property of the underlying baseline model, (b) lets us use a central-difference scheme for the discretization of all the operators in the model, which leads to a non-dissipative implementation that is crucial for the simulation of turbulent flows and acoustics. Furthermore, the provable strengths of the proposed model are: (a) the model maintains the boundedness property of the volume fraction field, which is a physical realizability requirement for the simulation of two-phase flows, (b) the proposed model is such that the transport of volume fraction field inherently satisfies the total-variation-diminishing property without having to add any flux limiters that destroys the non-dissipative nature of the scheme, (c) the proposed interface-regularization terms in the model do not spuriously contribute to the kinetic energy of the system and therefore does not affect the non-linear stability of the numerical simulation, (d) the model is consistent with the second law of thermodynamics. Finally, we present numerical simulations using the model and assess (a) the accuracy of evolution of the interface shape, (b) implementation of surface tension effects, (c) propagation of acoustics and their interaction with material interfaces, (d) the accuracy and robustness of the numerical scheme for simulation of complex high Reynolds number flows, and (e) performance and scalability of the method.

Keywords: phase-field method, compressible flows, two-phase flows, conservative, central-difference scheme

1. Introduction

Compressible two-phase flows are ubiquitous in nature and are of engineering interest. One of the primary applications of two-phase flows with compressible phases is in the study of underwater bubble acoustics. Prediction of bubble dynamics in turbulent seawater is of practical importance for the engineering analysis of naval systems. In ships, the air bubbles

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entrained by boundary layers and stern waves form an elongated wake that lasts for several kilometers downstream (Trevorrow et al., 1994, Fu et al., 2007, Stanic et al., 2009). Though the bubbles are tiny, with diameters of order 1 mm or less, they exhibit strong acoustic responses and hence the bubbly wake can be detected acoustically, which reveals the presence and position of the ship. The predictive modeling of bubble distributions in wakes, along with their acoustic response, has remained elusive and mostly confined to Reynolds-averaged Navier-Stokes (RANS) analyses because of the multiscale nature of the problem and the computational challenges associated with scalability and performance (Carrica et al., 1999, Culver and Trujillo, 2007). Hence, the current study is focused on developing a conservative numerical method that enables accurate treatment of the interaction of acoustics with gas-liquid interfaces (single and multiple bubbles) in compressible turbulent flow environments. This aids in investigating the current limitations and in developments of subgrid-scale models based on the Rayleigh-Plesset or Keller-Miksis equations used in RANS and large-eddy simulations (LES). The present paper deals with the development and verification of the numerical method, and the application of this to study for bubble acoustics in a realistic setting will be deferred to a future work.

Apart from bubble acoustics, applications of compressible two-phase flows also include super-critical flow regimes in high-pressure environments and liquid fuel injection systems. In compressible flows, thermodynamics plays an important role and adds one more level of difficulty to an already complex problem of two-phase flows, by imposing an additional requirement that the model should maintain thermodynamic consistency at the interface. Moreover, the numerical study of turbulent flows and acoustics requires stable, non-dissipative, and conservative numerical methods. To the best of our knowledge, the state-of-the-art techniques to simulate compressible two-phase flows lack many of these features. With this motivation, we have developed a diffuse-interface five-equation model for the simulation of two immiscible compressible fluids that has all the above favorable properties.

Compressible two-phase flows have been extensively studied for the last two decades (Saurel and Pantano, 2018), predominantly using diffuse-interface methods. Different diffuse-interface models present in the literature can be broadly classified into four major types: (a) The five-equation model (Kapila et al., 2001) solves two mass balance equations—one for each of the phases—a momentum equation, a total energy equation, and a volume fraction advection equation. This is the model that is most suitable for the simulation of two-phase non-reacting flows with immiscible fluids. More on this model will be described in Section 2. (b) The six-equation model is similar to the five-equation model but solves two energy equations, one for each of the phases. (c) The seven-equation model (Baer and Nunziato, 1986) solves two momentum equations and two energy equations and has two separate velocity fields for each of the phases. This is the most general of all the models since it includes non-equilibrium effects such as phase change and mass transfer. (d) The four-equation model (Abgrall, 1996) has no separate mass balance equations for each of the phases; instead, it solves a continuity equation, hence conserving only the total mass and not the individual mass of each phase. The volume fraction advection equation has also been replaced by a transport equation for the polytropic coefficient in this model.

The seven-equation model was first proposed by Baer and Nunziato (1986) for the simulation of detonation-to-deflagration transition in reactive granular materials and was later used by Sainsaulieu (1995) to simulate two-phase flows using an approximate Roe-type Re-
mann solver. Abgrall (1996) proposed the first four-equation model to simulate two ideal gases using Roe’s Riemann solver and derived an interface-equilibrium condition (IEC) to eliminate the spurious pressure oscillations that was observed at the interface. More on IEC can be found in Section 7. Further Saurel and Abgrall (1999a) extended this four-equation model with IEC for stiffened-gas equation of state (EOS) and also derived IEC for seven-equation model (Saurel and Abgrall, 1999b). A more recent use of the four-equation model can be seen in Johnsen and Ham (2012), Movahed and Johnsen (2013) where a weighted essentially non-oscillatory (WENO) scheme was used at the interfaces and shocks and a high-order central-difference scheme was used away from these, and was used to simulate Richtmyer-Meshkov instability.

The five-equation model was first proposed by Kapila et al. (2001) for the simulation of detonation-to-deflagration transition in granular materials and was later used by Allaire et al. (2002) to simulate two-phase flows. They also proposed the isobaric closure law that mimics the IEC for five-equation model and showed that the model can simulate two fluids with arbitrary EOSs. Further, Perigaud and Saurel (2005) extended this model to include capillary and viscous effects. More recently, Shukla et al. (2010), Tiwari et al. (2013) proposed interface-regularization (diffusion-sharpening) terms that keeps the interface sharp for long time integrations, thus increasing the accuracy of the simulation. The five-equation model has also been implemented on unstructured grids in Chiapolino et al. (2017).

Attempts to simulate compressible two-phase flows have also been made using sharp-interface methods; see Jemison et al. (2014) for the moment-of-fluid approach, Hermann (2016) for a geometric volume-of-fluid approach, Huber et al. (2015) and Pu et al. (2017) for a level-set method, and He et al. (2017) for an algebraic volume-of-fluid approach. Although, sharp-interface methods are more accurate than diffuse-interface methods, they are also more expensive. Moreover, the expensive function evaluation of the sharp-interface methods is localized at the interface, which results in load-balancing and parallel scalability issues. When it comes to compressible flows, diffuse-interface methods have an obvious advantage over sharp-interface methods. The volume of each phase is inherently not conserved in compressible flows; hence, the expensive interface reconstruction and the geometric advection step in sharp-interface methods to achieve discrete volume conservation are less useful. Moreover, one cannot achieve mass conservation of each phase using a sharp-interface method —with the exception of the moment-of-fluid method (Jemison et al. 2014) —whereas, depending on the choice of the model, a mass balance equation in each phase can be solved in a diffuse-interface method to discretely conserve the mass of each phase. For these reasons, in the current study, we choose to use a diffuse-interface method over a sharp-interface method. For a more detailed comparison between sharp-interface and diffuse-interface methods, see Mirjalili et al. (2017).

In summary, a five-equation model appears to be the preferred choice of diffuse-interface model for the simulation of compressible two-phase flows with immiscible fluids. Some of the limitations in the current state-of-the-art methods are as follows: (a) The study of acoustics and turbulent flows requires non-dissipative methods, but to the best of our knowledge, there is no previous implementation of compressible two-phase flows that is fully non-dissipative (central-difference schemes). (b) All the interface-regularization (diffusion-sharpening) terms used along with the five-equation model are in non-conservative form (Shukla et al. 2010, Tiwari et al. 2013, Garrick et al. 2017), and the conservative form of the regularization
terms are currently considered to be unstable.

Therefore, in the current paper we present a novel diffuse-interface model that tries to address and overcome above inherent limitations of the current state-of-the-art methods. Our model (a) can be solved using non-dissipative numerical methods (central-difference schemes) that is crucial for the simulation of turbulence and acoustics, (b) discretely conserves mass of each phase, total momentum, and total energy in the system, (c) maintains mechanical equilibrium and thermodynamic equilibrium across the interface (no spurious behavior in velocity and pressure fields), (d) maintains a steady interface thickness throughout the simulation, (e) maintains boundedness of the volume fraction field, which is a physical realizability requirement for the simulation of two-phase flows, (f) maintains total-variation-diminishing (TVD) property of the volume fraction field without having to add any flux limiters that destroys the non-dissipative nature of the underlying central-difference scheme.

In the present paper, we present the model for shock-free compressible region, but shocks in a high-Mach number regime can potentially be handled with the implementation of the localized artificial bulk viscosity approach (Mani et al., 2009; Kawai et al., 2010). Rest of the article is divided into 11 sections, where (i) Section 2 presents the diffuse-interface formalism and the proposed new model, (ii) Section 3 presents the derivation of the volume-fraction equation and the proof of boundedness and TVD properties, (iii) Section 4, 5 and 6 presents the derivation of mass, momentum and energy equations respectively, (iv) Section 7 presents the proof of IEC condition, (v) Section 8 presents the final model in full form including the surface tension and gravity terms, and (vi) Section 9 presents the numerical implementation and Section 10 presents all the simulation results followed by the summary of results and findings in Section 11 and concluding remarks in Section 12.

2. Governing equations and diffuse-interface formalism

A close-up view of the molecular picture of the interface between two-phases is schematically shown in Figure 1, where a denser fluid is shown in green and the lighter fluid is shown in red. If we volume average the phases, we obtain the volumetric representation of the interface between two fluids (also shown in Figure 1) which is of $O(nm)$ thick typically and can be represented using a volume fraction field on an Eulerian grid. For problems that are of engineering interest, interface between two fluids can be regarded as mostly sharp because of the inherent scale separation that exists between the interface thickness and the characteristic scales of the flow present in the problem. However, a diffuse-interface method is a computational model that represents sharp interfaces that are artificially made $\sim O(\Delta x)$ thick so that the gradients at the material interface can be resolved on an Eulerian grid. This has huge implications on the choice of numerical methods used to represent the interface, numerical stability and accuracy of the numerical simulation and hence has been the focus of study for over two decades.

With the above diffuse-interface formalism as the focus of the current work, we start with the well-known inviscid five-equation model of Allaire et al. (2002). This form of the model has a volume fraction advection equation [Eq. (1)], a mass balance equation for each of the phases $l$ [Eq. (2)], a momentum equation [Eq. (3)], and a total energy equation [Eq. (4)].

$$\frac{\partial \phi_1}{\partial t} + \vec{u} \cdot \nabla \phi_1 = 0,$$

(1)
Volumetric averaging
Interface
Molecular picture Volume fraction

\[ \frac{\partial \rho_l \phi_l}{\partial t} + \nabla \cdot (\rho_l \vec{u} \phi_l) = 0, \quad l = 1, 2, \] (2)

\[ \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u} + p I) = 0, \] (3)

and

\[ \frac{\partial \rho (e + k)}{\partial t} + \nabla \cdot (\rho H \vec{u}) = 0, \] (4)

where \( \phi_l \) is the volume fraction of phase \( l \) that satisfies the condition \( \sum_{l=1}^{2} \phi_l = 1 \), \( \rho_l \) is the density of phase \( l \), \( \rho \) is the total density defined as \( \rho = \sum_{l=1}^{2} \rho_l \phi_l \), \( \vec{u} \) is the velocity, \( p \) is the pressure, \( e \) is the specific mixture internal energy, which can be related to the specific internal energy of phase \( l \) \( e_l \) as \( e = \sum_{l=1}^{2} \rho_l e_l \), \( k = \frac{1}{2} u_i u_i \) is the specific kinetic energy, and \( H = e + k + p/\rho \) is the specific total enthalpy of the mixture.

[Allaire et al., 2002] showed that when this system is solved along with an isobaric closure law at the interface, one can achieve mechanical and thermodynamic equilibrium (Postulate 2.1) at the interface that results in stable numerical solutions and eliminates spurious oscillations at the interface.

Postulate 2.1. If \( u_i^k = u_0 \) and \( p_i^k = p_0 \) across the interface, any model or a numerical scheme that satisfies \( u_i^{k+1} = u_0 \) and \( p_i^{k+1} = p_0 \), \( \forall i \), is said to satisfy the interface equilibrium condition (IEC), where \( k \) is the timestep index and \( i \) is the grid index (see Abgrall, 1996).

It is generally known that the interface thickness increases with simulation time in a classical diffuse-interface method, reducing the accuracy of the solution for long-time integrations. Hence, [Shukla et al., 2010] and [Tiwari et al., 2013] proposed interface-regularization (diffusion-sharpening) terms to counter this thickening of the interface. However, the regularization terms are in non-conservative form, and they argued that their conservative form of the interface-regularization terms results in tangential fluxes, which leads to unphysical interface deformations.

