

High-order hybrid DG-FV framework for compressible multi-fluid problems on unstructured meshes

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ABSTRACT

In this work we extend the hybrid Discontinuous Galerkin/ Finite Volume framework, introduced in V. Maltsev, D. Yuan, K. W. Jenkins, M. Skote, P. Tsoutsanis, “Hybrid discontinuous Galerkin-finite volume techniques for compressible flows on unstructured meshes, Journal of Computational Physics 473 (2023)” [1], to multi-species problems involving gas-gas and gas-liquid systems. The numerical scheme achieves high order accuracy in smooth flow regions thanks to the DG discretisation, yet avoiding oscillations at material interfaces and shocks thanks to a FV type reconstruction. This strategy, as typically represented in literature, makes use of the so-called troubled cell indicators for the detection of numerical oscillations generated by an unlimited high-order scheme in presence of discontinuities, and enables a more dissipative scheme in the troubled cells only in order to suppress the spurious oscillations. As will be shown in a series of increasingly challenging test-cases, when applied to multi-species flows in the context of diffuse-interface models, the hybrid framework is able to limit the excessive material interface dissipation, characteristic of these interface-capturing methods, allowing at the same time a control over the amount of dissipation necessary to solve stiffer problems.

1. Introduction

Complex fluid flows involving compressible effects with multiple species and materials are almost ubiquitous in scientific and industrial applications, demanding for versatile and accurate solvers. Among the principal strategies for simulating multi-species flows, the diffuse interface model (DIM) formulation provides a simple and robust methodology with straightforward mass conservation properties. Contrarily to the other schemes under the Eulerian-Lagrangian framework, like the sharp interface methods (SIM), where the interfaces are treated like infinitely thin discontinuities and are numerically tracked or reconstructed, the DIM allows the interfaces to have a non-zero thickness. Thus, material interfaces are numerically diffused over a number of mesh elements, requiring a proper thermodynamic treatment of these diffused zone, where some artificial mixing take place as the interface evolves. A unique set of PDEs need to be solved, generally in the form of the complete seven-equation model of Baer and Nunziato [2,3], or the reduced six- [4,5] or five-equation models [6,7]. We refer to [8,9] for more details on each model. In this work, the five-equation model of Allaire [7] is used with isobaric closure for simulating two fluids with arbitrary equation of state (EOS). The five-equation model can be easily extended to account for additional physical phenomena, from capillarity effects [10], to the family of fluid-solid solver presented in [11–13] and systems involving the four states of matter [14]. However, the main drawback of DIM, i.e. the increasing with time interface diffusion due to numerical dissipation, often results in excessive smearing if not properly treated, and somewhat

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limited the adoption of these methods for computations of phenomena evolving on large time scales. Many attempts to remedy to excessive diffusion were proposed, in terms of interface sharpening [15], compression [16], and interface regularisation [17], where additional source terms are included in the governing equations. Some of the issues with these techniques are mass conservation, applicability to situations with dynamic collapse or generation of interfaces, and extension to three-dimensions. Alternatively, the interface diffusion can be limited by the adoption of a high-order discretisation scheme, and the recent advancements in high-order, non-oscillatory shock-capturing schemes for single-species flows, seems to have provided a valuable tool for improving simulation of flows with interfaces, as shown in [18–21]. Despite not having a physical regularisation like in the case of shock waves, the resolution of material interfaces greatly benefits from increasingly higher orders of accuracy, making use at the same time of non-oscillatory reconstruction schemes, mandatory in the presence of steep gradients.

In this work we show the performance of a unstructured, compressible, hybrid DG-FV scheme when applied to a number of multi-species flow problems with large pressure gradients, including gas-gas, and more challenging gas-liquid systems. The hybrid framework was recently introduced and discussed for the Euler equations in [1], and uses a modal DG [22] formulation in smooth flow regions.

Physical discontinuities and numerical oscillations are detected by a troubled cell indicator, enabling a CWENOZ reconstruction [23,24] which provides a non-oscillatory polynomial solution of the same order of the original unlimited DG schemes, and is substituted to the higher DG modes in the troubled cells only. It was shown in [1] that the hybrid schemes perform within a 40% computational overhead when large portions of the cells in the domain are deemed as troubled, and within the 5 – 10% range for more localised discontinuous features as often encountered in benchmarks using the Euler system of equations.

Hybrid FV/DG frameworks were recently studied in literature [25,26], also known as $P_N P_M$ schemes, where the higher order degrees of freedom M of the DG formulation are reconstructed via least square or Green-Gauss reconstruction from the underlying lower order degrees of freedom N , in order to decrease the computational cost of the original pure DG scheme. In this work, instead, the FV reconstruction is coupled to the DG method and enabled to stabilise the underlying DG method with a polynomial correction.

For the case of multi-species flows, a quasi-conservative DG formulation with a consistent discretisation for the volume fraction equation is employed. The troubled cell indicator is a combination of the physically admissible detector (PAD) [27–29], which checks whether the densities and equilibrium pressure are non-negative, and the Shock Detector (SD) which measures the jump in the solution among adjacent cells. In addition, the PAD checks if the volume fraction is neither less than zero or higher than unity, and a bound preserving limiter is also applied to the volume fractions, in the form introduced in [30], rescaling the out-of-range values at the quadrature points. The baseline five-equation model used in this work does not account for phase-transition effects, and the additional non-conservative term in the volume fraction advection equation that accounts for volume fraction variation of each phase during compression or expansion, also referred as Kapila's term, is not included to avoid the well-known numerical stiffness in proximity of the interface during strong expansion or compression. A solution is to adopt relaxed pressure-disequilibrium six-equation models, however, in order to achieve a good balance in computational costs, accuracy and simplicity we make use of the modified Schmidt model [31], which is used as a post-processing technique like in one-fluid models and is activated whenever the local pressure is lower than the saturation level. In this work this is used to avoid the large negative pressure that may occur for benchmarks like the underwater explosion when using the stiffened gas equation of state, which can cause instabilities and over-activation of the troubled cell indicator.

The implementation is performed in the open-source UCNS3D code [32], and the framework performance is assessed against 2D and 3D problems.

2. Governing equations and numerical framework

2.1. Five-equation model

The diffuse-interface model used in this work is the quasi-conservative five-equation model of Allaire et al. [7] and consists of two continuity equations Eq. (1) and Eq. (2), a momentum equation per dimension Eq. (3), an energy equation Eq. (4), and the non-conservative advection equation of the volume fraction of one of the two fluids Eq. (5) as given below

$$\frac{\partial(a_1 \rho_1)}{\partial t} + \nabla \cdot (a_1 \rho_1 \mathbf{u}) = 0, \quad (1)$$

$$\frac{\partial(a_2 \rho_2)}{\partial t} + \nabla \cdot (a_2 \rho_2 \mathbf{u}) = 0, \quad (2)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \mathbf{I}) = 0, \quad (3)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (E + p) \mathbf{u} = 0, \quad (4)$$

$$\frac{\partial a_1}{\partial t} + \mathbf{u} \cdot \nabla a_1 = 0, \quad (5)$$

where ρ is the density, $\mathbf{u} = (u, v, w)^T$ is the velocity, p is the pressure, E is the total energy and a_1 is the volume fraction of phase 1. The stiffened gas EOS is employed for closing the five-equation model, as it allows the treatment of fluids with vastly different thermodynamic properties and is widely used for gas-gas and gas-liquid problems. For the stiffened gas EOS, each fluid pressure is characterised by

$$p_i = (\gamma_i - 1)\rho_i \epsilon_i - \gamma_i \pi_{\infty,i}, \quad (6)$$

where γ_i is the heat capacity ratio for each material, and $\pi_{\infty,i} \geq 0$ is a reference pressure that is assigned the value $\pi_{\infty} = 0$ when referring to gases. The total mass is defined as:

$$\rho = \sum_i a_i \rho_i, \quad (7)$$

and $\rho \epsilon$ being

$$\rho \epsilon = \sum_i a_i \rho_i \epsilon_i, \quad (8)$$

where ϵ is the internal energy, with $\rho \epsilon = E - \frac{1}{2} \rho \mathbf{u} \mathbf{u}$, and in this work $1 \leq i \leq 2$. Assuming isobaric closure, the EOS for the mixture reads as

$$\xi = \frac{1}{\gamma - 1} = \sum_i \frac{a_i}{\gamma_i - 1}, \quad (9)$$

$$\frac{\pi_{\infty} \gamma}{\gamma - 1} = \sum_i a_i \frac{\pi_{\infty,i} \gamma_i}{\gamma_i - 1}, \quad (10)$$

$$p = (\gamma - 1) \rho \epsilon - \gamma \pi_{\infty}, \quad (11)$$

and the mixture sound of speed reads

$$c = \sqrt{\frac{\gamma(p + \pi_{\infty})}{\rho}}. \quad (12)$$

2.2. Discontinuous Galerkin method

In DG methods, higher orders of accuracy are attained by means of a high-order polynomial representation of the local element solution. Similarly to FV schemes, as the solution is discontinuous across the domain elements, the treatment of the flux may be dealt with numerically by introducing a Riemann solver.

We rewrite the governing equations Eqs. (1)–(5) as a conservative system with non-conservative source term, such

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot (\mathbf{F}(\mathbf{U})) = \mathbf{S}(\mathbf{U}) \nabla \cdot \mathbf{u}, \quad (13)$$

where we have rewritten the volume fraction advection equation Eq. (5) in an equivalent form

$$\frac{\partial a_1}{\partial t} + \nabla \cdot (a_1 \mathbf{u}) = a_1 \nabla \cdot \mathbf{u}. \quad (14)$$

Therefore, the vector of conserved variables, non-linear flux tensor, and source vector are defined respectively as

$$\mathbf{U} = \begin{bmatrix} a_1 \rho_1 \\ a_2 \rho_2 \\ \rho \mathbf{u} \\ E \\ a_1 \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} a_1 \rho_1 \mathbf{u} \\ a_2 \rho_2 \mathbf{u} \\ \rho \mathbf{u} \mathbf{u} + p \mathbf{I} \\ \mathbf{u}(E + p) \\ a_1 \mathbf{u} \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ a_1 \end{bmatrix}, \quad (15)$$

We consider first the conservative part of the system represented in Eq. (13), on a physical domain Ω consisting of any combination of conforming tetrahedral, hexahedral, prism or pyramids in 3D, and quadrilateral or triangular in 2D. All the elements are indexed by a unique mono-index i . The global solution is discretely approximated for each cell i by a set of locally continuous piecewise solutions $\mathbf{U}_i(\mathbf{x})$. The local approximation of the solution within each cell i , is given by a linear combination of a basis functions $\phi_i^k(\mathbf{x})$ as follows

$$\mathbf{U}_i(\mathbf{x}) = \sum_{k=0}^K \mathbf{U}_{h,i}^k \phi_i^k(\mathbf{x}). \quad (16)$$

The DG formulation is obtained multiplying the conservative part of Eq. (13) by a smooth test function $\psi(\mathbf{x})$, integrating over each element $V_i \in \Omega$ and performing an integration by parts

$$\int_{V_i} \psi(\mathbf{x}) \frac{\partial \mathbf{U}_i}{\partial t} dV = \int_{V_i} \nabla \psi(\mathbf{x}) \cdot \mathbf{F}(\mathbf{U}_i) dV - \oint_{S_i} \psi(\mathbf{x}) \mathbf{F}(\mathbf{U}_i) \cdot \mathbf{n} dS. \quad (17)$$

The vector $\mathbf{U}_{h,i}^k(t)$ denotes the unknown degrees of freedom of the solution that are advanced in time, and S_i is the boundary of V_i . Adopting a smooth test function from the same space of the basis function, thus $\psi_i^k(\mathbf{x}) = \phi_i^k(\mathbf{x})$, the DG formulation for each element i is given by

$$\sum_{k=0}^K \left(\int_{V_i} \phi_i^k(\mathbf{x}) \phi_i^b(\mathbf{x}) dV \right) \frac{d\mathbf{U}_{h,i}^k}{dt} = \int_{V_i} \nabla \phi_i^b(\mathbf{x}) \cdot \mathbf{F}(\mathbf{U}_i(\mathbf{x})) dV - \oint_{S_i} \phi_i^b(\mathbf{x}) \mathbf{F}(\mathbf{U}_i(\mathbf{x})) \cdot \mathbf{n} dS. \quad (18)$$

In this work a modal DG formulation is used, which allows for the same basis to be used for any element shape and avoids the underintegration errors often present in nodal implementations. Here the unknowns to be solved are the polynomial expansion coefficients, and a popular choice for the modal basis is the cell centered Taylor series expansion, as follows

$$\phi_i^k(\mathbf{x})|_{V_i} = \frac{(x - x_{c_i})^{p_k}}{h_i^{p_k}} \frac{(y - y_{c_i})^{q_k}}{h_i^{q_k}} \frac{(z - z_{c_i})^{r_k}}{h_i^{r_k}} - \frac{1}{|V_i|} \int_{V_i} \frac{(x - x_{c_i})^{p_k}}{h_i^{p_k}} \frac{(y - y_{c_i})^{q_k}}{h_i^{q_k}} \frac{(z - z_{c_i})^{r_k}}{h_i^{r_k}} dV, \quad (19)$$

where $0 \leq p_k + q_k + r_k \leq K$, $k = 1, \dots, K$ and K represents the number of degrees of freedom (DOF). For the first DOF $k = 0$, $\phi_i^0(\mathbf{x}) = 1$ holds. The index i ranges over the total number of elements, and $x_{c_i}, y_{c_i}, z_{c_i}$ are the coordinates of the cell centre of the considered element i . The basis functions are intentionally designed such that the higher-order modes vanish when integrating within the considered cell i , which is convenient when pursuing conservation and seamless interaction between DG and FV discretisation.

