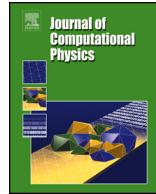




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Positivity-preserving and entropy-bounded discontinuous Galerkin method for the chemically reacting, compressible Euler equations. Part II: The multidimensional case

Eric J. Ching*, Ryan F. Johnson, Andrew D. Kercher

Laboratories for Computational Physics and Fluid Dynamics, U.S. Naval Research Laboratory, Washington, DC, 20375, United States of America



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ABSTRACT

In this second part of our two-part paper, we extend to multiple spatial dimensions the one-dimensional, fully conservative, positivity-preserving, and entropy-bounded discontinuous Galerkin scheme developed in the first part for the chemically reacting Euler equations. Our primary objective is to enable robust and accurate solutions to complex reacting-flow problems using the high-order discontinuous Galerkin method without requiring extremely high resolution. Variable thermodynamics and detailed chemistry are considered. Our multidimensional framework can be regarded as a further generalization of similar positivity-preserving and/or entropy-bounded discontinuous Galerkin schemes in the literature. In particular, the proposed formulation is compatible with curved elements of arbitrary shape, a variety of numerical flux functions, general quadrature rules with positive weights, and mixtures of thermally perfect gases. Preservation of pressure equilibrium between adjacent elements, especially crucial in simulations of multicomponent flows, is discussed. Complex detonation waves in two and three dimensions are accurately computed using high-order polynomials. Enforcement of an entropy bound, as opposed to solely the positivity property, is found to significantly improve stability. Mass, total energy, and atomic elements are shown to be discretely conserved.

1. Introduction

This paper is the second part of a series of two that introduces a fully conservative, positivity-preserving, and entropy-bounded discontinuous Galerkin (DG) method for simulating the multicomponent, chemically reacting, compressible Euler equations. In Part I [1], we addressed the one-dimensional case; here, we focus on the multidimensional case. The starting point of our methodology is the fully conservative, high-order scheme previously developed by Johnson and Kercher [2] that can maintain pressure equilibrium (in an approximate sense) in smooth regions of the flow or across material interfaces when the temperature is continuous. The generation of such oscillations is a major, well-known issue that inhibits fully conservative numerical schemes [3–5]. Nonconservative methods are a common alternative to circumvent this drawback. The fully conservative formulation in [2] instead maintains both pressure equilibrium and discrete conservation of mass and total energy through consistent evaluation of both the complex thermodynamics and the resulting semidiscrete form, as well as the proper choice of nodal basis. A series of complex multicomponent reacting flows was computed, including a three-dimensional reacting shear flow, which did not require additional stabilization to calculate.

* Corresponding author.

E-mail address: eric.ching@nrl.navy.mil (E.J. Ching).

Also simulated was a two-dimensional moving detonation wave. With artificial viscosity to stabilize the flow-field discontinuities, the correct cellular structure was predicted. However, a linear polynomial approximation and a very fine mesh were required to maintain robustness, illustrating the challenge of using high-order methods to achieve stable and accurate solutions to multidimensional detonation-wave problems on relatively coarse meshes. In light of this difficulty, we aim to develop a positivity-preserving and entropy-bounded DG method that can robustly and efficiently simulate complex reacting flows in multiple dimensions using high-order polynomial approximations.

1.1. Summary of Part I

In Part I [1], we introduced the groundwork to construct such a formulation. First, we established a minimum entropy principle satisfied by entropy solutions to the multicomponent Euler equations with chemical source terms, extending to the reacting case the proof by Gouasmi et al. [6] of a minimum entropy principle in the nonreacting case. This principle, which states that the spatial minimum of the specific thermodynamic entropy increases with time, is a critical component of the theoretical basis for the formulation. In the remainder of Part I [1], we introduced the mathematical framework in one spatial dimension that ensures the discrete solution satisfies the following: nonnegative species concentrations, positive density, positive pressure, and specific thermodynamic entropy bounded from below. We discussed how to maintain compatibility with the strategies devised in [2] to maintain approximate pressure equilibrium between adjacent elements. In addition, a two-point numerical state function was derived, as part of an entropy-stable DG scheme based on diagonal-norm summation-by-parts operators for treating stiff chemical reactions in the reaction step of an operator splitting procedure. Applying the coupled solver to canonical one-dimensional test cases, we demonstrated that the formulation can achieve robust and accurate solutions on relatively coarse meshes. Optimal high-order convergence in two smooth-flow problems was obtained. Furthermore, we found that the enforcement of only the positivity property (i.e., nonnegative concentrations and positive density and pressure) can fail to suppress large-scale nonlinear instabilities, but the added enforcement of an entropy bound significantly improves robustness, to a greater degree than in the monocomponent, calorically perfect case.

1.2. Contributions of Part II

In this paper, we extend the solver to two and three spatial dimensions. Our main contributions are as follows:

- The mathematical framework in Part I [1] is enhanced to account for curved, multidimensional elements of arbitrary shape. Our multidimensional extension further generalizes current multidimensional positivity-preserving/entropy-bounded DG schemes in the literature [7–10] by relaxing restrictions on the volume and surface quadrature rules, physical modeling, polynomial order of the geometric approximation, and/or numerical flux function. We also discuss how to deal with curved elements in the reaction step.
- We propose strategies to maintain compatibility with the procedures introduced in [2] to preserve pressure equilibrium, which is less straightforward than in one dimension. We compute the advection of a thermal bubble in two dimensions to determine whether pressure equilibrium can be maintained when using curved elements (not considered in [2]).
- We compute complex, large-scale detonation-wave problems in two and three dimensions with detailed chemistry. Enforcement of only the positivity property often fails to provide adequate stabilization (even with artificial viscosity), while enforcing an entropy bound enables robust calculations on coarse meshes.

1.3. Additional background

Positivity-preserving DG schemes have emerged in recent years as a popular numerical technique to simulate fluid flows in a robust manner. [1, Section 1] briefly reviews the history of the development of positivity-preserving and related entropy-bounded DG methods pioneered by Zhang and Shu [11,7] for the monocomponent, nonreacting Euler equations; here, we focus on the multidimensional aspect. The key idea in constructing such positivity-preserving/entropy-bounded schemes is to expand the element average of the solution as a convex combination of first-order three-point systems and pointwise values. Zhang and Shu [7] devised one such expansion on rectangular meshes based on tensor products of Gauss-Legendre and Gauss-Lobatto rules, which was later extended to straight-sided triangular elements [8] by utilizing triangle-rectangle transformations [12,13]. Lv and Ihme [9] introduced an expansion compatible with curved elements of arbitrary shape. The only restriction on the volume and surface quadrature rules is that the weights be positive; the surface quadrature points need not be part of the set of volume quadrature points, and the surface quadrature rules can be different among the faces of a given element, which is crucial for prismatic elements and p -adaptive calculations. However, the expansion in [9] relies on the Lax-Friedrichs numerical flux, and the resulting time-step-size constraint assumes a calorically perfect gas. Jiang and Liu [10] proposed an expansion that is compatible with certain polygonal elements and does not rely on the Lax-Friedrichs numerical flux, but the following assumptions are made: (a) for a given face, the geometric Jacobian and surface normal are constant and (b) the same surface quadrature rule is employed for each face. Said expansion can be viewed as a generalization of that by Zhang et al. [8] for straight-sided triangular elements. In this paper, we introduce an expansion that is compatible with:

- curved elements of arbitrary shape
- any invariant-region-preserving numerical flux

- any combination of volume and surface quadrature rules (which can differ among faces) with positive weights

Furthermore, no physics-based assumptions are placed on the resulting time-step-size constraint.

1.4. Outline

The remainder of this paper is organized as follows. The governing equations and basic DG discretization are reviewed in Sections 2 and 3, respectively. The following section presents the positivity-preserving and entropy-bounded multidimensional DG formulation for the transport step. Results for two-dimensional thermal-bubble advection and complex two- and three-dimensional moving detonation-wave simulations are given in Section 6. We close the paper with concluding remarks.

It is recommended that Part I [1] be read first since the formulation developed here relies on many of the key ideas introduced in detail in the first part. For conciseness, important concepts already discussed in Part I are only briefly summarized in this paper.

2. Governing equations

The governing equations are the compressible, multicomponent, chemically reacting Euler equations, written as

$$\frac{\partial \mathbf{y}}{\partial t} + \nabla \cdot \mathcal{F}(\mathbf{y}) - \mathcal{S}(\mathbf{y}) = 0 \quad (2.1)$$

where $t \in \mathbb{R}^+$ is time and $\mathbf{y}(x, t) : \mathbb{R}^d \times \mathbb{R}^+ \rightarrow \mathbb{R}^m$ is the conservative state vector, given by

$$\mathbf{y} = \left(\rho v_1, \dots, \rho v_d, \rho e_t, C_1, \dots, C_{n_s} \right)^T. \quad (2.2)$$

$\mathbf{x} = (x_1, \dots, x_d)$ denotes the physical coordinates, with d indicating the number of spatial dimensions, $\mathbf{v} = (v_1, \dots, v_d)$ is the velocity vector, e_t is the specific total energy, and C_i is the concentration of the i th species. ρ is the density, computed as

$$\rho = \sum_{i=1}^{n_s} \rho_i = \sum_{i=1}^{n_s} W_i C_i,$$

where ρ_i is the partial density and W_i is the molecular weight of the i th species. n_s is the total number of species, and $m = d + n_s + 1$ is the total number of state variables. $Y_i = \rho_i / \rho$ and $X_i = C_i / \sum_{i=1}^{n_s} C_i$ are the mass fraction and mole fraction, respectively, of the i th species. $\mathcal{F}(\mathbf{y}) : \mathbb{R}^m \rightarrow \mathbb{R}^{m \times d}$ in Equation (2.1) is the convective flux, the k th spatial component of which is defined as

$$\mathcal{F}_k^c(\mathbf{y}) = \left(\rho v_k v_1 + P \delta_{k1}, \dots, \rho v_k v_d + P \delta_{kd}, v_k (\rho e_t + P), v_k C_1, \dots, v_k C_{n_s} \right)^T, \quad (2.3)$$

where P is the pressure, computed as

$$P = R^0 T \sum_{i=1}^{n_s} C_i, \quad (2.4)$$

with T denoting the temperature and R^0 the universal gas constant. The total energy is given by

$$e_t = u + \frac{1}{2} \sum_{k=1}^d v_k v_k,$$

where u is the mixture-averaged specific internal energy, calculated as

$$u = \sum_{i=1}^{n_s} Y_i u_i,$$

with u_i indicating the specific internal energy of the i th species. In this work, we employ the thermally perfect gas model, with u_i approximated by a polynomial function of temperature as

$$u_i = \sum_{k=0}^{n_p+1} b_{ik} T^k, \quad (2.5)$$

based on the NASA curve fits [14,15]. The specific heats at constant volume and constant pressure, c_v and c_p , the specific enthalpy, h_i , and the specific thermodynamic entropy, s_i , of the i th species can be calculated by appropriately differentiating/integrating Equation (2.5). The mixture-averaged thermodynamic entropy, s , which will be important in subsequent sections, is given by

$$s = \sum_{i=1}^{n_s} Y_i s_i.$$

Finally, $\mathcal{S}(\mathbf{y}) : \mathbb{R}^m \rightarrow \mathbb{R}^m$ in Equation (2.1) is the chemical source term, given by

$$\mathcal{S}(y) = \left(0, \dots, 0, 0, \omega_1, \dots, \omega_{n_s}\right)^T, \quad (2.6)$$

where ω_i is the production rate of the i th species. Additional details on the thermodynamic relationships and chemical production rates can be found in Part I [1].

3. Discontinuous Galerkin discretization

Let $\Omega \subset \mathbb{R}^d$ be the computational domain, which is partitioned by \mathcal{T} , comprised of non-overlapping cells κ with boundaries $\partial\kappa$. Let \mathcal{E} denote the set of interfaces ϵ , with $\cup_{\epsilon \in \mathcal{E}} \epsilon = \cup_{\kappa \in \mathcal{T}} \partial\kappa$. At interior interfaces, there exists $\kappa^+, \kappa^- \in \mathcal{T}$ such that $\epsilon = \partial\kappa^+ \cap \partial\kappa^-$. n^+ and n^- denote the outward facing normal of κ^+ and κ^- , respectively, with $n^+ = -n^-$. The discrete subspace V_h^p over \mathcal{T} is defined as

$$V_h^p = \left\{ \mathbf{v} \in [L^2(\Omega)]^m \mid \forall \kappa \in \mathcal{T}, \mathbf{v}|_\kappa \in [\mathcal{P}_p(\kappa)]^m \right\}, \quad (3.1)$$

where, for $d = 1$, $\mathcal{P}_p(\kappa)$ is the space of polynomial functions of degree less than or equal to p in κ . For $d > 1$, the choice of polynomial space typically depends on the type of element [16].

The semi-discrete problem statement is as follows: find $y \in V_h^p$ such that

$$\sum_{\kappa \in \mathcal{T}} \left(\frac{\partial y}{\partial t}, \mathbf{v} \right)_\kappa - \sum_{\kappa \in \mathcal{T}} (\mathcal{F}(y), \nabla \mathbf{v})_\kappa + \sum_{\epsilon \in \mathcal{E}} (\mathcal{F}^\dagger(y^+, y^-, n), [\mathbf{v}])_\epsilon - \sum_{\kappa \in \mathcal{T}} (\mathcal{S}(y), \mathbf{v})_\kappa = 0 \quad \forall \mathbf{v} \in V_h^p, \quad (3.2)$$

where (\cdot, \cdot) denotes the inner product, $\mathcal{F}^\dagger(y^+, y^-, n)$ is the numerical flux, and $[\cdot]$ is the jump operator, defined such that $[\mathbf{v}] = \mathbf{v}^+ - \mathbf{v}^-$ at interior interfaces and $[\mathbf{v}] = \mathbf{v}^+$ at boundary interfaces. Due to the stiff chemical source terms, we employ second-order Strang splitting [17] over a given interval $(t_0, t_0 + \Delta t]$ as

$$\frac{\partial y}{\partial t} + \nabla \cdot \mathcal{F}(y) = 0 \text{ in } \Omega \times (t_0, t_0 + \Delta t/2], \quad (3.3)$$

$$\frac{\partial y}{\partial t} - \mathcal{S}(y) = 0 \text{ in } (t_0, t_0 + \Delta t], \quad (3.4)$$

$$\frac{\partial y}{\partial t} + \nabla \cdot \mathcal{F}(y) = 0 \text{ in } \Omega \times (t_0 + \Delta t/2, t_0 + \Delta t], \quad (3.5)$$

where Equations (3.3) and (3.5) are integrated in time with an explicit scheme, while Equation (3.4) is solved using a fully implicit, temporal DG discretization for ODEs. Additional discussion on operator splitting can be found in Part I [1].