In the current work, we propose a new set of interface-regularization (diffusion-sharpening) terms that are in conservative form and show that the numerical solution is stable for long-time integrations. We propose a model of the form given in Eqs. (5)–(8) along with the viscous terms, where the highlighted terms are the newly introduced interface-regularization
(diffusion-sharpening) terms. Equation (5) represents the modified volume fraction advection equation, Eq. (6) represents the modified mass balance equation for phase $l$, Eq. (7) represents the modified momentum equation, and Eq. (8) represents the modified total energy equation. If a general equation of state (EOS) for phase $l$ is written as $p_l = \alpha_l p + \beta_l$, where $\alpha_l$ and $\beta_l$ are constants, then by invoking the isobaric closure law for pressure in the mixture region ($p = p_1 = p_2$), the generalized mixture EOS can be written as in Eq. (9).

$$\frac{\partial \phi_1}{\partial t} + \vec{\nabla} \cdot (\vec{u} \phi_1) = \phi_1 (\vec{\nabla} \cdot \vec{u}) + \vec{\nabla} \cdot \vec{a}_1^1,$$  \hspace{1cm} (5)

$$\frac{\partial m_l}{\partial t} + \vec{\nabla} \cdot (\vec{u} m_l) = \vec{\nabla} \cdot \vec{R}_l, \quad l = 1, 2,$$  \hspace{1cm} (6)

$$\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} \vec{u} + p \vec{I}) = \vec{\nabla} \cdot \vec{\tau} + \vec{\nabla} \cdot (\vec{f} \otimes \vec{u}),$$  \hspace{1cm} (7)

$$\frac{\partial E}{\partial t} + \vec{\nabla} \cdot (\vec{u} E) + \vec{\nabla} \cdot (p \vec{u}) = \vec{\nabla} \cdot (\vec{f} k) + \vec{\nabla} \cdot (\vec{\tau} \cdot \vec{u}) + \sum_{l=1}^{2} \vec{\nabla} \cdot (\rho_l h_l \vec{a}_l),$$  \hspace{1cm} (8)

and

$$p = \rho c + \left( \frac{\phi_1}{\alpha_1} + \frac{1 - \phi_2}{\alpha_2} \right) \left( \frac{\gamma - 1}{\alpha_1} \right).$$  \hspace{1cm} (9)

In Eqs. (5)–(8), $\vec{a}_1 = \Gamma \{ \epsilon \vec{\nabla} \phi_1 - \phi_1 (1 - \phi_1) \vec{n} \}$ is the flux of the interface regularization term for phase 1, and it satisfies the condition $\vec{a}_1 = -\vec{a}_2$, $\vec{n} = \vec{\nabla} \phi / |\vec{\nabla} \phi|$ is the outward normal of the interface, and $\Gamma$ and $\epsilon$ are the interface parameters, where $\Gamma$ represents an artificial regularization velocity scale and $\epsilon$ represents an interface thickness scale (see Section 3 for a discussion on the choice of these parameters). $\vec{R}_l = \rho_0 \vec{a}_l$ is the flux of the regularization term in the mass equation for phase $l$, where $\rho_0$ is the characteristic density representing phase $l$ (see Section 4). $\vec{f} = \sum_{l=1}^{2} \vec{R}_l$ is the net mass regularization flux, $m_l = \rho_0 \phi_l$ is the mass per unit total volume for phase $l$, and $\rho = \sum_{l=1}^{2} m_l$ is the total density of the mixture. In Eq. (6), $m_l$ is written instead of $\rho_0 \phi_l$ only to show that $m_l$ is the variable being solved and not $\rho_l$ (see Section 4). Invoking Stoke’s hypothesis, the Cauchy stress tensor is written as $\vec{\tau} = 2\mu \vec{D} - 2\mu (\vec{\nabla} \cdot \vec{u}) \vec{I} / 3$, where $\mu$ is the dynamic viscosity of the mixture evaluated using the one-fluid mixture rule as $\mu = \sum_{l=1}^{2} \phi_l \mu_l$, $\vec{D} = \{ \vec{\nabla} \vec{u} + (\vec{\nabla} \vec{u})^T \}$ is the strain-rate tensor, and $E = \rho (c + k)$ is the total energy per unit volume. If each of the phases is assumed to follow a stiffened-gas EOS, then the constants in the EOS can be written as $\alpha = \gamma - 1$ and $\beta = -\gamma \pi$, where $\gamma$ is the polytropic coefficient and $\pi$ is the reference pressure. Values of $\gamma$ and $\pi$ are experimentally determined, and the values used in this work are listed in Table 1. Then, the speed of sound $c_l$ for phase $l$ can be written as

$$c_l = \sqrt{\gamma_l (\frac{p + \pi_l}{\rho_l})}.$$  \hspace{1cm} (10)

In Eq. (8), $h_l = e_l + p/\rho_l$ represents the specific enthalpy of the phase $l$ and can be expressed in terms of $\rho_l$ and $p$ using the EOS as

$$h_l = \frac{(p + \pi_l) \gamma_l}{\rho_l (\gamma_l - 1)}.$$  \hspace{1cm} (11)
All the newly added terms are in conservative form, and hence the mass of each phase, momentum, and total energy are discretely conserved in the simulation irrespective of the choice of the numerical scheme. Moreover, we choose to use a second-order central-difference scheme for all the discretizations in this study since low-order central-difference schemes are known to have some advantages for the simulation of turbulent flows (Moin and Verzicco, 2016) due to their (a) non-dissipative nature, (b) low aliasing error, (c) easy boundary treatment, (d) low cost, and (e) improved stability. The non-dissipative nature of these schemes is also crucial for the resolved simulation of acoustics.

Further, a systematic derivation of the newly introduced regularization terms, along with the mathematical proofs is described in the subsequent sections.

3. Volume fraction advection equation

If we denote the volume fraction of phase 1 $\phi_1$ as $\phi$, then the the volume fraction advection equation in Eq. (5) can be written as

$$\frac{\partial \phi}{\partial t} + \vec{\nabla} \cdot (\vec{u} \phi) = \phi (\vec{\nabla} \cdot \vec{u}) + \vec{\nabla} \cdot \left[ \Gamma \{ \epsilon \vec{\nabla} \phi - \phi (1 - \phi) \vec{n} \} \right]. \tag{12}$$

This equation is obtained by combining Eq. (1) and the reinitialization step of the conservative level-set method by Olsson and Kreiss (2005) and Olsson et al. (2007), and is also an extension of the incompressible version of the conservative diffuse-interface method introduced by Mirjalili et al. (2018). One can show that Eq. (12) also governs the advection of the volume fraction for phase 2; i.e., $\phi_2 = 1 - \phi$ also satisfies Eq. (12). Hence, both phases 1 and 2 are consistently transported.

3.1. Proof of boundedness of $\phi$

Since we choose to use a central-difference scheme to discretize all the system of equations in our model because of the well-known desirable properties, as already described in Section 2, this choice of the scheme could potentially create overshoots and undershoots in the $\phi$ field due to the dispersion errors. Hence, one needs to pick the values of the free parameters $\Gamma$ and $\epsilon$ such that $\phi$ is maintained between 0 and 1.

Mirjalili et al. (2018) showed that there exists a crossover line in the $\epsilon$-$\Gamma$ parameter space above which the boundedness of $\phi$ is guaranteed for an incompressible flow. We extend this analysis to show that the same criterion (Figure 2) is sufficient to maintain the boundedness of the $\phi$ field in a compressible flow setting, provided that the timestep restriction given in Eq. (14) for a one-dimensional setting and Eq. (20) for a three-dimensional setting is satisfied (Theorem 3.1).

**Theorem 3.1.** On a uniform one-dimensional grid, if $0 \leq \phi_i^k \leq 1$ is satisfied for $k = 0$, then $0 \leq \phi_i^k \leq 1$ holds $\forall k \in \mathbb{Z}^+$, where $k$ is the time-step index and $i$ is the grid index, provided

$$\frac{\epsilon}{\Delta x} \geq \frac{\langle |u|_{\text{max}} \rangle}{1} + 1 \tag{13}$$

and

$$\Delta t \leq \min_i \left[ \frac{1}{\max \{ (2\Gamma \epsilon) - (\frac{u_i^k - u_{i+1}^k}{\Delta x}), 0 \} } \right]. \tag{14}$$
are satisfied.

Proof. Consider the discretization of Eq. (12) on a one-dimensional uniform grid

\[
\phi_i^{k+1} = \phi_i^k + \Delta t \left[ - \frac{(u_{i+1}^k - u_i^{k-1})}{2\Delta x} \right] + \Delta t \left[ \Gamma \epsilon \left( \frac{\phi_{i+1}^k - 2\phi_i^k + \phi_{i-1}^k}{\Delta x^2} \right) - \Gamma \left\{ \frac{(1 - \phi_{i+1}^k)n_i^k + (1 - \phi_{i-1}^k)n_{i-1}^k}{2\Delta x} \right\} \right]
\]

(15)

where \( k \) represents the time index and \( i \) the grid index. This can be rearranged as

\[
\phi_i^{k+1} = \tilde{C}_i^{k-1} \phi_i^{k-1} + \tilde{C}_i^k \phi_i^k + \tilde{C}_i^{k+1} \phi_{i+1}^k,
\]

(16)

where \( \tilde{C}'s \) are coefficients given by

\[
\tilde{C}_i^{k-1} = \frac{\Delta t u_{i-1}^k}{2\Delta x} + \frac{\Delta t \Gamma \epsilon}{\Delta x^2} + \frac{\Delta t \Gamma}{2\Delta x} (1 - \phi_{i-1}^k)n_{i-1}^k,
\]

(17)

\[
\tilde{C}_i^k = -\frac{\Delta t u_{i+1}^k}{2\Delta x} + \frac{\Delta t \Gamma \epsilon}{\Delta x^2} - \frac{\Delta t \Gamma}{2\Delta x} (1 + \phi_{i+1}^k)n_i^k,
\]

(18)

and

\[
\tilde{C}_i^{k+1} = 1 + \frac{\Delta t}{2\Delta x} (u_{i+1}^k - u_i^{k-1}) - \frac{2\Delta t \Gamma \epsilon}{\Delta x^2}.
\]

(19)

Lemma 3.1.1. A scheme is said to be bounded if \( \tilde{C}'s \) are all positive (see Section 5.4.2 of Versteeg and Malalasekera [2007]).

For \( k = 0 \), it is given that \( 0 \leq \phi_i^k \leq 1 \) holds, which implies that \( (1 - \phi_{i-1}^k)n_{i-1}^k \geq -1 \).

Then \( \tilde{C}_i^{k-1} \geq \Delta t u_{i-1}^0/(2\Delta x) + \Delta t \Gamma \epsilon/(\Delta x^2) - \Delta t \Gamma/(2\Delta x) \geq -\Delta t / 2\Delta x (|u_{\text{max}}^0 + \Gamma| + \Delta t \Gamma \epsilon / \Delta x^2) \).

Now, invoking the condition in Eq. (13), we can show that \( \tilde{C}_i^{k-1} \geq 0 \) holds. Using similar arguments, we can show that \( \tilde{C}_i^{k+1} \geq 0 \) holds. Invoking the condition in Eq. (14), we can also show that \( \tilde{C}_i^k \geq 0 \) holds. Thus, Lemma 3.1.1 proves that \( 0 \leq \phi_i^k \leq 1 \) is satisfied. Now, by repeating the same procedure above, we can show that \( 0 \leq \phi_i^{k+1} \leq 1 \) is satisfied, provided

FIGURE 2. Region of boundedness as given by Eq. (13).
that $0 \leq \phi^k_i \leq 1$ is satisfied. Hence, using mathematical induction, $0 \leq \phi^k_i \leq 1$ is satisfied \( \forall k \in \mathbb{Z}^+ \), which concludes the proof.

\( \square \)

If $\phi$ is bounded, then $1 - \phi$ is also bounded. Hence, the volume fractions of both phases 1 and 2 are bounded. Now, generalizing Theorem (3.1) for three dimensions, the timestep restriction required for the boundedness of $\phi$ can be written as

$$
\Delta t \leq \min_i \left[ \frac{1}{\max \left\{ \left( \frac{6\Gamma \epsilon}{\Delta x^2} \right) - \left( \frac{\delta u_i}{\delta x_i} \right), 0 \right\}} \right],
$$

(20)

where $\delta/\delta x$ is the discrete derivative operator. The first term $(6\Gamma \epsilon/\Delta x^2)$ represents the diffusive Courant–Friedrichs–Lewy (CFL) condition of the interface, with $\Gamma \epsilon$ representing the diffusivity of the interface regularization and the second term $(\delta u_i/\delta x_i)$ represents the time constraint associated with the local dilation of the flow. If the flow is incompressible, the time-step constraint reduces to

$$
\Delta t \leq \frac{\Delta x^2}{6\Gamma \epsilon}.
$$

(21)

But, if the flow is expanding, the time-step constraint is less restrictive compared to an incompressible flow, and if the flow is compressing, the time-step constraint is more restrictive compared to an incompressible flow. However, the timestep restriction due to the acoustic CFL condition in the flow is usually more restrictive than the condition in Eq. (20) and hence it doesn’t add any additional time-step restriction on the flow.

3.2. Proof of total-variation-diminishing property of $\phi$

Boundedness property of $\phi$ is very important since it maintains $\phi$ between the physical values of 0 and 1 throughout the simulation. However, $\phi$ can still develop oscillations without going unbounded. But we need $\phi$ to be a smooth field that takes a value of 0 and 1 in the pure single phase regions away from the interface and a smooth variation in between in the mixture regions. Hence we seek a stronger nonlinear stability condition, the total-variation-diminishing (TVD) property for $\phi$.

Total variation of an arbitrary function $f$ is defined as the sum of 2 times all the local maxima of $f$, $-2$ times all the local minima of $f$ and $1$ times the boundary value of $f$, if that is a local maximum and $-1$ times of it, if that is a local minimum. Similarly, a numerical approximation of the total variation of $f$ is given by

$$
TV = \sum_{-\infty}^{\infty} |f_{i+1} - f_i|
$$

(22)

where $i$ is the grid index. Below we show that the criterion in Eq. (23) in addition to being bounded is sufficient to maintain the TVD property of the $\phi$ field for compressible flows in a one-dimensional setting and the criterion is Eq. (26) for a three-dimensional setting (Theorem 3.2). We thus want to emphasize that the $\phi$ field satisfies the TVD property without having to add any additional flux limiters that is typically done in the literature to achieve this property (Laney [1998]), which would destroy the non-dissipative property of the numerical method and is detrimental to the simulation of turbulent flows and acoustics.
Theorem 3.2. On a uniform one-dimensional grid, if $0 \leq \phi^k_i \leq 1$ is satisfied, then $\phi^k_i$ is said to satisfy the total-variation diminishing property (TVD), where $k \in \mathbb{Z}^+$ is the time-step index and $i$ is the grid index, provided

$$\phi^k \text{ is bounded}$$

and

$$\frac{2\Gamma \epsilon}{\Delta x^2} \geq \max_i \left\{ \frac{u^k_{i+1} - u^k_{i-1}}{\Delta x} \right\}, \quad (23)$$

are satisfied.