We have resorted to this basis function since we want to be able to handle arbitrary unstructured meshes and element shapes, and therefore the integration of the basis functions in physical space requires the decomposition of elements into triangles or tetrahedra. This strategy has been previously documented in other studies [33,34], and the resulting mass matrix for each cell is given by

$$M_{bk} = \int_{V_i} \phi_i^b(\mathbf{x}) \phi_i^k(\mathbf{x}) dV, \quad \text{with } b = 0, 1, \dots, K \text{ and } k = 0, 1, \dots, K. \quad (20)$$

The non-uniquely defined intercell fluxes in Eq. (18) are determined in the same manner as in the FV framework, i.e. with an exact or approximate Riemann solver [22]. The semi-discrete system can be written as

$$M_{bk} \frac{d\mathbf{U}_{h,i}^k}{dt} = \sum_{g=1}^{N_v} \omega_g \mathbf{F}(\mathbf{U}_i(\mathbf{x}_{i,g})) \cdot \nabla \phi_i^b(\mathbf{x}_{i,g}) |V_i| - \sum_{h=1}^{N_f} \sum_{\alpha=1}^{N_{qp}} \tilde{F}^{n_{im}} \left(\mathbf{U}_{im,L}^n(\mathbf{x}_{im,\alpha}, t), \mathbf{U}_{im,R}^n(\mathbf{x}_{im,\alpha}, t) \right) \omega_\alpha \cdot \phi_i^b |S_{im}|, \quad (21)$$

where $\tilde{F}^{n_{im}}$ is the numerical flux normal to the interface between cell i and cell m . N_f is the number of faces, N_v is the number of the volume Gaussian quadrature points, N_{qp} is the number of face quadrature points, and $|S_{im}|$ is the surface area of the considered face. $\mathbf{U}_{im,L}^n(\mathbf{x}_{im,\alpha}, t)$ and $\mathbf{U}_{im,R}^n(\mathbf{x}_{im,\alpha}, t)$ are the discontinuous solutions for cell i and cell m at the prescribed face Gaussian quadrature points respectively; while $\mathbf{x}_{im,\alpha}$ and ω_α , and $\mathbf{x}_{i,g}$ and ω_g correspond to different face and volume Gaussian integration points and weights respectively.

Eq. (21) can be written as

$$\mathbf{M}_i \frac{d\mathbf{U}_i}{dt} + \mathbf{R}_i(\mathbf{U}_i) = 0, \quad (22)$$

where $\mathbf{U}_i$ is the approximate solution, $\mathbf{M}_i$ is the mass matrix and $\mathbf{R}_i(\mathbf{U}_i)$ is the residual vector.

2.3. Non-conservative equation

The term on the RHS of Eq. (14) is treated as a source term and following the approach of Johnsen and Colonius [18] it is numerically approximated as surface integral, rather than a volume one. In addition, the velocity used in the integration of the source term must be compatible with the velocity used in the integration of the convective fluxes, and is approximated by the estimate provided by the Riemann as detailed in Appendix A:

$$\int_{V_i} a_1 \nabla \cdot \mathbf{u} dV \approx \int_{V_i} a_1 dV \cdot \int_{\partial V_i} (u_n)^{Riem.} dS. \quad (23)$$

Therefore, the extended form for the non-conservative equation reads

$$M_{bk} \frac{d\mathbf{U}_{h,i}^k}{dt} = \sum_{g=1}^{N_v} \omega_g \mathbf{F}(\mathbf{U}_i(\mathbf{x}_{i,g})) \cdot \nabla \phi_i^b(\mathbf{x}_{i,g}) |V_i| - \sum_{h=1}^{N_f} \sum_{\alpha=1}^{N_{qp}} \left(\tilde{F}^{n_{im}} \left(\mathbf{U}_{im,L}^n(\mathbf{x}_{im,\alpha}, t), \mathbf{U}_{im,R}^n(\mathbf{x}_{im,\alpha}, t) \right) - \mathbf{a}_{i,1}^n \cdot u_n^{Riem}(\mathbf{x}_{f,l}) \right) \omega_\alpha \cdot \phi_i^b |S_{im}|. \quad (24)$$

2.4. FV reconstruction

The CWENOZ scheme employed in this study follows the implementation of Tsoutsanis and Dumbser [35] and uses the combination of an optimal (high-order) polynomial p_{opt} with lower-order polynomials. The optimal polynomial is built from the central stencil, while the lower-order polynomials employ the directional stencils. When the variation of the solution is smooth, the optimal polynomial is recovered and therefore the desired-order of accuracy is obtained. In the presence of discontinuous data, at least one of the lower-order polynomials arising from the directional stencils could contain smooth data, hence essentially reducing the oscillations in the computed solution, which is of great importance in situations of shock interaction with material interfaces. The directional stencils employ the Type3 definition which includes one directional stencil per element face as detailed in the work by Tsoutsanis [34]. The optimal polynomial is defined as follows

$$p_{opt}(\xi, \eta, \zeta) = \sum_{s=1}^{s_t} \lambda_s p_s(\xi, \eta, \zeta), \quad (25)$$

where s is the stencil index. The value $s = 1$ corresponds to the central stencil, $s = 2, 3$, and so on, represents the directional stencils. s_t is the total number of stencils and λ_s is the linear coefficients for each stencil, whose sum is equal to 1. The p_1 polynomial is not computed directly, but obtained by subtracting the lower-order polynomials from the optimum polynomial

$$p_1(\xi, \eta, \zeta) = \frac{1}{\lambda_1} \left(p_{opt}(\xi, \eta, \zeta) - \sum_{s=2}^{s_t} \lambda_s p_s(\xi, \eta, \zeta) \right). \quad (26)$$

The CWENOZ reconstruction polynomial is given as a non-linear combination of all the polynomials in the following manner

$$p(\xi, \eta, \zeta)^{cwenoZ} = \sum_{s=1}^{s_t} \omega_s p_s(\xi, \eta, \zeta), \quad (27)$$

where ω_s correspond to the non-linear weights assigned to each polynomial, and in regions with smooth data $\omega_s \approx \lambda_s$, hence obtaining the high-order approximation from the central stencil. In regions of discontinuous solutions the reconstructed solution will be mostly influenced from the lower-order polynomials of the directional stencils. The non-linear weight ω_s is defined as

$$\omega_s = \frac{\tilde{\omega}_s}{\sum_{s=1}^{s_t} \tilde{\omega}_s} \quad \text{where} \quad \tilde{\omega}_s = \lambda_s \left(1 + \frac{\tau}{\epsilon + SI_s} \right), \quad (28)$$

where the definition of global oscillation indicator has been used

$$\tau = \left(\frac{\sum_{s=2}^{s_t} |SI_s - SI_1|}{s_t - 1} \right)^b. \quad (29)$$

The smoothness indicator SI_m is given by

$$SI_s = \sum_{1 \leq |\beta| \leq r_{V'_0}} \int (D^\beta p_s(\xi, \eta, \zeta))^2 (d\xi, d\eta, d\zeta), \quad (30)$$

where β is a multi-index, r is the polynomial's order, λ_m is the linear weight. The value set to prevent division by zero of $\epsilon = 10^{-6}$ is used, with $b = 4$ and D being the derivative operator. The smoothness indicator is a quadratic function of the degrees of freedom (a_k^s) and Eq. (30) can be rewritten as

$$SI_s = \sum_{k=1}^K a_k^s \left(\sum_{q=1}^K \mathcal{O}I_{kq} a_q^s \right), \quad (31)$$

where the oscillation indication matrix $\mathcal{O}I_{kq}$ is computed with

$$\mathcal{O}I_{kq} = \sum_{1 \leq |\beta| \leq r_{V'_0}} \int (D^\beta \phi_k(\xi, \eta, \zeta)) (D^\beta \phi_q(\xi, \eta, \zeta)) (d\xi, d\eta, d\zeta), \quad (32)$$

which can be precomputed and stored at the beginning of the simulation. For the directional stencils and their corresponding polynomials we employ $r = 1$ to obtain 2nd-order of accuracy, and any arbitrary order of accuracy for the polynomial associated with the central stencil. The linear weights are computed by firstly assigning the non-normalised linear weight for the central stencil λ'_1 an arbitrary value, and then normalising this as follows

$$\lambda_1 = 1 - \frac{1}{\lambda'_1}, \quad (33)$$

with the linear weights associated with lower-order polynomials being equal and provided by the following expression

$$\lambda_s = \frac{1 - \lambda_1}{s_t - 1}, \quad (34)$$

where s_t is the total number of stencils. The FV reconstruction on unstructured meshes of the present algorithm used in UCNS3D [32,36] follows the approaches of Tsoutsanis et al. [35,37–39], and Titarev et al. [40] that have been previously applied to smooth and discontinuous flow problems [34–56]. Thus, every element in the domain that are not triangular in 2D or tetrahedral in 3D is first decomposed in elementary triangular or tetrahedral elements respectively. The stencils are built by adding neighbouring elements recursively, up to a number of elements $M = 2K$ determined by the number of polynomial coefficients K . All the polynomials reconstructed on each element of each stencil satisfy the requirement of matching the cell averages of the solution $\mathbf{U}_m$:

$$\int_{V_m} p^{cwenoZ}(\mathbf{x}) d\mathbf{x} = |V_m| \bar{\mathbf{U}}_0 + \sum_{k=1}^K \int_{V_m} \tilde{a}_k \phi_k d\mathbf{x} = |V_m| \bar{\mathbf{U}}_m, \quad m = 1, \dots, M, \quad (35)$$

and this condition is satisfied due to the employed basis function, as defined in Eq. (19). The limited reconstructed DOFs are referred as $\tilde{a}$. Defining the following quantities:

$$A_{mk} \equiv \int_{V_m} \phi_k dxdydz, \quad b_m \equiv |V_m|(\bar{\mathbf{U}}_m - \bar{\mathbf{U}}_0), \quad (36)$$

Eq. (35) can be rearranged in a matrix form as

$$\sum_{k=1}^K A_{mk} a_k = b_m, \quad m = 1, 2, \dots, M. \quad (37)$$

The resulting overdetermined system is solved by a least-squares approach using a QR decomposition [57] and for speeding up the computation we pre-store the Moore-Penrose pseudo-inverse of A_{mk} . From this point forward the order of the scheme will be defined by a number next to the type of the scheme, thus the nomenclature $P2 - CWENOZ3$ refers to a 3^{rd} order hybrid DG/FV scheme for example.

2.5. Volume fraction bound preserving limiter

One of the key requirements to successfully solve the five-equation diffuse interface model is that the volume fractions a_1 should remain bounded in the range $[0, 1]$ during the whole simulation time. Unlimited higher-order schemes such as the DG method are prone to generate overshoots and undershoots of physical quantities. In addition, the CWENOZ scheme, not being a total variation diminishing reconstruction, cannot guarantee a well behaved solution, and small volume fraction bound violation can undermine the correct evolution of material interfaces. In order to reduce the oscillation, a bound-preserving limiter, as introduced in [58], is here adopted. This limiter consists of checking the value of the volume fraction at every Gaussian quadrature point $a_{i,1}(\mathbf{x}_{f,l})$, and compute a scaling factor θ_i as

$$\theta_i = \begin{cases} \frac{\bar{a}_1^n - m}{\bar{a}_1^n - a_{i,1}(\mathbf{x}_{f,l})} & \text{if } a_{i,1}^n(\mathbf{x}_{f,l}) < m, \\ 1 & \text{if } a_{i,1}(\mathbf{x}_{f,l}) \in [m, M], \\ \frac{M - \bar{a}_1^n}{a_{i,1}^n(\mathbf{x}_{f,l}) - \bar{a}_1^n} & \text{if } a_{i,1}(\mathbf{x}_{f,l}) > M. \end{cases} \quad (38)$$

where the barred variables refer to cell averaged values. The volume fraction at the quadrature points are then scaled with

$$\tilde{a}_{i,1}(\mathbf{x}_{f,l}) = \bar{a}_1^n + \theta_i(a_{i,1}(\mathbf{x}_{f,l}) - \bar{a}_1^n), \quad (39)$$

where the scaling $\theta = \min_i \{\theta_i\}$ is activated only if the volume fraction a_1 exceeds the lower or higher threshold values, m and M respectively, defined as $m = \epsilon$, $M = 1 - \epsilon$, with $\epsilon = 10^{-12}$ being a small positive constant. In the same way, the limiter is applied also to partial densities of both phases. In this case the scaling factor $\theta_{i,k}$ for materials $k = 1, 2$, takes the value of unity if $\rho_{i,k} a_{i,k}(\mathbf{x}_{f,l}) > m$ and

$$\theta_{i,k} = \frac{(\bar{\rho}_k a_k)^n - m}{(\rho_k a_k)^n - (\rho_{i,k} a_{i,k})^n(\mathbf{x}_{f,l})}, \quad (40)$$

otherwise. The partial densities at each quadrature point are then modified similarly to Eq. (39). This limiter is applied after verifying the unlimited DG solution, and in the event the CWENOZ scheme fails to provide a well behaved solution. It has to be stressed that once the volume fraction has been modified at a quadrature point, the total energy need to be update accordingly as illustrated in [59], retaining the initial cell average quantity and thus preserving mass, momentum and energy conservation.

2.6. Cavitation model

To prevent the occurrence of negative pressures, which can be mistakenly permitted by the stiffened gas EOS in the presence of intense expansion waves, a distinct treatment of cavitation is necessary. This issue arises because the existing system of equations fails to accurately capture cavitation. In this work we adopt the modified Schmidt model [60,61] as a post processing technique at the end of every Runge-Kutta stage, and at each pressure check, the allowed values for pressure must follow

$$P = \begin{cases} SG EOS & \text{if } P \geq P_{sat}, \\ P_{sat} + P_{1,2} \cdot \log A & \text{if } P_\epsilon < P < P_{sat}, \\ P_\epsilon & \text{if } P < P_\epsilon. \end{cases} \quad (41)$$

As suggested in [60], we impose a value for saturation pressure of $P_{sat} = 2000$ Pa, which is chosen to ensure that the pressure value in the cavitation region is below the pressure in the surrounding regions and always non-negative. To avoid negative pressure, a cut-off is applied if the pressure goes below $P_\epsilon = 10^{-5}$. The values for $P_{1,2}$ and A can be determined by

$$P_{1,2} = \frac{\rho_1 c_1^2 \rho_2 c_2^2 (\rho_1 - \rho_2)}{(\rho_1^2 c_1^2 - \rho_2^2 c_2^2)} \quad (42)$$

$$A = \frac{\rho_1 c_1^2 \rho_2 c_2^2 (\rho_2 + a_1 (\rho_1 - \rho_2))}{(\rho_2 (\rho_1^2 c_1^2 - a_1 (\rho_1^2 c_1^2 - \rho_2^2 c_2^2)))}.$$

It is assumed that the values ρ_1, ρ_2, c_1, c_2 are constant and here refers to density and speed of sound of gas and liquid respectively, at saturation level for air-water mixtures. This model is expected to perform better than a pure cut-off model which neglects phase transition and imposes the pressure to be equal to a constant saturation pressure whereas the detected pressure value is below a certain threshold value, often resulting in conservation violation. It is also expected to perform better than the original Schmidt model, which still allows for negative pressure values in cavitation zones with a large vapor to liquid density ratio (larger than 10^{-5}).