The volume and surface terms in Equation (3.2) are evaluated with a quadrature-free approach [18,19]. A nodal basis is employed, such that the element-local polynomial approximation of the solution is given by

$$y_\kappa = \sum_{j=1}^{n_b} y_j(x_j) \phi_j, \quad (3.6)$$

where n_b is the number of basis functions, $\{\phi_1, \dots, \phi_{n_b}\}$ are the basis functions, and $\{x_1, \dots, x_{n_b}\}$ are the node coordinates. The nonlinear convective flux in the second and third integrals in Equation (3.2) can be approximated as

$$\mathcal{F}_\kappa \approx \sum_{k=1}^{n_c} \mathcal{F}(y_\kappa(x_k)) \varphi_k, \quad (3.7)$$

where $n_c \geq n_b$ and $\{\varphi_1, \dots, \varphi_{n_c}\}$ is a set of polynomial basis functions that may be different from those in Equation (3.6). As discussed by Johnson and Kercher [2], pressure equilibrium within and between elements can be approximately maintained under either of the following conditions:

- $n_c = n_b$ and the integration points are in the set of solution nodes
- If $n_c > n_b$ (i.e., over-integration), then the flux interpolation in Equation (3.7) is replaced with

$$\mathcal{F}_\kappa \approx \sum_{k=1}^{n_c} \mathcal{F}(\tilde{y}_\kappa(x_k)) \varphi_k, \quad (3.8)$$

where $\tilde{y} : \mathbb{R}^m \times \mathbb{R} \rightarrow \mathbb{R}^m$ is a modified state defined as

$$\tilde{y}(y, \tilde{P}) = \left(\rho v_1, \dots, \rho v_d, \tilde{\mu}(C_1, \dots, C_{n_s}, \tilde{P}) + \frac{1}{2} \sum_{k=1}^d \rho v_k v_k, C_1, \dots, C_{n_s} \right)^T. \quad (3.9)$$

$\tilde{\mu}$ is a modified internal energy is evaluated from the unmodified species concentrations and a polynomial approximation of the pressure that interpolates onto the span of $\{\phi_1, \dots, \phi_{n_b}\}$ as

$$\tilde{P}_\kappa = \sum_{j=1}^{n_b} P(y_\kappa(x_j)) \phi_j.$$

Standard over-integration typically fails to preserve pressure equilibrium, resulting in the generation of spurious pressure oscillations that can lead to solver divergence. On the other hand, employing the modified flux interpolation (3.8) in both the volume and surface flux integrals in Equation (3.2) achieves pressure equilibrium both internally and between adjacent elements (except in severely underresolved computations, in which appreciable deviations from pressure equilibrium are inevitable).

As discussed in Part I [1], the linear-scaling limiter used to enforce the positivity property and entropy boundedness does not completely eliminate small-scale nonlinear instabilities, particularly in the vicinity of flow-field discontinuities. Therefore, the artificial dissipation term [16]

$$-\sum_{\kappa \in \mathcal{T}} (\mathcal{F}^{\text{AV}}(y, \nabla y), \nabla v)_\kappa, \quad (3.10)$$

where $\mathcal{F}^{\text{AV}}(y, \nabla y) = v_{\text{AV}} \nabla y$, is added to the LHS of Equation (3.2). v_{AV} is the artificial viscosity, computed as [2]

$$v_{\text{AV}} = (C_{\text{AV}} + S_{\text{AV}}) \left(\frac{h^2}{p+1} \left| \frac{\partial T}{\partial y} \cdot \frac{\mathcal{R}(y, \nabla y)}{T} \right| \right),$$

where S_{AV} is a shock sensor based on intra-element variations [20], C_{AV} is a user-defined coefficient, h is the element size, and $\mathcal{R}(y, \nabla y)$ is the strong form of the residual (2.1). This artificial viscosity formulation was used to successfully dampen nonphysical oscillations near flow-field discontinuities in a variety of multicomponent-flow simulations [1,2]. Other types of artificial viscosity or limiters can be employed as well. Note that the integral (3.10) vanishes for $v \in V_h^0$, which will be important in Section 4. For further details on the basic DG discretization, boundary-condition implementation, and conditions under which pressure oscillations are generated, we refer the reader to [2].

4. Transport step: entropy-bounded discontinuous Galerkin method in multiple dimensions

In this section, we extend the one-dimensional positivity-preserving/entropy-bounded DG scheme presented in Part I to multiple dimensions.

4.1. Preliminaries

We first review the geometric mapping from reference space to physical space, as well as volumetric and surface quadrature rules. The minimum entropy principle is then summarized. Finally, a first-order three-point system, which is a building block for the general multidimensional, high-order scheme, is discussed.

4.1.1. Geometric mapping

Consider the mapping $x(\xi) : \hat{\kappa} \rightarrow \kappa$, with $\hat{\kappa}$ denoting the reference element, given by

$$x(\xi) = \sum_{m=1}^{n_g} x_{\kappa,m} \Phi_m(\xi),$$

where $\xi \in \mathbb{R}^d$ are the reference coordinates, $x_{\kappa,m}$ is the physical coordinate of the m th node of κ , Φ_m is the m th basis function for the geometry interpolation, and n_g is the number of basis functions. The unit (or bi-unit) square and right triangle with unit (or bi-unit) side length are common reference elements for quadrilateral and triangular elements, respectively. The local solution approximation can then be written as

$$y_\kappa = \sum_{j=1}^{n_b} y_\kappa(x_j) \phi_j(\xi), \quad x = x(\xi) \in \kappa, \quad \forall \xi \in \hat{\kappa}.$$

Let $\partial\kappa^{(f)}$ be the f th face of κ . The geometric mapping $x(\zeta^{(f)}) : \hat{\epsilon} \rightarrow \partial\kappa^{(f)}$ for interfaces, where $\zeta^{(f)} \in \mathbb{R}^{d-1}$ are the reference coordinates and $\hat{\epsilon}$ is the reference face, is given by

$$x(\zeta^{(f)}) = \sum_{m=1}^{n_{g,f}^d} x_{\kappa,m}^{(f)} \Phi_m^{(f)}(\zeta^{(f)}),$$

where $x_{\kappa,m}^{(f)}$ is the physical coordinate of the m th node of $\partial\kappa^{(f)}$, $\Phi_m^{(f)}$ is the m th basis function, and $n_{g,f}^d$ is the number of basis functions. The reference face can also be mapped to the reference element (i.e., $\xi(\zeta^{(f)}) : \hat{\epsilon} \rightarrow \hat{\kappa}$).

4.1.2. Quadrature rules

Consider a volumetric quadrature rule with points ξ_v and positive weights w_v that satisfy $\sum_{v=1}^{n_q} w_v = |\hat{\kappa}|$, where $|\hat{\kappa}|$ is the volume of the reference element. The volume integral over κ of a generic function, $g(x)$, can be evaluated as

$$\int_{\kappa} g(x) dx = \int_{\hat{\kappa}} g(x(\xi)) |J_{\kappa}(\xi)| d\xi \approx \sum_{v=1}^{n_q} g(x(\xi_v)) |J_{\kappa}(\xi_v)| w_v,$$

where J_{κ} is the geometric Jacobian and $|J_{\kappa}|$ is its determinant. The integral evaluation is exact if $g(x)$ is a polynomial and the quadrature rule is sufficiently accurate. Similarly, let ζ_l and w_l^{∂} be the points and positive weights of a surface quadrature rule, with $\sum_{l=1}^{n_q^{\partial}} w_l^{\partial} = |\hat{\epsilon}|$, where $|\hat{\epsilon}|$ is the surface area of the reference face. The surface integral over $\partial\kappa^{(f)}$ of a generic function can be evaluated as

$$\int_{\partial\kappa^{(f)}} g(x) ds = \int_{\hat{\epsilon}} g(x(\zeta^{(f)})) |J_{\partial\kappa}^{(k)}(\zeta^{(f)})| d\xi \approx \sum_{l=1}^{n_q^{\partial}} g(x(\zeta_l^{(f)})) |J_{\partial\kappa}^{(f)}(\zeta_l^{(f)})| w_{f,l}^{\partial} = \sum_{l=1}^{n_q^{\partial}} g(x(\zeta_l^{(f)})) v_{f,l}^{\partial},$$

where $v_{f,l}^{\partial} = |J_{\partial\kappa}^{(f)}(\zeta_l^{(f)})| w_{f,l}^{\partial}$ and $J_{\partial\kappa}^{(f)}$ is the surface Jacobian. The integral evaluation is again exact if $g(x)$ is a polynomial and the quadrature rule is sufficiently accurate. The closed surface integral over $\partial\kappa$ of a generic function is evaluated as

$$\int_{\partial\kappa} g(x) ds = \sum_{f=1}^{n_f} \int_{\partial\kappa^{(f)}} g(x) ds = \sum_{f=1}^{n_f} \int_{\hat{\epsilon}} g(x(\zeta^{(f)})) |J_{\partial\kappa}^{(f)}(\zeta^{(f)})| d\xi \approx \sum_{f=1}^{n_f} \sum_{l=1}^{n_q^{\partial,f}} g(x(\zeta_l^{(f)})) v_{f,l}^{\partial},$$

where a different quadrature rule can be employed for each face. n_f , the number of faces, is allowed to change among elements, but a slight abuse of notation is done for simplicity.

Given that, as mentioned in Section 3, a quadrature-free approach [18,19] is employed in this work to evaluate the integrals in Equation (3.2), the reader may question why quadrature rules are reviewed in such detail. As in Part I, the first step in our analysis in Section 4.2 is to take $\mathbf{v} \in V_h^0$ in Equation (3.2) to obtain the scheme satisfied by the element averages, which remains the same whether a quadrature-based or quadrature-free approach is employed. Furthermore, in Section 4.2 we present our analysis in terms of a quadrature-based approach for consistency with previous studies on positivity-preserving and/or entropy-bounded DG methods.

4.1.3. Minimum entropy principle

Let $U(y) : \mathbb{R}^m \rightarrow \mathbb{R}$ be a given convex (mathematical) entropy function and $\mathcal{F}^s(y) : \mathbb{R}^m \rightarrow \mathbb{R}^d$ the corresponding spatial entropy flux. Satisfaction of the entropy inequality

$$\frac{\partial U}{\partial t} + \nabla \cdot \mathcal{F}^s \leq 0, \quad (4.1)$$

distinguishes physical solutions from nonphysical solutions when discontinuities are present. Specifically, *entropy solutions* are those that satisfy (4.1) for all entropy/entropy-flux pairs. $U = -\rho s$ and $\mathcal{F}^s = -\rho s \mathbf{v}$ form a common, admissible entropy/entropy-flux pair for the multicomponent Euler equations [6,21].

The minimum entropy principle, which states that the spatial minimum of the specific thermodynamic entropy is non-decreasing in time, follows from a particular choice of entropy/entropy-flux pair,

$$(U, \mathcal{F}^s) = (-\rho f_0(s), -\rho \mathbf{v} f_0(s)), \quad (4.2)$$

where $f_0(s) = \min \{s - s_0, 0\}$. Although $f_0(s)$ is not a smooth function of s , it can be written as the limit of a sequence of smooth functions, $f_0(s) = \lim_{\epsilon \rightarrow 0} f_{\epsilon}(s)$, where $f_{\epsilon}(s)$ is given by [6]

$$f_{\epsilon}(s) = \frac{1}{\epsilon} \int_{-\infty}^{\infty} f_0(s - \xi) \frac{\exp\left(-\frac{\xi^2}{\epsilon^2}\right)}{\sqrt{\pi}} d\xi, \quad \epsilon > 0.$$

According to the minimum entropy principle, we have, for $|x| \leq R$,

$$s(x, t) \geq s_0 = \operatorname{Ess\ inf}_{|x| \leq R + v_{\max} t} s(x, 0), \quad (4.3)$$

where $R > 0$ and v_{\max} is the maximum speed in the domain at $t = 0$. The inequality (4.3) was first proved by Tadmor [22] for the monocomponent Euler equations. It was recently generalized to the multicomponent, nonreacting Euler equations by Gouasmi et al. [6] and then extended to the reacting case in Part I [1].

4.1.4. First-order three-point system

Let \mathcal{G}_{σ} be the following set:

$$\mathcal{G}_{\sigma} = \left\{ y \mid C_1 > 0, \dots, C_{n_s} > 0, \rho u^* > 0, s \geq \sigma \right\}, \quad (4.4)$$

where $\sigma \in \mathbb{R}$ and u^* is the “shifted” internal energy [23],

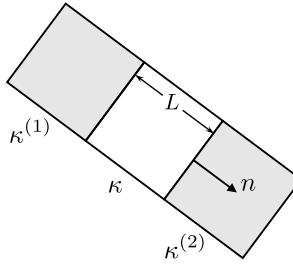


Fig. 4.1. Schematic of a rotated three-point system in the multidimensional setting (Equation (4.9)).

$$u^* = u - u_0 = u - \sum_{i=1}^{n_s} Y_i b_{i0}, \quad (4.5)$$

such that $u^* > 0$ if and only if $T > 0$, provided $c_{v,i} > 0$, $i = 1, \dots, n_s$ [21]. Note that $y \in \mathcal{G}_\sigma$ implies $P(y) > 0$. By the quasi-concavity of $s(y)$ (which follows from the convexity of the entropy function $U = -\rho s$ [24]) and concavity of $\rho u^*(y)$ [1] with respect to the state, for a given σ , \mathcal{G}_σ is a convex set. Note that \mathcal{G}_σ is similar to the corresponding set of admissible states in [25,26], but with the addition of the entropy constraint. Under the assumption that the exact solution to the classical Riemann problem with initial data

$$y(x, 0) = \begin{cases} y_1, & x < 0 \\ y_2, & x > 0 \end{cases}$$

is an entropy solution that preserves positivity, \mathcal{G}_σ is an invariant set [27,28,1]. Specifically, $y_1, y_2 \in \mathcal{G}_\sigma$ implies that the average of the exact Riemann solution over a domain that includes the Riemann fan is also in \mathcal{G}_σ .

Consider the one-dimensional three-point system,

$$y_\kappa^{j+1} = y_\kappa^j - \frac{\Delta t}{h} \left[\mathcal{F}^\dagger \left(y_\kappa^j, y_{\kappa^{(1)}}^j, -1 \right) + \mathcal{F}^\dagger \left(y_\kappa^j, y_{\kappa^{(2)}}^j, 1 \right) \right], \quad (4.6)$$

which corresponds to a $p = 0$, one-dimensional, element-local DG discretization with forward Euler time stepping, where j indexes the time step, h is the element size, and $\kappa^{(1)}$ and $\kappa^{(2)}$ are the elements to the left and right of κ , respectively. If \mathcal{F}^\dagger is an *invariant-region-preserving* numerical flux, then $y_\kappa^j, y_{\kappa_L}^j, y_{\kappa_R}^j \in \mathcal{G}_\sigma$ implies $y_\kappa^{j+1} \in \mathcal{G}_\sigma$ under the condition [10]

$$\frac{\Delta t \lambda}{h} \leq \frac{1}{2}, \quad (4.7)$$

where λ is an upper bound on the maximum wave speed of the system. In particular, y_κ^{j+1} then satisfies [10,29]

$$s(y_\kappa^{j+1}) \geq \min \left\{ s(y_{\kappa_L}^j), s(y_{\kappa^{(1)}}^j), s(y_{\kappa^{(2)}}^j) \right\}. \quad (4.8)$$

Examples of invariant-region-preserving fluxes are the Godunov, Lax-Friedrichs, HLL, and HLLC fluxes (see [10]).

