Diffuse Interface Modeling of Compressible Multiphase Flows using an Adaptive Mesh Refinement Library

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Abstract
In this work, a diffuse interface method is developed using an unstructured adaptive mesh refinement (AMR) library for orthogonal Cartesian grids. The compressible multicomponent Euler equations, i.e. the quasi-conservative five-equation model including capillary effects, is discretized by the finite-volume method, which utilizes a fifth-order weighted essentially non-oscillatory (WENO) reconstruction procedure. The finite-volume method is complemented by a modified Harten-Lax-Van Leer Contact (HLLC) approximate Riemann solver which is used to upwind the fluxes on cell faces. Surface tension effects are integrated into the governing equations by virtue of the continuum surface force (CSF) model, whereas local interface curvature is calculated by utilizing second-order accurate height functions. The excessive numerical smearing of the material interface is limited to a narrow band of cells by employing the THINC reconstruction. The temporal integration is carried out by a three stage, third-order strong stability-preserving (SSP) Runge-Kutta scheme. Several one and two-dimensional benchmark problems are performed to verify the implementation and robustness of the method. The efficient utilization of AMR increases the resolution of small-scale flow features while keeping the computational cost feasible.
Introduction

The simulation of compressible multiphase flows involves accurately capturing the presence and interaction of material interfaces, shocks and rarefaction waves. To this end, numerical modeling is categorized based on the treatment of the interface. Sharp interface methods [1, 2, 3, 4] aim to treat the phase interface as a discontinuity. However these methods require elaborate means of treating the jump in physical quantities, which increases the complexity of the implementation.

Diffuse interface methods extend standard shock capturing algorithms to take into account the transport of the material interface. The drawback of these approaches is the inherent smearing of the phase interface due to numerical dissipative errors, especially in the presence of high density ratios. Many approaches exist to counter this numerical dissipation such as application of anti-diffusion fluxes [5], iterative compression methods [6, 7] and the tangent hyperbola for interface capturing (THINC) reconstruction method [8]. In this paper we extend the work of [9] to utilize the high resolution weighted essentially non-oscillatory (WENO) scheme [10, 11] for the reconstruction of the solution variables in an adaptive mesh refinement (AMR) framework in order to efficiently resolve discontinuities. The excessive smearing of material interfaces is alleviated by employing the THINC reconstruction. Additionally, the height function method [12] originally proposed for sharp interfaces is extended to account for the smearing of interface region over a number of cells.

Governing Equations

In this work, the evolution of compressible multicomponent flows is described by the quasi-conservative five-equation model [13] including capillary effects [14, 15]. The governing equations in a compact notation read

$$\partial_t Q + \nabla \cdot F(Q) = S(Q, \nabla Q),$$

where the vector of conserved quantities \(Q\), tensorial flux function \(F\) and source vector \(S\) are

\[
Q = \begin{pmatrix} \alpha_1 \rho_1 \\ \alpha_2 \rho_2 \\ \rho u \\ \rho E \\ \alpha_1 \end{pmatrix}, \quad
F = \begin{pmatrix} \alpha_1 \rho_1 u \\ \alpha_2 \rho_2 u \\ \rho \left( \rho u \otimes u + p I \right) \\ \rho (pE + p)u \\ \alpha_1 u \end{pmatrix}, \quad
S = \begin{pmatrix} 0 \\ 0 \\ \sigma \kappa \nabla \alpha_1 \\ \sigma \kappa \nabla \alpha_1 \cdot u \\ \alpha_1 \nabla \cdot u \end{pmatrix},
\]

Here, \(\alpha_i\) is the volume fraction of the components, \(\rho_i\) the mass density of the components, \(\rho\) the mixture density, \(u\) the velocity vector, \(E\) the total mixture energy per unit mass, \(p\) the pressure, \(I\) the identity matrix, \(\kappa\) the local interface curvature and \(\sigma\) the surface tension coefficient. The total energy \(E\), internal energy \(e\) and kinetic energy per unit mass are related by

$$E = e + \frac{1}{2} \rho \cdot u.$$ Capillary effects are considered by means of the continuum surface force (CSF) [16] model, which aims to approximate surface tension forces at fluid interfaces as volumetric forces. The effects of viscosity, heat conductivity and gravity are not considered in this work.