2.7. Troubled cell indicators

In this work, a FV type reconstruction is performed in the regions presenting oscillations of physical quantities, as typically resulting from the application of unlimited high-order schemes in proximity of physical discontinuities or steep gradients. The detection of undesired numerical instabilities is performed by means of the so-called troubled cell indicator and is of paramount importance for a good trade-off between accuracy, stability and computational efficiency. A variety of troubled cell indicators are available in literature, from the KXRCF detector presented in [62], to the PAD and NAD detectors employed in [51,63,64] for the *a posteriori* MOOD framework. In this work we use a combination of the PAD detector and a shock detector, which measures the jump in the solution between adjacent cells, specifically adapted to multispecies problems.

The PAD detector, when applied to multispecies problems, checks at every Gaussian quadrature point of each domain element, whether the boundary extrapolated values of the volume fractions are bounded in the range $[0, 1]$, the partial densities are non-negative, and that the pressure values are admissible

1. $0 < a_i < 1$,
2. $(a\rho)_i > 0$,
3. $p_i > -\pi_{\infty_i}$.

For all these variables the PAD indicator also checks that none of these variable presents *NaN* values. The PAD is coupled to a shock detector (SD), defined as

$$\frac{\sum_{n=1}^N \left| \frac{1}{V_0} \int_{V_0} U_0(\mathbf{x}) dV - \frac{1}{V_n} \int_{V_n} U_n(\mathbf{x}) dV \right|}{\max_{n \in \{0 \dots N\}} \left\{ \frac{1}{V_n} \left| \int_{V_n} U_n(\mathbf{x}) dV \right| \right\}} > C_k, \quad (43)$$

which measures the relative jump in the solution between adjacent cell, using the cell averaged values. The threshold value C_k is usually considered to be unity unless otherwise specified, and the quantities being checked by the SD detector are partial densities, pressure and volume fraction.

2.8. Hybrid scheme and implementation

The adoption of a modal DG scheme allows the easy hybridisation with a FV type framework, where the unlimited DG solution is checked at every RK stage of each time step, and the underlying FV type reconstruction is enabled in the cells that are deemed troubled by the solution checking criteria. For the troubled cells only, the reconstructed polynomial is substituted to the original DG solution

$$\mathbf{U}_i(\mathbf{x}, t) = \mathbf{U}_0 + \sum_{k=1}^K \mathbf{U}_{h,i}^k(t) \phi_i^k(\mathbf{x}) = \mathbf{U}_0 + \sum_{k=1}^K \tilde{a}_k \phi_k(\mathbf{x}), \quad (44)$$

where the first degree of freedom assigned with index $j, k = 0$ ensures conservation, since the higher-order terms $j, k = 1, 2, \dots, K$ cancel out when integrated within the considered cell due to the employed basis. Since the same basis is used for both DG and FV we simply set $U_{h,i}^j = \tilde{a}_k$, where $\tilde{a}_k$ are the CWENOZ reconstructed polynomial coefficients as defined in Sec. 2.4.

Algorithm 1: Pre-store geometry based information.

```

for every element  $\Omega_i$  in the domain do
  for every volume quadrature point  $\mathbf{x}_k$  of element  $\Omega_i$  do
    compute mass matrix;
    assemble reconstruction stencil;
  end
  compute and prestore inverse of mass matrix;
  establish communications requirements for stencil elements;
  establish communications requirements for surface quadrature points;
end

```

The general procedure for solving the five-equation model with the presented hybrid framework can be briefly summarised in two different blocks. The first, summarised in Algorithm 1, includes the operations that are performed only once and the stored in memory for the duration of the simulation, which includes the computation of the mass matrix and its inverse, the assembly of the reconstruction stencils and establishing the communication requirements across each processor. In order to evolve the solution in time, the unlimited DG solution is first computed and its validity checked by the troubled cell indicator. If the FV reconstruction is activated, suggesting for the presence of steep gradients due to shock waves or material interfaces in the targeted cell, the bound preserving limiter is also applied to enforce boundedness of volume fraction solution, but only the in presence of contact surfaces. The validity of the solution is then checked again with the indicator, and if it is still not well behaved, the reconstruction is performed with a decreased order as illustrated in Algorithm 2, down to a 2^{nd} order MUSCL reconstruction if necessary.

Algorithm 2: Advance in time\stage.

```

for every Runge-Kutta stage do
  for every element  $\Omega_i$  in the domain do
    for every face  $f_j$  of element  $\Omega_i$  do
      for every surface quadrature point  $\mathbf{x}_{f,k}$  of face  $f_j$  do
        compute unlimited DG solution;
        check solution with PAD & NAD-SD detector;
      end
    end
    while troubled cell for element  $\Omega_i == 1$  do
      reconstruct DOFs with CWENOZ scheme;
      replace higher DG DOFs with FV DOFs;
      apply bound preserving limiter;
      check solution with PAD & NAD-SD detector;
    end
    check if pressure below saturation point;
    extrapolate solution at qps.  $\mathbf{x}_{f,k}$  and compute numerical fluxes;
  end
end

```

2.9. Fluxes & time advancement

The flux approximation and temporal discretisation techniques are shared between the FV and DG methods. For the inviscid fluxes, the approximate HLLC (Harten-Lax-van Leer-Contact) Riemann solver of Toro [65] is employed as detailed in Appendix A, unless otherwise stated. The solution is advanced in time by a third-order TVD Runge-Kutta method

$$\mathbf{U}_i^{(n+1/3)} = \mathbf{U}_i^n + \Delta t M^{-1} R_i(\mathbf{U}), \quad (45)$$

$$\mathbf{U}_i^{n+2/3} = \frac{3}{4} \mathbf{U}_i^n + \frac{1}{4} \mathbf{U}_i^{(n+1/3)} + \frac{1}{4} \Delta t M^{-1} R_i(\mathbf{U}^{(n+1/3)}), \quad (46)$$

$$\mathbf{U}_i^{n+1} = \frac{1}{3} \mathbf{U}_i^n + \frac{2}{3} \mathbf{U}_i^{(n+2/3)} + \frac{2}{3} \Delta t M^{-1} R_i(\mathbf{U}^{(n+2/3)}), \quad (47)$$

and the time step Δt is selected according to

$$\Delta t = \text{CFL} \frac{1}{2r+1} \min_i \left(\frac{h_i}{S_i} \right), \quad (48)$$

Table 1

Convergence studies for the hybrid DG/FV scheme on different meshes. The e_{L^∞} and e_{L^2} error norms, and related convergence orders, are computed comparing the final profile after one period advection with the initial solution. The time coefficient is normalised with respect to the lowest order scheme on coarsest mesh of the same typology.

Var.	h	$P2$					$P3$				
Quadrilateral mesh		e_{L^∞}	$\mathcal{O}_{L^\infty}$	e_{L^2}	$\mathcal{O}_{L^2}$	time	e_{L^∞}	$\mathcal{O}_{L^\infty}$	e_{L^2}	$\mathcal{O}_{L^2}$	time
a_1	1/8	4.57E-05	-	4.65E-05	-	1.000	3.34E-07	-	2.52E-07	-	2.128
	1/16	3.31E-06	3.79	3.65E-06	3.67	5.757	6.37E-09	5.71	4.50E-09	5.81	19.434
	1/32	2.60E-07	3.67	2.80E-07	3.70	38.651	4.05E-10	3.98	2.29E-10	4.30	188.729
	1/64	9.88E-09	4.72	8.16E-09	5.09	288.073	2.48E-11	4.02	1.27E-11	4.17	1192.602
$\rho_1 a_1$	1/8	4.65E-04	-	3.29E-04	-	1.000	2.17E-06	-	1.64E-06	-	2.128
	1/16	1.69E-05	4.79	1.20E-05	5.75	6.231	2.17E-08	6.64	1.56E-08	6.71	19.434
	1/32	7.60E-07	4.47	5.39E-07	4.48	38.651	1.32E-09	4.03	9.34E-10	4.06	188.729
	1/64	5.26E-08	3.85	4.21E-08	3.68	288.073	8.64E-11	3.93	7.11E-11	3.71	1192.602
Triangular mesh		e_{L^∞}	$\mathcal{O}_{L^\infty}$	e_{L^2}	$\mathcal{O}_{L^2}$	time	e_{L^∞}	$\mathcal{O}_{L^\infty}$	e_{L^2}	$\mathcal{O}_{L^2}$	time
a_1	1/8	4.48E-05	-	1.53E-05	-	1.000	6.75E-07	-	1.95E-07	-	2.989
	1/16	5.45E-06	3.04	1.15E-06	3.73	6.841	4.63E-08	3.87	9.50E-09	4.36	21.786
	1/32	5.74E-07	3.25	1.09E-07	3.41	53.684	2.40E-09	4.27	4.46E-10	4.41	165.996
	1/64	9.23E-08	2.64	1.12E-08	3.28	410.127	2.77E-10	3.12	3.10E-11	3.85	1296.700
$\rho_1 a_1$	1/8	3.14E-04	-	1.07E-04	-	1.000	4.86E-06	-	1.38E-06	-	2.989
	1/16	3.82E-05	3.04	8.08E-06	3.73	6.841	3.39E-07	3.84	6.98E-08	4.31	21.786
	1/32	4.02E-06	3.25	7.60E-07	3.41	53.684	1.90E-08	4.15	3.98E-09	4.13	165.996
	1/64	6.46E-07	2.64	7.84E-08	3.28	410.127	1.16E-09	4.03	2.43E-10	4.04	1296.700
Hybrid mesh		e_{L^∞}	$\mathcal{O}_{L^\infty}$	e_{L^2}	$\mathcal{O}_{L^2}$	time	e_{L^∞}	$\mathcal{O}_{L^\infty}$	e_{L^2}	$\mathcal{O}_{L^2}$	time
a_1	1/8	3.70E-04	-	6.08E-05	-	1.000	6.88E-06	-	1.69E-06	-	2.375
	1/16	2.54E-05	3.86	7.03E-06	3.11	8.027	7.03E-07	3.29	1.13E-07	3.91	19.874
	1/32	4.83E-06	2.40	9.18E-07	2.94	66.463	7.79E-08	3.18	8.13E-09	3.79	199.252
	1/64	6.65E-07	2.86	9.88E-08	3.22	444.843	5.76E-09	3.76	4.79E-10	4.08	1501.665
$\rho_1 a_1$	1/8	2.59E-03	-	4.26E-04	-	1.000	4.81E-05	-	1.18E-05	-	2.375
	1/16	1.78E-04	3.86	4.92E-05	3.11	8.027	4.92E-06	3.29	7.89E-07	3.91	19.874
	1/32	3.38E-05	2.40	6.43E-06	2.94	66.463	5.45E-07	3.18	5.69E-08	3.79	199.252
	1/64	4.65E-06	2.86	6.88E-07	3.22	444.843	4.01E-08	3.76	3.37E-09	4.08	1501.665

where S_i is an estimate of the maximum in absolute value of the propagation speed in the cell V_i , h_i is a characteristic length of the element V_i and CFL refers to the Courant-Friedrichs-Lewy condition.

All the volume/surface/line integrals are approximated by Gaussian quadrature rule suitable for the order of polynomial employed [66]. All the schemes developed are implemented in the UCNS3D CFD code [32] which is written in object-oriented Fortran 2008, employing MPI message passing interface (MPI), and the Open Multi-Processing (OpenMP) application programming interface (API), and the reader is referred to [50,67] for more details on implementation and performance benchmarks. The computational times reported in each case are obtained for the same hardware (and compilation settings) and normalised with respect to a reference setup for the same hardware so that the performance of various algorithms under identical hardware can be appreciated.

3. Results and discussion

3.1. Multispecies convergence test

For the verification of the designed order of spatial accuracy for the numerical schemes developed, a multi-species advection test similar to the one employed by Wong and Lele [68] is used. In this test a smooth volume fraction profile of two gases is advected for one period in a periodic computational domain. The initial condition is given by

$$(\rho_1, \rho_2, u, v, p, a_1) = (7, 1, 1, 0, 1/1.4, 0.5 + 0.25 \sin(2\pi(x - 0.5))). \quad (49)$$

The 2D computational domain is defined by $[0, 1]^2$, and the convergence test is performed on uniform quadrilateral, triangular and hybrid quadrilateral-triangular meshes, each with 8, 16, 32 and 64 edges per side resolution, and the simulation is run for a time of $t_f = 1$. The two gases selected are nitrogen and helium with specific heats 1.4 and 1.66 respectively. The numerical errors e_{L^2} and the e_{L^∞} are computed as follows

$$e_{L^2} = \sqrt{\frac{\sum_i \int_{\Omega_i} (\mathbf{U}_e(x, t_f) - \mathbf{U}_c(x, t_f))^2 dV}{\sum_i |\Omega_i|}}, \quad (50)$$

$$e_{L^\infty} = \mathcal{M}ax \left| \mathbf{U}_e(x, t_f) - \mathbf{U}_c(x, t_f) \right|, \quad (51)$$

where $\mathbf{U}_c(x, t_f)$ and $\mathbf{U}_e(x, t_f)$ are the computed and exact solutions at the end of the simulation $t_f = 1.0$. The exact solution $\mathbf{U}_e(x, t_f)$ being given by the initial condition itself at $t = 0$. The simulations were performed using a $CFL = 0.5$ that was the minimum sufficient to obtain the theoretical order of convergence on all the meshes. The wallclock time per simulation is normalised with respect to the fastest time taken for a simulation on the coarsest mesh of the same typology with the lowest order under examinations. The convergence orders for 3rd and 4th order hybrid scheme are presented in Table 1 for the volume fraction a_1 and

Table 2

Initial conditions for the isolated gas-water material interface advection.

Location	ρ_1	ρ_2	u	v	p	γ	π_∞	a_1
$0.25 < x < 0.75$	1.0	1000	2	0	1	1.4	0	1.0
$x < 0.25, x > 0.75$	1.0	1000	2	0	1	4.4	6000	0

Table 3

Initial conditions for the 2D gas-liquid Riemann problem.