Next, we analyze a general three-point system in the multidimensional setting:

$$y_\kappa^{j+1} = y_\kappa^j - \frac{\Delta t}{L} \left[\mathcal{F}^\dagger \left(y_\kappa^j, y_{\kappa^{(1)}}^j, n \right) + \mathcal{F}^\dagger \left(y_\kappa^j, y_{\kappa^{(2)}}^j, -n \right) \right], \quad (4.9)$$

where a schematic of this three-point system is given in Fig. 4.1. To analyze the classical Riemann problems associated with the interfaces, we introduce a rotated coordinate system with orthonormal basis $\{n, t_1, \dots, t_{d-1}\}$. With this change of basis and letting x^\parallel denote the coordinate in the n -direction, the projected (homogeneous) governing equations are given by [30]

$$\frac{\partial y}{\partial t} + \frac{\partial}{\partial x^\parallel} (n \cdot \mathcal{F}(y)) = 0, \quad (4.10)$$

with

$$y = \left(\rho v^\parallel, \rho v_1^\perp, \dots, \rho v_{d-1}^\perp, \rho e_t, C_1, \dots, C_{n_s} \right)^T$$

and

$$n \cdot \mathcal{F}(y) = \left(\rho (v^\parallel)^2 + P, \rho v^\parallel v_1^\perp, \dots, \rho v^\parallel v_{d-1}^\perp, v^\parallel (\rho e_t + P), v^\parallel C_1, \dots, v^\parallel C_{n_s} \right)^T,$$

where the velocity is expanded as

$$\begin{aligned} v &= (v^\parallel, v_1^\perp, \dots, v_{d-1}^\perp) \\ &= (v \cdot n, v \cdot t_1, \dots, v \cdot t_{d-1}). \end{aligned}$$

An equivalent system is

$$\left\{ \begin{array}{l} \frac{\partial \rho_1}{\partial t} + \frac{\partial}{\partial x_1} (\rho_1 v^\parallel) = 0 \\ \vdots \\ \frac{\partial \rho_{n_s}}{\partial t} + \frac{\partial}{\partial x_1} (\rho_{n_s} v^\parallel) = 0 \\ \frac{\partial v^\parallel}{\partial t} + v^\parallel \frac{\partial}{\partial x_1} (v^\parallel) + \frac{1}{\rho} \frac{\partial P(\rho, s)}{\partial x_1} = 0 \\ \frac{\partial v_1^\perp}{\partial t} + v^\parallel \frac{\partial}{\partial x_1} (v_1^\perp) = 0 \\ \vdots \\ \frac{\partial v_{d-1}^\perp}{\partial t} + v^\parallel \frac{\partial}{\partial x_1} (v_{d-1}^\perp) = 0 \\ \frac{\partial s}{\partial t} + v^\parallel \frac{\partial}{\partial x_1} (s) = 0 \end{array} \right., \quad (4.11)$$

where the last equation is the entropy transport equation (see [1, Section 4]). The Jacobian of (4.11) is

$$\left(\begin{array}{ccccccccc} v^\parallel & 0 & 0 & \rho_1 & 0 & \dots & 0 & 0 & 0 \\ 0 & \ddots & 0 & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & v^\parallel & \rho_{n_s} & 0 & 0 \dots & 0 & 0 & 0 \\ \frac{1}{\rho} \frac{\partial P}{\partial \rho} & \dots & \frac{1}{\rho} \frac{\partial P}{\partial \rho} & v^\parallel & 0 & 0 \dots & 0 & \frac{1}{\rho} \frac{\partial P}{\partial s} & \\ 0 & \dots & 0 & 0 & v^\parallel & 0 & \dots & 0 & \\ \vdots & \ddots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & 0 & \dots & 0 & v^\parallel & 0 & 0 \\ 0 & \dots & 0 & 0 & 0 & \dots & 0 & v^\parallel & 0 \end{array} \right),$$

which does not depend on $v^\perp = (v_1^\perp, \dots, v_{d-1}^\perp)$. The exact solution of the classical Riemann problem associated with (4.10) with initial data

$$y(x^\parallel, 0) = \begin{cases} y_1, & x^\parallel < 0 \\ y_2, & x^\parallel > 0 \end{cases}$$

can then be obtained in two steps [30,31, Chapter 4.8]. The first step is to solve the one-dimensional classical Riemann problem associated with the equations

$$\frac{\partial y^\parallel}{\partial t} + \frac{\partial \mathcal{F}(y^\parallel)}{\partial x^\parallel} = 0, \quad (4.12)$$

where

$$y^\parallel = (\rho_1, \dots, \rho_{n_s}, \rho v^\parallel, \rho e_t^\parallel)^T$$

and

$$\mathcal{F}(y^\parallel) = (\rho_1 v^\parallel, \dots, \rho_{n_s} v^\parallel, \rho (v^\parallel)^2 + P, v^\parallel (e_t^\parallel + P))^T,$$

with $e_t^\parallel = e_t - (v^\parallel)^2 / 2$. The second step is to solve

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho v_1^\perp \\ \vdots \\ \rho v_{d-1}^\perp \end{pmatrix} + \frac{\partial}{\partial x^\parallel} \begin{pmatrix} \rho v^\parallel v_1^\perp \\ \vdots \\ \rho v^\parallel v_{d-1}^\perp \end{pmatrix} = 0.$$

See [30] and [31, Chapter 4.8] for more information. Notice that

$$\rho(y) = \rho(y^\parallel), \quad \rho u^*(y) = \rho u^*(y^\parallel), \quad s(y) = s(y^\parallel),$$

$$C_i(y) = C_i(y^\parallel), \quad i = 1, \dots, n_s.$$

Consequently, since \mathcal{G}_σ is an invariant set for (4.12), it is also an invariant set for the projected equations (4.10). The invariant-region-preserving numerical fluxes for the one-dimensional three-point system (4.6) can then be shown to be invariant-region-preserving for the rotated (quasi-one-dimensional) three-point system (4.9). Specifically, as in [10] for the one-dimensional case, the RHS of (4.9) can be rewritten as a convex combination of y_κ^j and exact-Riemann-solution averages. As such, if y_κ^j , $y_{\kappa^{(1)}}^j$, and $y_{\kappa^{(2)}}^j$ in (4.9) are in \mathcal{G}_σ , then y_κ^{j+1} is also in \mathcal{G}_σ under the time-step-size constraint

$$\frac{\Delta t \lambda}{L} \leq \frac{1}{2},$$

where λ is an upper bound on the maximum wave speed of the system. Note that a multidimensional scheme has not yet been analyzed; such analysis will be performed in the following subsection. Throughout this work, we employ the HLLC numerical flux [31].

The analysis of the rotated three-point system (4.9) is essential for the construction of a positivity-preserving and entropy-bounded high-order DG scheme on arbitrary, curved elements. Specifically, as we demonstrate in Section 4.2, the element average of the solution at the $(j+1)$ th time step, \bar{y}_κ^{j+1} , can be decomposed into a convex combination of both pointwise values of $y_\kappa^j(x)$ and three-point systems involving pointwise values of $y_\kappa^j(x)$. Therefore, with the aid of a simple limiting procedure to ensure that said pointwise values of $y_\kappa^j(x)$ are in \mathcal{G}_σ , \bar{y}_κ^{j+1} will also be in \mathcal{G}_σ under a time-step-size constraint.

4.2. Entropy-bounded, high-order discontinuous Galerkin method in multiple dimensions

We are now in a position to derive a time-step constraint that ensures that the evolved element average is in \mathcal{G} . The average of y_κ is given by

$$\bar{y}_\kappa = \frac{1}{|\kappa|} \int_{\kappa} y dx, \quad (4.13)$$

where $|\kappa|$ is the volume of κ . Let ∂D_κ be the set of surface integration points used to evaluate the surface integrals in Equation (3.2) (i.e., the numerical flux terms), defined as

$$\partial D_\kappa = \bigcup_{f=1}^{n_f} \left\{ x(\zeta_l^{(f)}) \mid l = 1, \dots, n_{q,f}^\partial \right\}.$$

As discussed by Lv and Ihme [9], given a sufficiently accurate quadrature rule, the element average can be expanded as

$$\begin{aligned} \bar{y}_\kappa &= \sum_{v=1}^{n_q} \frac{|J_\kappa(\xi_v)| w_v}{|\kappa|} y_\kappa(\xi_v), \\ &= \sum_{v=1}^{n_q} \theta_v y_\kappa(\xi_v) + \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \theta_{f,l} y_\kappa(\xi(\zeta_l^{(f)})). \end{aligned} \quad (4.14)$$

If $\partial D_\kappa \subseteq \{x(\xi_v), v = 1, \dots, n_q\}$, i.e., this set of volume quadrature points contains the surface integration points, then we can simply take

$$\theta_v = \begin{cases} \frac{|J_\kappa(\xi_v)| w_v}{|\kappa|} & x(\xi_v) \notin \partial D_\kappa \\ 0 & x(\xi_v) \in \partial D_\kappa \end{cases}$$

and

$$\theta_{f,l} = \frac{|J_\kappa(\xi(\zeta_l^{(f)}))| w_{f,l}}{|\kappa| N_{f,l}},$$

where $w_{f,l}$ is the volume quadrature weight corresponding to the volume quadrature point that satisfies $\xi_v = \xi(\zeta_l^{(f)})$ and $N_{f,l}$ denotes the number of faces belonging to κ shared by the given point. If $\partial D_\kappa \not\subseteq \{x(\xi_v), v = 1, \dots, n_q\}$, we can instead take

$$\theta_v = \frac{|J_\kappa(\xi_v)| w_v}{|\kappa|} - \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \theta_{f,l} \psi_v(\xi(\zeta_l^{(f)})),$$

where $\{\psi_1, \dots, \psi_{n_d}\}$ is a set of Lagrange basis functions, with $n_b \leq n_d \leq n_q$, whose interpolation nodes are located at a subset of the n_q quadrature points, while $\psi_v = 0$ for $v = n_d + 1, \dots, n_q$, such that

$$\begin{aligned} \sum_{v=1}^{n_q} \theta_v y_\kappa(\xi_v) &= \sum_{v=1}^{n_q} \left[\frac{|J_\kappa(\xi_v)| w_v}{|\kappa|} - \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \theta_{f,l} \psi_v(\xi(\zeta_l^{(f)})) \right] y_\kappa(\xi_v) \\ &= \sum_{v=1}^{n_q} \frac{|J_\kappa(\xi_v)| w_v}{|\kappa|} y_\kappa(\xi_v) - \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \theta_{f,l} \sum_{v=1}^{n_q} y_\kappa(\xi_v) \psi_v(\xi(\zeta_l^{(f)})) \\ &= \sum_{v=1}^{n_q} \frac{|J_\kappa(\xi_v)| w_v}{|\kappa|} y_\kappa(\xi_v) - \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \theta_{f,l} y_\kappa(\xi(\zeta_l^{(f)})). \end{aligned}$$

$\theta_{f,l}$ will be related to a time-step-size constraint later in this section. Note that $\sum_{v=1}^{n_q} \theta_v + \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}} \theta_{f,l} = 1$. The positivity of the quadrature weights guarantees the existence of positive values of $\theta_{f,l}$ that yield $\theta_v \geq 0$ [9]. Since $\sum_v \theta_v + \sum_f \sum_l \theta_{f,l} = 1$, the RHS of Equation (4.14) is a convex combination of y_κ evaluated at a set of points in κ . Let $\kappa^{(f)}$ denote the f th neighbor of κ , and let D_κ be the set of points at which the solution is evaluated in Equation (4.14),

$$D_\kappa = \partial D_\kappa \bigcup \{x(\xi_v), v = 1, \dots, n_q\} = \bigcup_{f=1}^{n_f} \left\{ x\left(\zeta_l^{(f)}\right), l = 1, \dots, n_{q,f}^\partial \right\} \bigcup \{x(\xi_v), v = 1, \dots, n_q\}.$$

Without loss of generality, we assume that the n_f th face is such that $N = \max_f \{n_{q,f}^\partial\} = n_{q,n_f}^\partial$ and define $v_{f,l}^\partial$ as

$$v_{f,l}^\partial = \begin{cases} |J_{\partial\kappa}^{(f)}(\zeta_l)| w_{f,l}^\partial, & l = 1, \dots, n_{q,f}^\partial \\ 0, & l = n_{q,f}^\partial + 1, \dots, N \end{cases}, \quad (4.15)$$

such that

$$\sum_{f=1}^{n_f} \sum_{l=1}^N v_{f,l}^\partial = \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} v_{f,l}^\partial = \sum_{f=1}^{n_f} |\partial\kappa^{(f)}| = |\partial\kappa|,$$

where $|\partial\kappa|$ is the surface area of κ and $|\partial\kappa^{(f)}|$ is the surface area of the f th face. Standard flux interpolation, as in Equation (3.7), is assumed here. In Section 4.2.2, we will account for the modified flux interpolation in Equation (3.8). Taking $\mathbf{v} \in V_h^0$ in Equation (3.2), the scheme satisfied by the element averages can then be expanded as

$$\begin{aligned} \bar{y}_\kappa^{j+1} &= \bar{y}_\kappa^j - \frac{\Delta t}{|\kappa|} \sum_{f=1}^{n_f} \int_{\partial\kappa^{(f)}} \mathcal{F}^\dagger \left(y_\kappa^j, y_{\kappa^{(f)}}^j, n \right) ds \\ &= \bar{y}_\kappa^j - \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \frac{\Delta t v_{f,l}^\partial}{|\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_{\kappa^{(f)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \end{aligned} \quad (4.16)$$

$$\begin{aligned} &= \sum_{v=1}^{n_q} \theta_v y_\kappa^j (\xi_v) + \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \left[\theta_{f,l} y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right) - \frac{\Delta t v_{f,l}^\partial}{|\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_{\kappa^{(f)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right] \\ &= \sum_{v=1}^{n_q} \theta_v y_\kappa^j (\xi_v) + \sum_{f=1}^{n_f-1} \sum_{l=1}^{n_{q,f}^\partial} \theta_{f,l} A_{f,l} + \sum_{l=1}^{N-1} \theta_{n_f,l} B_l + \theta_{n_f,N} C. \end{aligned} \quad (4.17)$$

Note that the volume quadrature rule used to expand \bar{y}_κ^j need not be explicitly used to evaluate any integrals in Equation (3.2). Equation (4.16) and thus Equation (4.17) still hold for the quadrature-free approach [18,19] employed in this work since the weights w_v , $w_{f,l}$, and $w_{f,l}^\partial$ can be taken to be the integrals of the basis functions over the reference element/face, corresponding to a generalized Newton-Cotes quadrature rule [32]. Consequently, θ_v , $\theta_{f,l}$, and $v_{f,l}^\partial$ can be treated in the same manner as in a quadrature-based approach. Notice that \bar{y}_κ^{j+1} in Equation (4.17) is expressed as a convex combination of $A_{f,l}$, B_l , C , and pointwise values $y_\kappa^j(x_v)$. $A_{f,l}$, B_l , and C in Equation (4.17) are given by

$$\begin{aligned} A_{f,l} &= y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right) - \frac{\Delta t v_{f,l}^\partial}{\theta_{f,l} |\kappa|} \left[\mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_{\kappa^{(f)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right. \\ &\quad \left. + \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right) \right], \end{aligned} \quad (4.18)$$

for $f = 1, \dots, n_f - 1$, $l = 1, \dots, n_{q,f}^\partial$;

$$\begin{aligned} B_l &= y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) \\ &\quad - \frac{\Delta t v_{n_f,l}^\partial}{\theta_{n_f,l} |\kappa|} \left[\mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_{\kappa^{(n_f)}}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(n_f)} \right) \right) \right. \\ &\quad \left. + \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(n_f)} \right) \right) \right] \end{aligned}$$

$$\begin{aligned}
& - \sum_{f=1}^{n_f-1} \frac{\Delta t v_{f,l}^\partial}{\theta_{n_f,l} |\kappa|} \left[\mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right. \\
& \quad \left. + \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right) \right], \tag{4.19}
\end{aligned}$$

for $l = N - 1$; and

$$\begin{aligned}
C &= y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) \\
&\quad - \frac{\Delta t v_{n_f,N}^\partial}{\theta_{n_f,N} |\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), n \left(\zeta_N^{(n_f)} \right) \right) \\
&\quad - \sum_{l=1}^{N-1} \frac{\Delta t v_{n_f,l}^\partial}{\theta_{n_f,N} |\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(n_f)} \right) \right) \\
&\quad - \sum_{f=1}^{n_f-1} \frac{\Delta t v_{f,N}^\partial}{\theta_{n_f,N} |\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_N^{(f)} \right) \right), n \left(\zeta_N^{(f)} \right) \right) \\
&\quad - \sum_{f=1}^{n_f-1} \sum_{l=1}^{N-1} \frac{\Delta t v_{f,l}^\partial}{\theta_{n_f,N} |\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right). \tag{4.20}
\end{aligned}$$