Closure of the compressible five-equation model is achieved by providing a set of mixture rules and a suitable equation of state. Thermodynamically consistent mixture rules ensure that numerical diffusion does not introduce spurious oscillations in the transitional region which would otherwise deteriorate stability. The mixture rules [13] for the volume fraction, density and internal energy are given by

$$1 = \sum_i \alpha_i, \quad (3a)$$
$$\rho = \sum_i \alpha_i \rho_i, \quad (3b)$$
$$\rho e = \sum_i \alpha_i \rho_i e_i. \quad (3c)$$

In this work, the stiffened equation of state (EOS) [17] is used,

$$\rho e = \frac{1}{\gamma - 1} p + \frac{\gamma \pi}{\gamma - 1}, \quad (4)$$

where \(\gamma\) and \(\pi\) are material parameters of the mixture. The mixture rules for the EOS parameters [13] read

$$\frac{1}{\gamma - 1} = \sum_i \alpha_i \frac{1}{\gamma_i - 1}, \quad (5a)$$
$$\frac{\gamma \pi}{\gamma - 1} = \sum_i \alpha_i \gamma_i \pi_i. \quad (5b)$$

The mixture speed of sound is

$$c = \sqrt{\frac{\gamma(p + \pi)}{\rho}}. \quad (6)$$

Numerical Methods

Spatial Discretization

An adaptive mesh refinement (AMR) algorithm is used to concentrate the computational effort on regions with large local gradients, such as shocks, contact discontinuities and material interfaces. To minimize the computational overhead associated with block- and patch-based AMR, a novel three-dimensional unstructured AMR method for Cartesian orthogonal meshes [18] is utilized. Nonetheless, the spatial discretization in this work is given...
on a two-dimensional Cartesian mesh with uniform mesh spacing for the sake of brevity. The spatial discretization of the five-equation model by the conservative finite-volume method [19] reads

\[
\frac{dQ_{i,j}}{dt} + \frac{1}{\Delta x} (\hat{F}_{i+1/2,j} - \hat{F}_{i-1/2,j}) + \frac{1}{\Delta y} (\hat{G}_{i,j+1/2} - \hat{G}_{i,j-1/2}) = S_{i,j} \tag{7a}
\]

where \( Q_{i,j} \) and \( S_{i,j} \) are the volume-averaged vector of conserved quantities and source vector, and \( \hat{F}_{i\pm1/2,j} \) and \( \hat{G}_{i,j\pm1/2} \) are numerical fluxes, which approximate the face-averaged physical flux integrated by the mid-point rule [20]. As pointed out by Coralic and Colominus [21], usage of the mid-point rule is only second-order accurate and deteriorates the desired high-order properties. In order to reach genuinely high-order accuracy, they emphasized the importance of utilizing a computationally demanding Gaussian quadrature rule [22]. However, Zhang et al. [20] demonstrated that for non-smooth problems with shocks, both methods yield comparable results, despite their difference in accuracy and computational cost.

The HLLC approximate Riemann solver [23] is utilized to upwind the numerical flux at the faces based on the reconstructed left and right states,

\[
\hat{F}_{i+1/2} = \hat{P}_{i+1/2}^{HLLC}(Q_{i+1/2}^L, Q_{i+1/2}^R), \tag{8}
\]

where \( L \) and \( R \) denote the state vector reconstructed from the left and right side of a face, respectively. Surface tension effects are taken into account by employing the modified HLLC solver of Garrick et al. [14], which also performs an upwinding on the volume fraction and face-normal velocity to achieve a consistent discretization of the source term associated with the CSF model.