Location	ρ_1	ρ_2	u	v	p	γ	π_∞	a_1
Left-state	1.241	0	0	0	2.753	1.4	0	1.0
Right-state	0	0.991	0	0	$3.059 \cdot 10^{-4}$	5.5	1.505	0

phasic density $\rho_1 a_1$ of material 1. For both variables, and all mesh typology, the hybrid scheme is able to achieve a convergence order close to the theoretical one. It has to be noted the exponential increase in computational time, especially for the highest order on the finest meshes, due to the large number of DOFs evolved, as typically experienced with this type of discretisation, where the 3rd order scheme provides a good balance between accuracy and computational costs.

3.2. Isolated material interface

In this test case the accuracy and non-oscillatory properties of the framework are verified during the advection at constant velocity of a sharp gas-water material interface. The interface is advected in a 2D computational domain $[0, 1]^2$, and at the final time $t_f = 2$ the position of the interface coincides with the initial position. Thus the interface at the initial instant is used as reference, and the initial conditions are defined in Table 2, following the set up proposed by [59].

The computations are performed on a uniform quadrilateral and triangular mesh, with a resolution of 64 edges per side. Fig. 1 shows the results obtained with the hybrid framework on the mesh composed of triangular elements, compared at final time against the reference solution, corresponding to the profile at time $t = 0$, and the solution obtained with a pure FV with CWENOZ reconstruction of the same order. The final profile obtained with the hybrid $P2 - CWENOZ3$ scheme is sensibly less diffused than the one with the pure FV scheme. As required for consistency in the interface advection, pressure and velocity are uniform and constant across the interface, where only minute oscillations, close to machine precision, are observed for the normalised pressure. It is reported in literature [18,39] that within the pure FV context, the WENO reconstruction has to be performed with respect to the primitive variables in order to preserve non-oscillatory solution across material interfaces with different γ . In the current implementation of the hybrid framework, we were able to suppress the oscillations at the interface by adopting more stringent criteria for the troubled cell detection. For the present test case only, an additional NAD detector in the form of *relaxed* MOOD type detector proposed in [28], was tested *a priori* fashion with the following parameters:

$$\min_{y \in \mathcal{V}_i} (U^n(y)) - \delta \leq U(x) \leq \max_{y \in \mathcal{V}_i} (U^n(y)) + \delta, \quad (52)$$

where the margin δ is defined as:

$$\delta = \max(10^{-8}, 10^{-6} \cdot [\max_{y \in \mathcal{V}_i} (U^n(y)) - \min_{y \in \mathcal{V}_i} (U^n(y))]), \quad (53)$$

where $\mathcal{V}_i$ refers to the group of von Neumann neighbours of the target cell. With the use of the criteria defined above, we were able to suppress the oscillations at the interface without having to resort to a primitive reconstruction of the troubled cells, although we remark the importance of applying the detection criteria to the primitive variables. The contours of volume fraction primary cell values are shown in Fig. 2 at final time, and on the relatively coarse meshes specified above, the hybrid scheme is able to preserve a fairly good representation of the material interface, within 2-3 mesh points.

3.3. Gas-liquid Riemann problem

The two-dimensional set up of the gas-water Riemann problem proposed in [69] is here studied. Highly compressed air is considered for the left state, while the right state is occupied by water at atmospheric pressure, and the parameters for the initial conditions are listed in Table 3.

The 2D domain $[-1, 1]^2$ is discretised by a triangular mesh consisting of 64 edges per side resolution, and the discontinuity is initially placed at $x = 0$. The simulation is carried out until the final time $t_f = 0.2$, employing the 2nd and 3rd order $P1 - MUSCL2/P2 - CWENOZ3$ schemes respectively, where the former make use of MUSCL type reconstruction for the troubled cells, whilst the latter uses the CWENOZ type reconstruction. The problem consists of a left moving rarefaction wave, and a right moving shock wave and material interface. Both the schemes being used provide good agreement with the reference solution, showed in Fig. 3, correctly capturing the waves present in the problem, and without generating excessive oscillation at this coarse resolution.

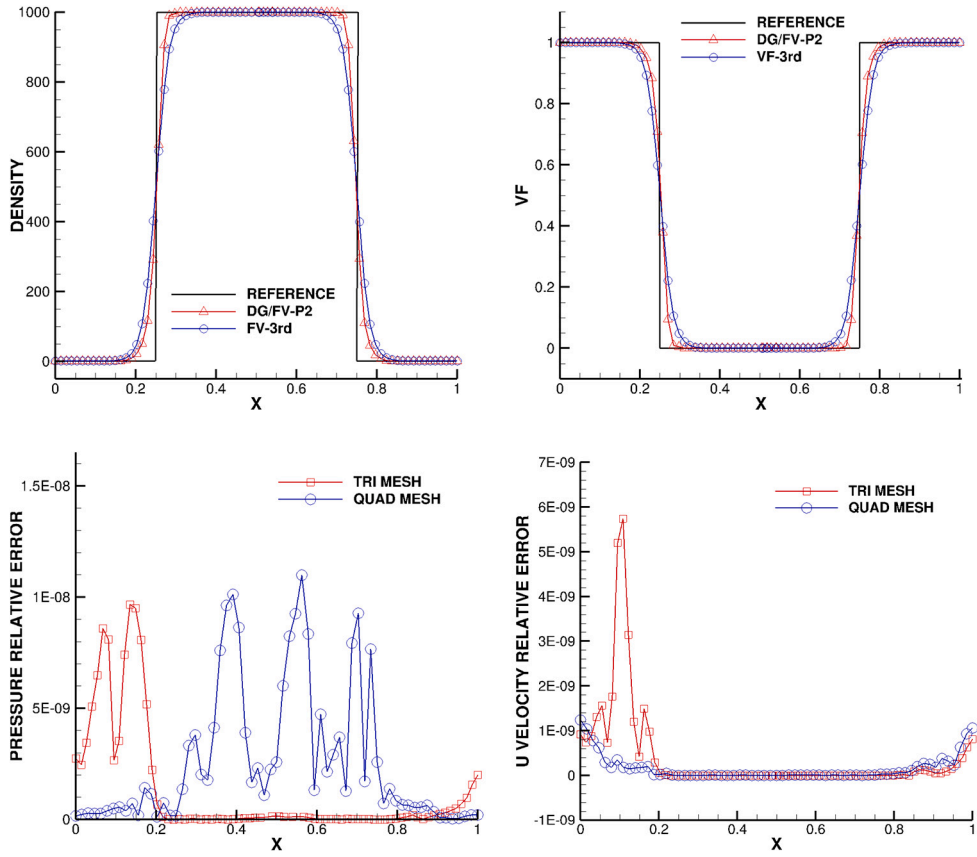


Fig. 1. Plots of density (top left), volume fraction (top right), pressure relative error (bottom left), and U velocity relative error (bottom right) for the isolated material interface advection test case.

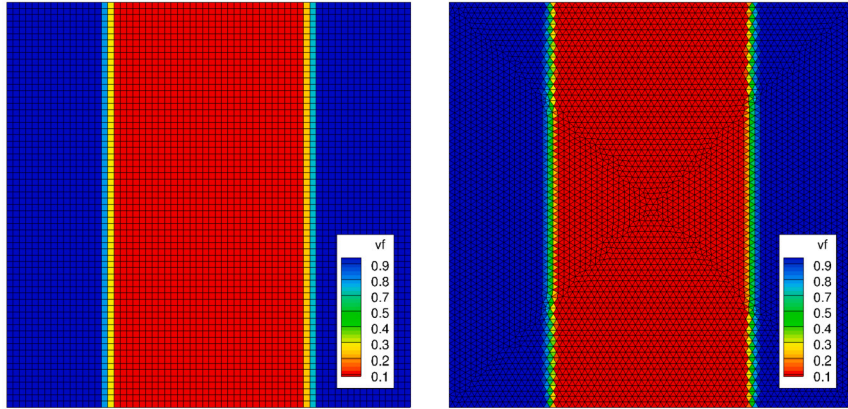


Fig. 2. Cell primary value contours of volume fractions after one period advection on uniform quadrilateral and triangular meshes computed with the 3rd order DG/FV scheme.

3.4. Helium Bubble-Shock wave interaction in air

The accuracy of the hybrid scheme is then assessed against the widely used benchmark consisting of the interaction of a weak shock wave in air and a helium bubble. The helium bubble is initially contaminated by air, with 28% concentration in mass of air, and the initial conditions are defined as in Table 4.

The computations are performed on a coarse 2D mesh composed of triangular elements, characterised by an average element edge length in the shock bubble interaction zone of $e_c \approx D_b/35$, and on a hybrid unstructured finer mesh $e_f \approx D_b/120$, where D_b refers to the bubble diameter. On both meshes slip-wall boundary conditions are applied to top and bottom boundaries, and inflow and outflow are applied to right and left of the domain respectively. The final simulation time is $t_f = 983 \mu s$, and the evolution of volume

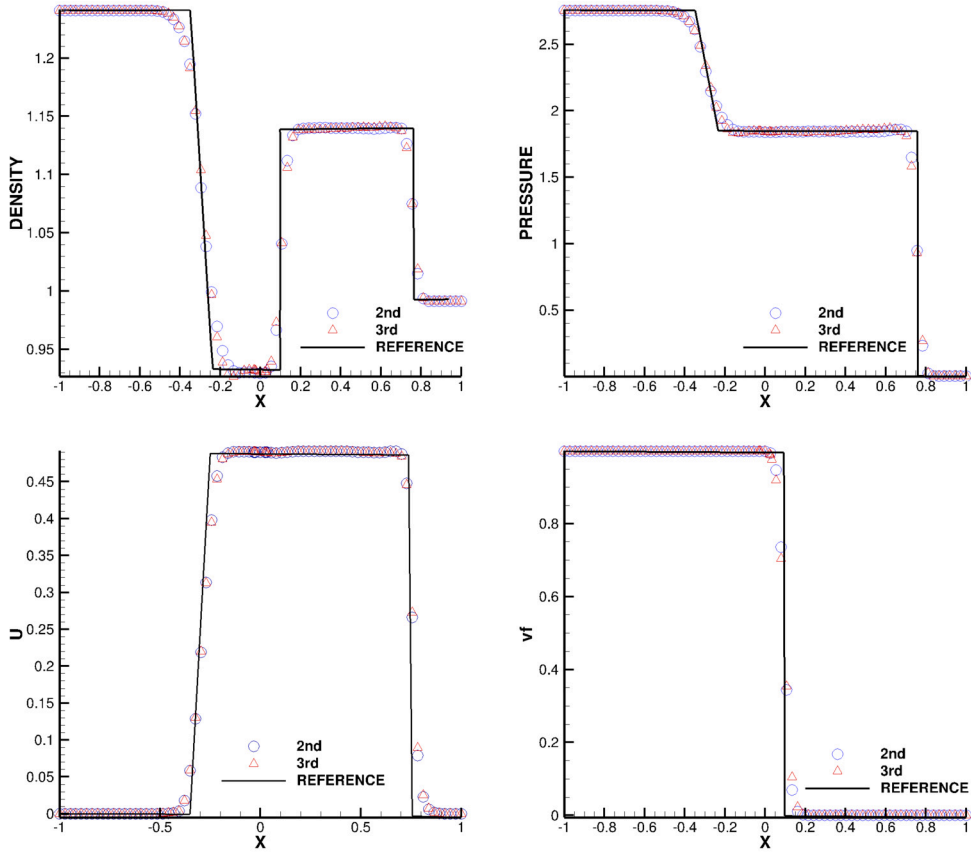


Fig. 3. Plots of density (top left), pressure (top right), velocity (bottom left), and volume fraction (bottom right) for the gas-liquid Riemann problem.

Table 4

Initial Conditions for the helium bubble shock wave test case.

Location	$a_1 \rho_1$	$a_2 \rho_2$	u	v	p	a_1
Post-shock	0.0	1.204	0	0	101325	0
Pre-shock	0.0	1.658	-114.49	0	159060	0
Bubble	0.158	0.061	0	0	101325	0.95

fraction and density gradient magnitude on the finer grid, computed with the 3rd order hybrid $P2-CWENO3$ scheme, are shown in Fig. 4. The time evolution shows the left-moving shock wave impinging on the helium bubble and the hybrid scheme is able to capture the correct flow pattern, in accordance with experiments and other numerical applications. The onset of Kelvin-Helmoltz instabilities at the interface, triggered by baroclinic effects, are finely captured and greatly benefits from the increased accuracy of the hybrid scheme. It is to be remarked that this test case has no converged solution, as it is an inviscid case solved by using the Euler set of equations and it is here used to assess the diffusivity of the framework. In this sense, the comparison with the computations performed with a pure FV reconstruction scheme of the same order on the coarser and finer grids as shown in Fig. 5, highlights how compared to the hybrid scheme, the pure FV scheme results in much more diffuse material interface at the final time. As a form of validation with other works and experimental results, the evolution of the position for upstream, jet and downstream interfaces is illustrated in Fig. 6, showing a good agreement with reference [70], where a front-tracking/ghost fluid method has been used.

A 3D configuration of the problem has also been considered, and is tested on a coarse 3D mesh with an average edge length in proximity of the bubble interface of $e_{3D} \approx D_b/25$ resulting in a domain of approximately 390'000 cells composed of hexahedral and tetrahedral elements. The simulation is run with the hybrid $P2-CWENO3$ and $P4-CWENO5$ schemes as shown in Fig. 7 for different time stamps, and the dynamic of the shock-bubble interaction resemble closely the one found in the 2D setup, although the profiles are more diffused due to the very coarse resolution adopted. The comparison of the volume fraction contours at the final time, with the pure FV CWENO3 scheme is illustrated in Fig. 8.