The above expansion relies on the conservation property of the numerical flux:

$$\mathcal{F}^\dagger (y_1, y_2, n) = -\mathcal{F}^\dagger (y_2, y_1, -n).$$

$A_{f,l}$ in Equation (4.18) takes the form of the three-point system (4.9). Invoking the identity

$$y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) = \sum_{f=1}^{n_f} \frac{|\partial \kappa^{(f)}|}{|\partial \kappa|} y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), \tag{4.21}$$

B_l can be rewritten as

$$\begin{aligned}
B_l &= \frac{|\partial \kappa^{(n_f)}|}{|\partial \kappa|} \left\{ y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) - \frac{\Delta t v_{n_f,l}^\partial |\partial \kappa|}{\theta_{n_f,l} |\kappa| |\partial \kappa^{(n_f)}|} \left[\mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(n_f)} \right) \right) \right. \right. \\
&\quad \left. \left. + \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(n_f)} \right) \right) \right] \right\} \\
&\quad + \sum_{f=1}^{n_f-1} \frac{|\partial \kappa^{(f)}|}{|\partial \kappa|} \left\{ y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) - \frac{\Delta t v_{f,l}^\partial |\partial \kappa|}{\theta_{n_f,l} |\kappa| |\partial \kappa^{(f)}|} \left[\mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right. \right. \\
&\quad \left. \left. + \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right) \right] \right\}, \tag{4.22}
\end{aligned}$$

for $l = 1, \dots, N - 1$. The RHS of Equation (4.22) is a convex combination of three-point systems and, if some $v_{f,l}^\partial$ are zero, the pointwise value $y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right)$. To analyze C , we invoke the following identities:

$$y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) = \sum_{f=1}^{n_f} \sum_{l=1}^N \frac{v_{f,l}^\partial}{|\partial \kappa|} y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right)$$

and

$$\begin{aligned}
\sum_{f=1}^{n_f} \sum_{l=1}^N v_{f,l}^\partial \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) &= \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}} v_{f,l}^\partial \mathcal{F} \left(y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) \right) \cdot n \left(\zeta_l^{(f)} \right) \\
&= \int_{\partial \kappa} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) \right) \cdot n ds
\end{aligned}$$

$$= \int_{\kappa} \nabla \cdot \mathcal{F}^{\dagger} \left(y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) \right) dx \\ = 0,$$

where the first line is due to the consistency property of the numerical flux and the second line assumes sufficient accuracy of the surface quadrature rule. C in Equation (4.20) can then be rewritten as

$$C = \frac{v_{n_f, N}^{\partial}}{|\partial\kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) - \frac{\Delta t |\partial\kappa|}{\theta_{n_f, N} |\kappa|} \left[\mathcal{F}^{\dagger} \left(y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), n \left(\zeta_N^{(n_f)} \right) \right) \right. \right. \\ \left. \left. + \mathcal{F}^{\dagger} \left(y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_N^{(n_f)} \right) \right) \right] \right\} \\ + \sum_{l=1}^{N-1} \frac{v_{n_f, l}^{\partial}}{|\partial\kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) - \frac{\Delta t |\partial\kappa|}{\theta_{n_f, N} |\kappa|} \left[\mathcal{F}^{\dagger} \left(y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(n_f)} \right) \right) \right. \right. \\ \left. \left. + \mathcal{F}^{\dagger} \left(y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(n_f)} \right) \right) \right] \right\} \\ + \sum_{f=1}^{n_f-1} \frac{v_{f, N}^{\partial}}{|\partial\kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) - \frac{\Delta t |\partial\kappa|}{\theta_{n_f, N} |\kappa|} \left[\mathcal{F}^{\dagger} \left(y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_{\kappa}^j \left(\xi \left(\zeta_N^{(f)} \right) \right), n \left(\zeta_N^{(f)} \right) \right) \right. \right. \\ \left. \left. + \mathcal{F}^{\dagger} \left(y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_N^{(f)} \right) \right) \right] \right\} \\ + \sum_{f=1}^{n_f-1} \sum_{l=1}^{N-1} \frac{v_{f, l}^{\partial}}{|\partial\kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) - \frac{\Delta t |\partial\kappa|}{\theta_{n_f, N} |\kappa|} \left[\mathcal{F}^{\dagger} \left(y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(n_f)} \right) \right) \right. \right. \\ \left. \left. + \mathcal{F}^{\dagger} \left(y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(n_f)} \right) \right) \right] \right\},$$

which is a convex combination of three-point systems (regardless of whether some $v_{f, l}^{\partial}$ are zero). As such, \bar{y}_{κ}^{j+1} is a convex combination of the following components:

- Pointwise values, $y_{\kappa}^j(x_v)$, in κ
- Three-point systems involving pointwise values, $y_{\kappa}^j(\xi(\zeta_l^{(f)}))$ and $y_{\kappa^{(f)}}^j(\xi(\zeta_l^{(f)}))$, along $\partial\kappa$
- If some $v_{f, l}^{\partial}$ are zero, pointwise values, $y_{\kappa}^j(\xi(\zeta_l^{(n_f)}))$, along $\partial\kappa$

The above results lead to the following theorem, where we use y_{κ}^- to denote the exterior state along $\partial\kappa$.

Theorem 1. If $y_{\kappa}^j(x) \in \mathcal{G}_{\sigma}$, $\forall x \in D_{\kappa}$, and $y_{\kappa}^{-, j} \in \mathcal{G}_{\sigma}$, $\forall x \in \partial D_{\kappa}$, with

$$\sigma \leq \min \left\{ \min \left\{ s(y_{\kappa}^j(x)) \mid x \in D_{\kappa} \right\}, \min \left\{ s(y_{\kappa}^{-, j}(x)) \mid x \in \partial D_{\kappa} \right\} \right\}, \quad (4.23)$$

then \bar{y}_{κ}^{j+1} in Equation (4.16) is also in \mathcal{G}_{σ} under the constraint

$$\frac{\Delta t \lambda}{|\kappa|} \leq \frac{1}{2} \min \left\{ L_A, L_B, L_C \right\}, \quad (4.24)$$

$$L_A = \min \left\{ \frac{\theta_{f, l}}{v_{f, l}^{\partial}} \mid f = 1, \dots, n_f - 1, l = 1, \dots, n_{q, f}^{\partial} \right\}, \\ L_B = \min \left\{ \frac{\theta_{n_f, l}}{v_{f, l}^{\partial}} \frac{|\partial\kappa^{(f)}|}{|\partial\kappa|} \mid f = 1, \dots, n_f, l = 1, \dots, \min \left\{ n_{q, f}^{\partial}, N - 1 \right\} \right\}, \\ L_C = \frac{\theta_{n_f, N}}{|\partial\kappa|},$$

and the conditions

$$\begin{cases} \theta_v \geq 0, & v = 1, \dots, n_q \\ \theta_{f,l} > 0, & f = 1, \dots, n_f, l = 1, \dots, n_{q,f}^\partial. \end{cases} \quad (4.25)$$

Proof. The proof follows similar logic to that of the one-dimensional version in Part I [1, Theorem 1]. The constraint $\Delta t \lambda / |\kappa| \leq L_A / 2$ ensures that $A_{f,l}$ (Equation (4.18)) is in \mathcal{G}_σ , the constraint $\Delta t \lambda / |\kappa| \leq L_B / 2$ ensures that B_l (Equation (4.22)) is in \mathcal{G}_σ , and the constraint $\Delta t \lambda / |\kappa| \leq L_C / 2$ ensures that C (Equation (4.20)) is in \mathcal{G}_σ . It follows from Equation (4.17) that \bar{y}_κ^{j+1} is in \mathcal{G}_σ . \square

Remark 2. A direct result of Theorem 1 is that

$$s(\bar{y}_\kappa^{j+1}) \geq \min \left\{ \min \left\{ s(y_\kappa^j(x)) \mid x \in D_\kappa \right\}, \min \left\{ s(y_\kappa^{-j}(x)) \mid x \in \partial D_\kappa \right\} \right\}.$$

Remark 3. Theorem 1 applies to mixtures of thermally perfect gases, curved elements of arbitrary shape, any invariant-region-preserving numerical flux, and any combination of volume and surface quadrature rules (which can differ among faces), thus generalizing previous positivity-preserving and/or entropy-bounded schemes in the literature.

Remark 4. A simple linear-scaling limiter, described in Section 4.2.1, is directly applied to enforce $y_\kappa^{j+1}(x) \in \mathcal{G}_{s_{b,\kappa}}$, $\forall x \in D_\kappa$, where s_b is a lower bound on the specific thermodynamic entropy. Motivated by the minimum entropy principle (4.3), s_b is computed in this work in an element-local manner as

$$s_{b,\kappa}^{j+1}(y) = \min \left\{ s(y^j(x)) \mid x \in \bigcup_{f=1}^{n_f} D_{\kappa^{(f)}} \bigcup D_\kappa \right\}, \quad (4.26)$$

which is an approximation of the minimum entropy over κ and the neighboring elements. An alternative to the local entropy bound in Equation (4.26) is the following global entropy bound:

$$s_b(y) = \min \left\{ s(y(x)) \mid x \in \bigcup_{\kappa \in \mathcal{T}} D_\kappa \right\}. \quad (4.27)$$

It was demonstrated that the local entropy bound (4.26) can more effectively dampen nonlinear instabilities [1], particularly when the entropy varies significantly throughout the domain. Additional information on these local and global entropy bounds can be found in Part I [1]. This completes the construction of a positivity-preserving, entropy-bounded, high-order DG scheme.

Remark 5. As discussed in Part I [1], in practice, we loosen some of the above requirements. First, the maximum wave speed at a given point is simply approximated as $|v| + c$, where c is the speed of sound. Simple algorithms to compute bounds on the wave speeds exist for the monocomponent case [30,33]; extending these to the multicomponent, thermally perfect case may indeed be worthy of future investigation. A similar comment can be made for most invariant-region-preserving numerical fluxes, which often require wave-speed estimates. Second, we revise the definition of \mathcal{G}_σ as

$$\mathcal{G}_\sigma = \left\{ y \mid \rho > 0, \rho u^* > 0, C_1 \geq 0, \dots, C_{n_s} \geq 0, \chi_\sigma \geq 0 \right\}, \quad (4.28)$$

where $\chi_\sigma = \rho s - \rho \sigma$ (introduced in [10]), which is concave, and the species concentrations are permitted to be equal to zero, given that requiring only positive concentrations would preclude the calculation of practical problems. However, it is important to note that if $C_i = 0$ for some i , the specific thermodynamic entropy, s , becomes ill-defined and the entropy functions $U = -\rho s$ and $U = -\rho f_e(s)$ lose convexity [6,41]. Nevertheless, by making use of $0 \log 0 = 0$ [21, Chapter 6], ρs remains well-defined. We did not face any issues associated with relaxing these two requirements in this study.

In the case that $\partial D_\kappa \not\subseteq \{x(\xi_v), v = 1, \dots, n_q\}$, as described by Lv and Ihme [9], an optimization problem can be solved for each element in a pre-processing step to maximize the RHS of (4.24). They also introduced another simpler but more restrictive approach that reformulates the time-step-size constraint as

$$\frac{\Delta t \lambda}{L} \leq \frac{1}{2} B,$$

where L is a proposed length scale and B is tabulated in [9] for common element shapes and quadrature rules. The constraint (4.24) can be reformulated in a similar manner, utilizing the values of B in [9]. These values of B naturally apply to the quadrature-free approach [18,19] employed in this work since, as previously mentioned, $\theta_{f,l}$ and $v_{f,l}^\partial$ can be treated in the same manner between quadrature-free and quadrature-based approaches. Here, instead of explicitly accounting for the constraint (4.24), we simply prescribe the time-step size according to a user-prescribed CFL based on the acoustic time scale, which is often less restrictive than the constraint (4.24). Note that the condition (4.24) is sufficient but not necessary for \bar{y}_κ^{j+1} to be in \mathcal{G}_σ . Therefore, as recommended by Zhang [34], larger time-step sizes can be initially taken and, if $\bar{y}_\kappa^{j+1} \notin \mathcal{G}_\sigma$, the time step can be restarted with smaller Δt . In this study, this backtracking strategy is needed only during the first time steps of the two-dimensional, $p = 1$ and three-dimensional,

$p = 2$ detonation-wave simulations in Sections 6.2 and 6.3. We also neglect the artificial-viscosity formulation when determining the time-step size. In principle, however, the artificial viscosity may need to be bounded to maintain stability.

If the faces are straight-sided (i.e., the surface Jacobian, $J_{\partial\kappa}^{(f)}$, and the normal, n , are constant over any $\partial\kappa^{(f)}$, for all f) and identical surface quadrature rules are employed for each face, the time-step-size constraint (4.24) can be simplified. Equation (4.17) can instead be written as

$$\begin{aligned}\bar{y}_\kappa^{j+1} &= \bar{y}_\kappa^j - \sum_{f=1}^{n_f} \sum_{l=1}^{n_q^\partial} \frac{\Delta t v_{f,l}^\partial}{|\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_{\kappa^{(f)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \\ &= \sum_{v=1}^{n_q} \theta_v y_\kappa^j \left(\xi_v \right) + \sum_{f=1}^{n_f} \sum_{l=1}^{n_q^\partial} \left[\theta_{f,l} y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right) - \frac{\Delta t v_{f,l}^\partial}{|\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_{\kappa^{(f)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right] \\ &= \sum_{v=1}^{n_q} \theta_v y_\kappa^j \left(\xi_v \right) + \sum_{f=1}^{n_f-1} \sum_{l=1}^{n_q^\partial} \theta_{f,l} A_{f,l} + \sum_{l=1}^{n_q^\partial} \theta_{n_f,l} B_l,\end{aligned}\quad (4.29)$$

where $v_{f,l}^\partial$ is now defined as

$$v_{f,l}^\partial = |\partial\kappa^{(f)}| \hat{w}_l^\partial,$$

with \hat{w}_l^∂ denoting normalized weights such that $\sum_l \hat{w}_l^\partial = 1$. $A_{f,l}$ in Equation (4.29) is still of the form (4.18) for $f = 1, \dots, n_f - 1$, $l = 1, \dots, n_q^\partial$, while B_l is given by

$$\begin{aligned}B_l &= y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) \\ &\quad - \frac{\Delta t v_{n_f,l}^\partial}{\theta_{n_f,l} |\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_{\kappa^{(n_f)}}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(n_f)} \right) \right) \\ &\quad - \sum_{f=1}^{n_f-1} \frac{\Delta t v_{f,l}^\partial}{\theta_{n_f,l} |\kappa|} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right)\end{aligned}$$

for $l = 1, \dots, n_q^\partial$. With the identity

$$\begin{aligned}\sum_{f=1}^{n_f} |\partial\kappa^{(f)}| \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) &= \sum_{f=1}^{n_f} |\partial\kappa^{(f)}| \mathcal{F} \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) \right) \cdot n \left(\zeta_l^{(f)} \right) \\ &= \int_{\partial\kappa} \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) \right) \cdot n ds \\ &= \int_{\kappa} \nabla \cdot \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) \right) dx \\ &= 0,\end{aligned}$$

B_l can be rewritten as

$$\begin{aligned}B_l &= \frac{|\partial\kappa^{(n_f)}|}{|\partial\kappa|} \left\{ y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) - \frac{\Delta t \hat{w}_l^\partial |\partial\kappa|}{\theta_{n_f,l} |\kappa|} \left[\mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_{\kappa^{(n_f)}}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(n_f)} \right) \right) \right. \right. \\ &\quad \left. \left. + \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), -n \left(\zeta_l^{(n_f)} \right) \right) \right] \right\} \\ &\quad + \sum_{f=1}^{n_f-1} \frac{|\partial\kappa^{(f)}|}{|\partial\kappa|} \left\{ y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) - \frac{\Delta t \hat{w}_l^\partial |\partial\kappa|}{\theta_{n_f,l} |\kappa|} \left[\mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right. \right. \\ &\quad \left. \left. + \mathcal{F}^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right) \right] \right\}.\end{aligned}$$

B_l is therefore a convex combination of three-point systems. The time-step-size constraint can then be modified as

$$\frac{\Delta t \lambda}{|\kappa|} \leq \frac{1}{2} \min \{ L_A, L_B \}, \quad (4.30)$$

$$L_A = \min \left\{ \frac{\theta_{f,l}}{|\partial\kappa^{(f)}| \hat{w}_l^\partial} \middle| f = 1, \dots, n_f - 1, l = 1, \dots, n_q^\partial \right\},$$

$$L_B = \min \left\{ \frac{\theta_{n_f,l}}{|\partial\kappa| \hat{w}_l^\partial} \middle| f = 1, \dots, n_f, l = 1, \dots, n_q^\partial \right\},$$

which is similar to that in [10].