In order to achieve a high-order accurate spatial discretization, the weighted essentially non-oscillatory (WENO) reconstruction scheme [10, 11] is used to recover the left and right states. The basic idea of WENO schemes is to apply low-dissipative, high order stencils in smooth flow regions, while applying a non-linear convex combinations of low-order stencils in regions near discontinuities. As pointed out by several authors [24, 21, 14], either the primitive states or their projection into characteristic space should be used as the preferred choice of reconstructed variables to avoid the introduction of spurious oscillations. Despite providing an excellent methodology for shock-capturing schemes, WENO reconstruction does not circumvent the excessive smearing of material interfaces. To this end, the tangent of hyperbola for interface capturing (THINC) scheme is used in regions near material interfaces as a building block for the reconstruction of sub-grid discontinuities within control volumes [25, 8, 9]. The algebraic THINC scheme aims to interpolate a diffuse material interface by a locally defined sigmoid type function. From that, the reconstruction of the volume fraction at the cell faces follows to

\[
\alpha_{i+1/2}^K = \begin{cases} 
\frac{1}{2} (1 + \tanh(\beta_1(\sigma_i + \tilde{x}_i))) & \text{if } K = L, \\
\frac{1}{2} (1 + \tanh(\beta_{i+1}\tilde{x}_{i+1})) & \text{if } K = R,
\end{cases}
\]

where \( \sigma_i \equiv \text{sign}(\alpha_{i+1} - \alpha_{i-1}) \) is the sign of the volume fraction gradient, the parameter \( \beta_i \) controls the interface thickness parameter in sharpness with respect to the current control volume. The latter is uniquely determined from the volume fraction and the definition of the hyperbolic tangent function, see Garrick et al. [26] and the references therein. Once the volume-fraction has been sharpened, the remaining variables need to be treated in a consistent manner. In this work, we follow Garrick et al. [9] and perform the THINC reconstruction after transforming the conservative variables into the primitive variables. The THINC reconstruction is applied on all control volumes which contain the diffuse material interface. In practice, those control volumes are identified by volume fractions which satisfy \( \alpha_j \in (\epsilon, 1 - \epsilon) \), where \( \epsilon = 1 \times 10^{-4} \), and fulfill the monotonicity constraint \( (\alpha_{i+1} - \alpha_i)(\alpha_i - \alpha_{i-1}) > 0 \). In regions, where the conditions are not fulfilled, the reconstruction is done by WENO.

The genuinely one-dimensional hyperbolic tangent function is applied to multi-dimensional problems by scaling the interface thickness parameter in accordance to the orientation of the material interface,

\[
\beta_i = \beta |n^T_i| + 0.01,
\]

and likewise for the other coordinate directions. Here, \( n = (n^x, n^y)^T \) denotes the normal vector perpendicular to the material interface. The normal vector is obtained by differentiating a mollified volume-fraction field [6, 14], which, by construction principal, has the same normal vector as the original volume-fraction field. Throughout this work we use \( \beta = 3.0 \), which essentially limits the interface thickness between two and three cells and circumvents excessive smearing of material interfaces.

**Temporal Discretization**

The spatial discretization (7) yields a system of ordinary differential equations (ODEs). Introducing the discrete differential operator \( \mathcal{R} \) yields the com-
\[ \frac{dQ_{i,j}}{dt} = R(Q_{i,j}), \quad (9) \]

where, for ease of notation, the subscripts are dropped subsequently. The system of ODEs \((9)\) is evolved in time by utilizing a low-storage variant \([27]\) of the three stage, third-order strong stability-preserving Runge-Kutta scheme of Shu and Osher \([28]\),

\[
Q^{(1)} = Q^{(0)} + \Delta t R(Q^{(0)}), \quad (10a)
\]

\[
Q^{(2)} = \frac{3}{4} Q^{(0)} + \frac{1}{4} Q^{(1)} + \frac{1}{4} \Delta t R(Q^{(1)}), \quad (10b)
\]

\[
Q^{(3)} = \frac{1}{3} Q^{(0)} + \frac{2}{3} Q^{(2)} + \frac{2}{3} \Delta t R(Q^{(2)}), \quad (10c)
\]

where \(Q^{(0)} = Q^n\) and \(Q^{(3)} = Q^{n+1}\). The maximum timestep size is limited by the CFL condition,

\[
\Delta t = CFL \times \min(\Delta t_c, \Delta t_\sigma), \quad (11)
\]

where \(\Delta t_c\) is the convective \([29]\) and \(\Delta t_\sigma\) the capillary \([30, 16]\) timestep criterion.