3.5. Shock-induced collapse of gas bubble in water

In this test case we consider the time evolution of a gas bubble in water impacted by a planar right-moving shock wave. Due to the initial set-up of the problem the gas bubble undergoes a shock induced collapse, involving very-high pressure, providing a

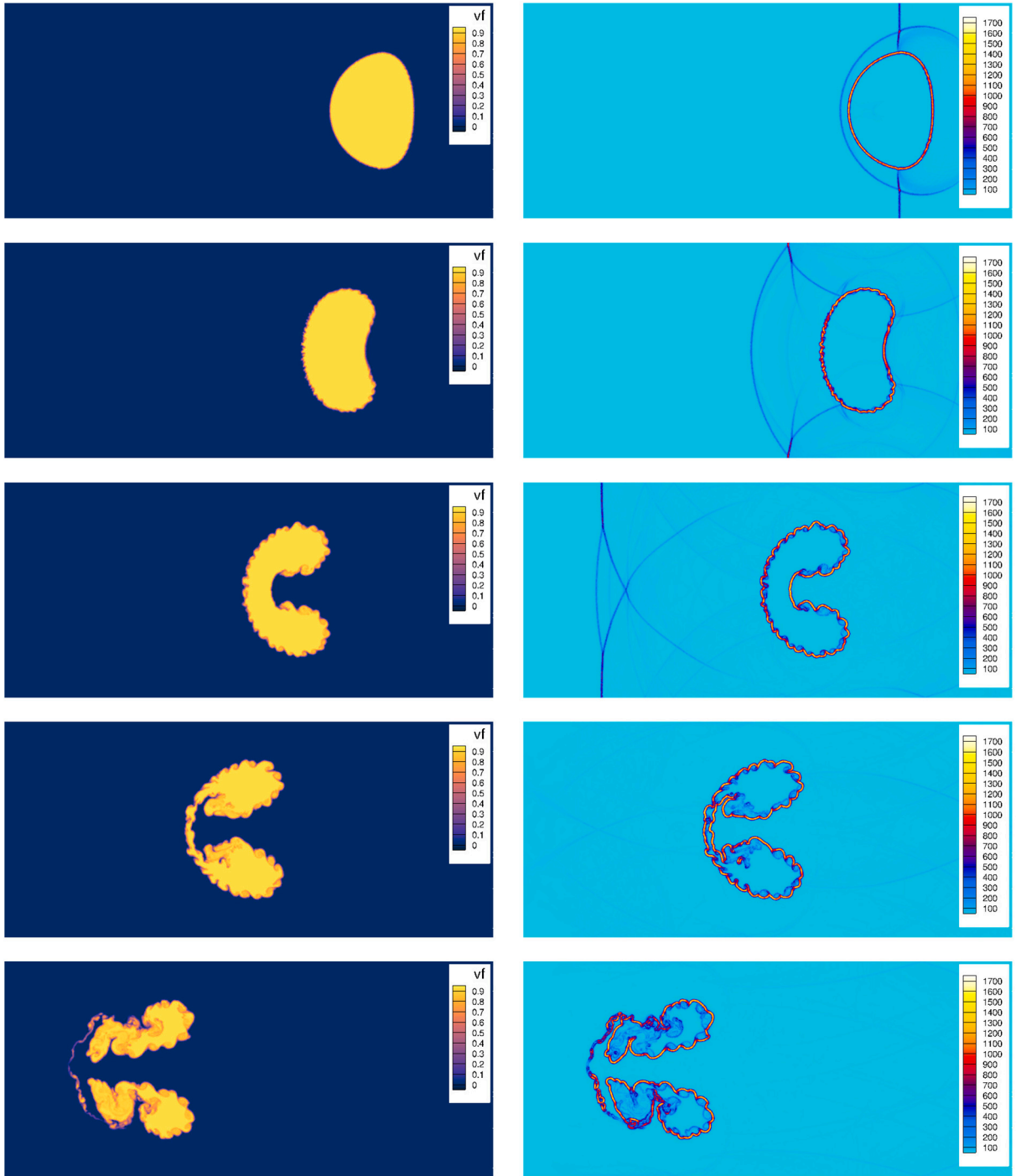


Fig. 4. Evolution of volume fraction (*left*) and density gradient magnitude (*right*) for the interaction with shock of helium bubble in air test case computed with the hybrid $P2 - CWENOZ3$ scheme. Time stamps from top to row to bottom: $t = 124 \mu s$, $t = 234 \mu s$, $t = 425 \mu s$, $t = 617 \mu s$, $t = 983 \mu s$.

good benchmark for multi-species numerical methods. The right-moving shock is a strong shock $M_{sh} = 1.72$, defined by the initial conditions specified in Table 5

The gas bubble is placed at the center of a square domain $[0, 0.024]^2$, and the shock front is initially placed at $x = 0.0066$ m. Non-reflecting boundary conditions are prescribed at the left and right boundaries of the domain, and Euler-slip wall conditions are prescribed for top and bottom boundaries. The mesh resolution is coarser than the ones used in other studies, with an average cell length of $e_m \approx D_b/80$. The final simulation time is $t = 6.2 \mu s$, and the bubble evolution is shown in Fig. 9 at different time stamps.

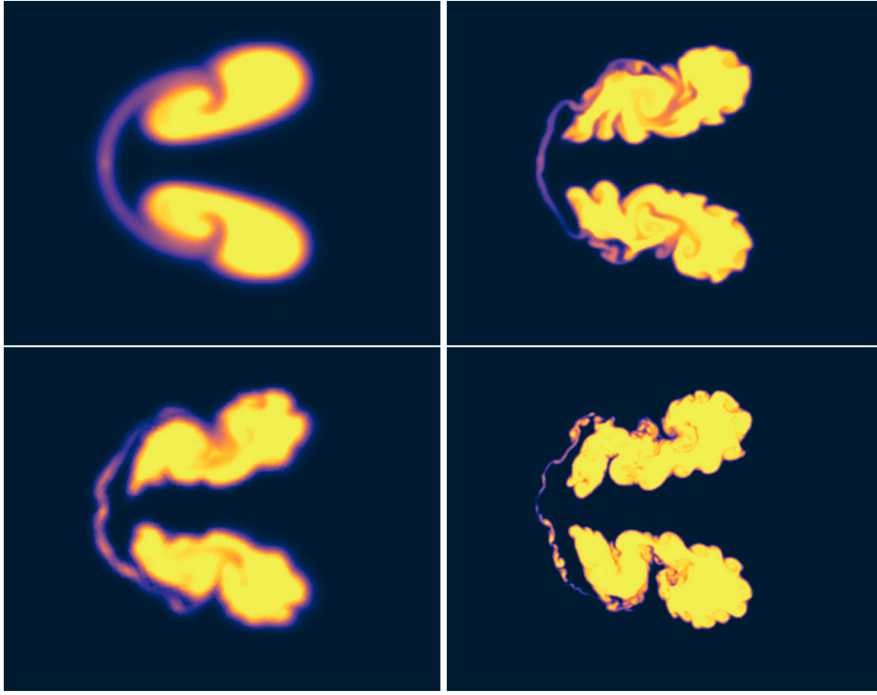


Fig. 5. Computed results for helium bubble in air shock wave interaction. The results represent the volume fraction of helium bubble at final time $t = 983 \mu s$, on a coarse mesh on the *left* column, and on a finer mesh on the *right* column. In the top row are shown the results obtained with a 3rd order CWENO scheme (*left*) and a 5th order CWENO scheme (*right*), in the bottom row are shown the results obtained with a hybrid $P2 - CWENOZ3$ scheme.

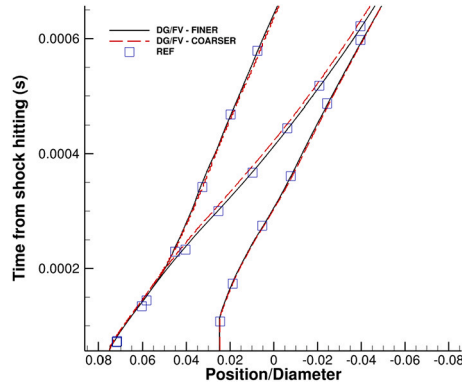


Fig. 6. Bubble interface locations after shock hitting computed on coarser and finer meshes, and compared with reference [70].

Table 5

Initial conditions for gas bubble in water test case.

Location	ρ	u	v	p	γ	π_∞	a_1
Post-shock	1323.65	681.058	0	$1.9 \cdot 10^9$	4.4	$6 \cdot 10^8$	0
Pre-shock	1000	0	0	$1 \cdot 10^5$	4.4	$6 \cdot 10^8$	0
Bubble	1	0	0	10^5	1.4	0	1

The evolution of pressure in time is represented in Fig. 11. The bubble collapse is initiated as the incident shock travels and gets transmitted across the gas bubble. The upstream surface gets accelerated as a result of the rarefaction and generates a water jet. In accordance with other studies, two pressure peaks are registered at times $t \approx 4.0 \mu s$ and $t = 5.0 \mu s$, the former of lower magnitude, as the water jet crosses the stationary bubble downstream front, inducing a high-pressure blast wave. The second pressure peak is more intense, as the blast wave interacts with the remaining bubble fragments, and is a metric of good use for comparison with other studies. The peak registered is of 7.2 GPa being in line with the values obtained in [71], and approximately 1.4 GPa higher than the peak measured with a pure FV scheme of the same order on the same mesh resolution, thanks to the increased number of DOFs being evolved with the hybrid DG/FV scheme.

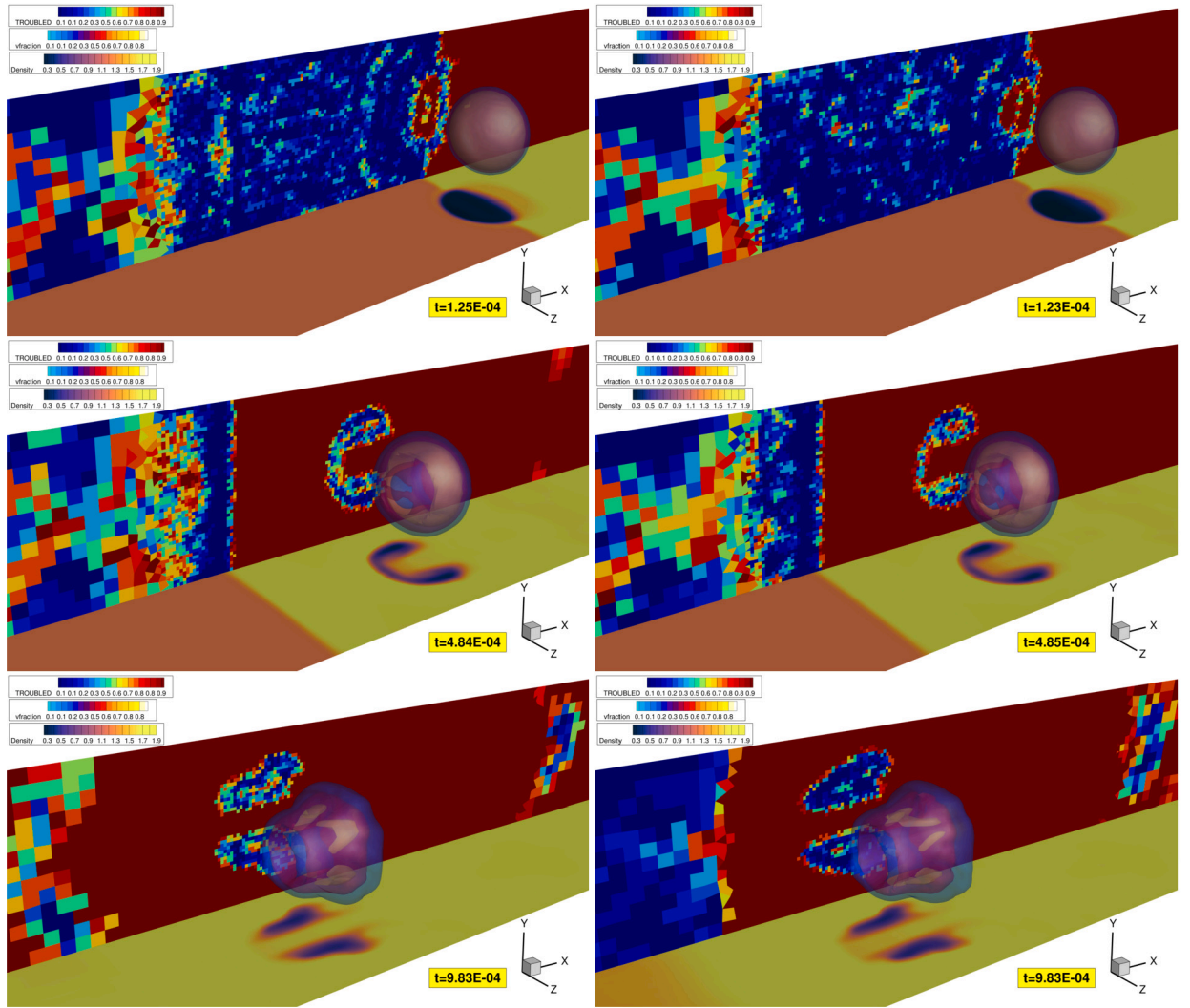


Fig. 7. Iso-surface of volume fraction, and contour plots of density and troubled cells slices at the middle of the computational domain at different instants with a DG-FV P2 scheme (left) and a DG-FV P4 scheme (right) for the 3D Helium Bubble-Shock wave interaction problem.

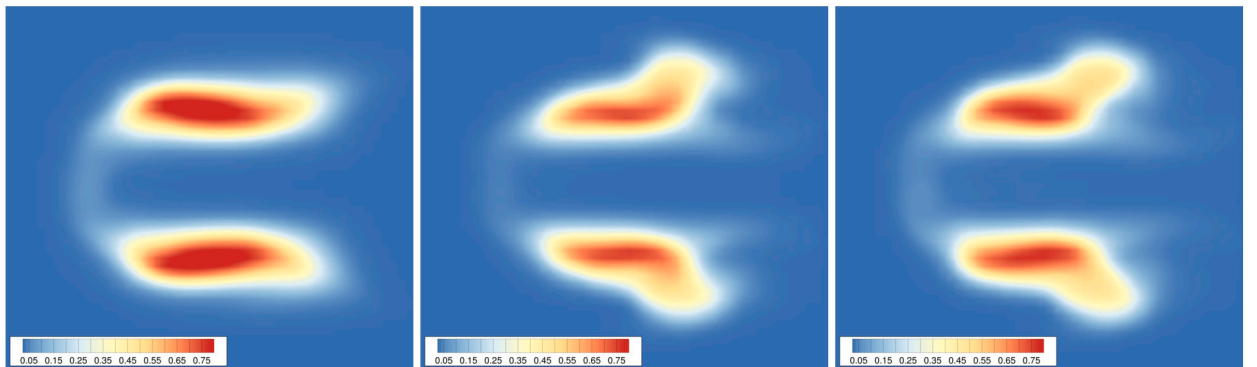


Fig. 8. Contour plots of volume fraction at $t = t_{final}$ with a CWENO3 scheme (left), DG-FV P2 scheme (middle) and a DG-FV P4 scheme (right) for the 3D Helium Bubble-Shock wave interaction problem.

