Diffuse-interface capturing methods for compressible multiphase fluid flows and elastic-plastic deformation in solids: Part I. Methods

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1. Motivation and objectives

Compressible multiphase fluid flow and multiphase elastic-plastic deformation of solid materials with strength are important phenomena in many engineering applications, including shock compression of condensed matter, detonations and shock-material-interface interactions, impact welding, high-speed fuel atomization and combustion, and cavitation and bubble collapse motivated by both mechanical and biomedical systems. The numerical simulation of multiphase compressible flow and material deformation presents several new challenges in addition to those associated with analogous single-phase simulations. These modeling complications include but are not limited to (1) representing the phase interface on an Eulerian grid; (2) resolving discontinuities in quantities at the interface, especially for high-density ratios; (3) maintaining conservation of (a) the mass of each phase, (b) the mixture momentum, and (c) the total energy of the system; and (4) achieving an accurate mixture representation of the interface for maintaining thermodynamic equilibria.

With these numerical challenges in mind, we choose to pursue the single-fluid approach (Kataoka 1986), in which a single set of equations is solved to describe all of the phases in the domain, as opposed to a multifluid approach, which requires solving a separate set of equations for each of the phases. We are presented with various choices in terms of the system of equations that can be used to represent a compressible multiphase system. In this work, we employ a multicomponent system of equations (a four-equation model) that assumes spatially local pressure and temperature equilibria, including at locations within the diffuse material interface (Shyue 1998; Venkateswaran *et al.* 2002; Marquina & Mulet 2003; Cook 2009). Relaxing the assumption of temperature equilibrium, Allaire *et al.* (2002) and Kapila *et al.* (2001) developed the five-equation model that has proven successful for a variety of applications with high density ratios, strong compressibility effects, and phases with disparate equations of state (EOS), and has been widely adopted for the simulation of compressible two-phase flows (Shukla *et al.* 2010; So *et al.* 2012; Ansari & Daramizadeh 2013; Shukla 2014; Coralic & Colonius 2014; Tiwari *et al.* 2013; Perigaud & Saurel 2005; Wong & Lele 2017; Chiapolino *et al.* 2017; Garrick *et al.* 2017*a*,*b*; Jain *et al.* 2018, 2020a). This modeling strategy will be explored in the future, with the goal of quantifying the advantages of either modeling approach using the same numerical methods and problem set.

For representing the interface on an Eulerian grid, we use an interface-capturing method, as opposed to an interface-tracking method, due to the natural ability of the former method to simulate dynamic creation of interfaces and topological changes. See Mirjalili *et al.* (2017) for a recent review on various interface-capturing methods for

two-phase flows. Interface-capturing methods can be classified into sharp-interface and diffuse-interface methods. In this work, we choose to use diffuse-interface methods (Saurel & Pantano 2018) for modeling the interface between compressible materials. This choice is due to the natural advantages that the diffuse-interface methods offer over the sharp-interface methods, such as ease of representation of the interface, low cost, good conservation properties, and parallel scalability.

One challenge of diffuse-interface capturing of material interfaces is the tendency of the interface to diffuse over time. Unlike shock waves, in which the convective characteristics sharpen the shock over time, material interfaces (like contact discontinuities) do not sharpen naturally; therefore, diffuse capturing of material interfaces requires an active balance between interface sharpening and diffusion to maintain the appropriate interface thickness over time. The severity of this problem is reduced when employing high-order low-dissipation schemes, and the problem can be completely eliminated with the use of explicit interface regularization (diffusion and sharpening) terms that result in constant interface thickness throughout the simulation.

This brief explores three popular diffuse-interface-capturing methods. The first approach (referred to as the LAD approach) is based on the localized-artificial-diffusivity (LAD) method (Cook 2007; Subramaniam *et al.* 2018; Adler & Lele 2019), in which localized, nonlinear diffusion terms are added to the individual phase mass transport equations and coupled with the other conservation equations. This method conserves the mass of individual phases, mixture momentum, and total energy of the system due to the conservative nature of the diffusion terms added to the system of equations and results in no net mixture-mass transport. This method is primarily motivated by applications involving miscible, multicomponent, single-phase fluids, but it has been successfully adapted for multiphase applications. The idea behind this approach is to effectively add species diffusion in the selected regions of the domain to properly resolve the interface on the grid and to prevent oscillations due to discontinuities in the phase mass equations. High-order compact derivative schemes can be used to discretize the added diffusion terms without resulting in distortion of the shape of the interface over long-duration time advancement. However, one drawback of this approach is that the interface thickness increases with time due to the lack of sharpening fluxes that act against the diffusion. This method is therefore most effective for problems in which the interface is in compression (such as shock/material-interface interactions with normal alignment). However, the deficiency of this method due to the lack of a sharpening term is evident for applications in which the interface between immiscible materials undergoes shear or expansion/tension. LAD formulations have also been examined in the context of five-equation models, in which localized diffusion is also added to the volume fraction transport equation (Aslani & Regele 2018).

The second approach (referred to as the gradient-form approach) is based on the quasi-conservative method proposed by Shukla *et al.* (2010), in which diffusion and sharpening terms (together called regularization terms) are added for the individual phase volume fraction transport equations and coupled with the other conservation equations (Tiwari *et al.* 2013). This method only approximately conserves the mass of individual phases, mixture momentum, and total energy of the system due to the non-conservative nature of the regularization terms added to the system of equations. In contrast to the LAD approach, this method can result in net mixture-mass transport, which can sharpen or diffuse the mixture density; depending on the application, this may be an advantageous or disadvantageous property. The primary advantage of this method is that the regu-

larization terms are insensitive to the method of discretization; they can be discretized using high-order compact derivative schemes without distorting the shape of the interface over long-duration time advancement. However, the non-conservative nature of this approach results in poor performance of the method for certain applications. For example, premature topological changes and unphysical interface behavior can be observed when the interfaces are poorly resolved (exacerbating the conservation error) and subjected to shocks that are not aligned with the interface.