**Computation of Curvature**

The height function (HF) technique \([12]\) utilizes a geometric approach for estimating the surface curvature from well-resolved volume fractions. The position of the interface is recovered from discrete sums of the volume fraction along the direction of the maximum component of the normal vector, i.e.

\[
H_{i,j} = \left\{ \begin{array}{ll}
\sum_{i'=-n_{HF}}^{i+n_{HF}} \phi_{i',j} \Delta x & \text{if } |n_{i,j}^x| > |n_{i,j}^y|, \\
\sum_{j'=-n_{HF}}^{j+n_{HF}} \phi_{i,j'} \Delta y & \text{if } |n_{i,j}^y| > |n_{i,j}^x|,
\end{array} \right. 
\]

where \((2n_{HF} + 1)\) denotes the total height of the HF columns. Once an approximation of the interface position is determined, the surface curvature can be evaluated by

\[
\kappa_{i,j} = \left\{ \begin{array}{ll}
\frac{\partial_y H_{i,j}}{(1 + \partial_y H_{i,j}^2)^{3/2}} & \text{if } |n_{i,j}^x| > |n_{i,j}^y|, \\
\frac{\partial_x H_{i,j}}{(1 + \partial_x H_{i,j}^2)^{3/2}} & \text{if } |n_{i,j}^y| > |n_{i,j}^x|,
\end{array} \right. 
\]

where the partial derivatives of the HF columns are discretized using second-order central differences.

Traditionally, the HF technique has been used mostly in conjunction with sharp-interface methods, where the HF column heights are commonly set to \(n_{HF} = 3\). To compensate the increased thickness of the material interface for diffuse-interface methods, we use \(n_{HF} = 5\) for interfaces which are spread out across approximately three cells, which produces reasonable approximations to the curvature for canonical test problems.

By construction principle, the HF technique only provides an approximation of the curvature at control volumes, which intersect the interface. Consequently, a redistribution scheme, which extrapolates the curvature values at the interface to its neighborhood is needed. Therefore, the iterative fast sweeping method (FSM) \([31]\) is utilized to extrapolate the curvature by an upwind discretization of the spatial differential operators and the systematic and alternating ordering of Gauss-Seidel iterations.

**Numerical results**

The following section discusses some of the verification test cases performed with the present method. In all test cases, until otherwise stated explicitly, the volume fraction field \(\alpha_1\) is initialized in accordance to the hyperbolic tangent function of the THINC reconstruction, which results in an initially smooth material interface.

**Curvature Verification**

The curvature computation using the HF technique is verified by calculating the curvature of a two-dimensional column under mesh-refinement. The curvature error is calculated with the volume fraction field \(\alpha_1\) initialized both with a sharp jump and as a smooth field with \(\beta = 3.0\). The convergence of the computed curvature for both these initial fields is given in Figure 1. For this idealized symmetric test problem with the column center located at the center of the domain, the HF technique approximates the curvature with second order accuracy for both the sharp and smooth initial fields.