Proof. Following the proof of Theorem 3.1, discretizing the Eq. (12) on a one-dimensional uniform grid, we can arrive at the form

$$\phi^{k+1}_i = \tilde{C}^k_{i-1} \phi^k_{i-1} + \tilde{C}^k_i \phi^k_i + \tilde{C}^k_{i+1} \phi^k_{i+1}, \quad (24)$$

where $k$ represents the time index and $i$ the grid index and $\tilde{C}$’s are coefficients given in Eqs. (17-19).

Lemma 3.2.1. A scheme is said to be TVD if $\tilde{C}$’s are all positive and additionally $\tilde{C}^k_i$ is $\leq 1$ (Harten, 1983).

Following the proof of Theorem 3.1 if $\tilde{C}$’s are all positive, $\phi^k$ is bounded. Additionally, if $\tilde{C}^k_i$ is $\leq 1$, invoking Eq. (19), we have $1 + (\Delta t/(2\Delta x))(u^k_{i+1} - u^k_{i-1}) - 2\Delta t \Gamma \epsilon/(\Delta x^2) \leq 1$. Rearranging this, we arrive at the condition

$$\frac{2\Gamma \epsilon}{\Delta x^2} \geq \max_i \left\{ \frac{u^k_{i+1} - u^k_{i-1}}{\Delta x} \right\}, \quad (25)$$

which concludes the proof.

Now, generalizing Theorem 3.2 for three dimensions, the condition required for the total-variation-diminishing property of $\phi$ can be written as

$$\frac{6\Gamma \epsilon}{\Delta x^2} \geq \max_i \left\{ \frac{\delta u^k_i}{\delta x_i} \right\}, \quad (26)$$

If the flow is incompressible, this condition is trivially satisfied always. Therefore, boundedness implies TVD and vice-versa for an incompressible flow. But for compressible flows, it depends on the local dilatation of the flow. If the flow is compressing, then the dilation term is negative and therefore the above condition in Eq. (26) is again trivially satisfied. But high regions of compression adds constraint on the time-step size to maintain boundedness property (as described in Section 3.1) which is a requirement for TVD. On the other hand, if the flow is expanding, then this brings in an additional constraint on the value of $\Gamma$ for a given $\epsilon$ and $\Delta x$ given by Eq. (26). However, for all the simulations present in this work, time-step size given by acoustic CFL and the constraint on $\Gamma$ given by Eq. (13) was sufficient to maintain the boundedness and TVD properties for $\phi$ field (see Section 10 for the values of $\Gamma$, $\epsilon$ and $\Delta t$ used for various simulations in this work).
Figure 3. A schematic of a one-dimensional drop in a compressible flow, showing the typical flow conditions that could violate boundedness and TVD criteria and the consequence of the violation. Solid lines are the \( \phi \) field before and after the violation of the criterion. Small arrows around the dashed line shows the flow behavior and the dashed line is the location where the criterion is violated.

Summarizing Theorems 3.1 and 3.2, assuming that the constraints for an incompressible flow (Eq. (13) and Eq. (21)) are already satisfied in a compressible flow, high regions of compression might violate both TVD and boundedness properties if the constraint on time-step size \( \Delta t \) (Eq. 20) is not satisfied and high regions of expansion might violate TVD property if the constraint on \( \Gamma \) (Eq. 26) is not satisfied. Typical flow conditions and the consequence when the \( \phi \) field violates TVD and boundedness criteria in a compressible flow setting are schematically shown in Figure 3.

4. Mass balance equation

We employ a phenomenological approach to derive the mass balance equation for phase 1 [Eq. (6)]. Similar to Section 3.1, let \( \phi = \phi_1 \). Then, the mass per unit total volume of phase 1, is given by \( m_1 = \rho_1 \phi_1 \). Now, starting with the mass balance equation of the form

\[
\frac{\partial \rho_1 \phi}{\partial t} + \vec{\nabla} \cdot (\rho_1 \vec{u} \phi) = \vec{\nabla} \cdot \left[ \rho_1 \Gamma \left\{ \epsilon \vec{\nabla} \phi - \phi (1 - \phi) \vec{n} \right\} \right],
\]

one can see that in the incompressible limit (\( \rho_1 \rightarrow \rho_{01}, \vec{\nabla} \cdot \vec{u} = 0 \)), it is consistent with the volume fraction advection equation (Eq. (12)), where the characteristic density of phase 1 \( \rho_{01} \) is indeed the density of phase 1 in the incompressible limit. But one main disadvantage of this formulation is that it requires explicit computation of \( \rho_1 \). Typically, \( m_1 = \rho_1 \phi \) are solved together, and to obtain \( \rho_1 \), one should use \( \rho_1 = \phi_1 / \phi \), which results in inaccurate values of \( \rho_1 \) at the interface due to round-off errors (that stem from division by a small number). To overcome this, we use a form of the equation

\[
\frac{\partial \rho_1 \phi}{\partial t} + \vec{\nabla} \cdot (\rho_1 \vec{u} \phi) = \vec{\nabla} \cdot \left[ \rho_{01} \Gamma \left\{ \epsilon \vec{\nabla} \phi - \phi (1 - \phi) \vec{n} \right\} \right].
\]
This form of the equation also satisfies the same consistency condition in the limit of incompressibility and is similar to the one proposed in Eq. (27). Hence, we use this form of the mass equation since it does not require explicit computation of $\rho_1$. Now, writing Eq. (28) in terms of $m$, we get Eq. (6).

Further, summing up Eq. (6) for phases 1 and 2, we can derive the modified version of the continuity equation given by

$$ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = \nabla \cdot \vec{f}, $$

where $\vec{f} = \sum_{l=1}^{2} R_l = \sum_{l=1}^{2} \rho_0 \vec{a}_l$ is the net mass-regularization flux. The mass-regularization flux for phase $l$, $R_l = \rho_0 \vec{a}_l$ in Eq. (6), can be intuitively thought to be a weighted version of the interface-regularization flux $\vec{a}_l$ for phase $l$, where the weight is the characteristic density of the phase $\rho_0$. This scaling of the flux is employed such that the timescales of regularization of the $\phi$ and $\rho_l$ fields are similar.

The regularization terms are crucial in maintaining consistency between the mass and volume fraction fields. Figure 4 shows the effect of regularization terms on all the quantities being solved. Hence, if the volume fraction field is modified, reorganization of the mass is required to maintain consistency between the $\rho$ and $\phi$ fields, which is essentially achieved with the use of the regularization terms.

5. Momentum equation

Since the momentum of each of the phases is not individually conserved due to exchange of momentum at the interface, it is most efficient to write a single momentum equation for both phases. One can start with the momentum equation of the form

$$ \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u} + p \vec{1}) = 0, $$

in the inviscid limit. Taking the dot product of this equation with $\vec{u}$, and utilizing the modified continuity equation (Eq. (29)), results in the kinetic energy transport equation of the form

$$ \frac{\partial \rho k}{\partial t} + \nabla \cdot (\rho \vec{u} k) + k(\nabla \cdot \vec{f}) + \nabla \cdot (\vec{u} p) - p(\nabla \cdot \vec{u}) = 0, $$

where, the non-conservative term $k(\nabla \cdot \vec{f})$ represents the spurious contribution to the kinetic energy, which stems from the regularization of the interface. Having a spurious non-conservative term in the kinetic energy equation, even in the continuous form, is a sign that
the solutions of this model could potentially be spurious. This allusion is correct since the form of the momentum equation in Eq. (30) does not satisfy the IEC.

Now, let’s consider the modified version of momentum equation (Eq. (7)) in the inviscid limit

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \{ (\rho \vec{u} - \vec{f}) \otimes \vec{u} + p \mathbf{1} \} = 0. \quad (32)$$

Taking the dot product of this equation with $\vec{u}$ and utilizing the modified continuity equation (Eq. (29)), results in the kinetic energy transport equation of the form

$$\frac{\partial \rho k}{\partial t} + \nabla \cdot \{ (\rho \vec{u} - \vec{f})k \} + \nabla \cdot (\vec{u} p) - p(\nabla \cdot \vec{u}) = 0, \quad (33)$$

where there are no non-conservative terms that spuriously contribute to the kinetic energy. Additionally, the form of momentum equation in Eq. (7) also satisfies IEC (see Section 7), thus reinforcing the fact that the solution is not spuriously affected by regularization of the interface. This consistency correction to the momentum is crucial for compressible flows, without which the spurious momentum (or velocity) contribution to kinetic energy naturally leads to blow-up of the solver for any pair of fluids (especially in a non-dissipative numerical method). However, this consistency requirement is not as severe for incompressible flows and has been used for the simulation of low-density ratio flows at low Reynolds number ($Re$) without this correction (Mirjalili et al., 2018). This could be due to the enforcement of the divergence-free condition for the velocity, which stabilizes the solver in the process of projecting the velocity field on to a divergence-free field.

6. Energy equation: entropy conservation form

Entropy is not conserved in a diffuse-interface method even in the inviscid limit due to the regularization of the interface (irreversible process), which leads to the reorganization of mass, momentum, and potentially also energy, as illustrated in Figure 4. Entropy should only be conserved if the interface is already perfectly regular and the effects of all the regularization terms are identically zero. Thus, we seek to achieve approximate entropy conservation instead of exact conservation and derive the conservative form of the regularization terms in the energy equation with the constraint that it should satisfy the IEC. We first look at the case of exact entropy conservation and show that it doesn’t satisfy the IEC, and then look at the case where the IEC is satisfied and then state that entropy is not conserved as was expected for an irreversible process (second law of thermodynamics).

**Lemma 6.1.** Let $s_l$ be the physical entropy and $T_l$ be the temperature of phase $l$. Then the form of the internal energy equation that satisfies (entropy conservation)

$$\sum_{l=1}^{2} \left[ \rho_l \phi_l T_l \frac{Ds_l}{Dt} \right] = 0 \quad (34)$$

in the inviscid limit is

$$\frac{\partial p}{\partial t} + \nabla \cdot (\rho \vec{u} e) + \nabla \cdot (p \vec{u}) - \vec{u} \cdot \nabla p = \sum_{l=1}^{2} \left\{ h_l \nabla \cdot (\rho_l \tilde{a}_l) \right\}. \quad (35)$$
Proof. Let the internal energy equation be of the form
\[
\frac{D\rho e}{Dt} + \rho h(\vec{\nabla} \cdot \vec{u}) + X = 0, \quad (36)
\]
where \( X \) is the unknown term to be determined. Expressing the internal energy in terms of phase quantities
\[
\frac{D\rho e}{Dt} = \sum_{l=1}^{2} \frac{D(\phi_l \rho e_l)}{Dt} = \sum_{l=1}^{2} \left[ \phi_l \frac{D(\rho e_l)}{Dt} + \rho e_l \frac{D\phi_l}{Dt} \right], \quad (37)
\]
we then use Gibb’s relation to get
\[
d(\rho e_l) = \rho_e d\rho_l + e_l d\rho_l = \rho_l T_l ds_l + h_l d\rho_l. \quad (38)
\]
Using this in Eq. (36) results in
\[
\sum_{l=1}^{2} \left[ \rho_l \phi_l T_l \frac{D s_l}{Dt} + \phi_l h_l \frac{D\rho_l}{Dt} + \phi_l h_l \rho_l (\vec{\nabla} \cdot \vec{u}) + \rho e_l \frac{D\phi_l}{Dt} \right] + X = 0. \quad (39)
\]
Now, using Eqs. (5)–(6), one obtains
\[
\sum_{l=1}^{2} \left[ \rho_l \phi_l T_l \frac{D s_l}{Dt} + h_l \vec{\nabla} \cdot (\rho_l \vec{a}_l) - p_l (\vec{\nabla} \cdot \vec{a}_l) \right] + X = 0. \quad (40)
\]
Hence, if \( X = \sum_{l=1}^{2} \{ p_l (\vec{\nabla} \cdot \vec{a}_l) - h_l \vec{\nabla} \cdot (\rho_l \vec{a}_l) \} \), then the condition in Eq. (34) is satisfied. Now, invoking the isobaric closure law (Section 2), \( \sum_{l=1}^{2} \{ p_l (\vec{\nabla} \cdot \vec{a}_l) \} = 0 \), and the proof is complete.

The internal energy equation of the form in Eq. (35) does not satisfy the IEC, which also alludes to the fact that the entropy is not conserved exactly in a diffuse-interface method with regularization terms. Since we now only seek approximate entropy conservation, we modify the regularization term in Eq. (35) such that it satisfies the IEC, and the conservative form of the regularization term is restored. Thus, we arrive at the final form of the internal energy equation (taking the \( h_l \) on the right-hand side of Eq. (35) inside the divergence operator)
\[
\frac{\partial \rho e}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} e) + \vec{\nabla} \cdot (p \vec{u}) - \vec{u} \cdot \vec{\nabla} p = \sum_{l=1}^{2} \vec{\nabla} \cdot (\rho_l h_l \vec{a}_l). \quad (41)
\]
In compressible flows, internal energy is not a conserved quantity due to the reversible exchange of compression/expansion work between internal and kinetic energies, but the sum of internal and kinetic energy is conserved. Hence, summing up the internal energy transport equation (Eq. (41)) and the kinetic energy transport equation (Eq. (33)), we obtain
\[
\frac{\partial E}{\partial t} + \vec{\nabla} \cdot (\vec{u} E) + \vec{\nabla} \cdot (p \vec{u}) = \vec{\nabla} \cdot (f \vec{k}) + \sum_{l=1}^{2} \vec{\nabla} \cdot (\rho_l h_l \vec{a}_l). \quad (42)
\]
Clearly, all the terms in this equation are in conservative form as desired, and since this equation was obtained by summing the forms of internal energy and kinetic energy equations that satisfied the IEC, this form of the total energy equation also satisfies the IEC. With the inclusion of viscous terms, we get the final form of the total energy transport equation in Eq. (8).
7. Interface equilibrium condition

In incompressible flows, the divergence-free condition constrains the velocity and pressure fields, and hence eliminates the possibility of spurious solutions at the interface (in the absence of surface tension forces). However, such a constraint in compressible flows is absent, and thus care must be taken in the implementation of any numerical scheme in order to avoid spurious solutions at the interface. The IEC provides a consistency condition to check and eliminate the forms of the model and the numerical discretizations that contribute spuriously to the solution.