4.2.1. Limiting procedure

The limiting procedure to enforce $y_\kappa^{j+1}(x) \in \mathcal{G}_{s_b}$, $\forall x \in D_\kappa$, is the same as in Part I. For completeness, we summarize it here. The $j+1$ superscript and κ subscript are dropped for brevity. $\bar{y}_\kappa^j(x)$ is assumed to be in \mathcal{G}_{s_b} . The limiting operator is of the same form as in [35], [34], [10], [29], and related papers.

- Positive density: if $\rho(x) > \epsilon$, $\forall x \in D_\kappa$, where $\epsilon > 0$ is a small number (e.g., $\epsilon = 10^{-10}$), then set $C_i^{(1)} = C_i = \sum_{j=1}^{n_b} C_i(x_j) \phi_j$, $i = 1, \dots, n_s$; otherwise, compute

$$C_i^{(1)} = \bar{C}_i + \theta^{(1)} (C_i - \bar{C}_i), \quad \theta^{(1)} = \frac{\rho(\bar{y}) - \epsilon}{\rho(\bar{y}) - \min_{x \in D} \rho(y(x))},$$

for $i = 1, \dots, n_s$.

- Nonnegative concentrations: if $C_i^{(1)}(x) \geq 0$, $\forall x \in D_\kappa$, then set $C_i^{(2)} = C_i^{(1)}$, $i = 1, \dots, n_s$; otherwise, compute

$$C_i^{(2)} = \bar{C}_i + \theta^{(2)} (C_i^{(1)} - \bar{C}_i), \quad \theta^{(2)} = \frac{\bar{C}_i}{\bar{C}_i - \min_{x \in D} C_i^{(1)}(x)}.$$

Let $y^{(2)} = (\rho v_1, \dots, \rho v_d, \rho e_t, C_1^{(2)}, \dots, C_{n_s}^{(2)})$.

- Positive temperature: if $\rho u^*(y^{(2)}(x)) > \epsilon$, $\forall x \in D_\kappa$, then set $y^{(3)} = y^{(2)}$; otherwise, compute

$$y^{(3)} = \bar{y} + \theta^{(3)} (y^{(2)} - \bar{y}), \quad \theta^{(3)} = \frac{\rho u^*(\bar{y}) - \epsilon}{\rho u^*(\bar{y}) - \min_{x \in D} \rho u^*(y^{(2)}(x))}.$$

The “positivity-preserving limiter” refers to the limiting procedure up to this point.

- Entropy constraint: if $\chi(y^{(3)}(x)) \geq 0$, $\forall x \in D_\kappa$, then set $y^{(4)} = y^{(3)}$; otherwise, compute

$$y^{(4)} = \bar{y} + \theta^{(4)} (y^{(3)} - \bar{y}), \quad \theta^{(4)} = \frac{\chi(\bar{y})}{\chi(\bar{y}) - \min_{x \in D} \chi(y^{(3)}(x))}.$$

The “entropy limiter” refers to the limiting procedure up to this point.

$y^{(4)}$ then replaces y as the solution. This limiting procedure is applied at the end of every RK stage. It is conservative and in general preserves the formal order of accuracy for smooth solutions [7,34,24,9,10]. Note that Step 1 may seem superfluous given Step 2; however, consider a two-species flow where both species concentrations are negative at the same point in D_κ . If Step 1 is neglected, Step 2 would limit the concentrations at that point to zero, resulting in zero density.

4.2.2. Modified flux interpolation

We now discuss how to account for over-integration with the modified flux interpolation in Equation (3.8). The scheme satisfied by the element averages becomes

$$\begin{aligned} \bar{y}_\kappa^{j+1} &= \bar{y}_\kappa^j - \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \frac{\Delta t v_{f,l}^\partial}{|\kappa|} \mathcal{F}^\dagger \left(\tilde{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \tilde{y}_{\kappa^{(k)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \\ &= \sum_{v=1}^{n_q} \theta_v y_\kappa^j(\xi_v) + \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \left[\theta_{f,l} y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right) - \frac{\Delta t v_{f,l}^\partial}{|\kappa|} \mathcal{F}^\dagger \left(\tilde{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \tilde{y}_{\kappa^{(f)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right] \\ &= \sum_{v=1}^{n_q} \theta_v y_\kappa^j(\xi_v) + \sum_{f=1}^{n_f-1} \sum_{l=1}^{n_{q,f}^\partial} \theta_{f,l} \tilde{A}_{f,l} + \sum_{l=1}^{N-1} \theta_{n_f,l} \tilde{B}_l + \theta_{n_f,N} \tilde{C}. \end{aligned} \tag{4.31}$$

Following the same steps as in Section 4.2, $\tilde{A}_{f,l}$, \tilde{B}_l , and \tilde{C} can be written as

$$\begin{aligned} \tilde{A}_{f,l} &= y_{\kappa}^j \left(\xi \left(\zeta_l^{(f)} \right) \right) - \frac{\Delta t v_{f,l}^\partial}{\theta_{f,l} |\kappa|} \left[\mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right. \\ &\quad \left. + \mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right) \right], \end{aligned} \quad (4.32)$$

$$\begin{aligned} \tilde{B}_l &= \frac{|\partial \kappa^{(n_f)}|}{|\partial \kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) - \frac{\Delta t v_{n_f,l}^\partial |\partial \kappa|}{\theta_{n_f,l} |\kappa| |\partial \kappa^{(n_f)}|} \left[\mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(n_f)} \right) \right) \right. \right. \\ &\quad \left. \left. + \mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(n_f)} \right) \right) \right] \right\} \\ &\quad + \sum_{f=1}^{n_f-1} \frac{|\partial \kappa^{(f)}|}{|\partial \kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right) - \frac{\Delta t v_{f,l}^\partial |\partial \kappa|}{\theta_{n_f,l} |\kappa| |\partial \kappa^{(f)}|} \left[\mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right. \right. \\ &\quad \left. \left. + \mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right) \right] \right\}, \end{aligned} \quad (4.33)$$

and

$$\begin{aligned} \tilde{C} &= \frac{v_{n_f,N}^\partial}{|\partial \kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) - \frac{\Delta t |\partial \kappa|}{\theta_{n_f,N} |\kappa|} \left[\mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), n \left(\zeta_N^{(n_f)} \right) \right) \right. \right. \\ &\quad \left. \left. + \mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_N^{(n_f)} \right) \right) \right] \right\} \\ &\quad + \sum_{l=1}^{N-1} \frac{v_{n_f,l}^\partial}{|\partial \kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) - \frac{\Delta t |\partial \kappa|}{\theta_{n_f,l} |\kappa|} \left[\mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), n \left(\zeta_l^{(n_f)} \right) \right) \right. \right. \\ &\quad \left. \left. + \mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(n_f)} \right) \right) \right] \right\} \\ &\quad + \sum_{f=1}^{n_f-1} \frac{v_{f,N}^\partial}{|\partial \kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) - \frac{\Delta t |\partial \kappa|}{\theta_{n_f,N} |\kappa|} \left[\mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right. \right. \\ &\quad \left. \left. + \mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right) \right] \right\} \\ &\quad + \sum_{f=1}^{n_f-1} \sum_{l=1}^{N-1} \frac{v_{f,l}^\partial}{|\partial \kappa|} \left\{ y_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right) - \frac{\Delta t |\partial \kappa|}{\theta_{n_f,N} |\kappa|} \left[\mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\xi \left(\zeta_l^{(f)} \right) \right) \right) \right. \right. \\ &\quad \left. \left. + \mathcal{F}^\dagger \left(\tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_N^{(n_f)} \right) \right), -n \left(\xi \left(\zeta_l^{(f)} \right) \right) \right) \right] \right\}. \end{aligned}$$

Unfortunately, the corresponding three-point systems are not necessarily of the type (4.9) since in general, $y_{\kappa}^j \left(\xi \left(\zeta_l^{(f)} \right) \right) \neq \tilde{y}_{\kappa}^j \left(\xi \left(\zeta_l^{(f)} \right) \right)$. The incompatibility is a result of expressing \bar{y}_{κ} as a convex combination of pointwise values of $y_{\kappa}(x)$ (as opposed to $\tilde{y}_{\kappa}(x)$). Since the element average of \tilde{y}_{κ} , denoted $\bar{\tilde{y}}_{\kappa}$, is not necessarily equal to \bar{y}_{κ} , \bar{y}_{κ} cannot be directly written as a convex combination of pointwise values of $\tilde{y}_{\kappa}(x)$. In the one-dimensional case, if the nodal set includes the endpoints, then this issue is circumvented since $y_{\kappa}^j(x_L) = \tilde{y}_{\kappa}^j(x_L)$ and $y_{\kappa}^j(x_R) = \tilde{y}_{\kappa}^j(x_R)$. However, the multidimensional case is more complicated. One simple approach, assuming that the nodal set includes surface points that can be used for integration, is as follows:

- Compute y_{κ}^{j+1} using over-integration with the modified flux interpolation (3.8).
- If $\bar{y}_{\kappa}^{j+1} \in \mathcal{G}_{s_b}$, then proceed to the next time step. This will typically be true since in general, $y_{\kappa}^j(x^{(f)}(\zeta_l)) \approx \tilde{y}_{\kappa}^j(x^{(f)}(\zeta_l))$ and the conditions laid out in Section 4.2 are not necessary for \bar{y}_{κ}^{j+1} to be in \mathcal{G}_{s_b} .
- In the rare case that $\bar{y}_{\kappa}^{j+1} \notin \mathcal{G}_{s_b}$, recompute y_{κ}^{j+1} with integration points that are in the nodal set, which effectively maintains pressure equilibrium. \bar{y}_{κ}^{j+1} is then guaranteed to be in \mathcal{G}_{s_b} since $y_{\kappa} = \tilde{y}_{\kappa}$ at the solution nodes.

Note that this would only need to be done for the surface integrals; since the second term in Equation (3.2) (i.e., the volumetric flux integral) does not factor into the scheme satisfied by the element averages, over-integration with the modified flux interpolation can be freely employed in said integral. Furthermore, if \bar{y}_{κ}^{j+1} satisfies the positivity property but $s(\bar{y}_{\kappa}^{j+1}) < s_b$ (and therefore $\bar{y}_{\kappa}^{j+1} \notin \mathcal{G}_{s_b}$),

then it may still be reasonable to proceed to the next time step, provided that $s(y_\kappa^j(x)) \ll s_b, \forall x \in D_\kappa$ (e.g., $s(y_\kappa^j(x)) < 0.95s_b, \forall x \in D_\kappa$). In Appendix A, we investigate the effect of over-integration on the frequency of limiter activation in a one-dimensional test case involving the advection of a low-density Gaussian wave.

It should also be noted that using over-integration with the modified flux interpolation (3.8), \bar{y}_κ^{j+1} is guaranteed to at least satisfy the positivity property under a different time-step-size constraint. To show this, let \mathcal{G} denote the set

$$\mathcal{G} = \left\{ y \mid C_1 \geq 0, \dots, C_{n_s} \geq 0, \rho > 0, \rho u^* > 0 \right\},$$

and, as a representative example, rewrite Equation (4.32) as

$$\tilde{A}_{f,l} = y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right) - \frac{\Delta t v_{f,l}^\theta}{\theta_{f,l} |\kappa|} \Delta F \left(\xi \left(\zeta_l^{(f)} \right) \right),$$

where

$$\begin{aligned} \dot{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right) &= y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right) - \frac{\Delta t v_{f,l}^\theta}{\theta_{f,l} |\kappa|} \left[F^\dagger \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right. \\ &\quad \left. + F^+ \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right) \right] \\ \Delta F \left(\xi \left(\zeta_l^{(f)} \right) \right) &= F^\dagger \left(\dot{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \dot{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \\ &\quad - F^+ \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \\ &\quad + F^+ \left(\dot{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \dot{y}_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right) \\ &\quad - F^+ \left(y_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), y_\kappa^j \left(\xi \left(\zeta_l^{(n_f)} \right) \right), -n \left(\zeta_l^{(f)} \right) \right). \end{aligned}$$

$\dot{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right)$ is expressed as a three-point system of the type (4.9) and is therefore in \mathcal{G} under the constraint (4.24). Then, according to Lemma (6) in Appendix B, $\tilde{A}_{f,l}$ is also in \mathcal{G} if

$$\frac{\Delta t}{|\kappa|} < \frac{\theta_{f,l}}{v_{f,l}^\theta \alpha^* \left(\dot{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \Delta F \left(\xi \left(\zeta_l^{(f)} \right) \right) \right)}, \quad (4.34)$$

where α^* is defined as in (B.1). Note that since the modified flux interpolation (3.8) does not alter species concentrations or momentum, α^* can actually be simplified as in Remark 7. In general, since $y_\kappa^j(x^{(f)}(\zeta_l)) \approx \dot{y}_\kappa^j(x^{(f)}(\zeta_l))$, ΔF and thus α^* are small, such that the constraint (4.34) is not restrictive. The same analysis can be performed for \tilde{B}_l and C to yield similar constraints on Δt . In practice, we do not find it necessary to explicitly account for these additional constraints.

Though not pursued in this work, in Appendix C, we present an alternative approach compatible with over-integration. Said approach utilizes an additional auxiliary polynomial to guarantee $\bar{y}_\kappa^{j+1} \in \mathcal{G}_{s_b}$ while employing the modified flux interpolation (3.8).

5. Reaction step

In this section, we briefly discuss the reaction step, most of which is independent of the number of spatial dimensions. Only the multidimensional considerations are detailed here; the reader is referred to Part I [1] for more information.

The element-local, semi-discrete form of Equation (3.4) is written as

$$\int_{\kappa} \mathbf{v}^T \frac{\partial \mathbf{y}}{\partial t} dx - \int_{\kappa} \mathbf{v}^T S(\mathbf{y}) dx = 0, \quad \forall \mathbf{v} \in V_h^P. \quad (5.1)$$

We approximate $S(\mathbf{y})$ locally as a polynomial in V_h^P as

$$S_\kappa \approx \sum_{j=1}^{n_b} S(y(x_j)) \phi_j,$$

giving the following spatially decoupled system of ODEs advanced at the solution nodes from $t = t_0$ to $t = t_f$:

$$\frac{d}{dt} y_\kappa(x_j, t) - S(y_\kappa(x_j, t)) = 0, \quad j = 1, \dots, n_b.$$

Suppose it can be guaranteed that

$$y_\kappa(x_j, t_f) \in \mathcal{G}_{s(y_\kappa(x_j, t_0))}, \quad j = 1, \dots, n_b. \quad (5.2)$$

With s_b now given by

$$s_b = \min_{j=1,\dots,n_b} s(y_\kappa(x_j, t_0)),$$

$\bar{y}_\kappa(t_f)$ is in \mathcal{G}_{s_b} under the following two conditions:

- The nodal set corresponds to the quadrature points of a rule with positive weights (e.g., Gauss-Lobatto nodes).
- Said quadrature rule is sufficiently accurate to compute \bar{y}_κ .