The third approach (referred to as the divergence-form approach) is based on the fully conservative method proposed by Jain *et al.* (2020a), in which diffusion and sharpening terms are added to the individual phase volume fraction transport equations and coupled with the other conservation equations. This method conserves the mass of individual phases, mixture momentum, and total energy of the system due to the conservative nature of the regularization terms added to the system of equations. Similar to the gradient-form approach and in contrast to the LAD approach, this method can result in net mixture-mass transport, which can sharpen or diffuse the mixture density. The primary challenge of this method is that one needs to be careful with the choice of discretization used for the regularization terms. Using a second-order finite-volume scheme (in which the nonlinear fluxes are formed on the faces), Jain *et al.* (2020a) showed that a discrete balance between the diffusion and sharpening terms is achieved, thereby eliminating the spurious behavior that was discussed by Shukla *et al.* (2010). The idea behind this is similar to the use of the balanced-force algorithm (Francois *et al.* 2006; Mencinger & Žun 2007) for the implementation of the surface-tension forces, in which a discrete balance between the pressure and surface-tension forces is necessary to eliminate the spurious current around the interface. The current study also demonstrates that appropriately crafted higher-order schemes may be used to effectively discretize the regularization terms. The method is free of premature topological changes and unphysical interface behavior present with the previous approach. However, due to the method of discretization, the anisotropy of the derivative scheme can more significantly distort the shape of the material interface over long-duration time advancement in comparison to the gradient-form approach; the severity of this problem is significantly reduced when using higher-order schemes.

Furthermore, several studies have emphasized the importance of providing physically consistent corrections to each of the governing equations associated with the interface regularization process. For example, Cook (2009), Tiwari *et al.* (2013), and Jain *et al.* (2020a) discuss physically consistent regularization terms for the LAD, gradient-form, and divergence-form approaches, respectively. The physically consistent regularization terms of Cook (2009), Tiwari *et al.* (2013), and Jain *et al.* (2020a) are derived in such a way that the regularization terms do not spuriously contribute to the kinetic energy and entropy of the system. This significantly improves the stability of the simulation, especially for flows with high density ratios. However, discrete conservation of kinetic energy and entropy is needed to show the stability of the methods for high-Reynolds-number turbulent flows (Jain & Moin 2020).

For modeling the solid-material deformation we employ a fully Eulerian method, as opposed to a fully Lagrangian approach (Benson 1992) or a mixed approach such as arbitrary-Lagrangian-Eulerian methods (Donea *et al.* 2004), because of its cost-effectiveness and accuracy for large deformations. There are various Eulerian approaches in the literature that differ in the way the deformation of the material is tracked. The popular methods employ the inverse deformation gradient tensor (Miller & Colella 2001; Ortega *et al.* 2014; Ghaisas *et al.* 2018), the left Cauchy-Green tensor (Sugiyama *et al.*

2010, 2011), the co-basis vectors (Favrie & Gavrilyuk 2011), the initial material location (Valkov *et al.* 2015; Jain *et al.* 2019), or other variants of these methods to track the deformation of the material in the simulation. In this work we use the inverse deformation gradient tensor approach because of its applicability to plasticity modeling. We introduce terms to maintain consistency of the interface regularization process with the kinematic equations describing the deformation of the solid, which have not been previously discussed.

In summary, the two main objectives of this brief are as follows. The first objective is to assess several diffuse-interface-capturing methods for compressible two-phase flows. The interface-capturing methods in this work will be used with a four-equation multicomponent model; however, they are readily compatible with a variety of other models, including the common five-, six-, or seven-equation models. The second objective is to extend these interface-capturing methods to the simulation of elastic-plastic deformation in solid materials with strength, including comparison of these methods in the context of modeling interfaces between solid materials. Section 2 describes the three diffuse-interface methods considered in this study, along with details of their implementation. The second brief (Jain *et al.* 2020b) of this two-part series discusses the application of these methods to a variety of problems including a shock/helium-bubble interaction in air, an advecting air bubble in water, a shock/air-bubble interaction in water, and a Richtmyer–Meshkov instability of an interface between copper and aluminum.

2. Theoretical and numerical model

2.1. *Governing equations*

The governing equations for the evolution of the multiphase flow or multimaterial continuum in conservative Eulerian form are described below, including the conservation of species mass (Eq. 2.1), total momentum (Eq. 2.2), and total energy (Eq. 2.3). These are followed by the kinematic equations that track material deformation, including the inverse deformation gradient tensor (Eq. 2.4), the elastic component of the inverse deformation gradient tensor (Eq. 2.5), and the plastic component of the inverse deformation gradient tensor (Eq. 2.6):

$$\underbrace{\frac{\partial \rho Y_m}{\partial t}}_{\substack{\text{local}\\ \text{derivative}}} + \underbrace{\frac{\partial u_k \rho Y_m}{\partial x_k}}_{\text{advection}} = -\underbrace{\frac{\partial \left(J_m^*\right)_i}{\partial x_i}}_{\substack{\text{artificial}\\ \text{diffusion}}} + \underbrace{J_m}_{\substack{\text{interface}\\ \text{regularization}}}, \tag{2.1}$$

$$\underbrace{\frac{\partial \rho u_i}{\partial t}}_{\substack{\text{local}\\ \text{derivative}}} + \frac{\partial}{\partial x_k}\left(\underbrace{u_k \rho u_i}_{\text{advection}} - \underbrace{\sigma_{ik}}_{\substack{\text{stress}\\ \text{source}}}\right) = \underbrace{\frac{\partial \tau_{ik}^*}{\partial x_k}}_{\substack{\text{artificial}\\ \text{diffusion}}} + \underbrace{F_i}_{\substack{\text{interface}\\ \text{regularization}}}, \tag{2.2}$$

$$\begin{aligned}\underbrace{\frac{\partial}{\partial t}\left[\rho\left(\epsilon + \frac{1}{2}u_j u_j\right)\right]}_{\substack{\text{local}\\ \text{derivative}}} + \frac{\partial}{\partial x_k}\left[\underbrace{u_k \rho\left(\epsilon + \frac{1}{2}u_j u_j\right)}_{\text{advection}} - \underbrace{u_i \sigma_{ik}}_{\substack{\text{stress}\\ \text{source}}}\right] \\ = \underbrace{\frac{\partial}{\partial x_k}\left(u_i \tau_{ik}^* - q_k^*\right)}_{\text{artificial diffusion}} + \underbrace{H}_{\substack{\text{interface}\\ \text{regularization}}},\end{aligned} \tag{2.3}$$