Lemma 7.1. The proposed conservative diffuse-interface model in Eqs. (5)-(8) satisfies the IEC defined in Postulate (2.1).

Proof. Part (a). Mechanical equilibrium: uniform velocity across the interface

Consider a one-dimensional second-order central discretization of the mass balance equation (Eq. (6)) on a uniform grid, assuming $u^k_i = u_0$

$$(\rho \phi^k_i)_{i+1} - (\rho \phi^k_i)_i = -\Delta t \left[ \frac{(\rho \phi^k_i)_{i+1} - (\rho \phi^k_i)_{i-1}}{2\Delta x} \right]^k u_0 + \Delta t \left[ \frac{R_{i,i+1} - R_{i,i-1}}{2\Delta x} \right]^k,$$  

where $k$ is the timestep and $i$ is the grid index. Now, consider a one-dimensional second-order central discretization of the momentum equation (Eq. (7)) on a uniform grid, assuming $u^k_i = u_0$ and $p^k_i = p_0$

$$(\rho u^k_i)_{i+1} - \rho^k_i u_0 = -\Delta t \left[ \frac{\rho_{i+1} - \rho_{i-1}}{2\Delta x} \right] u_0 + \Delta t \left[ \frac{\sum_{l=1}^2 R_{l,i+1} - \sum_{l=1}^2 R_{l,i-1}}{2\Delta x} \right] u_0.$$

Subtracting this from the sum of the discrete mass balance equations for phases 1 and 2 gives $u^{k+1}_i = u_0$.

Part (b). Thermodynamic equilibrium: uniform pressure across the interface

Consider a one-dimensional second-order central discretization of the internal energy equation (Eq. (41)) on a uniform grid, assuming $u^k_i = u_0$ and $p^k_i = p_0$ and using Eq. (11)

$$\sum_{l=1}^2 (\phi_l \rho_l e_l)^{k+1}_i - \sum_{l=1}^2 (\phi_l \rho_l e_l)^k_i = -\Delta t \sum_{l=1}^2 \left[ \frac{(p_l e_l \phi_l)_{i+1} - (p_l e_l \phi_l)_{i-1}}{2\Delta x} \right]^k u_0 + \Delta t \left[ \frac{\sum_{l=1}^2 R_{l,i+1} - \sum_{l=1}^2 R_{l,i-1}}{2\Delta x} \right] u_0.$$

"
and expressing \( e_i \) in terms of \( p_l \) using the EOS results in the discretized equation for pressure

\[
\begin{align*}
\left( \sum_{l=1}^{2} \phi_l \right)^k p_i^{k+1} - \left( \sum_{l=1}^{2} \phi_l \beta_l \right)^k p_0 + \left( \sum_{l=1}^{2} \phi_l \alpha_l \right)^k p_0 - \left( \sum_{l=1}^{2} \phi_l \beta_l \right)^k p_0 &+ \left( \sum_{l=1}^{2} \phi_l \alpha_l \right)^k p_0 - \left( \sum_{l=1}^{2} \phi_l \alpha_l \right)^k p_0
\end{align*}
\]

\[
= -\Delta t \left[ \frac{\sum_{l=1}^{2} \phi_l}{\alpha_l} p_0 - \left( \sum_{l=1}^{2} \phi_l \beta_l \right) i + \left( \sum_{l=1}^{2} \phi_l \beta_l \right) i - \left( \sum_{l=1}^{2} \phi_l \alpha_l \right) i - \left( \sum_{l=1}^{2} \phi_l \alpha_l \right) i \right] \frac{u_0}{2\Delta x} \right]^{k}
\]

\[
+ \Delta t \left[ \sum_{l=1}^{2} \left\{ \frac{p_0(1 + \alpha_l)}{\alpha_l} - \frac{\beta_l}{2\Delta x} \right\} \right]^{k}
\]

Now, let \( L(\phi_l) \) be a one-dimensional second-order central discretization of the volume fraction advection equation for phase \( l \) (Eq. (5)) on a uniform grid. Assuming \( u^k = u_0 \), and subtracting Eq. (46) from the equation \( \left( \sum_{l=1}^{2} L(\phi_l) \right) p_0 - \left( \sum_{l=1}^{2} L(\phi_l) \beta_l \right) \), results in

\[ p^{k+1} = p_0 \], which concludes the proof.

8. Full proposed model including the surface tension and gravity forces

We finally present the full proposed model in Eqs. (47)-(51) along with the viscous, surface tension and gravity terms, where the highlighted terms are the newly introduced interface-regularization (diffusion-sharpening) terms. We model the surface-tension force using the continuum surface force (CSF) method (Brackbill et al., 1992) as a volumetric body force in the momentum equation and the surface-tension energy term is included in the total-energy equation to consistently account for the exchange of surface energy and the kinetic energy in the flow (Perigaud and Saurel, 2005).

\[
\begin{align*}
\frac{\partial \phi}{\partial t} + \vec{\nabla} \cdot (\vec{u} \phi) &= \phi (\vec{\nabla} \cdot \vec{u}) + \vec{\nabla} \cdot \vec{a} \\
\frac{\partial m_i}{\partial t} + \vec{\nabla} \cdot (\vec{u} m_i) &= \vec{\nabla} \cdot \vec{R}_i, \quad i = 1, 2 \\
\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} \otimes \vec{u} + \vec{p} \mathbb{I}) &= \vec{\nabla} \cdot \vec{\tau} + \vec{\nabla} \cdot \left( \vec{f} \otimes \vec{u} \right) + \sigma \kappa \vec{\nabla} \phi_1 + \rho \vec{g} \\
\frac{\partial E}{\partial t} + \vec{\nabla} \cdot (\vec{u} E) + \vec{\nabla} \cdot (\rho \vec{u}) &= \vec{\nabla} \cdot \left( \vec{\tau} \cdot \vec{u} \right) + \vec{\nabla} \cdot \left( \vec{f} \otimes \vec{u} \right) + \sum_{i=1}^{2} \vec{\nabla} \cdot \left( \rho_i h_i \vec{a}_i \right) + \sigma \kappa \vec{u} \cdot \vec{\nabla} \phi_1 + \rho \vec{g} \cdot \vec{u} \\
p &= \rho e + \left( \frac{\phi \beta_1}{\alpha_1} + \frac{(1-\phi) \beta_2}{\alpha_2} \right) \left( \frac{\phi}{\alpha_1} + \frac{(1-\phi)}{\alpha_2} \right)
\end{align*}
\]

In Eqs. (47)-(51), \( \sigma \) is the surface-tension coefficient, \( \kappa = -\vec{\nabla} \cdot \vec{n} \) is the curvature of the interface and \( \vec{g} \) is the gravitational acceleration. For the convenience of the readers, the final model (Eqs. (47)-(51)) has been rewritten in Appendix A, where the highlighted modeling terms have been further expanded in terms of primitive variables and the mixture EOS has been expressed in terms of individual phase stiffened-gas EOS.
9. Numerical implementation

9.1. Numerical discretization

The choice of numerical method is very important in obtaining an accurate solution to the set of governing partial-differential equations (PDEs). In this work, we choose to use the fourth-order Runge-Kutta (RK4) time-stepping scheme and second-order central-differencing scheme for the discretization of all spatial operators. This choice of numerical scheme has some advantages for the simulation of turbulent flows and acoustics such as (a) non-dissipative nature, (b) low aliasing error, (c) easy boundary treatment, (d) low cost, and (e) improved stability as already explained in Section 2. Another highlight of this work is that, with the appropriate choice of $\Gamma$ and $\epsilon$, we can achieve the boundedness and TVD properties for the volume fraction field even with the use of central-difference scheme for all the spatial operators which would otherwise admit oscillatory solutions due to the associated dispersion errors.

A finite-volume collocated discretization strategy has been employed wherein all the variables are stored at cell centers and the fluxes are evaluated on the cell faces, and thus can be extended to arbitrary unstructured grids in a relatively straightforward manner. The choice of discretization of the non-linear sharpening term on the right-hand side (RHS) of the volume fraction advection equation (Eq. (47)) is crucial in achieving oscillation free, accurate solutions. Hence the discretization has been given in full detail in Appendix B. This non-linear sharpening term is also present in other equations which is more evident in the fully expanded form of the governing equations in Appendix A, and the above choice of discretization should be consistently used for this non-linear term in all the equations.

9.2. Performance and scalability

To verify the proposed model and the numerical method, we have written two versions of the in-house solver in C++ in two and three dimensions (CTR-DIs2D and CTR-DIs3D). These solvers can run on a parallel machine and the parallelization has been achieved using the Message Passing Interface (MPI) library, along with the arbitrary Cartesian-based domain decomposition capability. Both solvers has been optimized by using contiguous memory allocations for all the arrays to minimize cache misses. The number of communication calls has been minimized by the use of custom-defined MPI datatypes and by aggregating multiple message data into a single contiguous data. This increases the message size and decreases the number of communication calls and thereby achieving higher bandwidth and better parallel scalability. Additionally, all the communication is in synchronous non-blocking mode to hide latency and communication overhead which further increases the parallel scalability.

Apart from the performance improvement through solver optimization, diffuse-interface methods are inherently known to be cost effective and easily parallelizable compared to sharp-interface methods due to the absence of any expensive and localized geometric reconstruction of the interface, which could potentially result in load-balancing issues. The PDE-only nature of the diffuse-interface method results in well-balanced load throughout the domain and when combined with low-order central-difference schemes, gives rise to a low cost, robust and highly scalable method.

To evaluate the parallel-scaling efficiency of the in-house CTR-DIs3D solver, a strong-scaling test and a weak-scaling test has been performed on the Mira supercomputer at the
Argonne National Laboratory (ANL). The results from the strong-scaling test is shown in Figure 5. Ideal speedup and the actual speedup achieved are plotted against number of cores in the figure on the left. The numerical values in black (above the curve) are the number of cores and the numerical values in green (below the curve) represents the number of grid points per core. The actual time taken per time step (along with the numerical values in green, above the curve) and the ideal time per time step (along with the numerical values in black, below the curve) are plotted against the number of cores for the same simulation in the figure on the right. The results from the weak-scaling test is shown in Figure 6. Ideal time and the actual time taken are plotted against the number of cores. The numerical values in red (above the curve) are the number of cores and the numerical values in green (below the curve) represents the weak-scaling efficiency.

From the results it is evident that the weak scaling is almost ideal from 1 to $10^3$ cores, beyond which the efficiency drops to roughly 80% for $25K$ cores. The results from strong-scaling test shows an ideal behavior for large grid sizes per core and a drop in the scaling efficiency for grid sizes $\leq 12.5K$ per core due to a higher communication overhead compared to the time of computation for smaller grid sizes. This could be due to very small computational time per time step which is a result of highly optimized single-core performance of the solver and a low cost numerical method. However, the parallel scalability also depends on the underlying network topology of the machine on which the solver is being tested. Nevertheless, there is always a scope of improvement in optimizing the solver and in achieving better parallel scalability to obtain a highly performing code to save costs.

### 10. Results

In this section, multiple verification tests are presented that are used to assess the newly proposed model, the numerical discretization and the implementation. The verification tests used in this work can be broadly classified into (a) interface advection test cases, that test the accuracy of interface-capturing capability of the method, (b) surface tension test, that tests the accuracy of the implementation of the surface tension effects in the model, (c) acoustics test cases, that test the accuracy of propagation of acoustics and its interaction with material interfaces in the flow and (d) complex flows, that test the stability and robustness of the numerical scheme, and the accuracy of the method for high Reynolds number flows. In all the test cases, properties of the fluid used are that of air, water and kerosene, unless specified otherwise. The properties of the fluids in this study are listed in Table 1.

|        | air  | water | kerosene |
|--------|------|-------|----------|
| $\rho$ (kg/m$^3$) | 1.225 | 997   | 820      |
| $\mu$ (N/m$^2$)   | 0.0000181 | 0.00089 | 0.00164 |
| $\gamma$   | 1.4  | 4.4   | 4.4      |
| $\pi$ (MPa)    | 0    | 600   | 326.6    |
| $c$ (m/s)      | 338.1| 1627.4| 1324     |

**TABLE 1.** Properties of the fluids used in this work.
FIGURE 5. Strong scaling of the CTR-DIs3D solver on Mira supercomputer at Argonne National Laboratory. (a) Ideal speedup and the actual speedup achieved are plotted against number of cores. The numerical values in black (above the curve) are the number of cores and the numerical values in green (below the curve) represents the number of grid points per core. (b) The actual time taken per time step (along with the numerical values in green, above the curve) and the ideal time per time step (along with the numerical values in black, below the curve) are plotted against the number of cores for the same simulation.