With $\bar{y}_\kappa(t_f) \in \mathcal{G}_{s_b}$, the limiting procedure in Section 4.2.1 can then be applied to enforce $y_\kappa(x, t_f) \in \mathcal{G}_{s_b}$, $\forall x \in D_\kappa$ (unless $D_\kappa = \{x_j, j = 1, \dots, n_b\}$, in which case the limiting procedure is superfluous). However, if the geometric Jacobian is not constant, the quadrature rule may no longer be sufficiently accurate to compute \bar{y}_κ ; therefore, even if (5.2) is satisfied, $\bar{y}_\kappa(t_f)$ may not be in \mathcal{G}_{s_b} . One approach to guarantee $\bar{y}_\kappa(t_f) \in \mathcal{G}_{s_b}$ is to first expand y_κ as

$$y_\kappa = \sum_{i=1}^{n_a} y_\kappa(x_i) \Psi_i,$$

where $\{\Psi_1, \dots, \Psi_{n_a}\}$ is a basis of $V_h^{\hat{p}}$, with $n_a > n_b$ and $\hat{p} > p$, and then solve

$$\int_{\kappa} \mathbf{v}^T \frac{\partial y}{\partial t} dx - \int_{\kappa} \mathbf{v}^T \mathcal{S}(y) dx = 0, \quad \forall \mathbf{v} \in V_h^{\hat{p}} \quad (5.3)$$

for $y \in V_h^{\hat{p}}$. Following the same procedure as above, the resulting spatially decoupled system of ODEs is

$$\frac{d}{dt} y_\kappa(x_i, t) - \mathcal{S}(y_\kappa(x_i, t)) = 0, \quad i = 1, \dots, n_a. \quad (5.4)$$

Finally, L^2 projection is applied to project y from $V_h^{\hat{p}}$ to V_h^p . Since L^2 projection is a conservative operation, $\bar{y}_\kappa(t_f) \in \mathcal{G}_{s_b}$, where s_b is now given by

$$s_b = \min_{i=1,\dots,n_a} s(y_\kappa(x_i, t_0)).$$

The limiter can then be employed to enforce $y_\kappa(x, t_f) \in \mathcal{G}_{s_b}$, $\forall x \in D_\kappa$, unless $D_\kappa = \{x_i, i = 1, \dots, n_a\}$. Note that in [36] and [37], slightly modified ODEs are similarly solved at a generic set of quadrature points.

Each system of ODEs is solved in a spatially decoupled manner using a DG discretization in time. h -adaptivity in time is employed to ensure that the state at a given point is in \mathcal{G}_{s_b} , with a maximum of ten Newton iterations used to solve the nonlinear system at each sub-time-step. Since the remainder of the reaction step is identical to that in the one-dimensional case, we refer the reader to Part I [1] for further details on the temporal discretization.

6. Multidimensional results

First, we compute two-dimensional thermal-bubble advection to assess the ability of the proposed formulation to maintain pressure equilibrium on curved grids. Next, we present solutions to a two-dimensional moving detonation on a series of increasingly refined meshes over a range of polynomial orders. Finally, we present the solution to a three-dimensional, large-scale, moving detonation wave in order to demonstrate the utility of the proposed formulation. The SSPRK3 time integration scheme [38,39] is used in Section 6.1, while the SSPRK2 scheme is used in Sections 6.2 and 6.3. All simulations are performed using a modified version of the JENRE® Multiphysics Framework [40,2] that incorporates the developments and extensions described in this work.

6.1. Two-dimensional thermal-bubble advection

This flow configuration is a two-dimensional version of the one-dimensional thermal-bubble advection we computed in Part I [1]. The initial conditions are written as

$$\begin{aligned} (v_1, v_2) &= (1, 0) \text{ m/s}, \\ Y_{H_2} &= \frac{1}{2} \left[1 - \tanh \left(\sqrt{x_1^2 + x_2^2} - 10 \right) \right], \\ Y_{O_2} &= 1 - Y_{H_2}, \\ T &= 1200 - 900 \tanh \left(\sqrt{x_1^2 + x_2^2} - 10 \right) \text{ K}, \\ P &= 1 \text{ bar}. \end{aligned} \quad (6.1)$$

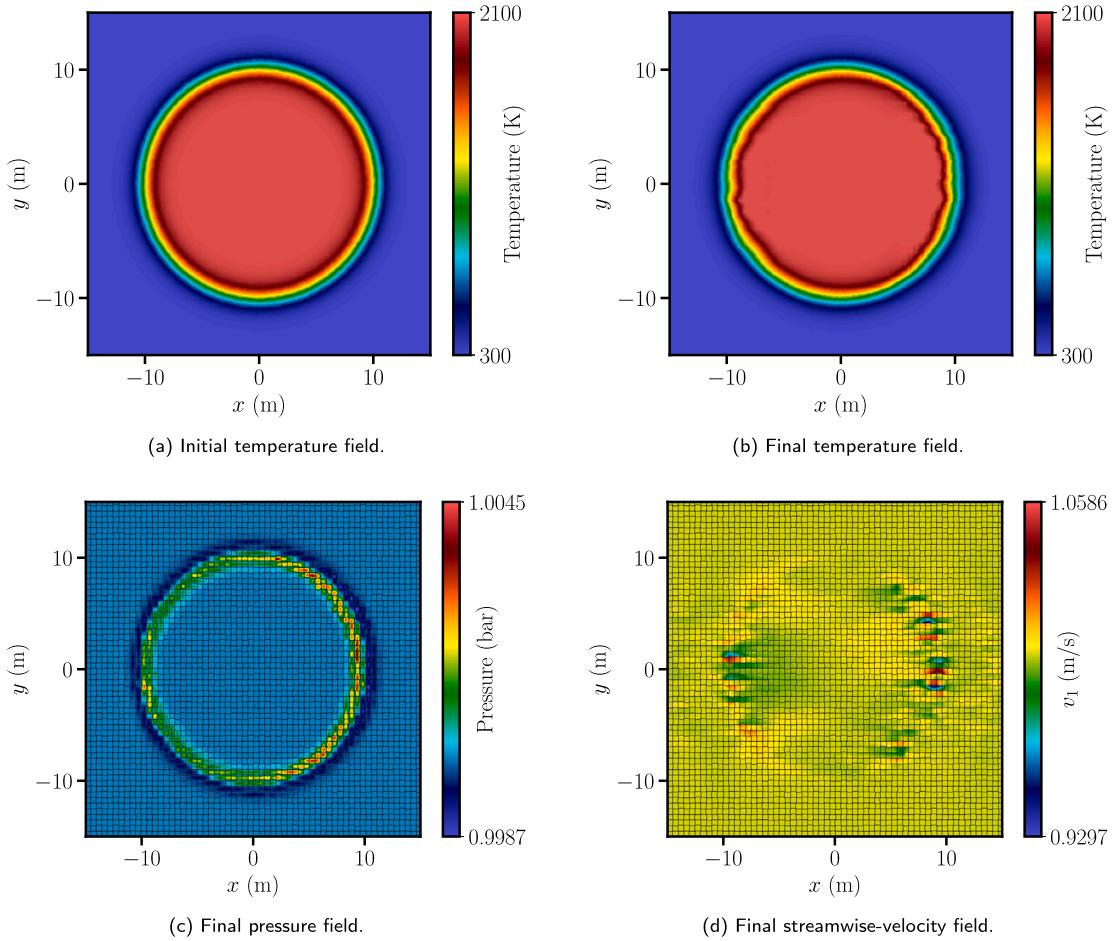


Fig. 6.1. $p = 1$ solution to two-dimensional thermal-bubble advection on a curved quadrilateral grid without artificial viscosity. The final time is $t = 50$ s, corresponding to one period. The colorbar minima and maxima for the pressure and velocity fields are the respective global minima and maxima. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

The thermodynamic relations for the hydrogen-oxygen mechanism used here are given by

$$\begin{aligned} \frac{W_{H_2} c_{p,H_2}(T)}{R^0} &= 3.47 - 0.220\hat{T} + 0.577\hat{T}^2 - 0.194\hat{T}^3 + 0.0210\hat{T}^4, \\ \frac{W_{H_2} h_{H_2}(T)}{R^0} &= \int \frac{W_{H_2} c_{p,H_2}(\tau) d\tau}{R^0} - 1028.7 \text{ K}, \quad \frac{W_{H_2} s_{H_2}^o}{R^0} = \int \frac{W_{H_2} c_{p,H_2}(\tau) d\tau}{R^0 \tau} - 4.00, \\ \frac{W_{O_2} c_{p,O_2}(T)}{R^0} &= 3.09 + 1.77\hat{T} - 0.911\hat{T}^2 + 0.243\hat{T}^3 - 0.0242\hat{T}^4, \\ \frac{W_{O_2} h_{O_2}(T)}{R^0} &= \int \frac{W_{O_2} c_{p,O_2}(\tau) d\tau}{R^0} - 992.9 \text{ K}, \quad \frac{W_{O_2} s_{O_2}^o}{R^0} = \int \frac{W_{O_2} c_{p,O_2}(\tau) d\tau}{R^0 \tau} + 6.57, \end{aligned}$$

where $\hat{T} = T/T_r$, with $T_r = 1000$ K, and τ is a dummy variable for T . The computational domain is $\Omega = (-25, 25) \text{ m} \times (-25, 25) \text{ m}$. Symmetry conditions are imposed along the top and bottom boundaries, while the left and right boundaries are periodic. The time-step size is prescribed according to $\text{CFL} = 0.4$ based on the acoustic time scale. The purpose of this test case is to determine whether the proposed formulation can maintain pressure equilibrium (in an approximate sense) when using multidimensional curved grids. Here, the curved elements are of quadratic geometric order. We first generate a uniform quadrilateral grid with 100 cells in each direction. At interior edges, the midpoint nodes are then slightly perturbed from their initial positions. We compute $p = 1$, $p = 2$, and $p = 3$ solutions without artificial viscosity up to $t = 50$ s, corresponding to one period.

Fig. 6.1 presents the $p = 1$ temperature, pressure, and streamwise-velocity distributions. The initial temperature field is also shown. The curved grid is superimposed on the pressure and velocity fields. Slight underresolution can be observed even in the initial temperature distribution. The pressure and velocity ranges given in Fig. 6.1 correspond to the actual respective minima and maxima in the corresponding solutions. Despite visible errors in the temperature and small deviations pressure and velocity

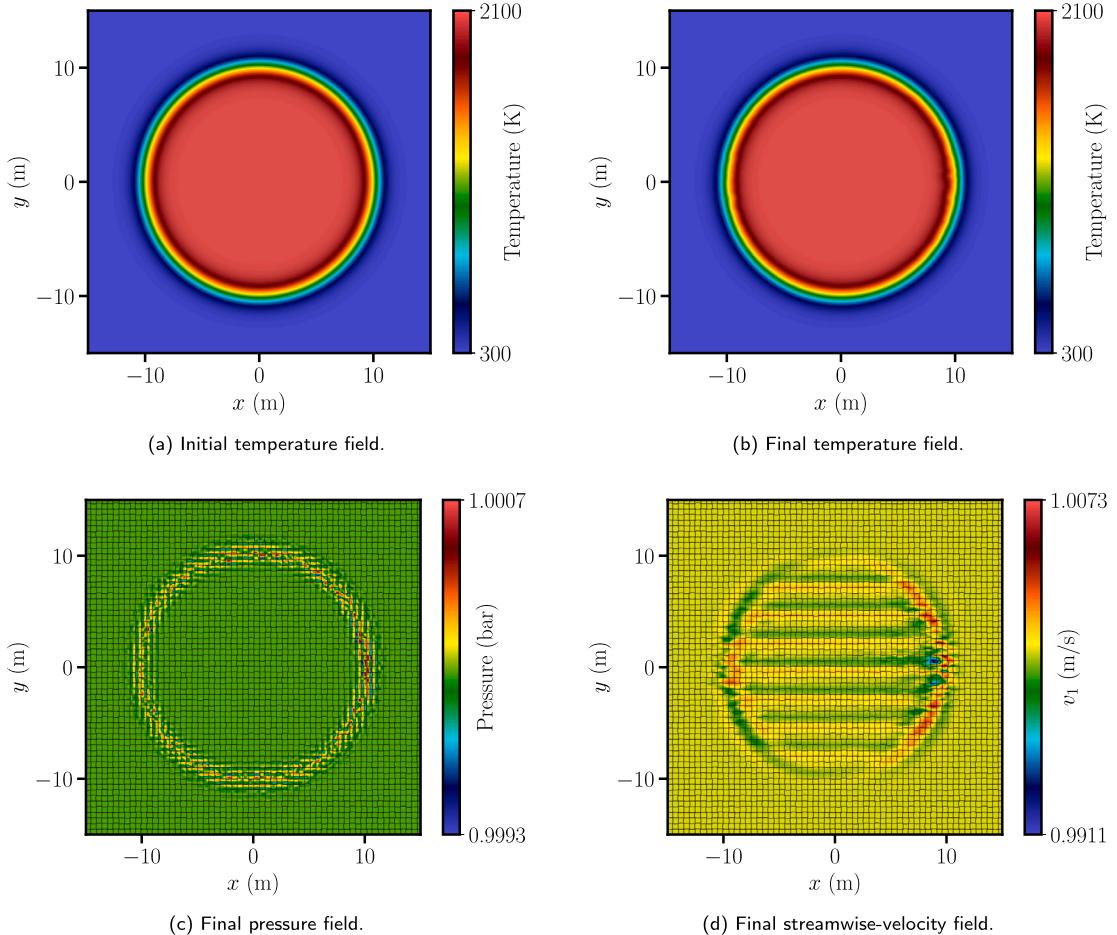


Fig. 6.2. $p = 2$ solution to two-dimensional thermal-bubble advection on a curved quadrilateral grid without artificial viscosity. The final time is $t = 50$ s, corresponding to one period. The colorbar minima and maxima for the pressure and velocity fields are the respective global minima and maxima.

equilibrium, the solution remains stable throughout the simulation. In contrast, with standard overintegration, the solver fails before $t = 0.06$ s. Note that it was previously found that spurious pressure oscillations still occur even when using entropy-stable (fully conservative) schemes and may be tied to spurious increases in thermodynamic entropy [41]. Here, with standard overintegration, such oscillations appear early in the simulation and grow rapidly in time, in turn causing substantial undershoots/overshoots in temperature and other quantities. The large-scale instabilities can cause failure by, for example, requiring a near-zero time-step size to maintain positivity and entropy boundedness or yielding temperatures at which the thermodynamic curve fits are nonsensical.

Figs. 6.2 and 6.3 display the $p = 2$ and $p = 3$ solutions, respectively. As the polynomial order increases, the profile of the thermal bubble is better maintained and the deviations from pressure and velocity equilibrium are decreased.