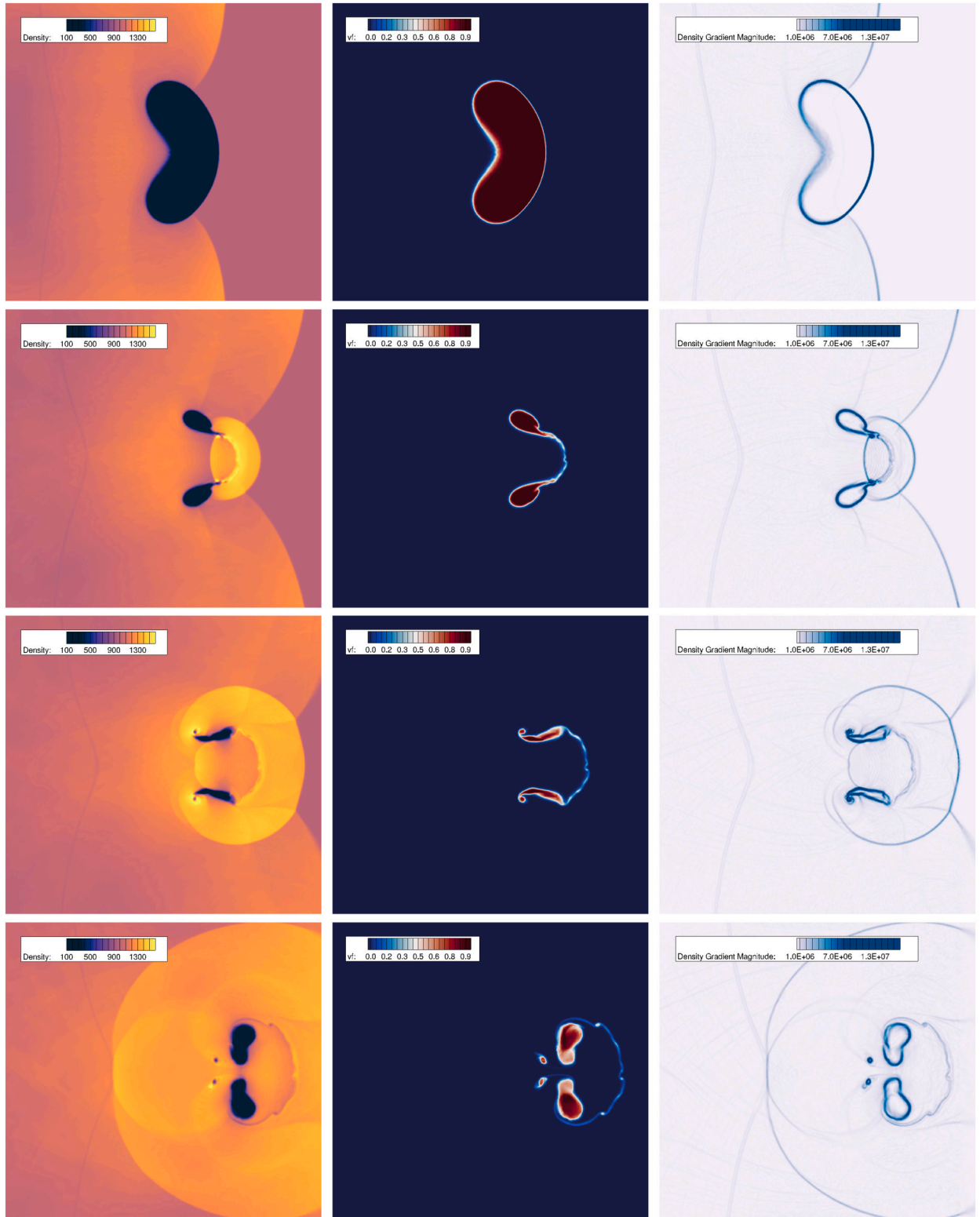


Fig. 9. Gas bubble shock induced collapse at time frames $t = 3.0$, $t = 4.1 \mu\text{s}$, $t = 4.7 \mu\text{s}$ and $t = 6.0 \mu\text{s}$ from left to right respectively. From top row to bottom row, volume fractions and density gradient magnitude, respectively, computed with the hybrid $P2 - CWENOZ3$ scheme.

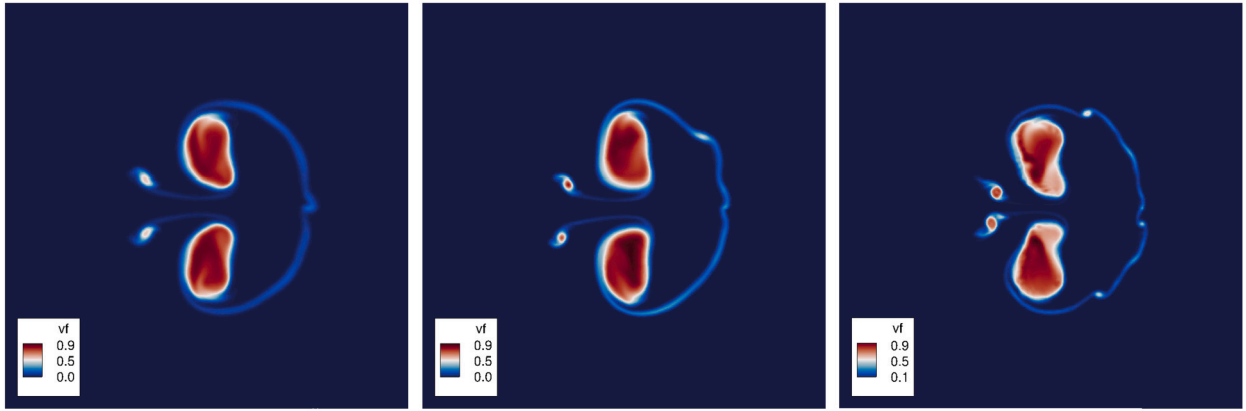


Fig. 10. Comparison of volume fraction contours at time $t = 6.0 \mu s$, computed with FV CWENO 5th order (left), hybrid $P1 - MUSCL2$ scheme (middle), and $P2 - CWENO3$ scheme (right).

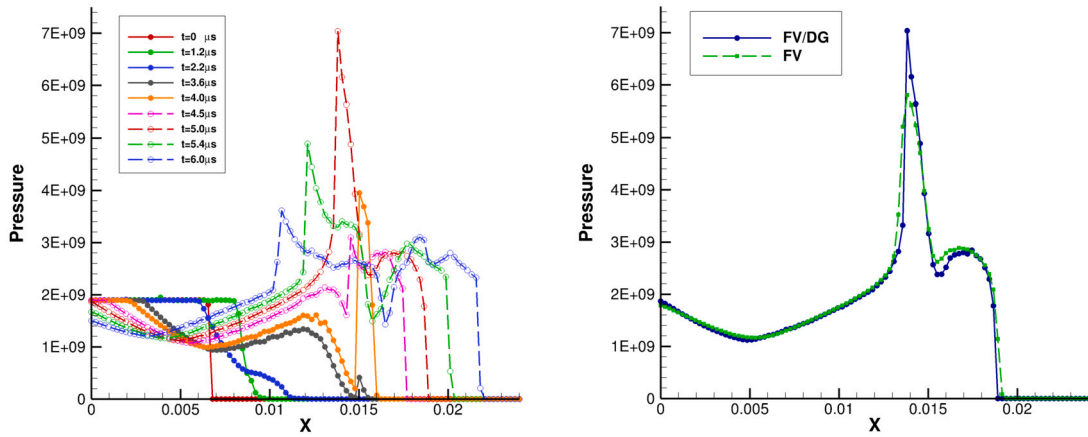


Fig. 11. Pressure evolution left, and comparison of pressure profiles at centerline between hybrid and pure FV scheme at time $t = 5 \mu s$.

Table 6

Initial conditions for shock induced 2D gas bubble array collapse in water test case.

Location	ρ	u	v	p	γ	π_∞	a_1
Post-shock	1323.65	0	681.058	$1.9 \cdot 10^9$	4.4	$6 \cdot 10^8$	0
Pre-shock	1000	0	0	$1 \cdot 10^5$	4.4	$6 \cdot 10^8$	0
Bubble	1	0	0	10^5	1.4	0	1

The effects of different discretisation orders and schemes on the final bubble shape are shown in Fig. 10, comparing the volume fraction contours at time $t = 6.0 \mu s$.

3.6. Shock-induced collapse of gas bubble array in water

This test case is a variation of Test Case 3.5 as we investigate here the shock induced collapse of an array of bubbles. This provides an useful benchmark to test the robustness of the numerical scheme, due to the high energy release as different waves interact after bubble collapse. The configuration being studied is a 2D triangular arrangement as introduced in [72], where two larger bubbles of radius $R_B = 0.0005m$ are located at the two bottom vertices and a smaller bubble of radius $R_b = 0.0002$ is located at the top vertex. The simulation is performed on a square domain $[0, 0.003]^2$, discretised by uniform quadrilateral elements with three resolutions $e_c \approx D_b/20$, $e_m \approx D_b/40$, $e_f \approx D_b/100$. The simulation is run until time $t_f = 1.2 \mu s$, with initial conditions as listed in Table 6.

The evolution of the density and pressure gradient contours, and troubled cells regions are represented in Fig. 12 at different times, and are qualitatively in line with [72]. It is of particular interest the dynamic of the central bubble collapse as it is highly dependent upon the initial arrangement, and we refer to [29,72] for a study of different configurations. For the set-up in use, corresponding to case I of [72], we measure a large pressure peak of $\approx 9.5GPa$ at time $t \approx 0.95 \mu s$ as the central bubble, already compressed by the incident shock, is hit by the water hammer shocks coming from the side bubbles, similar to the findings of [72]. The maximum pressure measured at different times on different mesh resolutions is shown in Fig. 13, where the grid sensitivity to this metric seems

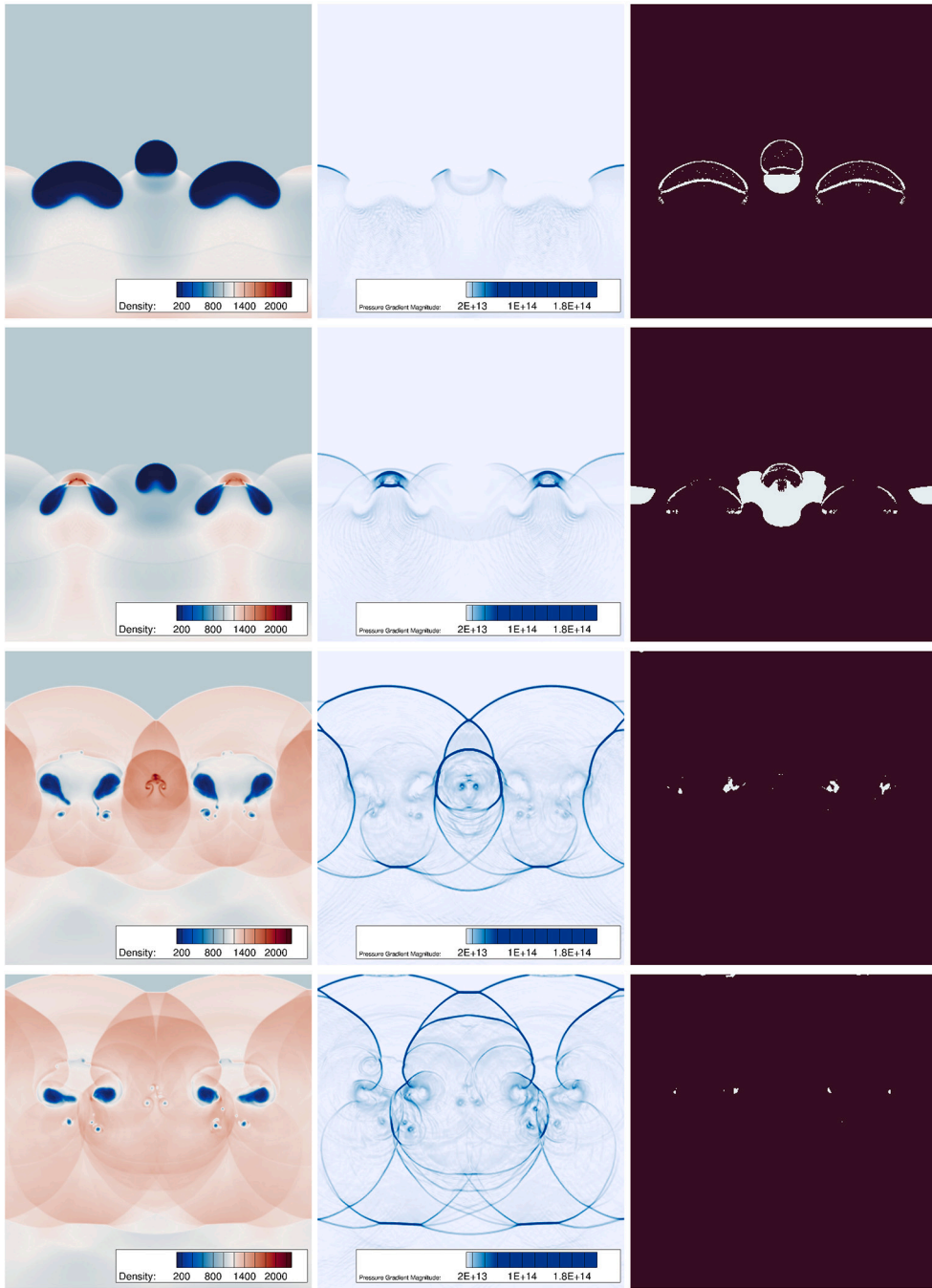


Fig. 12. Contours for the bubble array collapse in water with triangular arrangement. From left column to right, density, pressure gradient magnitude and troubled cells contours, from top row to bottom results at time: $t = 0.11 \mu\text{s}$, $t = 0.45 \mu\text{s}$, $t = 0.6 \mu\text{s}$, $t = 0.95 \mu\text{s}$, $t = 1.1 \mu\text{s}$.

to be minimal between medium and finer resolution, and similarly for the population of troubled cells. It has to be noted that since the incident shock is weakened by the interaction with secondary waves in the inner regions, the inner and outer lobes of the large bubbles have different evolution, and the asymmetry of these bubbles is more pronounced at later times after rebound.