FIGURE 6. Weak scaling of the CTR-DIs3D solver on Mira supercomputer at Argonne National Laboratory. (a) Ideal time and the actual time taken are plotted against the number of cores. The numerical values in red (above the curve) are the number of cores and the numerical values in green (below the curve) represents the weak scaling efficiency.
10.1. Initial conditions

One approach to set the initial values of $\phi$ is to start with a value of 1 in one phase and 0 in the other and to reinitialize the $\phi$ field using the equation

$$\frac{\partial \phi}{\partial \tau} = \vec{\nabla} \cdot \left\{ \epsilon \vec{\nabla} \phi - \phi(1-\phi)\vec{n} \right\}. \tag{52}$$

such that the $\phi$ field relaxes to the required equilibrium solution to the above equation. Alternatively, one could use an initial analytical profile to specify values for $\phi$ as

$$\phi = \frac{1}{2} \{1 + \tanh\left(\frac{x-x_0}{2\epsilon}\right)\}. \tag{53}$$

which is a one-dimensional equilibrium solution to Eq. (52), where $x_0$ is the desired location of the interface. In all the test cases in the present work, the initial profile of $\phi$ is analytically specified using Eq. (53) with an initial value of $\epsilon$ as $\epsilon_0 = \Delta x$, unless specified otherwise. Similarly, densities are initialized as $\rho_1 = \rho_{01} \phi$ and $\rho_2 = \rho_{02}(1-\phi)$, and viscosity as $\mu = \mu_1 \phi + \mu_2 (1-\phi)$. Velocity field $\vec{u}$ and pressure fields $p$ are initialized as desired and to initialize total energy, the internal energy $\rho e$ is first computed using Eq. (51) as

$$\rho e = p\left(\frac{\phi}{\alpha_1} + \frac{1-\phi}{\alpha_2}\right) - \left(\frac{\phi\beta_1}{\alpha_1} + \frac{(1-\phi)\beta_2}{\alpha_2}\right) \tag{54}$$

and then the total energy $E$ is computed by summing up the kinetic and internal energy contributions ($E = \rho \vec{u}^2/2 + \rho e$).

10.2. Interface advection tests

This section contains some standard test cases and newly proposed test cases to assess the accuracy of the shape of the interface computed using the proposed conservative diffuse-interface method in various simplified modeled flows that mimic complex real flow situations. The three test cases presented in this section are (a) drop in a shear flow, which is a standard test introduced by (Bell et al., 1989, Rider and Kothe, 1998) and has been extensively used in the literature (Tryggvason et al., 2011) to assess the accuracy of the interface in an incompressible shearing flow, (b) drop in a compressible shear flow is a new test case that we propose and use it to evaluate our model in terms of the accuracy of the shape of the interface being computed in a compressible shearing flow, and (c) star in a spiralling flow is also a new test case that we propose and use it to evaluate our model in terms of the accuracy in resolving sharp interfacial features in a compressible rotating flow. Additionally, test cases (b) and (c) also help in assessing the volume conservation properties of the method, and this is an important metric since the volume of individual phases are not inherently conserved in compressible flows.

10.2.1. Drop in a shear flow

Consider a two-dimensional computational square domain of dimensions $[0, 1] \times [0, 1]$. A circular drop of radius $R = 0.15$ is initially centered at $(0.5, 0.75)$. Since the quantity being assessed is the accuracy of the temporal evolution of the interface shape, which is computed by solving the volume fraction advection equation, the hydrodynamics can be decoupled
FIGURE 7. The enforced velocity field in the domain for the drop-in-a-shear-flow case at \( t = 0 \). The color field represents the magnitude of the velocity field and the lines represent the streamlines along with the arrows showing the direction of the flow.

from this test case by not solving the momentum and energy balance equations. Hence the velocity field is directly enforced in the domain at every time step as

\[
\begin{align*}
    u &= -\sin^2(\pi x)\sin(2\pi y)\cos(\pi t/T) \\
    v &= -\sin(2\pi x)\sin^2(\pi y)\cos(\pi t/T)
\end{align*}
\] (55)

where, \( T = 4 \) is the time period of the flow, \( t \) is the time coordinate, \( x \) and \( y \) are the spatial coordinates and \( u \) and \( v \) are the velocity components along \( x \) and \( y \) directions respectively. This test case is designed in such a way that the drop undergoes a shearing deformation until \( t = T/2 = 2 \) and the flow field is reversed due to the \( \cos(\pi t/T) \) term such that the initial drop shape should be recovered at \( t = T = 4 \). Since the velocity field \( \vec{u} \) is chosen to be incompressible, the drop undergoes deformation without changing the volume. The magnitude of the velocity field \( ||\vec{u}||_2 \) is plotted as a function of space in Figure 7 along with the streamlines at the initial time (\( t = 0 \)).

The domain was discretized using \( N_x \times N_y \) grid points and five different grid sizes (\( 32^2 \), \( 64^2 \), \( 128^2 \), \( 256^2 \) and \( 512^2 \)) were chosen to study the convergence of the error in the shape of the drop. The value of \( \epsilon = \Delta x \) and \( \Gamma = |u|_{max} \) were used in the simulation. Figure 8 shows the resultant shape of the drop obtained at half time (\( t = 2 \)) and at the final time (\( t = 4 \)) on five different grids. With an increase in the grid size, a clear convergence in the drop shape can be seen. Since at the final time, the drop is supposed to return to its original shape at \( t = 0 \), the “exact” final shape of the drop is known to be a circle, and hence the error in the “actual” shape of the drop obtained can be computed. We compute the error as

\[
NS_{\text{error}} = \frac{|\phi_f - \phi_i|}{N_x \times N_y}
\] (56)

where, \( NS_{\text{error}} \) is the cell-normalized shape error, \( \phi_f \) is the final volume fraction field, and \( \phi_i \) is the initial volume fraction field. The error \( NS_{\text{error}} \) is normalized by the grid size.
Figure 8. The computed drop shape ($\phi = 0.5$ contour) at half time of $t = 2$ (left) and at the final time of $t = 4$ on five different grid sizes: $32^2$, $64^2$, $128^2$, $256^2$ and $512^2$.

| Grid size    | $NS_{error}$ | $SE_{order}$ |
|--------------|--------------|--------------|
| $32 \times 32$ | 0.05344      |              |
| $64 \times 64$ | 0.02174      | 1.2290       |
| $128 \times 128$ | 0.004724    | 2.3010       |
| $256 \times 256$ | 0.001946    | 1.2139       |
| $512 \times 512$ | 0.0006397   | 1.5210       |

Table 2. Grid convergence of shape error for the case of drop in a shear flow.

$N_x \times N_y$ so that the error is independent of the grid size computed and can compared across simulations performed on different grid sizes. Alternatively, $\phi = 0.5$ contour can be chosen as the interface and can be used for the computation of the error. However, the volume enclosed (area in two dimensions) by $\phi = 0.5$ contour is not a conserved quantity in diffuse-interface method, and hence the error defined in Eq. (56) is often preferred over the other.

The computed shape error $NS_{error}$ on five different grids are listed in Table 2 along with the order of convergence $SE_{order}$. The shape error decreases with an increase in grid size, with an order of convergence roughly between 1 and 2.

10.2.2. Drop in a compressible shear flow

Consider a two-dimensional computational square domain of dimensions $[0,1] \times [0,1]$. A circular drop of radius $R = 0.15$ is initially centered at $(0.5,0.75)$. Since the proposed conservative diffuse-interface method can handle compressibility effects, the enforced velocity
field is composed of both solenoidal ($\vec{u}_s$) and dilatational ($\vec{u}_d$) components given by

$$u_s = -\sin^2(\pi x)\sin(2\pi y)\cos(\pi t/T)$$
$$v_s = -\sin(2\pi x)\sin^2(\pi y)\cos(\pi t/T)$$
$$u_d = (y - x)\cos(\pi t/T)$$
$$v_d = (-x - y + 1)\cos(\pi t/T)$$

(57)

where, $T = 2$ is the time period of the flow, $u_s$ and $v_s$ are the solenoidal velocity components along $x$ and $y$ directions respectively, and $u_d$ and $v_d$ are the dilatational velocity components along $x$ and $y$ directions respectively. The total enforced velocity $\vec{u}$ is therefore a sum of $\vec{u}_s$ and $\vec{u}_d$ in the domain at every time step. The dilatation is spatially uniform in the domain and is given by

$$\vec{\nabla} \cdot \vec{u} = -2\cos(\pi t/T)$$

(58)

This test case is designed in such a way that the drop undergoes a shearing deformation along with a uniform compression until $t = T/2 = 1$ and the flow field is reversed due to the $\cos(\pi t/T)$ term such that the initial drop shape and the volume should be recovered at $t = T = 2$. The compression ratio of the drop can be defined as

$$CR = \frac{V_i}{V_h} = 3.57$$

(59)

where, $V_i$ is the initial volume of the drop, and $V_h$ is the volume of the drop at $t = 1$. The magnitude of the velocity field $||\vec{u}||_2$ is plotted as a function of space in Figure 9 (left) along with the streamlines at the initial time ($t = 0$) and the temporal evolution of the volume of the drop is plotted in Figure 9 (right).

The domain was discretized using $N_x \times N_y$ grid points and five different grid sizes ($32^2$, $64^2$, $128^2$, $256^2$ and $512^2$) were chosen to study the convergence of the error in the shape and in the volume of the drop. The value of $\epsilon = \Delta x$ and $\Gamma = |u|_{\text{max}}$ were used in the simulation. Figure 10 shows the resultant shape of the drop obtained at half time ($t = 1$) and at the final time ($t = 2$) on five different grids. With an increase in the grid size, a clear convergence in the drop shape can be seen. Since at the final time, the drop is supposed to return to its original shape and volume at $t = 0$, the “exact” final shape and volume of the drop is known, and hence the error in the “actual” shape of the drop and the volume obtained can be computed. We compute the shape error as already defined in Eq. (56) and the volume error as

$$NV_{\text{error}} = \frac{V_f - V_i}{N_x \times N_y}$$

(60)

where, $NV_{\text{error}}$ is the cell-normalized volumetric error, and $V_f$ is the final volume of the drop. Similar to $NS_{\text{error}}$, $NV_{\text{error}}$ is normalized by the grid size $N_x \times N_y$ so that the error is independent of the grid size computed and can compared across simulations performed on different grid sizes. Additionally, we also define percentage change in volume of the drop as

$$\%V_{\text{error}} = \frac{V_f - V_i}{V_i} \times 100$$

(61)

that defines the percentage volumetric error, which is also independent of the grid size and can compared across simulations performed on different grid sizes. The computed shape error
FIGURE 9. (a) The enforced velocity field in the domain for the drop-in-a-compressible-shear-flow case at \( t = 0 \). The color field represents the magnitude of the velocity field and the lines represent the streamlines along with the arrows showing the direction of the flow, (b) Volume of the drop as a function of time, dashed line represents the initial volume of the drop used as a reference to show that the initial volume is recovered at final time \( t = 2 \).

FIGURE 10. The computed drop shape (\( \phi = 0.5 \) contour) at half time of \( t = 1 \) (left) and at the final time of \( t = 2 \) on five different grid sizes: \( 32^2 \), \( 64^2 \), \( 128^2 \), \( 256^2 \) and \( 512^2 \).
| Grid size   | NV<sub>error</sub>       | %V<sub>error</sub> | NS<sub>error</sub> | SE<sub>order</sub> |
|------------|-------------------------|-------------------|-------------------|-------------------|
| 32 × 32    | 2.0010 × 10<sup>-4</sup> | 0.2488            | 0.04529           |                   |
| 64 × 64    | 5.2806 × 10<sup>-6</sup>| 0.007213          | 0.01581           | 1.4317            |
| 128 × 128  | 1.2158 × 10<sup>-9</sup>| 1.7048 × 10<sup>-6</sup> | 0.003924          | 2.0153            |
| 256 × 256  | −2.1663 × 10<sup>-14</sup> | −3.0579 × 10<sup>-11</sup> | 0.0009728        | 2.01663           |
| 512 × 512  | 1.5266 × 10<sup>-15</sup> | 2.1584 × 10<sup>-12</sup> | 0.0002654        | 1.8329            |

**Table 3.** Grid convergence of shape and volumetric error for the case of drop in a compressible shear flow.

NS<sub>error</sub>, volume error NV<sub>error</sub> and percent volume change %V<sub>error</sub> on five different grids are listed in Table 3 along with the order of convergence SE<sub>order</sub> for the shape error. The shape error decreases with an increase in grid size, with an order of convergence approximately equal to 2, which is better than the incompressible case (Table 2). The absolute values of NS<sub>error</sub> are also smaller compared to the incompressible case, which could be due to the reduced volume of the drop that results in reduced shearing deformation. The volume error NV<sub>error</sub> and percent volume change %V<sub>error</sub> also decrease with an increase in grid size but at a much higher rate and NV<sub>error</sub> can be seen to have reached machine precision for 256<sup>2</sup> and 512<sup>2</sup> grid sizes even for compression ratio as high as CR = 3.57. This shows that the proposed method has good volume conservation properties.

### 10.2.3. Star in a spiralling flow

In this test case, a two-dimensional computational square domain ([−0.5, 0.5] × [−0.5, 0.5]) is used. A star shaped drop of radius \( R = 0.2(1 + \cos(4\theta)/4) \) is initially centered at (0, 0). Unlike the test case in Section 10.2.2, the enforced velocity field is composed of only the dilatational (\( \vec{u} = \vec{u}_d \)) components given by

\[
\begin{align*}
  u_d &= (y - x)\cos(\pi t/T) \\
  v_d &= (-x - y)\cos(\pi t/T)
\end{align*}
\]

where, \( T = 2 \) is the time period of the flow. However, the dilatation is spatially uniform in the domain and is same as in the test case in Section 10.2.2 and is given by the Eq. (58).

This test case is designed in such a way that the star undergoes a rotational motion along with a uniform compression until \( t = T/2 = 1 \) and the flow field is reversed due to the \( \cos(\pi t/T) \) term such that the initial star shape and the volume should be recovered at \( t = T = 2 \). The compression ratio in this test case is also 3.57. The magnitude of the velocity field \( ||\vec{u}||_2 \) is plotted as a function of space in Figure 11 along with the streamlines at the initial time (\( t = 0 \)).