$$\underbrace{\frac{\partial g_{ij}}{\partial t}}_{\substack{\text{local}\\\text{derivative}}} + \underbrace{\frac{\partial g_{ik}u_k}{\partial x_j}}_{\substack{\text{curl-free}\\\text{advection/strain}}} + \underbrace{u_k\left(\frac{\partial g_{ij}}{\partial x_k} - \frac{\partial g_{ik}}{\partial x_j}\right)}_{\substack{\text{non-zero curl}\\\text{advection/strain}}} = \underbrace{\frac{\zeta}{\Delta t}\left(\frac{\rho}{\rho_0\left|\boldsymbol{g}\right|} - 1\right)g_{ij}}_{\text{density compatibility}} + \underbrace{\frac{\partial}{\partial x_k}\left(g^*\frac{\partial g_{ij}}{\partial x_k}\right)}_{\text{artificial diffusion}} + \underbrace{K_{ij}}_{\substack{\text{interface}\\\text{regularization}}}, \tag{2.4}$$

$$\underbrace{\frac{\partial g^e_{ij}}{\partial t}}_{\substack{\text{local}\\\text{derivative}}} + \underbrace{\frac{\partial g^e_{ik}u_k}{\partial x_j}}_{\substack{\text{curl-free}\\\text{advection/strain}}} + \underbrace{u_k\left(\frac{\partial g^e_{ij}}{\partial x_k} - \frac{\partial g^e_{ik}}{\partial x_j}\right)}_{\substack{\text{non-zero curl}\\\text{advection/strain}}} - \underbrace{\frac{1}{2\mu\tau_{rel}}g^e_{ik}\sigma'_{kj}}_{\text{elastic-plastic source}} = \underbrace{\frac{\zeta^e}{\Delta t}\left(\frac{\rho}{\rho_0\left|\boldsymbol{g^e}\right|} - 1\right)g^e_{ij}}_{\text{density compatibility}} + \underbrace{\frac{\partial}{\partial x_k}\left(g^{e*}\frac{\partial g^e_{ij}}{\partial x_k}\right)}_{\text{artificial diffusion}} + \underbrace{K^e_{ij}}_{\substack{\text{interface}\\\text{regularization}}}, \tag{2.5}$$

$$\underbrace{\frac{\partial g^p_{ij}}{\partial t}}_{\substack{\text{local}\\\text{derivative}}} + \underbrace{u_k\frac{\partial g^p_{ij}}{\partial x_k}}_{\text{advection}} + \underbrace{\frac{1}{2\mu\tau_{rel}}g^p_{ik}g^e_{kl}\sigma'_{lm}\left(g^e\right)^{-1}_{mj}}_{\text{elastic-plastic source}} = \underbrace{\frac{\zeta^p}{\Delta t}\left(\frac{1}{\left|\boldsymbol{g^p}\right|} - 1\right)g^p_{ij}}_{\text{density compatibility}} + \underbrace{\frac{\partial}{\partial x_k}\left(g^{p*}\frac{\partial g^p_{ij}}{\partial x_k}\right)}_{\text{artificial diffusion}} + \underbrace{K^p_{ij}}_{\substack{\text{interface}\\\text{regularization}}}. \tag{2.6}$$

Here, t and $\boldsymbol{x}$ represent time and the Eulerian position vector, respectively. Y_m describes the mass fraction of each constituent material, m. The variables $\boldsymbol{u}$, ρ, ϵ, and $\underline{\boldsymbol{\sigma}}$ describe the mixture velocity, density, internal energy, and Cauchy stress, respectively, which are related to the species-specific components by the relations $\rho = \sum_{m=1}^{M}\phi_m\rho_m$, $\epsilon = \sum_{m=1}^{M}Y_m\epsilon_m$, and $\underline{\boldsymbol{\sigma}} = \sum_{m=1}^{M}\phi_m\underline{\boldsymbol{\sigma}}_m$, in which ϕ_m is the volume fraction of material m, and M is the total number of material constituents.

The right-hand-side terms describe the localized artificial diffusion (see also Section 2.5), including the artificial viscous stress, $\tau^*_{ik} = 2\mu^*S_{ik} + \left(\beta^* - 2\mu^*/3\right)\left(\partial u_j/\partial x_j\right)\delta_{ik}$, and the artificial enthalpy flux, $q^*_i = -\kappa^*\partial T/\partial x_i + \sum_{m=1}^{M}h_m\left(J^*_m\right)_i$, with strain rate tensor, $S_{ik} = \left(\partial u_i/\partial x_k + \partial u_k/\partial x_i\right)/2$, and temperature, T. The second term in the artificial enthalpy flux expression is the enthalpy diffusion term (Cook 2009), in which $h_m = \epsilon_m + p_m/\rho_m$ is the enthalpy of species m. The artificial Fickian diffusion of species m is described by $\left(J^*_m\right)_i = -\rho\left[D^*_m\left(\partial Y_m/\partial x_i\right) - Y_m\sum_k D^*_k\left(\partial Y_k/\partial x_i\right)\right]$.