**One-dimensional Gas-Liquid Interface Advection Problem**

The isolated interface advection problem proposed by Abgrall \([13]\) and used in various forms by several authors, e.g. \([24, 21, 9]\), illustrates the occurrence and severity of spurious oscillations at material interfaces. In this work, we follow Garrick et al. \([9]\) and advec a gas-liquid interface with the initial conditions

\[
\begin{pmatrix}
\alpha_2 p_1 \\
\alpha_2 p_2 \\
u \\
p \\
\alpha_1
\end{pmatrix}
= \begin{pmatrix}
0, 1, 0.5, 1, 0 \\
1000, 0, 0.5, 1, 1 \\
\end{pmatrix}^T, \quad x \in [-1, 0),
\]

\[
\begin{pmatrix}
\alpha_2 p_1 \\
\alpha_2 p_2 \\
u \\
p \\
\alpha_1
\end{pmatrix}
= \begin{pmatrix}
10, 0.5, 1, 1 \\
\end{pmatrix}^T, \quad x \in [0, 1].
\]

The non-dimensionalized material properties are \(\gamma_1 = 4.4, \pi_1 = 6000\) and \(\gamma_2 = 1.4, \pi_2 = 0\) \([9]\).
The numerical solution is evolved to $t = 4.00$ with CFL $= 0.6$ and uniform mesh spacing $\Delta x = 2.0/200$. We impose periodic boundary conditions to allow the interface to travel one period during the simulation time. The exact and numerical solution are given at the final time in Figure 2. Neither WENO5 nor WENO5-THINC reconstruction introduces spurious oscillations at the material interface, whereas only the latter is able to essentially preserves the interface thickness throughout the simulation time.

**One-dimensional Gas-Gas Shock-Interface Problem**

The interaction between a strong shockwave traveling towards a gas-gas interface [32, 21, 33, 9], is computed with the employed methodology. The non-dimensionalized initial conditions [32] are given by

\[
\begin{pmatrix}
\alpha_1 \rho_1 \\
\alpha_2 \rho_2 \\
u \\
p \\
\alpha_1
\end{pmatrix} = \begin{cases}
(0, 0.386, 26.59, 100, 0)^T, & x \in [-1, -0.8), \\
(0, 0.1, -0.5, 1, 0)^T, & x \in [-0.8, -0.2), \\
(1, 0, -0.5, 1, 1)^T, & x \in [-0.2, 1].
\end{cases}
\]

The non-dimensionalized material parameters are $\gamma_1 = 1.67$, $\gamma_2 = 1.4$ and $\pi_1 = \pi_2 = 0.0$. The numerical solution is evolved to $t = 0.07$ with CFL $= 0.6$ by utilizing both WENO5 and WENO5-THINC reconstruction. The uniform grid spacing is $h = 2.0/200$.

In Figure 3, the exact and numerical solution are given at final time. No spurious oscillations at the material interface are observable for both reconstruction schemes. However, as observed and noted by Coralic and Colonius [21] the high-order nature of the WENO reconstruction produces oscillations in the wake of the reflected shockwave. Furthermore, in conjunction with the high-order WENO5 reconstruction, only the characteristic reconstruction maintains an essentially oscillation-free shock-front in distinction to the primitive reconstruction.

**One-dimensional Gas-Liquid Riemann Problem**

In the following, a gas-liquid Riemann problem [21, 24, 14] which is used to model underwater explosions is considered. The non-dimensionalized initial conditions for the liquid and highly compressed gas are given by

\[
\begin{pmatrix}
\alpha_1 \rho_1 \\
\alpha_2 \rho_2 \\
u \\
p \\
\alpha_1
\end{pmatrix} = \begin{cases}
(0, 1.241, 0, 2.753, 0)^T, & x \in [-1, 0), \\
(0.991, 0, 0, 3.059 \cdot 10^{-4}, 1)^T, & x \in [0, 1],
\end{cases}
\]

with the non-dimensionalized material properties $\gamma_1 = 5.5$, $\pi_1 = 1.505$ and $\gamma_2 = 1.4$, $\pi_2 = 0$ [14]. Note, that for this Riemann problem the volume fraction $\alpha_1$ is initialized with a sharp jump. The numerical solution is evolved to $t = 0.2$ with CFL $= 0.6$ on a uniform mesh with grid spacing $\Delta x = 2.0/200$.

The exact and numerical solution is given in Figure 4 at final time. The latter is obtained by utilizing both WENO5 and WENO5-THINC reconstruction. Both approaches compare satisfactorily with previous findings [21, 24, 14]. The sharp initialization of the volume fraction does not introduce spurious oscillations at the material interface for this problem.