The domain was discretized using \( N_x \times N_y \) grid points and five different grid sizes (32<sup>2</sup>, 64<sup>2</sup>, 128<sup>2</sup>, 256<sup>2</sup> and 512<sup>2</sup>) were chosen to study the convergence of the error in the shape and in the volume of the star. The value of \( \epsilon = \Delta x \) and \( \Gamma = |u|_{\text{max}} \) were used in the simulation. Figure 12 shows the resultant shape of the star obtained at half time (\( t = 1 \)) and at the final time (\( t = 2 \)) on five different grids. With an increase in the grid size, a clear convergence in the star shape can be seen. Since at the final time, the star is supposed to return to its original shape and volume at \( t = 0 \), the “exact” final shape and volume of the star is known, and hence the error in the “actual” shape of the star and the volume obtained
FIGURE 11. The enforced velocity field in the domain for the star-in-a-spiralling-flow case at $t = 0$. The color field represents the magnitude of the velocity field and the lines represent the streamlines along with the arrows showing the direction of the flow.

FIGURE 12. The computed star shaped drop ($\phi = 0.5$ contour) at half time of $t = 1$ (left) and at the final time of $t = 2$ on five different grid sizes: $32^2$, $64^2$, $128^2$, $256^2$ and $512^2$. 
can be computed. We compute the shape error as already defined in Eq. (56), the volume error as defined in Eq. (60) and the percent change in volume as defined in Eq. (61). The computed shape error $N_{S_{\text{error}}}$, volume error $N_{V_{\text{error}}}$ and percent volume change $\%V_{\text{error}}$ on five different grids are listed in Table 4 along with the order of convergence $SE_{\text{order}}$ for the shape error.

The shape error decreases with an increase in grid size, with an order of convergence between 1 and 2 for grid sizes $128^2$ and higher. The absolute values of $N_{S_{\text{error}}}$ are also higher compared to the drop-in-a-compressible-shear-flow case, which could be due to the presence of sharp features in the star shaped drop. Interestingly, the sub-first order convergence for the shape error could be due to the total loss of the sharp interface features on the star for grid size $32^2$ and $64^2$ as can be seen in Figure 12. This shows that there exists a minimum grid size required to resolve the sharp interface features in the flow and is clearly not met for the grids $32^2$ and $64^2$ when the star is fully compressed at $t = 1$. A zoomed-in image of the star at $t = 1$ computed on $64^2$ grid is shown in Figure 13 (left) and on $128^2$ grid in Figure 13 (right) along with the meshes, and the star computed on $512^2$ grid is also shown as a reference. The sharp curved features have around 2 to 3 grid points and hence are not resolved on $64^2$ grid, however doubling the resolution results in a much better representation of the sharp features on $128^2$ grid. The volume error $N_{V_{\text{error}}}$ and percent volume change $\%V_{\text{error}}$ also decreases with an increase in grid size but at a much higher rate and $N_{V_{\text{error}}}$ can be seen to have reached machine precision for grid sizes $128^2$ and higher, and hence faster compared to the drop-in-a-compressible-shear-flow case.

10.2.4. Effect of interface thickness parameter $\epsilon$

As already discussed in Section 3.2, for all the simulations presented in this work, the time step size $\Delta t$ was chosen to satisfy acoustic CFL, and the criterion in the Eq. (13) was
| Grid size | $NV_{error}$ | $%V_{error}$ | $NS_{error}$ | $SE_{order}$ |
|-----------|-------------|-------------|-------------|----------|
| 32 × 32   | $-5.8102 \times 10^{-5}$ | $-0.04158$ | 0.04023     |          |
| 64 × 64   | $-1.0315 \times 10^{-8}$ | $-7.8079 \times 10^{-6}$ | 0.03803 | 0.5290   |
| 128 × 128 | $-2.0761 \times 10^{-14}$ | $-1.5943 \times 10^{-11}$ | 0.01255 | 1.5155   |
| 256 × 256 | $-3.067 \times 10^{-14}$ | $-2.3638 \times 10^{-11}$ | 0.004503 | 1.3929   |
| 512 × 512 | $7.6328 \times 10^{-15}$ | $5.8881 \times 10^{-12}$ | 0.001836 | 1.2261   |

### TABLE 4. Grid convergence of shape and volumetric error for the case of star in a spiralling flow.

used to define $\Gamma$ for a given $\epsilon$ and was enough to maintain boundedness and TVD properties since the additional criteria on $\Delta t$ in Eq. (20) and on $\Gamma$ in Eq. (26) were already satisfied and did not pose additional constraints. However, one needs to be aware that these criteria could potentially add additional restriction on $\Delta t$ and $\Gamma$ in more severe flow conditions such as flows that involve shocks (shock-interface and shock-turbulence interactions).

The $\Gamma$ parameter represents an artificial regularization velocity scale and the value of $\Gamma$ obtained from the criterion in Eq. (13) is such that the interface-regularization terms are the most stiff terms in the volume fraction advection equation. As a result, the interface is maintained as close as possible to the equilibrium shape at all times.

The $\epsilon$ parameter represents an interface thickness scale and the thickness of the interface is $\approx 2\epsilon$. Therefore as $\epsilon/\Delta x \to 0.5$, numerical solution of the diffuse-interface method reaches the limit of sharp-interface method, where the interface thickness is $\approx \Delta x$. However, from the Eq. (13), this requires that the $\Gamma/|u_{max}| \to \infty$ which is not practical since $\Delta t \to 0$ as $\Gamma$ approaches $\infty$ because of the criterion in Eq. (20). Therefore practically, one could reduce $\epsilon$ to an extent that the increase in $\Gamma$ doesn’t add any additional constraint on time step size $\Delta t$ already imposed by the physical CFL limits (acoustic, convective, viscous, and thermal) in the problem. The increase in $\Gamma$ not only adds additional constraint on the time step, but could potentially lead to artificial alignment of the interface along the grid (Chiodi and Desjardins, 2017) since an increase in the value of $\Gamma$ is equivalent to performing more reinitialization and hence the choice of $\epsilon$ and $\Gamma$ is a tradeoff between accuracy and cost.

Since $\epsilon$ is an important parameter that governs the accuracy of the method, we studied the effect of $\epsilon$ on the drop-in-a-shear-flow, drop-in-a-compressible-shear-flow and star-in-a-spiralling-flow cases. Decreasing the value of $\epsilon$ does not necessarily imply better accuracy, since it requires an increased value of $\Gamma$ which could reduce the accuracy. A value of $\epsilon = \Delta x$ and $\Gamma = |u_{max}|$ are used for all the test cases presented in this work. However, in this Section we use a value of $\epsilon = 0.75\Delta x$ and $\Gamma = 2|u_{max}|$ and compare the results against the results from Sections 10.2.1-10.2.3.

Table 5 lists the computed shape error $NS_{error}$, volume error $NV_{error}$ and percent volume change $%V_{error}$ on five different grids with $\epsilon = 0.75\Delta x$ and $\Gamma = 2|u_{max}|$. Compared to the simulations with $\epsilon = \Delta x$ and $\Gamma = |u_{max}$ presented in Tables 2 and 4, sharper interface (small $\epsilon$) simulations have similar shape error $NS_{error}$ but a significantly lower volume error $NV_{error}$ and percent volume change $%V_{error}$, i.e., the volume error $NV_{error}$ reaches machine precision values for much coarser grids and hence the accuracy is higher.
| Grid size | $NV_{error}$ | $%V_{error}$ | $NS_{error}$ | $SE_{order}$ |
|-----------|--------------|--------------|--------------|--------------|
| Drop in a shear flow |
| 32 × 32 | 0.06664 |
| 64 × 64 | 0.02848 | 1.1700 |
| 128 × 128 | 0.007160 | 1.9886 |
| 256 × 256 | 0.002564 | 1.3961 |
| 512 × 512 | 0.0005550 | 2.3101 |
| Drop in a compressible shear flow |
| 32 × 32 | $-1.9812 \times 10^{-4}$ | $-0.2597$ | 0.04561 |
| 64 × 64 | $3.2340 \times 10^{-7}$ | 0.0004485 | 0.01531 | 1.4897 |
| 128 × 128 | $1.8007 \times 10^{-11}$ | $2.5348 \times 10^{-8}$ | 0.003738 | 2.0477 |
| 256 × 256 | $-4.5797 \times 10^{-16}$ | $-6.4708 \times 10^{-13}$ | 0.0009116 | 2.05021 |
| 512 × 512 | $-1.1061 \times 10^{-14}$ | $1.5643 \times 10^{-11}$ | 0.0002558 | 1.7817 |
| Star in a spiralling flow |
| 32 × 32 | $-4.4604 \times 10^{-7}$ | $-0.0003296$ | 0.03939 |
| 64 × 64 | $9.0111 \times 10^{-13}$ | $6.8781 \times 10^{-10}$ | 0.03967 | 0.4964 |
| 128 × 128 | $-3.0503 \times 10^{-14}$ | $-2.3474 \times 10^{-11}$ | 0.01317 | 1.5064 |
| 256 × 256 | $-3.3584 \times 10^{-15}$ | $-2.5898 \times 10^{-12}$ | 0.004347 | 1.5144 |
| 512 × 512 | $-1.8707 \times 10^{-14}$ | $-1.4433 \times 10^{-11}$ | 0.001964 | 1.1068 |

TABLE 5. Grid convergence of shape error for the case of drop in a shear flow with $\epsilon = 0.75\Delta$ and $\Gamma = 2|u|_{\max}$. 
10.3. Surface tension test: Oscillating drop

This section contains a standard test case that is used to assess the accuracy of the model in simulating flows dominated by surface tension effects and has been previously used by (Perigaud and Saurel, 2005; Olsson et al., 2007; Li et al., 2012; Shukla, 2014; Garrick et al., 2017). Consider a two-dimensional computational square domain of dimensions $[-2, 2] \times [-2, 2]$. An initially ellipse shaped drop is placed at $(0, 0)$ at rest and the shape of the drop is given by the equation

$$
\frac{x^2}{1.25^2} + \frac{y^2}{0.8^2} = 1.
$$

The drop is initially perturbed from its equilibrium circular shape so that the surface tension forces deform the drop towards its equilibrium shape and the balance of inertia and surface tension forces results in an oscillating drop until all the energy (kinetic + surface tension) is lost due to viscous dissipation.

The properties of the fluid in the drop are $\rho_l = 1000$, $\mu_l = 8.9 \times 10^{-4}$, $\pi_l = 6000$ and $\gamma_l = 4.4$, and for the surrounding fluid are $\rho_g = 1$, $\mu_g = 1.81 \times 10^{-5}$, $\pi_g = 0$, $\gamma_g = 1.4$. The surface tension coefficient for the interface between the fluids is $\sigma = 1$. The domain was discretized using $N_x \times N_y$ grid points and three different grid sizes ($100^2$, $200^2$ and $400^2$) were chosen to study the convergence following Garrick et al. (2017). The value of $\epsilon = \Delta x$ and $\Gamma = |u|_{max}$ were used in the simulation. The total time of integration was $T_{tot} = 120$.

Figure 14 shows the computed global kinetic energy ($\int \rho ||\vec{u}||_2 dV$) on three different grids along with the results from Garrick et al. (2017) denoted as “g” in the legend. The total (kinetic + surface tension) energy $E_o$ is also shown in the Figure 14 as a reference that is a conserved quantity in this problem in the absence of viscous dissipation. However, the viscous dissipation is not zero but negligible due to small $\mu_l$ and $\mu_g$ values. Period of oscillation on all three grids are identical and are in good agreement with the results from Garrick et al. (2017).

Figure 14 also shows that the global kinetic energy doesn’t spuriously decay and is fairly constant throughout the simulation on all grids, indicating the non-dissipative nature of the scheme. Small differences in the global kinetic energy at later time in the simulation ($t > 100$) could be due to (a) physical viscous dissipation, (b) non-conservative surface tension model, and (c) spurious currents. However, the combined effect of these are still quite small and the results can be considered grid independent.

10.4. Acoustic test cases

In this section numerical tests are presented to assess the accuracy of the proposed diffuse-interface method for the simulation of propagation of acoustics and its interaction with material interfaces. The two test cases presented in this section are (a) pressure-driven bubble oscillation, that is used to evaluate the accuracy of the method in handling acoustic-bubble interactions and a similar test case has been presented in Huber et al. (2015) for an axisymmetric setup, (b) interaction of a plane acoustic wave with a flat interface, that is used to evaluate the accuracy of the method in capturing reflected and transmitted acoustic amplitudes across material interfaces and the their direction of propagation (angles they make with the interface normal).
10.4.1. Pressure-driven bubble oscillation

For the test case of pressure-driven bubble oscillation, we compare the results against the analytical solution of the Rayleigh-Plesset equation. In three dimensions, the Rayleigh-Plesset equation can be written as (Brennen, 2013)

$$\frac{P_B(t) - P_\infty(t)}{\rho} = R\ddot{R} + \frac{3}{2}(\dot{R})^2 + \frac{4\nu\dot{R}}{R} + \frac{2\sigma}{\rho R},$$  \hspace{1cm} (64)

where $P_B(t)$ is the uniform pressure inside the bubble, $P_\infty(t)$ is the liquid pressure at infinity, $R(t)$ is the radius of the bubble, $\rho$ is the liquid density, $\nu$ is the liquid kinematic viscosity, $\sigma$ is the surface tension, which is taken to be zero in this work, and each dot represents the $d/dt$. A two-dimensional Rayleigh-Plesset equation does not exist and cannot be derived due to the presence of a logarithmic singularity at infinity. However, a finite-domain analytical solution can still be derived and can be used to verify the numerical solution. Hence, we derive a two-dimensional equivalent of the Rayleigh-Plesset equation for finite-size domains (see Appendix C) as

$$\frac{P_B(t) - P_S(t)}{\rho} = \ln \left( \frac{S}{R} \right) \left\{ (\dot{R})^2 + R\ddot{R} \right\} + \left( \frac{R^2 - S^2}{2S^2} \right) (\dot{R})^2 + \frac{2\nu\dot{R}}{R} + \frac{\sigma}{\rho R},$$  \hspace{1cm} (65)

where $P_R$ and $P_S$ are the liquid pressures at the surface of the bubble ($r = R(t)$) and a finite distance from the center of the bubble $r = S$, respectively.