2.2. *Material deformation and plasticity model*

The kinematic equations that describe the deformation of the solid in the Eulerian framework employ the inverse deformation gradient tensor, $g_{ij} = \partial X_i/\partial x_j$, in which $\boldsymbol{X}$ and $\boldsymbol{x}$ describe the position of a continuum parcel in the material (Lagrangian) and spatial (Eulerian) perspectives, respectively. In this work, an inverse deformation gradient is tracked for each material constituent; however, it is possible to assume a single inverse deformation gradient for the entire mixture without loss of accuracy for specific scenarios (Ghaisas *et al.* 2017, 2018). Error associated with the latter approach is localized to the interface region and is often not significant (Subramaniam 2018). Following Miller & Colella (2001), a multiplicative decomposition of the total inverse deformation gradient tensor, $\underline{\boldsymbol{g}}$, into elastic, $\underline{\boldsymbol{g^e}}$, and plastic, $\underline{\boldsymbol{g^p}}$, components is assumed, $g_{ij} = g^p_{ik}g^e_{kj}$, reflecting

the assumption that the plastic deformation is recovered when the elastic deformation is reversed, $g^p_{ij} = g_{ik}\,(g^e)^{-1}_{kj}$. It is additionally assumed that the plastic deformation is volume preserving (Plohr & Sharp 1992), providing compatibility conditions for the inverse deformation gradient tensor determinants, $\left|\underline{\boldsymbol{g^p}}\right| = 1$ and $\left|\underline{\boldsymbol{g}}\right| = \left|\underline{\boldsymbol{g^e}}\right| = \rho/\rho_0$, in which ρ_0 represents the undeformed density and $|\cdot|$ represents the determinant operator. We also assume that the materials with strength are elastic perfectly plastic, in that the material yield stress is independent of strain and strain rate; thus, only the elastic component of the inverse deformation gradient tensor is necessary to close the governing equations. The plastic component of the inverse deformation gradient tensor, or the full tensor, can be employed to supply the plastic strain and strain rate necessary for more general plasticity models (Adler & Lele 2019).

Plastic deformation is incorporated into the numerical framework by means of a viscoelastic Maxwell relaxation model, which has been employed recently in several Eulerian approaches (Ndanou *et al.* 2015; Ortega *et al.* 2015; Ghaisas *et al.* 2018). The plastic relaxation timescale is described by

$$\frac{1}{\tau_{\text{rel}}} = \frac{1}{(\rho/\rho_0)\,\tau_0}\left[\frac{\mathrm{R}\left(\|\underline{\boldsymbol{\sigma}}'\|^2 - \frac{2}{3}\sigma_{\mathrm{Y}}^2\right)}{\mu^2}\right], \tag{2.7}$$

in which $\underline{\boldsymbol{\sigma}}' = \operatorname{dev}(\underline{\boldsymbol{\sigma}})$. The ramp function $R(x) = \max(x, 0)$ turns on plasticity effects only when the yield criterion is satisfied. In many cases, the elastic-plastic source term is stiff due to the small value of τ_{rel} relative to the convective deformation scales. To overcome this time step restriction, implicit plastic relaxation strategies are used based on the method of Favrie & Gavrilyuk (2011) and described by Ghaisas *et al.* (2018).

2.3. *Equations of state and constitutive equations*

A hyperelastic EOS, in which the elastic stress–strain relationship is compatible with a strain energy-density functional, is assumed to close the thermodynamic relationships in the governing equations. The internal energy, ϵ, is additively decomposed into a hydrodynamic component, ϵ_h, and an elastic component, ϵ_e. The hydrodynamic component is analogous to a stiffened gas, with

$$\epsilon = \epsilon_h(p, \rho) + \epsilon_e\left(\underline{\hat{\boldsymbol{g}}}\right), \qquad \epsilon_h = \frac{p + \gamma p_\infty}{(\gamma - 1)\,\rho}, \qquad \epsilon_e = \frac{\mu}{4\rho_0}\mathrm{tr}\left[\left(\underline{\hat{\boldsymbol{g}}} - \underline{\boldsymbol{I}}\right)^2\right], \tag{2.8}$$

in which $\underline{\hat{\boldsymbol{g}}} = |\underline{\boldsymbol{G^e}}|^{-1/3}\,\underline{\boldsymbol{G^e}}$, $\underline{\boldsymbol{G^e}} = \underline{\boldsymbol{g}}^{\boldsymbol{e}T}\underline{\boldsymbol{g}}^{\boldsymbol{e}}$, p is the pressure, p_∞ (with units of pressure) and γ (nondimensional) are material constants of the stiffened gas model for the hydrodynamic component of internal energy, and μ is the material shear modulus.In the case of compressible flow with no material strength, the model reduces to the stiffened gas EOS commonly employed for liquid/gas-interface interactions (Shukla *et al.* 2010; Jain *et al.* 2020a). With this EOS, the Cauchy stress, $\underline{\boldsymbol{\sigma}}$, satisfying the Clausius-Duhem inequality is described by

$$\underline{\boldsymbol{\sigma}} = -p\underline{\boldsymbol{I}} - \mu\frac{\rho}{\rho_0}\left\{|\underline{\boldsymbol{G^e}}|^{-2/3}\operatorname{dev}\left[\left(\underline{\boldsymbol{G^e}}\right)^2\right] - |\underline{\boldsymbol{G^e}}|^{-1/3}\operatorname{dev}\left(\underline{\boldsymbol{G^e}}\right)\right\}, \tag{2.9}$$

in which $\operatorname{dev}(\underline{\boldsymbol{G^e}})$ signifies the deviatoric component of the tensor: $\operatorname{dev}(\underline{\boldsymbol{G^e}}) = \underline{\boldsymbol{G^e}} - \frac{1}{3}\mathrm{tr}(\underline{\boldsymbol{G^e}})\,\underline{\mathbf{1}}$, with $\mathrm{tr}(\underline{\boldsymbol{G^e}})$ signifying the trace of the tensor and $\underline{\mathbf{1}}$ signifying the identity tensor. The elastic component of the internal energy, ϵ_e, is assumed to be isentropic. Therefore, the temperature, T, and entropy, η, are defined by the hydrodynamic stiffened

gas component of the EOS, as follows.

$$\begin{aligned} &\epsilon_h = C_v T \left(\frac{p + \gamma p_\infty}{p + p_\infty} \right), \qquad R = C_p - C_v, \qquad \gamma = \frac{C_p}{C_v}, \\ &\eta - \eta_0 = C_p \ln \left(\frac{T}{T_0} \right) + R \ln \left(\frac{p_0 + p_\infty}{p + p_\infty} \right). \end{aligned} \tag{2.10}$$

Here, η_0 is the reference entropy at pressure, p_0, and temperature, T_0.