6.2. Two-dimensional detonation wave

This test case is the two-dimensional extension of the one-dimensional hydrogen-oxygen detonation wave diluted in Argon presented in Part I [1]. The computational domain is $\Omega = (0, 0.45) \text{ m} \times (0, 0.06) \text{ m}$, with walls at the left, right, bottom, and top boundaries. An acoustic CFL value of 0.8 is used. Although the results presented here are obtained with the SSPRK2 time integration scheme, we have confirmed that the SSPRK3 scheme does not appreciably change the results. The detonation wave moves from left to right. To perturb the detonation, two high-temperature/high-pressure circular regions,

$$\begin{aligned} C_1 &= \left\{ x \left| \sqrt{(x_1 - 0.021)^2 + (x_2 - 0.015)^2} < 0.0025 \text{ m} \right. \right\}, \\ C_2 &= \left\{ x \left| \sqrt{(x_1 - 0.022)^2 + (x_2 - 0.044)^2} < 0.0025 \text{ m} \right. \right\}, \end{aligned}$$

are placed to the right of the initial detonation wave. The initial conditions are given by

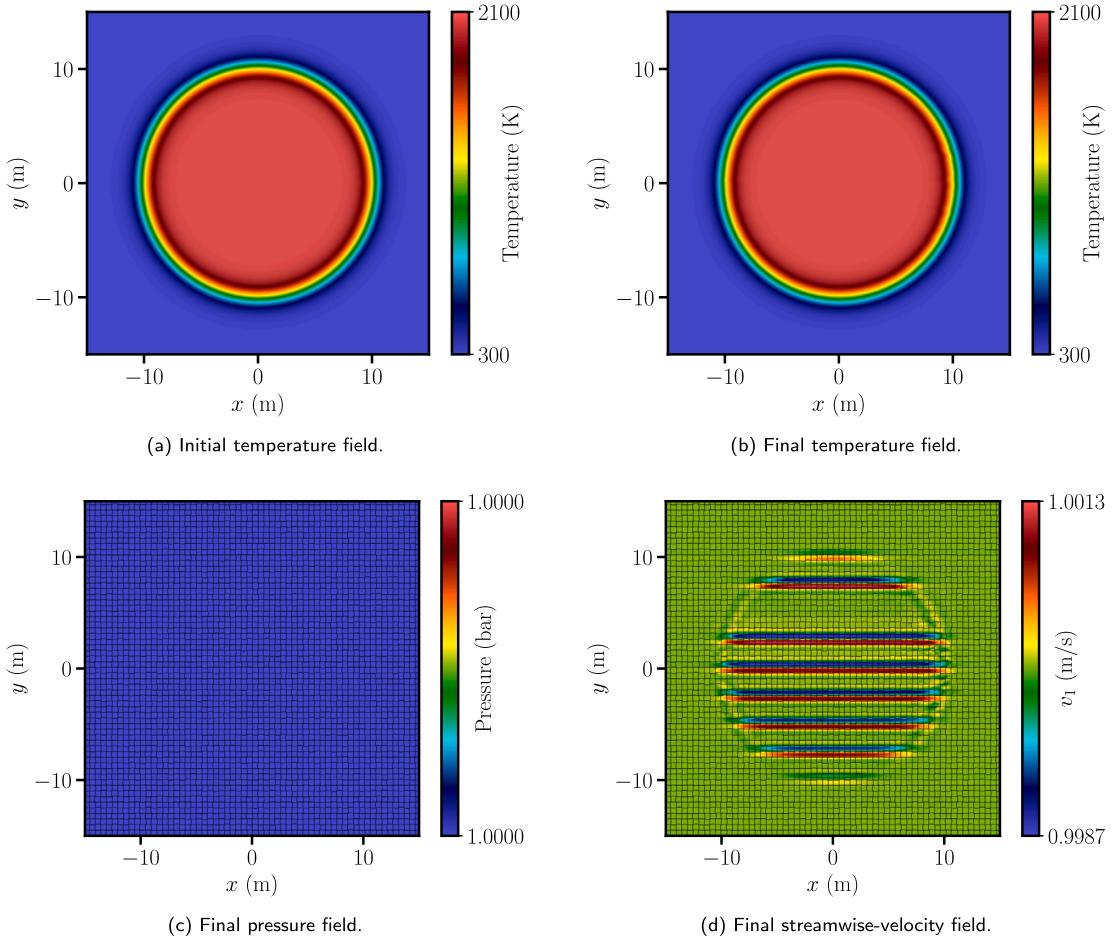


Fig. 6.3. $p = 3$ solution to two-dimensional thermal-bubble advection on a curved quadrilateral grid without artificial viscosity. The final time is $t = 50$ s, corresponding to one period. The colorbar minima and maxima for the pressure and velocity fields are the respective global minima and maxima.

$$\begin{aligned}
 (v_1, v_2) &= (0, 0) \text{ m/s}, \\
 X_{Ar} : X_{H_2O} : X_{OH} : X_{O_2} : X_{H_2} &= \begin{cases} 8 : 2 : 0.1 : 0 : 0 & x_1 < 0.015 \text{ m}, x \in C_1, x \in C_2, \\ 7 : 0 : 0 : 1 : 2 & \text{otherwise} \end{cases}, \\
 P &= \begin{cases} 5.50e5 \text{ Pa} & x_1 < 0.015 \text{ m}, x \in C_1, x \in C_2, \\ 6.67e3 \text{ Pa} & \text{otherwise} \end{cases}, \\
 T &= \begin{cases} 3500 \text{ K} & x_1 < 0.015 \text{ m}, x \in C_1, x \in C_2, \\ 300 \text{ K} & \text{otherwise} \end{cases}.
 \end{aligned} \tag{6.2}$$

No smoothing of the discontinuities in the initial conditions is performed. The thermodynamic fits and reaction-rate coefficients employed here and in the following subsection are provided in Appendix D.

This flow was also computed by Oran et al. [42], but with a slightly longer domain. Their simulations revealed a complex cellular structure wherein each cell is of size $0.055 \text{ m} \times 0.03 \text{ m}$. In addition, Houim and Kuo [43] and Lv and Ihme [36] simulated this case with a domain of height 0.03 m . In all the aforementioned simulations (not including those here), the solutions were initialized from a one-dimensional detonation.

In previous work, Johnson and Kercher [2] computed this flow with $p = 1$ and artificial viscosity for stabilization. Complex flow features, such as Kelvin-Helmholtz instabilities, pressure waves, and triple points, were well-captured, and the correct cellular structure was predicted. In particular, given that their domain height was 0.06 m , there were two cells in the vertical direction. However, a very fine mesh, with spacing $h = 9 \times 10^{-5} \text{ m}$, was required. Increasing h or p led to instabilities that could not be cured with the artificial viscosity, resulting in solver divergence. Although increasing p enhances the resolution, the solution also generally becomes more susceptible to spurious oscillations. Here, we aim to achieve robust solutions with $p \geq 1$ and relatively coarse meshes using the proposed entropy-bounded DG formulation. Gmsh [45] is used to generate unstructured triangular meshes with the following characteristic mesh sizes: $2h, 4h, 8h, 16h, 32h$, and $64h$.

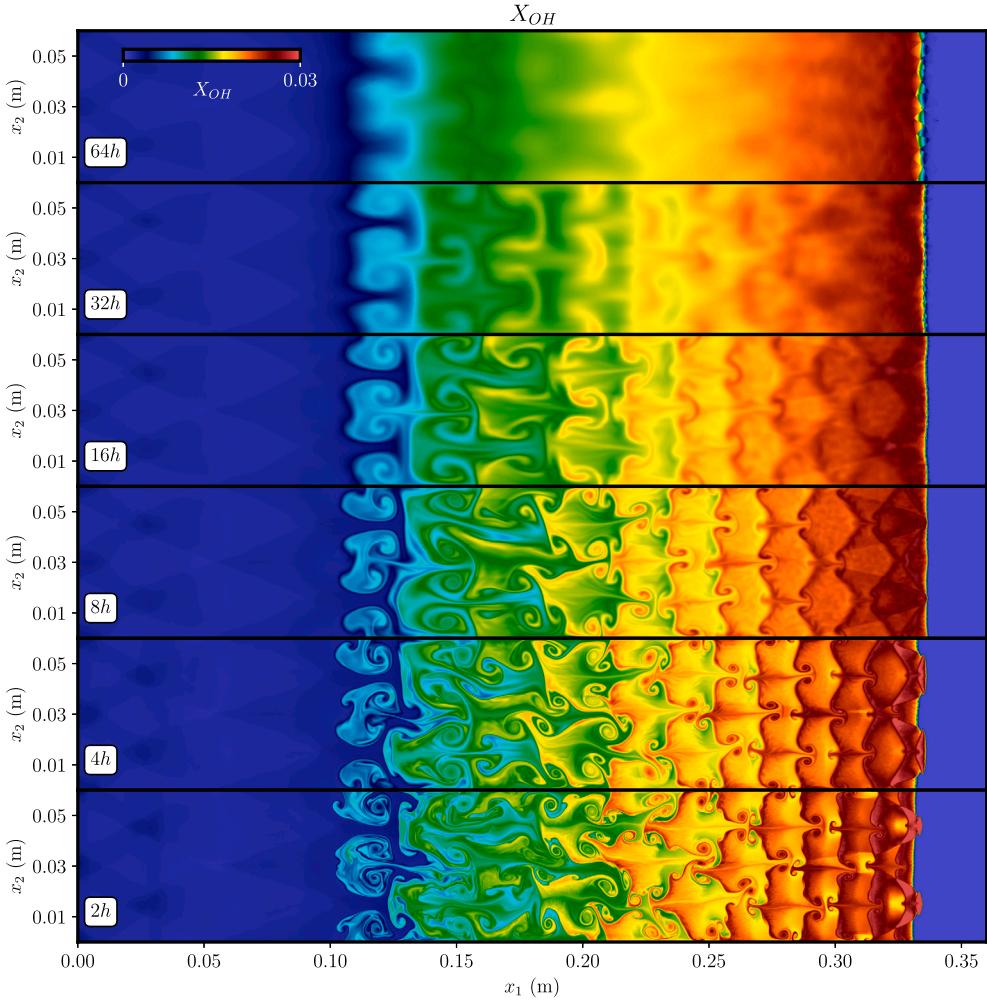


Fig. 6.4. OH mole-fraction field for a two-dimensional moving detonation wave at $t = 200 \mu\text{s}$, computed with $p = 2$ on a sequence of meshes, where $h = 9 \times 10^{-5} \text{ m}$. The initial conditions are given in Equation (6.2).

Fig. 6.4 displays the distribution of OH mole fraction obtained from $p = 2$ solutions at $t = 200 \mu\text{s}$ on a sequence of meshes. For $64h$, although the solution is stable, the post-shock flow is extremely smeared due to the exceedingly low resolution, and some spurious artifacts near the leading shock are present. Interestingly, the detonation-front location is nevertheless accurately predicted. For $32h$, despite evident smearing of the post-shock flow, the overall flow topology can be discerned. With each successive refinement of the mesh, the flow features behind the detonation front become sharper. For $4h$ and $2h$, the flow topology is very well-captured, including the triple points that connect the Mach stems and incident shock, the transverse waves traveling in the vertical directions, and the vortices that form behind the detonation front, demonstrating the ability of the developed entropy-bounded DG formulation to achieve accurate solutions to complex reacting flows. Furthermore, in all cases, the solution is stable throughout the simulation, illustrating the robustness of the proposed formulation.

Fig. 6.5 shows the maximum-pressure history, P^* , where $P^{*,j+1}(x) = \max \{ P^{j+1}(x), P^{*,j}(x) \}$, for the $p = 2$ solutions at $t = 200 \mu\text{s}$. This quantity reveals the expected diamond-like cellular structure, with two cells in the vertical direction. The $64h$ lacks any clear cellular structure due to the excessive smearing. However, detonation cells can be discerned in the $32h$ case, despite the coarse resolution. From $32h$ to $8h$, the cellular structure begins to dissipate towards the right of the domain, though it nevertheless remains intact. At $4h$ and $2h$, the detonation cells remain sharp throughout.

It remains to be seen how much smearing of the solution at and behind the detonation front is acceptable in a larger-scale configuration, although it is encouraging that the front location and cellular structure are overall well-predicted even with extremely coarse meshes. However, a thorough investigation of this matter is outside the scope of this study. Fig. 6.6 compares the solutions for $p = 1$, $p = 2$, and $p = 3$ on the $8h$ mesh, which has 123,466 cells. Some smearing of the flow field is observed in the $p = 1$ solution. Increasing p results in sharper predictions of the complex flow structures. Also included is a $p = 1$ solution on the $4h$, 488,772-cell mesh, which has slightly more degrees of freedom than the $p = 3, 8h$ solution. The flow near the detonation front is sharper in the $p = 1, 4h$ solution, while the vortical structures farther behind the detonation front are better resolved in the $p = 3, 8h$ solution. Note,

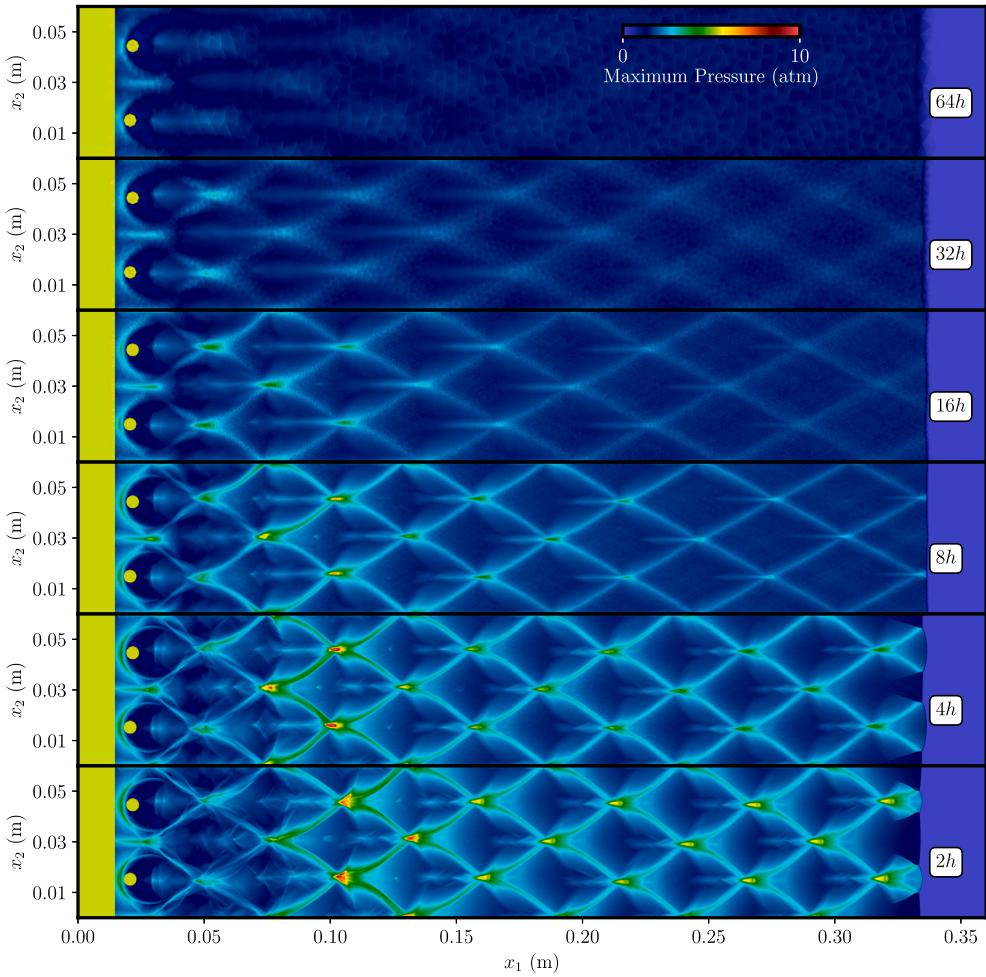


Fig. 6.5. Maximum-pressure history, P^* , where $P^{*,j+1}(x) = \max\{P^{j+1}(x), P^{*,j}(x)\}$, for a two-dimensional moving detonation wave at $t = 200 \mu\text{s}$ computed with $p = 2$ on a sequence of uniformly refined meshes, where $h = 9 \times 10^{-5} \text{ m}$. The initial conditions are given in Equation (6.2).

however, that a rigorous comparison among polynomial orders on the basis of accuracy vs. cost is left for future work; our goal here is to demonstrate (as in Figs. 6.5 and 6.6) that the proposed methodology can robustly compute accurate solutions using high-order polynomial approximations.