3.7. 3D shock-induced bubble array collapse in water

The extension to the third dimension of the previous test case is studied in this section. Five spherical bubbles in a pyramidal configuration are here considered as illustrated in Fig. 14, and were previously studied by Bempedelis and Ventikos [73] and Tsoutsanis et al. [29].

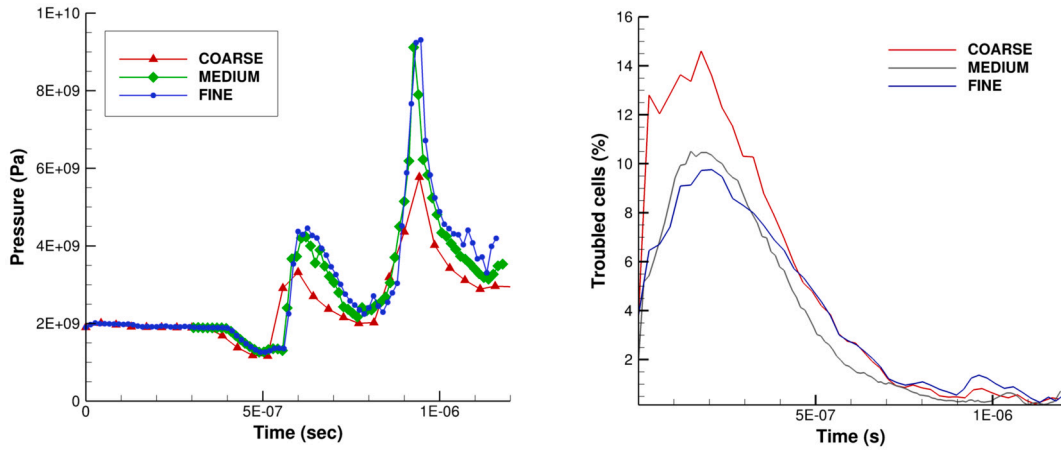


Fig. 13. Maximum pressure on different mesh resolutions (left), and troubled cell percentage in the domain (right).

Table 7

Initial conditions for shock induced 3D gas bubble array collapse in water test case.

Location	ρ	u	v	w	p	γ	π_∞	a_1
Post-shock	1323.65	0	681.058	0	$1.9 \cdot 10^9$	4.4	$6 \cdot 10^8$	0
Pre-shock	1000	0	0	0	$1 \cdot 10^5$	4.4	$6 \cdot 10^8$	0
Bubble	1	0	0	0	10^5	1.4	0	1

Table 8

Parameters of bubble array pyramidal arrangement.

#Bubble	radius [m]	x-coord. [m]	y-coord. [m]	z-coord. [m]
1	0.0002	0.0015	0.0015	0.0015
2	0.0005	0.00075	0.001	0.0015
3	0.0005	0.00225	0.001	0.0015
4	0.0005	0.0015	0.001	0.00075
5	0.0005	0.0015	0.001	0.00225

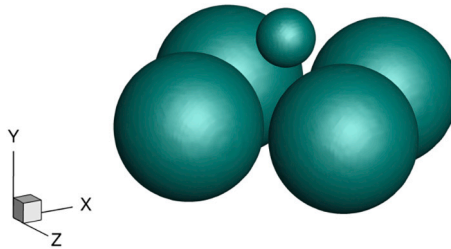


Fig. 14. Initial arrangement for array of bubbles in pyramidal configuration.

The computational domain is a cube with each face side extending from 0 to 0.0003m, and is discretised with a coarser and a finer mesh, counting approximately 1M and 3M hexahedral elements respectively. The initial conditions, reported in Table 7, are similar to the previous 2D set-up, and the details of the geometry of the pyramidal arrangement are illustrated in Table 8. The computations are performed with the 3rd order hybrid scheme.

The dynamic of the bubbles collapse, as depicted in Fig. 15 at different time stamps, is in line with previous work. As the main Mach 1.72 shock front impinges on the base bubbles, a first pressure peak due to the water hammer shock wave of the large bubbles is generated. The regions where the troubled cells are detected at different times when the main shock interacts with the bubbles are highlighted in Fig. 16. Observing Fig. 17 is evident that the first pressure peak is slightly anticipated to the one found in [73] likely due to the mismatch in the Mach number between [73] and the present work. A large pressure peak following the collapse of the smaller bubble, is experienced following the collapse of the central bubble. This peak is approximately 5 times larger than the one experienced in the 2D triangular configuration due to three-dimensional effects, and the contribution in the charging of the central bubble from the secondary waves that comes from the larger count of side bubbles.

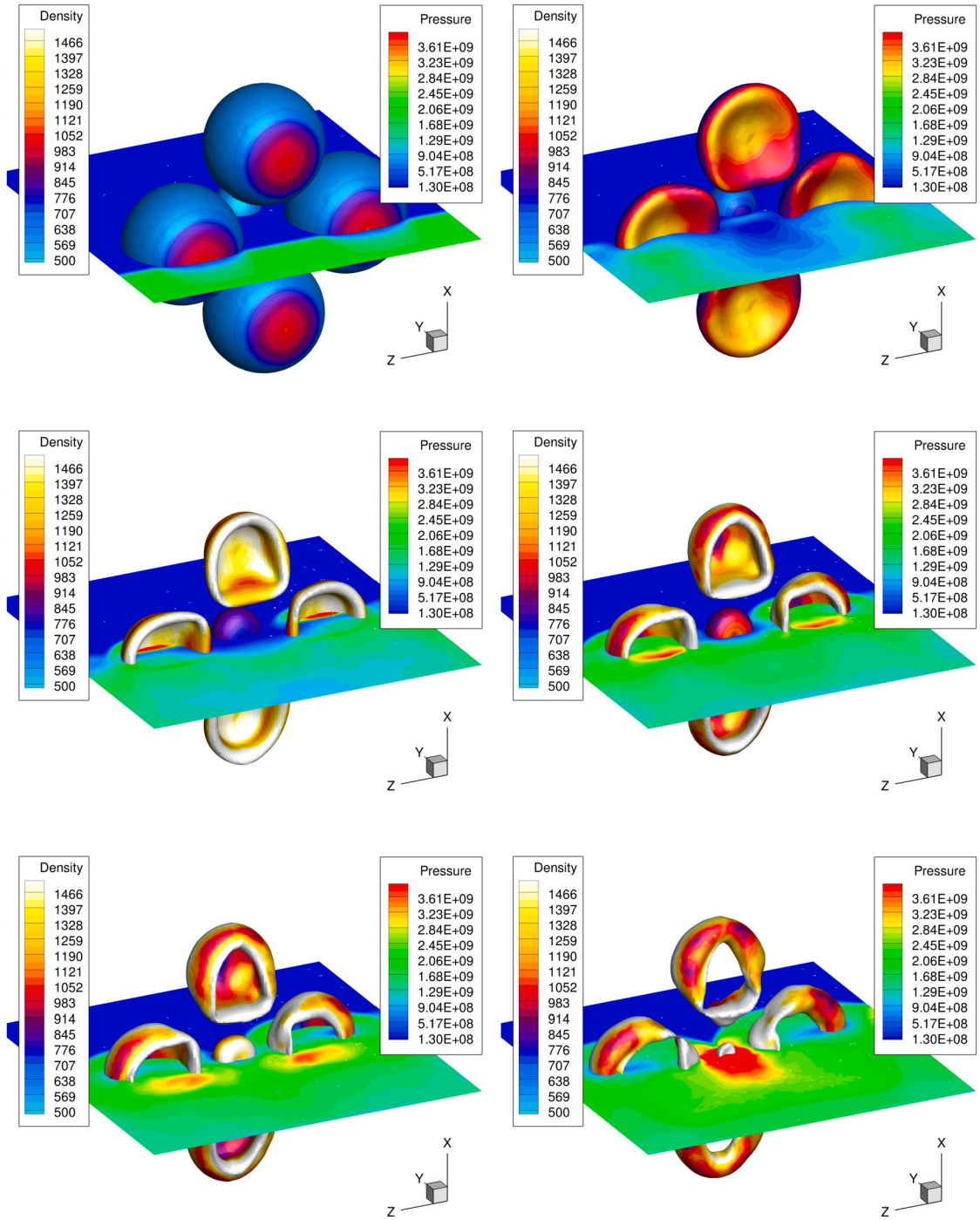


Fig. 15. Pressure slices at midspan and volume fraction iso-surfaces flooded by density contours for the bubble array collapse in water in pyramidal arrangement. From top to bottom row and left to right column in sequence, results at time $t = 0.20 \mu\text{s}$, $t = 0.50 \mu\text{s}$, $t = 0.72 \mu\text{s}$, $t = 0.80 \mu\text{s}$, $t = 0.85 \mu\text{s}$, $t = 0.95 \mu\text{s}$.

3.8. 2D underwater explosion

In this problem we consider the explosion of a gas bubble positioned under the sea level, as described in [71]. The initial conditions are summarized in Table 9, thus air is treated as perfect gas and water phase is modeled with the stiffened gas EOS. The computation is performed on a square $[-2, 2] \cdot [-1.5, 2.5]$ domain, and the air-water interface is placed at $y = 0$. The explosive gas bubble is initially positioned at coordinates $(0, -0.3)$, with a 0.12 radius. Wall boundary conditions are prescribed for the bottom side of the domain, and non-reflecting conditions are applied to the remaining sides.

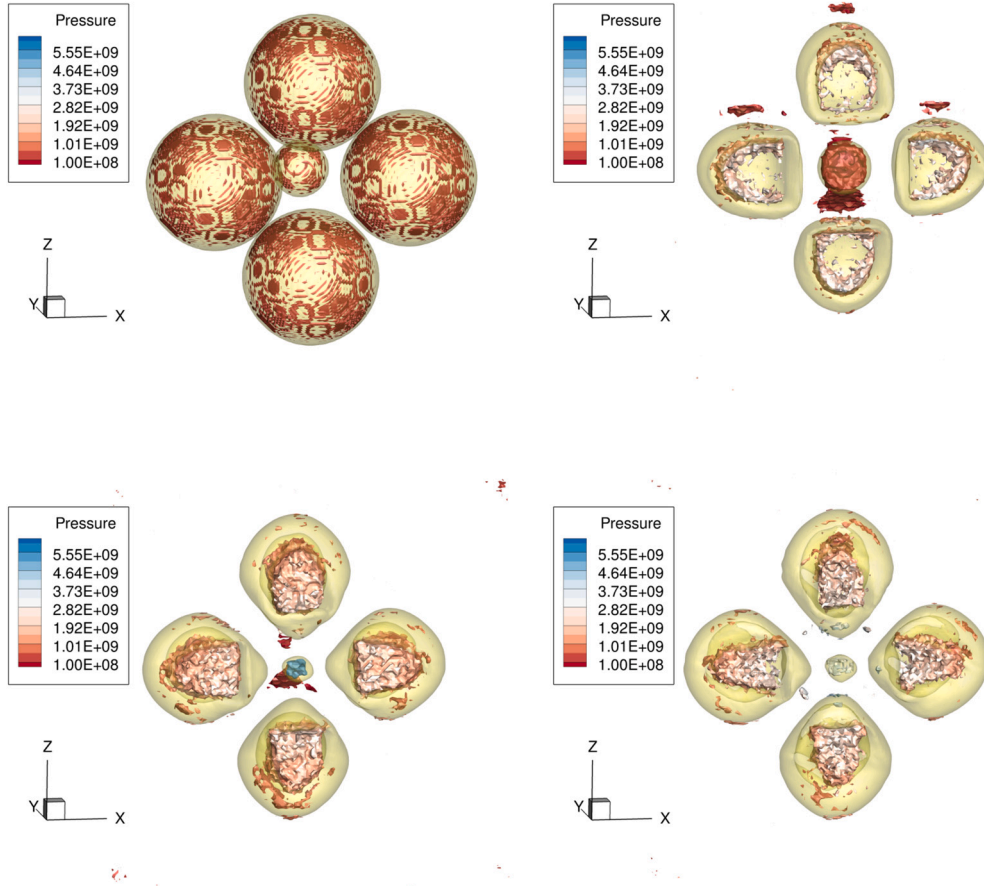


Fig. 16. Volume fraction iso-contours and troubled cells coloured by pressure contours at times $t = 0.01 \mu s$, $t = 0.45 \mu s$, $t = 0.90 \mu s$, $t = 0.95 \mu s$ from top to bottom row and left to right column in sequence.

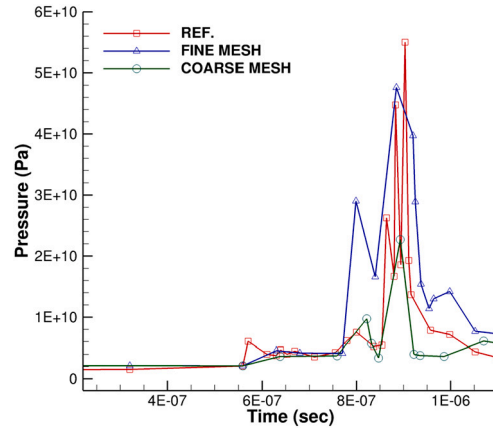


Fig. 17. Maximum pressure history for 3D bubble array collapse in pyramidal configuration, compared with reference [73].

Table 9

Initial conditions for 2D underwater explosion test case.