2.4. *Pressure and temperature equilibration method*

Many models for multiphase simulation assume that the thermodynamic variables are not in equilibrium, necessitating the solution of an additional equation for volume fraction transport (Shukla *et al.* 2010; Jain *et al.* 2020a). Our model begins with the assumption that both pressure and temperature remain in equilibrium between the phases. To achieve a stable equilibrium requires that all phases be present with non-negative volume fractions throughout the entire simulation domain. This is encouraged by initializing the problem with a minimum volume fraction (typically $\phi_{\min} \lesssim 10^{-6}$) and including additional criteria for volume fraction diffusion (Sections 2.6 and 3) or mass fraction diffusion (Section 2.5) based on out-of-bounds values of volume fraction and/or mass fraction. This equilibration method is stable in the well-mixed interface region, but can result in stability issues outside of the interface region, where the volume fraction of a material tends to become very small—a phenomenon exacerbated by high-order discretization methods. The equilibration method follows from Cook (2009) and Subramaniam *et al.* (2018). For a mixture of M species, we solve for $2M + 2$ unknowns, including the equilibrium pressure (p), the equilibrium temperature (T), the component volume fractions (ϕ_m), and the component internal energies (ϵ_m), from the following equations.

$$p = p_m, \qquad T = T_m, \qquad \sum_{m=1}^{M} \phi_m = 1, \qquad \sum_{m=1}^{M} Y_m \epsilon_m = \epsilon. \tag{2.11}$$

2.5. *Localized artificial diffusivity*

LAD methods have long proven useful in conjunction with high-order compact derivative schemes to provide necessary solution-adaptive and localized diffusion to capture discontinuities and introduce a mechanism for subgrid dissipation. Regardless of the choice of interface-capturing method, LAD is required in the momentum, energy, and kinematic equations, in all calculations, to provide necessary regularization. For instance, the artificial shear viscosity, μ^*, primarily serves as a subgrid dissipation model, whereas the artificial bulk viscosity, β^*, enables shock capturing, and the artificial thermal conductivity, κ^*, captures contact discontinuities. The artificial kinematic diffusivities (g^*, g^{e*}, g^{p*}) facilitate capturing of strain discontinuities, particularly in regions of sustained shearing.

When LAD is also used for interface regularization (to capture material interfaces), the artificial diffusivity of species m, D_m^*, is activated, in which the coefficient C_D controls the interface diffusivity and the coefficient C_Y controls the diffusivity when the mass fraction goes out of bounds. When using the volume-fraction-based approaches for interface regularization (Sections 2.6 and3), it is often unnecessary to also include the species LAD ($D_m^* = 0$); however, the species LAD seems to be necessary for some problems in conjunction with these other interface regularization approaches.

The diffusivities are described below, where the overbar denotes a truncated Gaussian filter applied along each grid direction; Δ_i is the grid spacing in the i direction; $\Delta_{i,\mu}$,

$\Delta_{i,\beta}$, $\Delta_{i,\kappa}$, Δ_{i,Y_m}, and $\Delta_{i,g}$ are weighted grid length scales in direction i; c_s is the linear longitudinal wave (sound) speed; H is the Heaviside function; and $\epsilon = 10^{-32}$:

$$\mu^* = C_\mu \rho \overline{\left| \sum_{k=1}^{3} \frac{\partial^r S}{\partial x_k^r} \Delta_k^r \Delta_{k,\mu}^2 \right|}, \qquad \Delta_{i,\mu} = \Delta_i, \tag{2.12}$$

$$\beta^* = C_\beta \rho f_{sw} \overline{\left| \sum_{k=1}^{3} \frac{\partial^r (\boldsymbol{\nabla} \cdot \boldsymbol{u})}{\partial x_k^r} \Delta_k^r \Delta_{k,\beta}^2 \right|}, \qquad \Delta_{i,\beta} = \Delta_i \frac{\left(\frac{\partial \rho}{\partial x_i} \right)^2}{\sum_{k=1}^{3} \left(\frac{\partial \rho}{\partial x_k} \right)^2 + \epsilon}, \tag{2.13}$$

$$\kappa^* = C_\kappa \frac{\rho c_s}{T} \overline{\left| \sum_{k=1}^{3} \frac{\partial^r \epsilon_h}{\partial x_k^r} \Delta_k^r \Delta_{k,\kappa} \right|}, \qquad \Delta_{i,\kappa} = \Delta_i \frac{\left(\frac{\partial \epsilon_h}{\partial x_i} \right)^2}{\sum_{k=1}^{3} \left(\frac{\partial \epsilon_h}{\partial x_k} \right)^2 + \epsilon}, \tag{2.14}$$

$$\begin{gathered} D_m^* = \max \left\{ C_D c_s \overline{\left| \sum_{k=1}^{3} \frac{\partial^r Y_m}{\partial x_k^r} \Delta_k^r \Delta_{k,D} \right|}, C_Y \overline{\frac{c_s}{2} \left(|Y_m| - 1 + |1 - Y_m| \right) \sum_{k=1}^{3} \Delta_{k,Y}} \right\}, \\ \Delta_{i,D} = \Delta_i \frac{\left(\frac{\partial Y_m}{\partial x_i} \right)^2}{\sum_{k=1}^{3} \left(\frac{\partial Y_m}{\partial x_k} \right)^2 + \epsilon}, \qquad \Delta_{i,Y} = \Delta_i \frac{\left| \frac{\partial Y_m}{\partial x_i} \right|}{\sqrt{\sum_{k=1}^{3} \left(\frac{\partial Y_m}{\partial x_k} \right)^2} + \epsilon}, \end{gathered} \tag{2.15}$$

$$g^* = C_g c_s \overline{\left| \sum_{k=1}^{3} \frac{\partial^r e^g}{\partial x_k^r} \Delta_k^r \Delta_{k,g} \right|}, \qquad \Delta_{i,g} = \Delta_i \frac{\left(\frac{\partial e^g}{\partial x_i} \right)^2}{\sum_{k=1}^{3} \left(\frac{\partial e^g}{\partial x_k} \right)^2 + \epsilon}, \tag{2.16}$$

$$f_{sw} = H\left(-\boldsymbol{\nabla} \cdot \boldsymbol{u}\right) \frac{\left(\boldsymbol{\nabla} \cdot \boldsymbol{u}\right)^2}{\left(\boldsymbol{\nabla} \cdot \boldsymbol{u}\right)^2 + \left(\boldsymbol{\nabla} \times \boldsymbol{u}\right)^2 + \epsilon}. \tag{2.17}$$