In this test case, an air bubble of diameter 4 $\mu$m is placed at the center of a square domain of size 10 $\mu$m $\times$ 10 $\mu$m (with coordinates $[-5,5]$ $\mu$m $\times$ $[-5,5]$ $\mu$m), as shown in
Figure 15. On all four sides of the domain, a Dirichlet boundary condition of the form $10^5\{1+0.1\sin(10\omega_c t)\}$ for the pressure and a Neumann boundary condition for the velocity are imposed, where $\omega_c = 10208967.75 \text{ s}^{-1}$ is the characteristic resonance frequency of the bubble [Minnaert, 1933]. The $\phi$ field is initialized with an analytical hyperbolic-tangent function (equilibrium solution of the volume fraction regularization term in Eq. (5)) given by $1 - 0.5\left[1 + \tanh\left\{\left(\sqrt{x^2 + y^2 - r}\right)/(2\epsilon_0)\right\}\right]$, where $r$ is the radius of the bubble.

The solution was numerically integrated for a total of 50 $\mu$s physical time. Four different grid sizes were chosen, $50^2$, $100^2$, $200^2$, and $400^2$, to study the convergence of the solution. The value of $\epsilon = 0.55\Delta x$ and $\Gamma = 10|u|_{\text{max}}$ were used in the simulation. Timesteps were chosen based on the acoustic CFL condition for the particular grid size. Results from the various grid sizes are shown in Figure 16 and are compared with the semi-analytical solution obtained from numerically integrating the ordinary differential equation in Eq. (65) along with the ideal-gas law, where the bubble area is computed as $\int \phi dV$ in the simulations. Figure 16 shows the bubble response at initial times (0 $\mu$s to 0.6 $\mu$s) and at later times (19.75 $\mu$s to 20 $\mu$s). The initial transient response of the bubble shows a clear convergence of the numerical solution to the analytical solution with the increase in grid size. Moreover, the solution is very accurate even on the coarsest grid for the bubble response at later times (Figure 16(b)). This test case also shows that the numerical solution is stable for long-time integrations.

10.4.2. Interaction of a plane acoustic wave with a flat air-water interface: normal incidence

In this test case, a long three-dimensional domain of size $10 \mu m \times 0.1 \mu m \times 0.1 \mu m$ (with coordinates $[0, 10] \mu m \times [0, 0.1] \mu m \times [0, 0.1] \mu m$) is used, with a flat air-water interface located at $x = 5 \mu m$, as shown in Figure 17. The $\phi$ field is initialized with the analytical function $1 - 0.5\left[1 + \tanh\left\{(x-x_0)/(2\epsilon_0)\right\}\right]$, where $x_0$ is the location of the interface. The domain
is filled with air for $x < 5 \ \mu m$ and water for $x > 5 \ \mu m$. Perfectly reflecting wall boundary conditions are imposed on the domain face at $x = 0 \ \mu m$, and periodic boundary conditions are imposed for the faces at $y = 0 \ \mu m$, $y = 0.1 \ \mu m$, $z = 0 \ \mu m$, and $z = 0.1 \ \mu m$. For the wall at $x = 10 \ \mu m$, a Dirichlet boundary condition of the form $10^5\{1 - 0.5 \sin(\omega t)\}$ for the pressure and a Neumann boundary condition for the velocity are imposed for $t < 614.5 \ ps$, where $\omega = 2\pi c/\lambda$, $\lambda = 1 \ \mu m$ and $c$ is the speed of sound in water. Later, it is switched to a perfectly reflecting wall boundary conditions for $t > 614.5 \ ps$ such that a half-wave is generated at the boundary and its propagation in the domain can be monitored.

The solution was numerically integrated for a total of $1 \ \mu s$ physical time. A grid of size $1000 \times 10 \times 10$ was used in this simulation along with the timestep size of $\Delta t = 1 \ ps$. The value of $\epsilon = \Delta x$ and $\Gamma = |u|_{max}$ were used in the simulation. Results from the simulation are shown in Figure 18. The pressure along $x$ is plotted at various times for $y = z = 0.05 \ \mu m$. The acoustic wave interacts with the air-water interface and reflects back, as can be seen from the results at 3 ns, 3.5 ns and 4 ns. Clearly, nothing gets transmitted across the interface, and
the reflected wave amplitude is approximately equal to the incident wave amplitude but the wave is flipped. This behavior of reflection and transmission of an acoustic wave across a flat air-water interface can be predicted using linear acoustic theory. The reflection coefficient is given by \( R = \frac{(Z_a - Z_w)}{(Z_a + Z_w)} = -0.999516 \), and the transmission coefficient is given by \( T = \frac{2Z_a}{(Z_a + Z_w)} = 4.8 \times 10^{-3} \), where \( Z_a \) and \( Z_w \) are the acoustic impedance for air and water, respectively. \( R \) being roughly equal to \(-1\) indicates that the reflected wave amplitude is the same as the incident wave amplitude and the wave is flipped. \( T \) being roughly equal to 0 indicates that nothing gets transmitted across the interface. Hence, the numerical solution is in good agreement with the theoretical prediction. Solutions at 6.5 ns and 12.5 ns also show the pressure-doubling behavior at the wall, which is again predicted by the theory (Blackstock, 2000).

10.4.3. Interaction of a plane acoustic wave with a flat air-water interface: oblique incidence

In this test case, a two-dimensional domain of size 10 \( \mu \text{m} \times 10 \mu \text{m} \) (with coordinates \([0, 10] \mu \text{m} \times [0, 10] \mu \text{m}\)) is used, with a flat interface that is aligned along the principal diagonal of the domain, as shown in Figure 19. The \( \phi \) field is initialized with the analytical function \( 1 - 0.5 \left[ 1 + \tanh \left\{ (10^{-5} - x - y)/(2\epsilon_0) \right\} \right] \). The domain is filled with water below the interface (medium 2) and kerosene above the interface (medium 1). A Dirichlet boundary condition of the form \( 10^5 \{1 - 0.5 \sin(\omega t)\} \) for pressure, where \( \omega = 2\pi c/\lambda \), \( \lambda = 2 \mu \text{m} \) and \( c \) is the speed of sound in kerosene, is imposed on the right domain boundary for \( t < 755.297 \) ps.
such that a half-wave is generated and propagates into the domain along the boundary normal so that the incident acoustic wave on the interface makes an angle $\theta_i = 45^\circ$.

A grid of size $1000 \times 1000$ was used in this simulation along with the time-step size of $\Delta t = 5$ ps. The value of $\epsilon = \Delta x$ and $\Gamma = |u|_{max}$ were used in the simulation. Results from the simulation are shown in Figure 20. The pressure field is plotted at time $t = 6$ ns. The acoustic wave interaction with the water-kerosene interface results in a reflected wave and a transmitted wave. The behavior of reflection and transmission of an oblique acoustic wave across a flat interface can be predicted using linear acoustic theory. The angle of the transmitted wave with the interface $\theta_t$ is given by the Snell’s law of refraction

$$\frac{\sin (\theta_i)}{c_1} = \frac{\sin (\theta_t)}{c_2}$$

where $c_1$ and $c_2$ are the speeds of sound in medium 1 and 2, and the angle of reflection $\theta_r$ is same as the angle of incidence $\theta_i$ (Pierce and Beyer, 1990). In this problem $c_1 = 1324 \text{ m/s}$ and $c_2 = 1627.4 \text{ m/s}$ and since $c_2/c_1 > 1$, $\theta_t$ only exists if $|\sin (\theta_i)| < 1$. Therefore, $\exists$ a critical angle $\theta_c$

$$\theta_c = \arcsin \left( \frac{c_1}{c_2} \right) = 54.5^\circ$$

such that $\forall \theta_i > \theta_c \implies \theta_r$ and the incident wave results in total internal reflection. Hence $\theta_i = 45^\circ$ is chosen in this problem such that there is no total internal reflection. From Eq. (66), the angle of the transmitted wave is $\theta_t = 60.358^\circ$ and the angle of the reflected wave is $\theta_r = 45^\circ$. In Figure 20, three arrows along incident, reflected and transmitted waves are plotted based on the theoretical prediction of $\theta_t$ and $\theta_r$ for the given $\theta_i$. The numerical solution is thus in good agreement with the theoretical prediction.
FIGURE 20. The pressure field (in Pa) at time $t = 6$ ns. Solid line is the interface, dashed lines represent interface normal, and three arrows represent the direction of propagation of incident, reflected and transmitted waves that are at an angle $\theta_i$, $\theta_r$ and $\theta_t$ respectively, with the interface normal.
10.5. Complex flow: Three-dimensional Rayleigh-Taylor instability

In this section, we present the simulation of late-time growth of a three-dimensional single-mode Rayleigh-Taylor instability and validate the accuracy of the proposed diffuse-interface method. This simulation also helps in evaluating the robustness of the numerical scheme to simulate complex high Reynolds number flows. In this test case, we compare the results against a previous numerical study by Liang et al. (2016) where they used a lattice Boltzmann multiphase model with multiple-relaxation-time collision operator for their simulation and also validate our method by comparing against an experimental study by Wilkinson and Jacobs (2007).

It is known that the three-dimensional Rayleigh-Taylor instability at sufficiently high Reynolds numbers, undergoes four stages of development (Sharp, 1983) (a) linear growth stage, where the amplitude of the perturbation grows exponentially with time until it reaches \( \approx O(\lambda) \), where \( \lambda \) is the wavelength of the initial perturbation, (b) terminal velocity growth stage, where the perturbation grows nonlinearly with the heavy fluid (referred to as spike) and light fluid (referred to as bubble) penetrating into each other at a constant velocity, (c) reacceleration stage, where the spike rolls up along the sides to form a mushroom structure due to Kelvin-Helmholtz instability (Glimm et al., 2002; Ramaprabhu et al., 2006; Wilkinson and Jacobs, 2007), and (d) chaotic development stage, where the spike breaks up resulting into a turbulent and chaotic mixing of the fluids (Ramaprabhu et al., 2012). For the two-dimensional Rayleigh-Taylor instability and the growth stages, see Wei and Livescu (2012). See Zhou (2017) for an extensive review and recent developments on the single and multi-mode Rayleigh-Taylor instability induced flow and turbulence.

Following Liang et al. (2016), we use a three-dimensional computational domain of size \( 12\lambda \times \lambda \times \lambda \), where \( \lambda = 1 \) (with dimensions \([-6, 6] \times [-0.5, 0.5] \times [-0.5, 0.5]\)). Initially, a square-mode perturbation

\[
h(y, z) = 0.05\lambda\{\cos(ky) + \cos(kz)\}
\]

is imposed at the midplane \((x = 0)\), where \( k = (2\pi)/\lambda \) is the wavenumber. The \( \phi \) field is initialized with the analytical function \( 1 - 0.5\left[1 + \tanh\left\{(h(y, z) - x)/(2\epsilon_0)\right\}\right] \). The domain is filled with heavy fluid for \( x < h(y, z) \) and lighter fluid for \( x > h(y, z) \). A no-slip Dirichlet boundary condition is imposed on the walls at \( x = 0 \) and \( x = 12 \), and periodic boundary conditions are imposed for the faces at \( y = -0.5, y = 0.5, z = -0.5, \) and \( z = 0.5 \).

The properties of the heavy fluid are \( \rho_l = 1, \mu_l = 10^{-3}, \pi_l = 30 \) and \( \gamma_l = 1.4 \), and of the light fluid are \( \rho_g = 0.74, \mu_g = 0.74 \times 10^{-3}, \pi_g = 40 \) and \( \gamma_g = 1.4 \). The dynamic viscosities are chosen in such a way that the kinematic viscosity is same for heavy and light fluid \( \nu_l = \nu_g = 10^{-3} \). The surface tension coefficient for the interface between the fluids is \( \sigma = 0 \) and the imposed gravitational force is \( \vec{g} = 1\vec{x} \). The relevant non-dimensional numbers in this problem are Atwood number

\[
A_t = \frac{(\rho_l - \rho_g)}{(\rho_l + \rho_g)} \approx 0.15,
\]

and Reynolds number

\[
Re = \frac{\lambda U}{\nu} = 1000,
\]
where \( U = \sqrt{g\lambda} = 1 \) is the velocity scale in the problem and the characteristic time scale can be defined as

\[
\tau = \frac{1}{\sqrt{A_t g k}} \approx 1
\]  
(71)

The solution was numerically integrated for a total of 15 \( \tau \). A grid of size \( 1200 \times 100 \times 100 \) \((\Delta = \lambda/100)\) was used in this simulation along with the timestep size of \( \Delta t = 0.001 \). Two other grid sizes \( \Delta = \lambda/50 \) and \( \Delta = \lambda/25 \) were also used to study the convergence of the solution. The value of \( \epsilon = \Delta x \) and \( \Gamma = |u|_{\text{max}} \) were used in the simulation. Results from the simulation are shown in Figure 21 at various times \( (t/\tau) \). The spike and bubble penetrate into each other as the time evolves. The roll-up of the spike due to the Kelvin-Helmholtz instability and the formation of mushroom-like structure can be seen at \( t = 5.8 \tau \). The roll-ups further shrink until \( t = 9.7 \tau \) as the spike penetrates, eventually leading to a more chaotic behavior at \( t = 13.6 \tau \) and the formation of small drops. Symmetry is maintained in the simulation at all times, which indicate that the small scale structures are well captured. A similar observation was made by Liang et al. (2016), Wei and Livescu (2012), however Ramaprabhu et al. (2012) reported the break of symmetry at late times in the simulation.