**Two-dimensional Gas-Gas Shock-Interface Problem**

To demonstrate the utilization of AMR in conjunction with the WENO5-THINC method, a simulation of a two-dimensional gas-gas shock-interface problem was performed with the present model. The problem consists of a helium column ($\rho_1 = 0.138$, $\gamma_1 = 1.667$, $\pi_1 = 0.0$), which is impacted by a planar shock-wave traveling with $Ma = 1.22$ in air ($\rho_2 = 1.0$, $\gamma_2 = 1.4$, $\pi_2 = 0.0$). Here, we follow Meng et al. [30] and non-dimensionalize the variables by the initial droplet diameter and the post-shock parameters of air. The numerical simulation is performed on the computational domain $(x, y) \in [-1.5, 3.5] \times [-2.5, 2.5]$ with zero-order extrapolation non-reflective boundary conditions [19] imposed on all boundaries. The spatial discretization is carried out with static grid spacing $\Delta x = \Delta y = 5/150$ on the coarsest level, while AMR dynamically in-
creases the local resolution by two additional levels. With each successive level, the resolution is doubled in each spatial direction. The numerical solution is evolved to non-dimensional time $t = 4.0$ with CFL = 0.4.

Numerical Schlieren images and density distribution are given in Figure 5 at different time instances. To highlight the increased resolution due to AMR, the density distribution with the instantaneous resolution is given in Figure 6. The utilized numerical method is capable of resolving both shocks and material interfaces, while AMR provides an increased resolution in the vicinity of discontinuities and small-scale flow structures.

**Conclusion**

We have presented an improvement over the five-equation model based finite volume approach for compressible multiphase flows [9], replacing the second-order accurate spatial fluxes with a high-resolution WENO scheme [10, 11] and the finite-difference based curvature calculation with a modification to the standard height function curvature calculation [12], within the context of a cell-based adaptive mesh refinement (AMR) framework [18]. The THINC reconstruction [8, 9] has been utilized to sharpen the diffuse material interface without compromising the conservation properties. Verification test cases indicate that the combination of WENO and THINC reconstruction controls the numerical smearing of the interface better than a standard WENO implementation. The presented curvature calculation also converges with second order in the infinity norm.

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**References**


*Finite Volume Methods for Hyperbolic Problems.*


[22] V.A. Titarev and E.F. Toro.


Numerical simulations of non-spherical bubble collapse with applications to shockwave lithotripsy, 2008.

Figure 2. Solution of the one-dimensional gas-liquid interface advection problem (12) at $t = 4.00$ for (a) density, (b) pressure error, (c) velocity error and (d) volume fraction with grid spacing $\Delta x = 2.0/200$. Given is the exact solution (----) and the numerical solution which utilizes the WENO5 (□) and WENO5-THINC (■) reconstruction.
Figure 3. Solution of the one-dimensional gas-gas shock-interface problem (13) at $t = 0.07$ for (a) density, (b) pressure, (c) velocity and (d) volume fraction with grid spacing $h = 2.0/200$. Given is the exact solution (---) and the numerical solution which utilizes the WENO5 (○) and WENO5-THINC (■) reconstruction.
Figure 4. Solution of the one-dimensional gas-liquid Riemann problem (14) at $t = 0.20$ for (a) density, (b) pressure, (c) velocity and (d) volume fraction with grid spacing $\Delta x = 2.0/200$. Given is the exact solution (—) and the numerical solution which utilizes the WENO5 (□) and WENO5-THINC (■) reconstruction.
Figure 5. Numerical solution of the two-dimensional gas-gas shock-interface problem. Given are numerical Schlieren images (upper half-plane), logarithmically scaled in range from 0.01 to 1.00, and the density distribution (lower half-plane) with the instantaneous grid resolution at different time steps.
Figure 6. Numerical solution of the two-dimensional gas-gas shock-interface problem. Given are the density distribution with the instantaneous grid resolution at different time steps.