Here, $S = \sqrt{S_{ij} S_{ij}}$ is a norm of the strain rate tensor, S, and $e^g = \sqrt{\frac{2}{3} e_{ij}^g e_{ji}^g}$ is a norm of the Almansi finite-strain tensor associated with the g equations, $e_{ij}^g = \frac{1}{2} \left(\delta_{ij} - g_{ki} g_{kj} \right)$. The other artificial kinematic diffusivities, g^{e*} and g^{p*}, are obtained in the same manner as g^*, but with the Almansi strain based on only the elastic or plastic component of the inverse deformation gradient tensor, respectively. We observe that LAD is not strictly necessary to ensure stability for the g^e equations; in fact, it has not been included in previous simulations (Ghaisas *et al.* 2018; Subramaniam *et al.* 2018), because the elastic deformation is often small relative to the plastic deformation, but LAD is necessary to provide stability for the g and g^p equations, especially when the interface is re-shocked, resulting in sharper gradients in the plastic (and total) deformation relative to the elastic deformation. The form for LAD is identical between the three sets of deformation equations, except for the choice of Almansi finite-strain norm, which is chosen to reflect the component of deformation associated with the specific set of equations. Typical values

for the model coefficients are $\zeta^e = \zeta^p = 0.5$, $\zeta = \zeta^p\zeta^e = 0.25$, $C_\mu = 2 \times 10^{-3}$, $C_\beta = 1$, $C_\kappa = 1 \times 10^{-2}$, $C_D = 3 \times 10^{-3}$, $C_Y = 1 \times 10^2$, and $C_g = 1.0$; these values are used in the subsequent simulations unless stated otherwise. However, these coefficients often need to be specifically tailored to the problem; for example, the bulk viscosity coefficient can be increased to more effectively capture strong shocks in materials with large stiffening pressures.

2.6. *Fully conservative divergence-form approach to interface regularization*

In this approach, interface regularization is achieved with the use of diffusion and sharpening terms that balance each other. This results in constant interface thickness during the simulation, unlike the LAD method, in which the interface thickness increases over time due to the absence of interface sharpening fluxes. All regularization terms are constructed in divergence form, resulting in a method that conserves the mass of individual species as well as the mixture momentum and total energy.

Following Jain *et al.* (2020a), we consider the implied volume fraction transport equation for phase m, with the interface regularization volume fraction flux $(a_m)_k$,

$$\frac{\partial \phi_m}{\partial t} + u_k \frac{\partial \phi_m}{\partial x_k} = \frac{\partial \left(a_m\right)_k}{\partial x_k}. \tag{2.18}$$

In this work, this equation is not directly solved, because the volume fraction is closed during the pressure and temperature equilibration process (Section 2.4), but the action of this volume fraction flux is consistently incorporated into the system through the coupling terms with the other governing equations. We employ the coupling terms proposed by Jain *et al.* (2020a) for the mass, momentum, and energy equations, and propose new consistent coupling terms for the kinematic equations.

Using the relationship of density (ρ) and mass fraction (Y_m) to component density (ρ_m) and volume fraction (ϕ_m) for material m ($\rho Y_m = \rho_m \phi_m$, with no sum on repeated m), we can describe the interface regularization term for each material mass transport equation,

$$J_m = \frac{\partial \left(a_m\right)_k \rho_m}{\partial x_k}, \qquad \text{with no sum on repeated } m. \tag{2.19}$$

Consistent regularization terms for the momentum and energy equations follow,

$$F_i = \frac{\partial \left(a_m\right)_k \rho_m u_i}{\partial x_k} \qquad \text{and} \qquad H = \frac{\partial}{\partial x_k}\left\{\left(a_m\right)_k \left[\frac{1}{2}\rho_m u_j u_j + \left(\rho h\right)_m\right]\right\}, \tag{2.20}$$

in which the enthalpy of species m is described,

$$\left(\rho h\right)_m = e_m \rho_m + p_m, \qquad \text{with no sum on repeated } m. \tag{2.21}$$

Consistent regularization terms for the kinematic equations take the form

$$K_{ij} = \frac{1}{\rho}\frac{\partial \left(a_m\right)_k \left(\rho_m\right) g_{ij}}{\partial x_k}, \tag{2.22}$$

from which K^e_{ij} or K^p_{ij} may be obtained similarly by replacing g_{ij} with g^e_{ij} or g^p_{ij}, respectively.

The volume fraction interface regularization flux for phase m is described by

$$(a_m)_k = \Gamma \left[\underbrace{\epsilon \frac{\partial \phi_m}{\partial x_k}}_{\substack{\text{interface} \\ \text{diffusion}}} - \underbrace{s_m \left(\hat{n}_m\right)_k}_{\substack{\text{interface} \\ \text{sharpening}}} \right] L_m + \underbrace{\Gamma^* \epsilon D_b \frac{\partial \phi_m}{\partial x_k}}_{\substack{\text{out-of-bounds} \\ \text{diffusion}}}, \qquad \text{with no sum on repeated } m, \tag{2.23}$$

with the interface sharpening term

$$s_m = \begin{cases} \left(\phi_m - \phi_m^\epsilon\right) \left(1 - \sum_{\substack{n=1 \\ n \neq m}}^{M} \phi_n^\epsilon - \phi_m\right), & \text{for } \phi_m^\epsilon \leq \phi_m \leq \sum_{\substack{n=1 \\ n \neq m}}^{M} \phi_n^\epsilon \\ 0, & \text{else} \end{cases}, \tag{2.24}$$