Location	ρ	u	v	p	γ	π_∞	a_1
air	1.225	0	0	101325	1.4	0	1
shocked gas	1250	0	0	10^9	1.4	0	1
water	1000	0	0	101325	4.4	$6 \cdot 10^8$	0

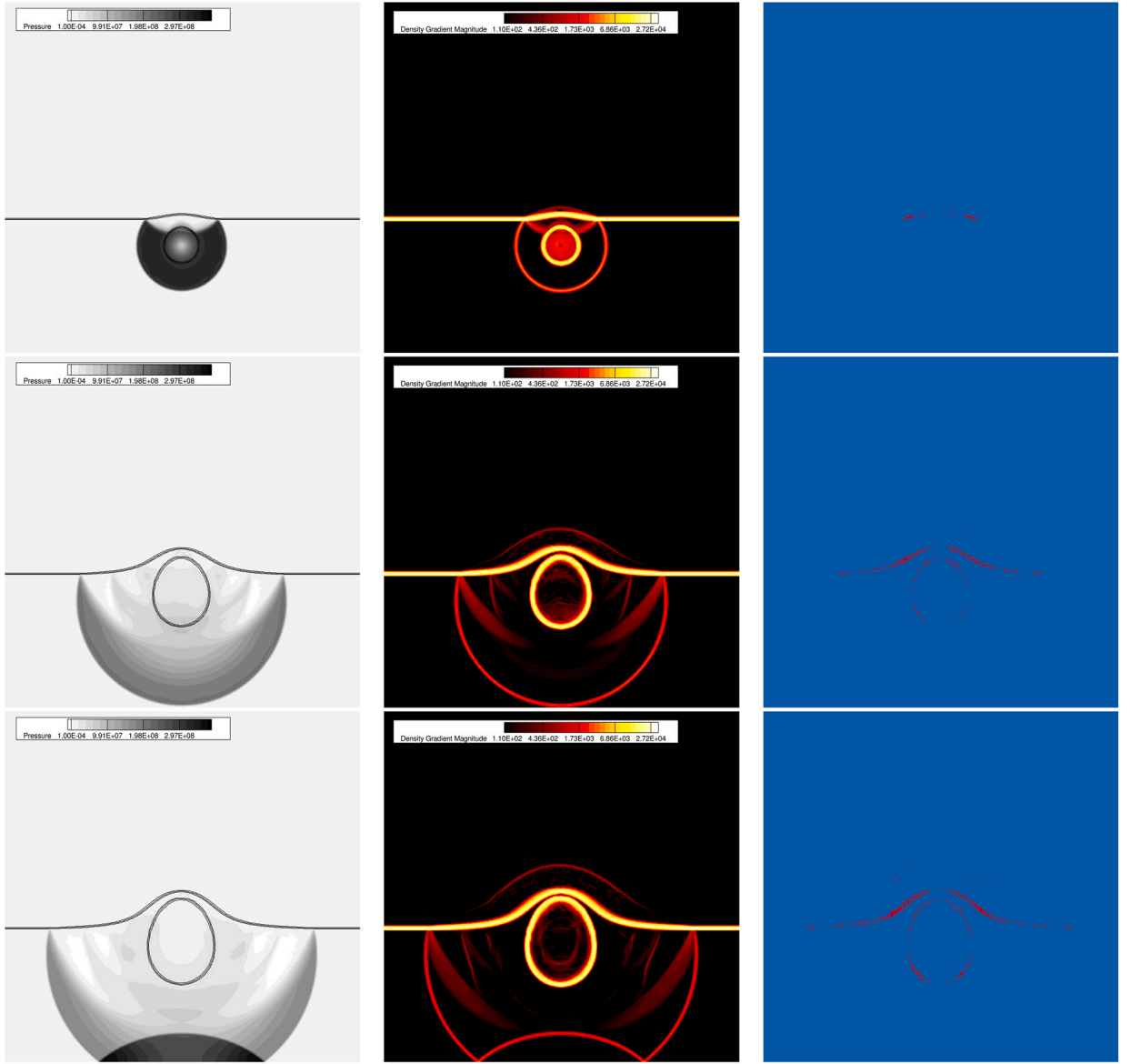


Fig. 18. From left to right column: Pressure, density gradient magnitude and troubled cells contours respectively. From top row to bottom, times: $t = 0.2$ ms, $t = 0.6$ ms, $t = 1$ ms.

Following the high difference in pressure between surrounding water and detonation bubble, as the simulation starts, a strong main shock is emitted from the bubble and moves radially throughout the water phase. Simultaneously, an expansion wave propagates radially inward the bubble. As the main shock hits the free-surface, a reflected rarefaction wave is generated and travels below the surface level, and a weak transmitted shock can be observed above the sea level, as shown in the sequence in Fig. 18. When the expansion wave reaches the explosion region, the upper side of the bubble is accelerated upwards and grows in shape until only a thin layer of water separates the air above sea level and detonation products, and is expected to break in several small fragments at later times.

Cavitation is also expected to occur near free surface as the reflected rarefaction wave expands in water, and is captured by the modified Schmidt cavitation model used in this study. The adoption of the cavitation model is here suggested to avoid the occurrence of regions with negative pressure allowed by the stiffened gas EOS, which would also cause the over-activation of the troubled cell detector.

We compare the performance of the hybrid $P1 - MUSCL2$ and $P2 - CWENO3$ with the pure FV scheme using a 5^{th} order CWENO reconstruction at time $t = 2$ ms in Fig. 19. Qualitatively, whilst the hybrid 2^{nd} order scheme shows a thin water layer between explosion products and free surface, that seems as diffused as the one provided by the 5^{th} order FV CWENO scheme, the 3^{rd} order hybrid scheme is able to preserve a sharper interface.

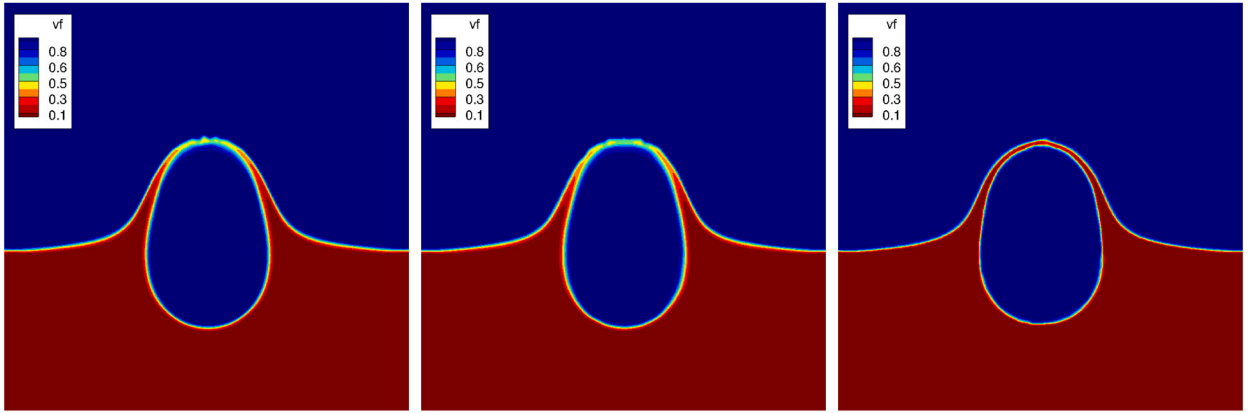


Fig. 19. Comparison of volume fraction contours at time $t = 2ms$, computed with FV CWENO 5^{th} order (left), hybrid $P1 - MUSCL2$ scheme (middle), and $P2 - CWENOZ3$ scheme (right).

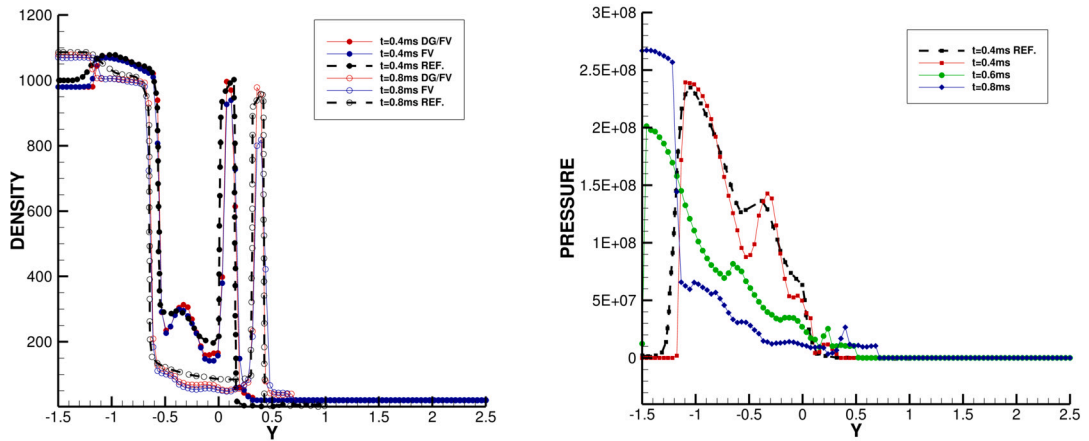


Fig. 20. Density and pressure profiles at different time, compared with reference [74].

For a more qualitative study, in Fig. 20 we compare the values of density and pressure obtained with the 3^{rd} order hybrid scheme, with reference [74] where anti-diffusion terms are included in the governing equations. Both density and pressure profile are in close agreement with [74], and the better performance of the hybrid scheme with respect to the pure FV scheme is confirmed as it better preserves the maximum density values at time $t = 0.8ms$.

4. Conclusions

With the present work we demonstrated the application of a hybrid DG/FV framework for the solution of multispecies flows with resolved material interfaces, including gas-gas and gas-liquid systems. The main objective of this study is to limit the interface dissipation typical of diffuse interface models, and to render this method appealing to be used on fairly coarse meshes, without the necessity of additional anti-diffusive or sharpening terms. As opposite, our strategy is to employ a classical high order DG method in smooth flow regions, while activating a more dissipative, non-oscillatory, same accuracy order FV scheme in regions with steep gradients such as material interfaces and shock waves. The CWENOZ-FV reconstruction, in conjunction with the DG method demonstrated to render the method stable in presence of interface with large pressure and density gradients, or interfaces interacting with shock waves, thanks to the reduced size directional stencils, which increases the chance to find a smooth stencil in those challenging flow regions. Several test cases demonstrated that the hybrid framework greatly improved the material interface resolution at later times, whereas a pure FV scheme on the same mesh resolution usually presents overly diffused interfaces. The hybrid scheme, as expected, comes with a computational overhead to the pure FV method, while this is generally negligible compared to a pure DG scheme due to the minimal additional cost introduced by the FV reconstruction in the benchmarks here considered, being it activated only in localised physical discontinuities. This considered, in our opinion the hybrid DG/FV framework proposes a robust, easy to extend and accurate platform to simulate multispecies flows in compressible medium, without necessity for very refined meshes as typically required by interface capturing methods.

Future work will aim to include more sophisticated cavitation and phase transition models, and effects of viscosity.

CRediT authorship contribution statement

Vadim Maltsev: Writing – review & editing, Writing – original draft, Validation, Software, Conceptualization. **Martin Skote:** Writing – review & editing, Writing – original draft, Funding acquisition. **Panagiotis Tsoutsanis:** Writing – review & editing, Writing – original draft, Software, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data relating to the results in this manuscript are available at the Cranfield Online Research Data Repository (DOI: <https://doi.org/10.17862/cranfield.rd.25109453>).

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Appendix A. HLLC Riemann solver

At cell interfaces, the numerical flux determined by the HLLC approximate solver is determined as:

$$\mathbf{F}^{HLLC} = \begin{cases} \mathbf{F}^L & \text{if } 0 \leq s^L \\ \mathbf{F}_{*L} & \text{if } s^L \leq 0 \leq s_* \\ \mathbf{F}_{*R} & \text{if } s_* \leq 0 \leq s^R \\ \mathbf{F}^R & \text{if } s^R < 0. \end{cases} \quad (\text{A.1})$$

Left and right fluxes, $K = L$ and $K = R$ respectively, and correspondent fluxes in the starred regions are defined as:

$$\mathbf{F}^K = \begin{bmatrix} a_1^K \rho_1^K u_n^K \\ a_2^K \rho_2^K u_n^K \\ \rho^K u^K u_n^K + p^K n_x \\ \rho^K v^K u_n^K + p^K n_y \\ \rho^K w^K u_n^K + p^K n_z \\ u_n^K (E^K + p^K) \\ a_1^K u_n^K \end{bmatrix}, \quad \mathbf{F}_*^K = \frac{s^K - u_n^K}{s^K - s_*} \begin{bmatrix} a_1^K \rho_1^K s_* \\ a_2^K \rho_2^K s_* \\ \rho^K u^K s_* + \frac{s^K - u_n^K}{s^K - s_*} p^K n_x + s^K \rho^K (s_* - u_n^K) n_x \\ \rho^K v^K s_* + \frac{s^K - u_n^K}{s^K - s_*} p^K n_y + s^K \rho^K (s_* - u_n^K) n_y \\ \rho^K w^K s_* + \frac{s^K - u_n^K}{s^K - s_*} p^K n_z + s^K \rho^K (s_* - u_n^K) n_z \\ s_* (E^K + p^K) + s^K \rho^K (s_* - u_n^K) s_* \\ a_1^K u_* \end{bmatrix}.$$

The wave speeds are estimated with:

$$s^L = \min(\hat{u}_n - \hat{c}_n, u^L - c^L), \quad s^R = \max(\hat{u}_n + \hat{c}_n, u^R + c^R), \quad (\text{A.2})$$

for left and right states respectively, where Einfeldt's generalised formulation for speed of sound $\hat{c}_n$ and Roe average for velocity $\hat{u}_n$ are used [75]:

$$\hat{c}^2 = \frac{c_L^2 \cdot \sqrt{\rho_L} + c_R^2 \cdot \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} + \frac{1}{2} \frac{\sqrt{\rho_L} \sqrt{\rho_R}}{(\sqrt{\rho_L} + \sqrt{\rho_R})^2} (u_R - u_L)^2, \quad \hat{u} = \frac{u_L \cdot \sqrt{\rho_L} + u_R \cdot \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (\text{A.3})$$

In the star regions, the wave speed is computed using Batten's formula [76]:

$$s_* = \frac{p^R - p^L + \rho^L u_n^L (s^L - u_n^L) - \rho^R u_n^R (s^R - u_n^R)}{\rho^L (s^L - u_n^L) - \rho^R (s^R - u_n^R)}. \quad (\text{A.4})$$

Ultimately, the velocity used for the computation of the source term in the volume fraction advection equation is obtained from:

$$(u_n)^{Riemm} = \begin{cases} u_n^L & \text{if } 0 \leq s^L \\ u_n^L + s^L \left(\frac{s^L - u_n^L}{s^L - s_*} - 1 \right) & \text{if } s^L \leq 0 \leq s_* \\ u_n^R + s^L \left(\frac{s^R - u_n^R}{s^R - s_*} - 1 \right) & \text{if } s_* \leq 0 \leq s^R \\ u_n^R & \text{if } s^R < 0. \end{cases} \quad (\text{A.5})$$

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