To further quantify the Rayleigh-Taylor growth at late times, we define non-dimensional bubble and spike velocities as

\[
Fr_b = \frac{u_b}{\sqrt{A_t g k \frac{1}{1 + A_t}}}, \quad Fr_s = \frac{u_s}{\sqrt{A_t g k \frac{1}{1 - A_t}}},
\]  
(72)

where \( Fr_b \) and \( Fr_s \) are the bubble and spike Froude numbers, \( u_b \) and \( u_s \) are the velocity of the bubble and spike fronts. Figure 22 shows the plot of bubble and spike Froude number as a function of time for three grid sizes \( \Delta = \lambda/25 \), \( \Delta = \lambda/50 \), and \( \Delta = \lambda/100 \) and along with the results by Liang et al. (2016). The four distinct growth stages exhibited by the Rayleigh-Taylor instability induced flow can be clearly seen in Figure 22 as (a) the linear growth stage for \( t \leq 2 \), (b) the terminal velocity growth stage for \( 2 \geq t \leq 6 \), (c) the reacceleration stage for \( 6 \geq t \leq 10 \), and (d) the chaotic mixing stage for \( t \geq 10 \). The results from grid sizes \( \Delta = \lambda/50 \) and \( \Delta = \lambda/100 \) are in a good agreement, showing the grid convergence of the results. Our results are also in fair agreement with the results of Liang et al. (2016) for the bubble Froude number, however there is a small disagreement for the spike Froude number at the late-time chaotic mixing stage. Moreover, the results from Liang et al. (2016) exhibit an oscillatory behavior throughout all four growth stages in the simulation, which could be a numerical artefact.

Figure 23 shows the plot of \( Fr_b \) and \( Fr_s \) as a function of non-dimensional bubble and spike heights \( (h_b/\lambda \) and \( h_s/\lambda)\) along with the experimental results of Wilkinson and Jacobs (2007). Note that the experimental results are limited to the first three stages of the flow and the numerical solution is in agreement with the experiments for all stages, thus validating the diffuse-interface method. The dashed lines in Figure 23 shows the second stage terminal velocity for bubble and spike predicted by the potential flow model of Goncharov (2002)

\[
u_b = \sqrt{\frac{2A_t g}{k(1 + A_t)}}, \quad u_s = \sqrt{\frac{2A_t t}{k(1 - A_t)}},
\]  
(73)

and expressed in terms of Froude numbers \( (Fr_b = 0.564 \) and \( Fr_s = 0.656) \) using Eq. (72).
FIGURE 21. Interface evolution and the volumetric rendering of the velocity field in a Rayleigh-Taylor instability induced flow for $A_t = 0.15$ and $Re = 1000$ at various times $t/\tau$. 
FIGURE 22. Bubble and spike Froude number as a function of time on three different grid sizes ($\Delta = \lambda/25$, $\lambda/50$, and $\lambda/100$). Results from Liang et al. (2016) is also shown and is denoted as "l" in the legend.

FIGURE 23. Froude number vs non-dimensional height for (a) bubble, (b) spike. Symbols are the experimental results of Wilkinson and Jacobs (2007). Dashed line represents the analytical solution of the potential flow model by Goncharov (2002).
11. Summary of the results and findings

Performance and scalability tests in Section 9.2 showed that the proposed diffuse-interface method, due to its PDE-only nature results in a low cost, highly scalable method and showed ideal weak scaling from 1 to $10^3$ cores and a good strong scaling for up to 6.25 K grid points per core. Interface advection tests in Section 10.2 showed an overall convergence between 1 and 2 for the interface shape and was found to be dependent on the features (sharp or smooth) of the interface. The volume error was shown to drop to machine precision with an increase in grid size, showing excellent volume conservation properties of the method. We also showed that the choice of interface parameters $\epsilon$ and $\Gamma$ results in a trade-off between accuracy and cost, and the most optimum choice would be to use $\epsilon = \Delta x$ and $\Gamma = |u|_{\text{max}}$ for most situations. Surface tension tests in Section 10.3 showed that the surface tension dynamics were captured accurately in the present method and that the non-dissipative nature of the numerical scheme resulted in highly accurate solutions even for very coarse grids. Acoustic test cases in Section 10.4 showed that the method was accurate in capturing bubble-acoustic interactions and was stable for long-time numerical integration. Results also showed that the numerical simulations were in good agreement with the linear acoustic theory, thus verifying the method. Complex flow simulations in Section 10.5 showed that the numerical scheme was robust in simulating high Reynolds number flows. Further, the results from the numerical simulations showed good agreement with the experiment results, thus validating the method.

12. Conclusion

In the present work, we proposed a novel conservative diffuse-interface method for the simulation of compressible two-phase flows. The proposed method discretely conserves the mass of each phase, momentum and total energy of the system. The advantages of the newly proposed interface-regularization terms compared to the state-of-the-art methods are that it (a) maintains the conservative property of the underlying baseline model, (b) lets us use a central-difference scheme for the discretization of all the operators in the model, which leads to a non-dissipative implementation that is crucial for the simulation of turbulent flows and acoustics.

Furthermore, we proved that our model maintains the boundedness property of the volume fraction field, which is a physical realizability requirement for the simulation of two-phase flows. We also proved that our model inherently satisfies the total-variation-diminishing property for the transport of volume fraction field without having to add any flux limiters that destroys the non-dissipative nature of the scheme. We showed that the proposed interface-regularization terms in the model do not spurious contribute to the kinetic energy of the system and therefore does not affect the non-linear stability of the numerical simulation, and the modeling terms in the energy equation are consistent with the second law of thermodynamics.

Finally, we presented a wide variety of numerical simulations and tests using the model to assess, evaluate, verify and validate the newly developed diffuse-interface method for (a) the accuracy of evolution of the interface shape, (b) implementation of surface tension effects, (c) propagation of acoustics and their interaction with material interfaces, (d) the accuracy and robustness of the numerical scheme for simulation of complex high Reynolds number flows, and (e) performance and scalability.
Appendix A: Expanded form of the model

Expanding all the terms from the full form of the model presented in Section 8 the volume fraction equation can be written as

\[ \frac{\partial \phi_1}{\partial t} + \nabla \cdot (\vec{u} \phi_1) = \phi_1 (\nabla \cdot \vec{u}) + \nabla \cdot \left[ \Gamma \left\{ \epsilon \nabla \phi_1 - \phi_1 (1 - \phi_1) \vec{n}_1 \right\} \right], \quad (74) \]

the mass balance equations for phase \( l \) can be written as

\[ \frac{\partial \rho_l \phi_l}{\partial t} + \nabla \cdot (\rho_l \vec{u} \phi_l) = \nabla \cdot \left[ \rho_0 l \Gamma \left\{ \epsilon \nabla \phi_l - \phi_l (1 - \phi_l) \vec{n}_l \right\} \right], \quad l = 1, 2, \quad (75) \]

the momentum balance equation can be written as

\[ \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u} + p \vec{1}) = \nabla \cdot (\tau + \sigma \kappa \nabla \phi_1 + \rho \vec{g}) \]

\[ + \nabla \cdot \left[ \sum_{l=1}^{2} \rho_0 l \Gamma \left\{ \epsilon \nabla \phi_l - \phi_l (1 - \phi_l) \vec{n}_l \right\} \otimes \vec{u} \right], \quad (76) \]

the total energy equation can be written as

\[ \frac{\partial E}{\partial t} + \nabla \cdot (\vec{u} E) + \nabla \cdot (p \vec{u}) = \sigma \kappa \vec{u} \cdot \nabla \phi_1 + \nabla \cdot (\tau \cdot \vec{u}) + \rho \vec{g} \cdot \vec{u} \]

\[ + \nabla \cdot \left[ \sum_{l=1}^{2} \rho_0 l \Gamma \left\{ \epsilon \nabla \phi_l - \phi_l (1 - \phi_l) \vec{n}_l \right\} \right] \]

\[ + \sum_{l=1}^{2} \nabla \cdot \left[ \rho_l h_l \Gamma \left\{ \epsilon \nabla \phi_l - \phi_l (1 - \phi_l) \vec{n}_l \right\} \right], \quad (77) \]

and the mixture EOS as

\[ p = \rho e - \sum_{l=1}^{2} \frac{\phi_l \gamma_l \gamma_l}{\gamma_l - 1} \frac{\phi_l}{\sum_{l=1}^{2} \phi_l}. \quad (78) \]

Appendix B: Finite-volume discretization for \( \phi \)

The choice of discretization scheme for the non-linear sharpening term on RHS of the volume fraction advection equation (Eq. (47)) is crucial in achieving oscillation free, accurate solutions to the full governing equations. Hence the discretization for this term has been presented in full detail here.

Consider the finite volume representation of the grid as shown in Figure 24 where stars represent cell centers and circles represent cell-face centers. Now discretizing the non-linear sharpening term in the volume fraction advection equation on a two-dimensional finite-volume grid

\[ \frac{\partial \phi}{\partial t} + \nabla \cdot (\vec{u} \phi) = \phi (\nabla \cdot \vec{u}) + \Gamma \epsilon \nabla^2 \phi - \Gamma \left[ \frac{\phi_e (1 - \phi_n) \vec{n}_e - \phi_w (1 - \phi_w) \vec{n}_w}{\Delta x} \right] \]

\[ - \Gamma \left[ \frac{\phi_n (1 - \phi_n) \vec{n}_n - \phi_s (1 - \phi_s) \vec{n}_s}{\Delta x} \right] \quad (79) \]
where \( \vec{n}_e \), is the normal on the east cell-face center and is obtained by a linear interpolation between \( \vec{n}_E \) and \( \vec{n}_P \) (normals evaluated on neighboring cell centers) as

\[
\vec{n}_e = \frac{1}{2} \{ \vec{n}_P + \vec{n}_E \}
\]  

where \( \vec{n}_E \) is the normal on the east cell center and can be represented in terms of its components as

\[
\vec{n}_E = \frac{\nabla \phi_E}{|\nabla \phi_E|} = n_{xE} \hat{i} + n_{yE} \hat{j}
\]  

where \( n_{xE} \) is the \( x \) component of \( \vec{n}_E \) and is approximated using the second-order central-differencing representation for the gradients of \( \phi \) as

\[
n_{xE} = \frac{\frac{\partial \phi}{\partial x}_{E} |_{E}}{\left\{ \left( \frac{\partial \phi}{\partial x}_{E} |_{E} \right)^2 + \left( \frac{\partial \phi}{\partial y}_{E} |_{E} \right)^2 \right\}^{1/2}} = \frac{\phi_{EE} - \phi_P}{2\Delta x} \left\{ \left( \frac{\phi_{EE} - \phi_P}{2\Delta x} \right)^2 + \left( \frac{\phi_{NE} - \phi_{SE}}{2\Delta y} \right)^2 \right\}^{1/2}
\]  

and \( n_{yE} \) is the \( y \) component of \( \vec{n}_E \) and is evaluated similar to \( n_{xE} \). Similarly, \( \vec{n}_P \) is the normal evaluated on the current cell center and is computed similar to \( \vec{n}_E \).

**Appendix C: Two-dimensional Rayleigh-Plesset equation for a cylindrical bubble**

Typically, the Rayleigh-Plesset equation is derived by integrating the mass and momentum conservation equations in the liquid region around the bubble. The liquid is assumed to be incompressible, and the bubble is assumed to oscillate in only the first volumetric mode, which is axisymmetric in nature. Now, balancing the mass in the liquid region between the radius of the bubble, \( R(t) \), and a distance \( r \) from the center of the bubble, we can write the radial velocity at a radius \( r \) as

\[
u(r, t) = \frac{R(t) \ dR(t)}{r \ dt}.
\]  

Starting with the radial component of the incompressible Navier-Stokes equation in polar coordinates
\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} = - \frac{1}{\rho} \frac{\partial p}{\partial r} + \nu \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) \right\} - \frac{u}{r^2}, \tag{84}
\]

and substituting for the velocity from Eq. (83), we obtain

\[
\frac{1}{r} \left\{ \left( \frac{dR(t)}{dt} \right)^2 + R(t) \frac{d^2 R(t)}{dt^2} \right\} - \frac{R^2(t)}{r^3} \left( \frac{dR(t)}{dt} \right)^2 = - \frac{1}{\rho} \frac{\partial p}{\partial r}. \tag{85}
\]

This equation is valid in the liquid region, and hence can be integrated from the surface of the bubble, \( R(t) \). If we integrate this to infinity, we encounter a logarithmic singularity unlike in the three-dimensional Rayleigh-Plesset equation. To avoid this, we integrate Eq. (85) to a finite distance \( S \) from the center of the bubble and obtain

\[
\frac{P_R(t) - P_S(t)}{\rho} = \ln \left\{ \frac{S}{R(t)} \right\} \left\{ \left( \frac{dR(t)}{dt} \right)^2 + R(t) \frac{d^2 R(t)}{dt^2} \right\} + \left( \frac{R^2(t) - S^2}{2S^2} \right) \left( \frac{dR(t)}{dt} \right)^2, \tag{86}
\]

where \( P_R \) and \( P_S \) are the liquid pressures at the surface of the bubble \( r = R \) and \( r = S \), respectively. Now, balancing the pressure, viscous, and surface tension forces at the surface of the bubble

\[
0 = -P_R(t) + 2 \mu \frac{\partial u}{\partial r} (R(t), t) + P_B(t) - \frac{\sigma}{R(t)}, \tag{87}
\]

and substituting in Eq. (86), we obtain the two-dimensional equivalent of the Rayleigh-Plesset equation for the finite-size circular domain

\[
\frac{P_B(t) - P_S(t)}{\rho} = \ln \left( \frac{S}{R} \right) \left\{ (\dot{R})^2 + R \ddot{R} \right\} + \left( \frac{R^2 - S^2}{2S^2} \right) (\dot{R})^2 + \frac{2 \nu \dot{R}}{R} + \frac{\sigma}{\rho R}. \tag{88}
\]

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