in which ϕ_m^ϵ denotes the minimum allowable volume fraction for phase m; this floor promotes physically realizable solutions to the pressure and temperature equilibria, which would otherwise not be well behaved if the mass or volume fraction exceeded the physically realizable bounds between zero and one. We assume $\phi_m^\epsilon = 1 \times 10^{-6}$ unless stated otherwise. The optional mask term,

$$L_m = \begin{cases} 1, & \text{for } \phi_m^\epsilon \leq \phi_m \leq \sum_{\substack{n=1 \\ n \neq m}}^{M} \phi_n^\epsilon \\ 0, & \text{else} \end{cases}, \tag{2.25}$$

localizes the interface diffusion and interface sharpening terms to the interface region, restricting the application of the non-compactly discretized terms to the interface region. Unlike the gradient-form approach, this mask in the divergence-form approach is not necessary for stability, as demonstrated by Jain *et al.* (2020a). The interface normal vector for phase m is given by

$$\left(\hat{n}_m\right)_k = \frac{\partial \phi_m}{\partial x_k} \Big/ \left| \frac{\partial \phi_m}{\partial x_i} \right|, \qquad \left| \frac{\partial \phi_m}{\partial x_i} \right| = \sqrt{\frac{\partial \phi_m}{\partial x_i} \frac{\partial \phi_m}{\partial x_i}}, \qquad \text{with no sum on repeated } m. \tag{2.26}$$

The out-of-bounds diffusivity, described by

$$D_b = \overline{\left[1 - \phi_m / \left(\phi_m^\epsilon\right)^b\right]_{\text{max over } m;\text{ no sum}}}, \qquad b = \frac{1}{2}, \tag{2.27}$$

maintains $\phi_m \gtrsim \phi_m^\epsilon$. The overbar denotes the same filtering operation as applied to the LAD diffusivities. A user-specified length scale, $\epsilon \approx \Delta x$, typically on the order of the grid spacing, controls the equilibrium thickness of the diffuse interface. The velocity scale, $\Gamma \approx u_{max}$ controls the timescale over which the interface diffusion and interface sharpening terms drive the interface thickness to equilibrium. The velocity scale for the out-of-bounds volume fraction diffusivity is also specified by the user, with $\Gamma^* \gtrsim \Gamma$. Volume fraction compatibility is enforced by requiring that $\sum_{m=1}^{M} (a_m)_k = 0$.

2.7. *Quasi-conservative gradient-form approach to interface regularization*

As with the divergence-form approach, the interface regularization in this approach is achieved with the use of diffusion and sharpening terms that balance each other. Therefore, this method also results in constant interface thickness during the simulation. Shukla *et al.* (2010) discuss disadvantages associated with the divergence-form approach due to the numerical differentiation of the interface normal vector. The numerical error of these terms can lead to interface distortion and grid imprinting due to the anisotropy of the

derivative scheme. Ideally, we would like to have a regularization method that is conservative and that does not require any numerical differentiation of the interface normal vector. However, starting with the assumption of conservation, for nonzero regularization flux, we see that numerical differentiation of the interface normal vector can only be avoided in the limit that the divergence of the interface normal vector goes to zero. This limit corresponds to the limit of zero interface curvature, which cannot be avoided in multidimensional problems. Therefore, this illustrates that a conservative method cannot be constructed for multidimensional applications without requiring differentiation of the interface normal vector; the non-conservative property (undesirable) of the gradient-form approach is a necessary consequence of the circumvention of interface-normal differentiation (desirable). This is demonstrated below, in which the phase subscript has been dropped.

$$\frac{\partial}{\partial x_k}\left\{\Gamma\left[\epsilon\frac{\partial\phi}{\partial x_k}+\phi\left(1-\phi\right)\hat{n}_k\right]\right\}=\frac{\partial}{\partial x_k}\left(\Gamma\epsilon\frac{\partial\phi}{\partial x_k}\right)+\frac{\partial\Gamma\phi\left(1-\phi\right)}{\partial x_k}\hat{n}_k+\Gamma\phi\left(1-\phi\right)\frac{\partial\hat{n}_k}{\partial x_k}$$
$$\underset{\nabla\cdot\vec{\boldsymbol{n}}\rightarrow 0}{\longrightarrow}\hat{n}_k\frac{\partial}{\partial x_k}\left\{\Gamma\left[\epsilon\left|\frac{\partial\phi}{\partial x_j}\right|+\phi\left(1-\phi\right)\right]\right\}, \tag{2.28}$$

in which the final expression is obtained in the limit of $\nabla\cdot\vec{\boldsymbol{n}}\rightarrow 0$.

Following Shukla *et al.* (2010), we arrive at an implied volume fraction transport equation for phase m, with the interface regularization volume fraction term α_m,

$$\frac{\partial\phi_m}{\partial t}+u_k\frac{\partial\phi_m}{\partial x_k}=\left(n_m\right)_k\frac{\partial\alpha_m}{\partial x_k}. \tag{2.29}$$

Unlike the divergence-form approach, the gradient-form approach requires no numerical differentiation of interface normal vectors, but it consequently results in conservation error. Like the divergence-form approach, this volume fraction transport equation is not directly solved, because the volume fraction is closed during the pressure and temperature equilibration process (Section 2.4), but the action of the volume fraction regularization term is consistently incorporated into the system of equations for mass, momentum, energy, and kinematic quantities through quasi-conservative coupling terms.

We employ an interface regularization term for each component mass transport equation consistent with the interface regularization volume fraction term,

$$J_m=\left(n_m\right)_k\frac{\partial\alpha_m\rho_m}{\partial x_k},\qquad\text{with no sum on repeated } m. \tag{2.30}$$

Because of the assumption of pressure and temperature equilibrium (volume fraction is a derived variable—not an independent state variable), it is important to form mass transport regularization terms consistently with the desired volume fraction regularization terms. In the method of Tiwari *et al.* (2013), the terms do not need to be fully consistent (e.g., the component density is assumed to be slowly varying); the terms only need to produce similar interface profiles in the limit of $\Gamma\rightarrow\infty$ (Shukla *et al.* 2010), because the volume fraction is an independent state variable. Following the assumption of Tiwari *et al.* (2013) that the velocity, specific energy, and kinematic variables (but not the mixture density) vary slowly across the interface, the stability of the method is improved by further relaxing conservation of the coupled equations. For example, the consistent regularization term for the momentum equation reduces to

$$F_i=\sum_m\left(n_m\right)_k\frac{\partial\alpha_m\rho_m u_i}{\partial x_k}\approx\sum_m\left(n_m\right)_k\frac{\partial\alpha_m\rho_m}{\partial x_k}u_i. \tag{2.31}$$

Similarly, the consistent regularization term for the energy equation reduces to

$$H = \sum_m (n_m)_k \frac{\partial}{\partial x_k}\left[\alpha_m \rho_m \left(\frac{1}{2}u_j u_j + h_m\right)\right] \approx \sum_m (n_m)_k \frac{\partial \alpha_m \rho_m}{\partial x_k}\left(\frac{1}{2}u_j u_j + h_m\right). \tag{2.32}$$

Consistent regularization terms for the kinematic equations take the form

$$K_{ij} = \sum_m (n_m)_k \frac{1}{\rho}\frac{\partial \alpha_m (\rho_m) g_{ij}}{\partial x_k} \approx \sum_m (n_m)_k \frac{1}{\rho}\frac{\partial \alpha_m (\rho_m)}{\partial x_k} g_{ij}, \tag{2.33}$$

from which K^e_{ij} or K^p_{ij} may be obtained similarly by replacing g_{ij} with g^e_{ij} or g^p_{ij}, respectively.

The volume fraction interface regularization flux for phase m is defined by

$$\alpha_m = \Gamma\left(\underbrace{\epsilon\left|\frac{\partial \phi_m}{\partial x_i}\right|}_{\substack{\text{interface}\\ \text{diffusion}}} - \underbrace{s_m}_{\substack{\text{interface}\\ \text{sharpening}}}\right)\mathscr{L}_m, \qquad \text{with no sum on repeated } m. \tag{2.34}$$

The volume fraction out-of-bounds diffusion term employed in the divergence-form approach (Eq. 2.23) is also active in the gradient-form approach. The gradient-form discretization of this term (including an equivalent volume fraction out-of-bounds term in Eq. 2.34) exhibits poor stability away from the interface, whereas the divergence-form approach does not. Following Shukla *et al.* (2010) and Tiwari *et al.* (2013), a necessary mask term blends the interface regularization terms to zero as the volume fraction approaches the specified minimum or maximum, thereby avoiding instability of the method away from the interface, where the calculation of the surface normal vector may behave spuriously and lead to compounding conservation error,

$$\mathscr{L}_m = \begin{cases} \tanh\left[\left(\dfrac{s_m}{\phi^{\mathscr{L}}_m}\right)^2\right], & \text{for } \phi^\epsilon_m \le \phi_m \le \sum_{\substack{n=1\\ n\neq m}}^{M} \phi^\epsilon_n \\ 0, & \text{else} \end{cases}, \tag{2.35}$$

in which $\phi^{\mathscr{L}}_m \approx 1 \times 10^{-2}$ is a user-specified value controlling the mask blending function. Other variables are the same as defined in the context of the divergence-form approach.

2.8. *High-order numerical method*

The equations are discretized on an Eulerian Cartesian grid. Time advancement is achieved using a five-stage, fourth-order, Runge-Kutta method, with an adaptive time step based on a Courant–Friedrichs–Lewy (CFL) condition. Other than the interface regularization terms for the divergence-form approach, all spatial derivatives are computed using a high-resolution, penta-diagonal, tenth-order, compact finite-difference scheme. This scheme is applied in the domain interior and near the boundaries in the cases of symmetry, anti-symmetry, or periodic boundary conditions. Otherwise, boundary derivatives are reduced to a fourth-order, one-sided, compact difference scheme.

The interface sharpening and interface diffusion regularization terms in the divergence-form approach are discretized using node-centered derivatives, for which the fluxes to be differentiated are formed at the faces (staggered locations); linear terms (e.g., ϕ_i) are interpolated from the nodes to the faces, where the nonlinear terms are formed [e.g., $\phi_{i+1/2}\left(1-\phi_{i+1/2}\right)$]. Here, we refer to the finite-difference grid points as nodes.

All variables are stored at the nodes (collocated). If the nonlinear fluxes are not formed at the faces, poor stability is observed for node-centered finite-difference schemes of both compact and non-compact varieties due to the nonlinear interface sharpening term. Both second-order and sixth-order (non-compact) discretization schemes are examined for these terms. The second-order scheme recovers the finite-volume approach successfully employed by Jain *et al.* (2020a), whereas the higher-order scheme provides increased resolution and formal accuracy; however, discrete conservation is not guaranteed. The out-of-bounds diffusion is discretized using the high-order compact scheme for all interface regularization approaches.

A spatial dealiasing filter is applied after each stage of the Runge-Kutta algorithm to each of the conservative and kinematic variables to remove the top 10% of the grid-resolvable wavenumber content, thereby mitigating against aliasing errors and numerical instability in the high-wavenumber range, which is not accurately resolved by the spatial derivative scheme. The filter is computed using a high-resolution, penta-diagonal, eighth-order, compact Padé filter, with cutoff parameters described by Ghaisas *et al.* (2018).

3. Concluding remarks

The second brief (Jain *et al.* 2020b) of this two-part series examines the application of these methods to a variety of problems, including (1) advection of an air bubble in water, (2) shock interaction with a helium bubble in air, (3) shock interaction and the collapse of an air bubble in water, and (4) Richtmyer–Meshkov instability of a copper–aluminum interface. The primary objective of this work is to compare these three methods in terms of their ability to maintain constant interface thickness throughout the simulation; simulate high-density-ratio interfaces; conserve mass, momentum, and energy; and maintain accurate interface shape for long-time integration. Comparison of the different implicit treatments of subgrid phenomena is also of interest. For the application of these methods to large-scale simulations of engineering interest, it is rarely practical to use hundreds of grid points to resolve the diameter of a bubble/drop. Therefore, the limit of relatively coarse grid resolution, which is more representative of the true performance of these methods, is examined in the second part of this brief series.

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