It is worth noting that the entropy limiter, as opposed to solely the positivity-preserving limiter, significantly improves the stability of these calculations. Specifically, throughout each simulation, the entropy limiter maintains a minimum temperature of around 300 K. Without it, however, the temperature can dip significantly below 300 K, where the curve fits for thermodynamic properties are no longer valid. Consequently, the nonlinear solver in the reaction step can slow down significantly and even stall. As an example, for $p = 2$, $64h$, the simulation with the entropy limiter is over 14 times less expensive than a corresponding simulation with only the positivity-preserving limiter. In other types of flows, these errors in temperature may pollute the solution in different ways as well. This further highlights not only the numerical difficulties of calculating multicomponent, reacting flows with realistic thermodynamics, but also the advantages of using the entropy limiter in simulations of such flows.

Additional diagnostics are obtained for the $p = 2$, $32h$ calculation as a representative example. Fig. 6.7 displays the time-step size at every step. At the beginning of the simulation, large variations in the time-step size are observed due to start-up effects and the onset of high-temperature chemical reactions. The time-step size then gradually increases and eventually oscillates around a steady value, reflecting the periodic manner in which the triple-point tracks collide with each other and reflect from the walls. At each time step, only one DGODE sub-step is required (i.e., no h -adaptivity in time is needed).

Fig. 6.8 presents the percent error in mass, energy, and atom conservation for $p = 3$, $64h$ as a representative example, calculated every $0.200 \mu\text{s}$ (for a total of 1000 samples). Specifically, N_O , N_H , and N_{Ar} denote the total numbers of oxygen, hydrogen, and argon atoms in the mixture. The error profiles oscillate around $10^{-13}\%$ due to minor numerical-precision issues. Overall, the errors remain close to machine precision, confirming that the entropy-bounded DG formulation is conservative. Fig. 6.8 also shows the error in mass conservation (calculated every time step) for a solution computed using a commonly employed clipping procedure in

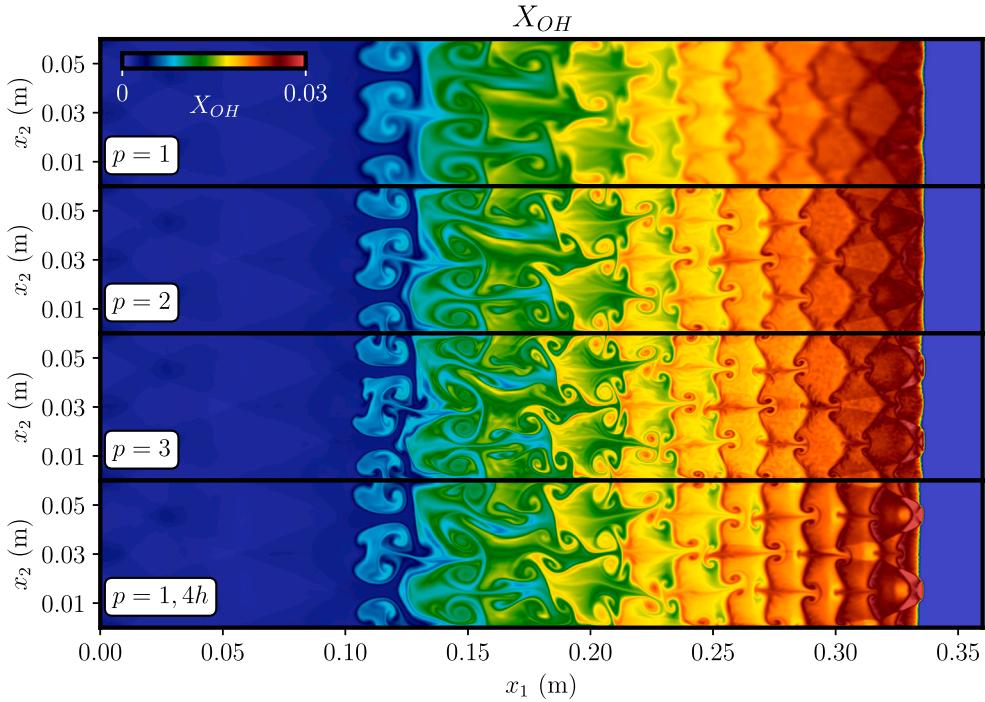


Fig. 6.6. OH mole-fraction field for a two-dimensional moving detonation wave at $t = 200 \mu\text{s}$ computed with the $8h$ mesh, where $h = 9 \times 10^{-5} \text{ m}$, using the following polynomial orders: $p = 1$, $p = 2$, and $p = 3$. Also included is a $p = 1$ solution on the $4h$ mesh. The initial conditions are given in Equation (6.2).

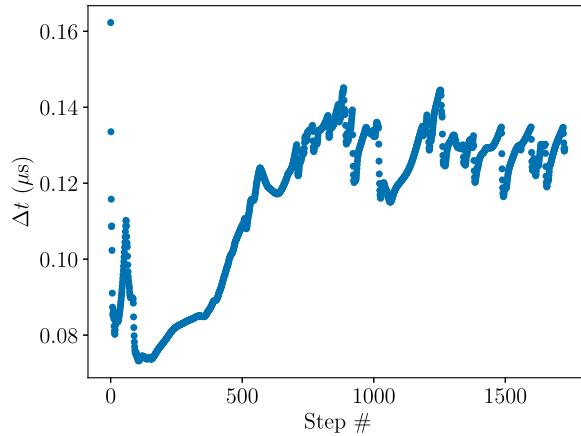


Fig. 6.7. Variation of time-step size for the $p = 2$, $32h$ calculation. The initial conditions for this two-dimensional hydrogen detonation problem are given in Equation (6.2).

which negative species concentrations are set to zero, instead of the limiting procedure described in Section 4.2.1. Although artificial viscosity is still employed, the error increases rapidly until the solver diverges.

Finally, we recompute the $p = 2$, $64h$ case with curved elements of quadratic geometric order. In particular, high-order geometric nodes are inserted at the midpoints of the vertices of each element. At interior edges, the midpoint nodes are then slightly perturbed from their initial positions. These perturbations are performed only for $x > 0.05 \text{ m}$ to guarantee identical initial conditions. We intentionally run this low-resolution case to ensure extensive activation of the limiter and aggressively test the robustness of the formulation when curved elements are employed. The distributions of OH mole fraction are given in Fig. 6.9 for both the linear and curved meshes. Though slight mesh imprinting can be observed for the curved mesh, likely due to the lower-quality elements, the two solutions are extremely similar and remain stable throughout. This result confirms that the proposed formulation is indeed compatible with nonlinear elements.

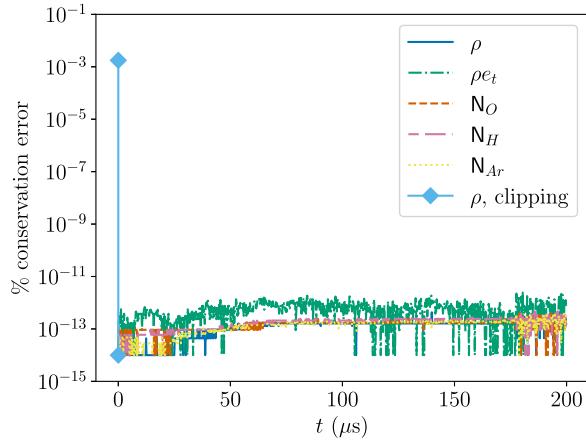


Fig. 6.8. Percent error in mass, energy, and atom conservation for $p = 3$, $64h$, where $h = 9 \times 10^{-5}$ m. The initial conditions for this two-dimensional hydrogen detonation problem are given in Equation (6.2). Also included is the error in mass conservation for a solution computed using a commonly employed clipping procedure in which negative species concentrations are set to zero instead of the limiting procedure described in Section 4.2.1.

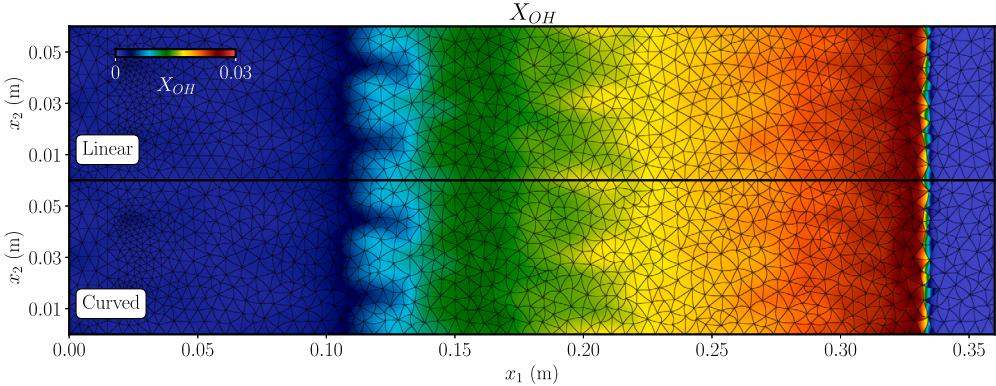


Fig. 6.9. OH mole-fraction field for a two-dimensional moving detonation wave at $t = 200$ μ s computed with $p = 2$ and $64h$, where $h = 9 \times 10^{-5}$ m, on linear and curved meshes. The curved mesh, which is of quadratic order, is obtained by inserting high-order geometric nodes into the linear mesh and then perturbing the inserted nodes. The initial conditions are given in Equation (6.2).

6.3. Three-dimensional detonation wave

This test case is the three-dimensional extension of the two-dimensional detonation wave computed in Section 6.2. The computational domain is $\Omega = (0, 0.3)$ m \times $(0, 0.03)$ m \times $(0, 0.03)$ m, with walls at all boundaries. To reduce computational and memory demands, the size of the domain in the x_1 - and x_2 -directions is smaller than in Section 6.2. An acoustic CFL value of 0.8 is used. Although the results presented here are obtained with the SSPRK2 time integration scheme, we have confirmed that the SSPRK3 scheme does not appreciably change the results. The initial conditions are given by

$$\begin{aligned} (v_1, v_2) &= (0, 0) \text{ m/s}, \\ X_{Ar} : X_{H_2O} : X_{OH} : X_{O_2} : X_{H_2} &= \begin{cases} 7 : 0 : 0 : 1 : 2 & x_1 \geq 0.015 \text{ m}, x \in C \\ 8 : 2 : 0.1 : 0 : 0 & \text{otherwise} \end{cases}, \\ P &= \begin{cases} 6.67\text{e}3 \text{ Pa} & x_1 \geq 0.015 \text{ m}, x \in C \\ 5.50\text{e}5 \text{ Pa} & \text{otherwise} \end{cases}, \\ T &= \begin{cases} 300 \text{ K} & x_1 \geq 0.015 \text{ m}, x \in C \\ 3500 \text{ K} & \text{otherwise} \end{cases}, \end{aligned} \quad (6.3)$$

where C represents a pocket of unburnt gas, similar to the two-dimensional configuration in [36], defined as

$$C = \left\{ x \left| \sqrt{(x_1 - 0.014)^2 + (x_2 - 0.015)^2 + x_3^2} < 0.005 \text{ m} \right. \right\}.$$

No smoothing of the discontinuities in the initial conditions is performed. The same type of diamond-like cellular structure is expected for this case, with one cell in the x_2 - and x_3 -directions [46,47]. Our objective with this demonstration test case is to

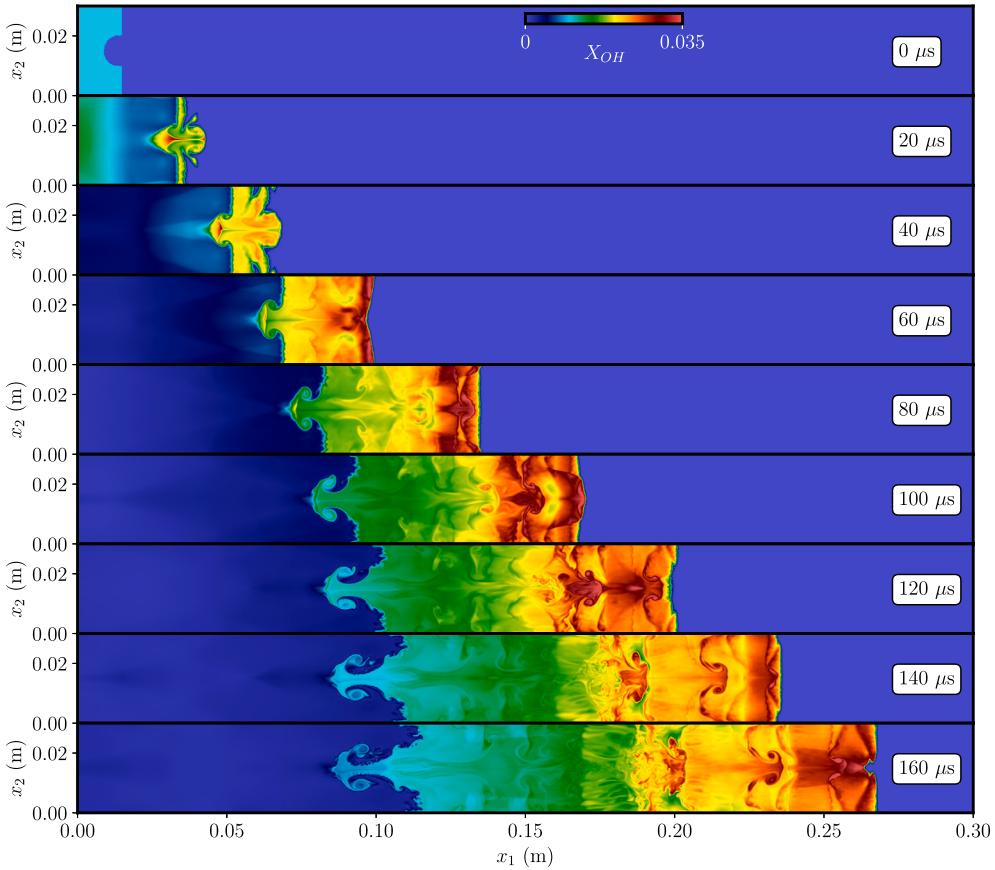


Fig. 6.10. X_{OH} distributions along the center $x_3 = 0.015$ mm plane for a three-dimensional moving detonation wave computed with $p = 2$ and $4.8h$, where $h = 9 \times 10^{-5}$ m. The initial conditions are given in Equation (6.3).

achieve an accurate solution to this complex, large-scale flow problem in a robust manner using high-order polynomials. We leverage previous studies that detail the physics of this flow configuration [46,47]. Based on the results in Section 6.2, we select $p = 2$ and a characteristic mesh spacing of $4.8h$, in order to balance accuracy with computational and memory costs. These choices result in an unstructured mesh containing approximately 15 million tetrahedral elements.

Figs. 6.10 and 6.11 display the X_{OH} and temperature distributions, respectively, along the center $x_3 = 0.015$ mm plane as the detonation front traverses the domain. At early times, transverse waves, a large induction zone, and a high-temperature, highly reactive region are present as a result of the initialization. As the detonation is established, the flow field behind the detonation front becomes characterized by unsteady, multidimensional flow features, such as vortical structures, wave interactions and reflections, and Kelvin-Helmholtz instabilities. In the vicinity of the detonation front, transverse waves traveling in the vertical directions and triple points can be observed. Some small-scale numerical instabilities are present, but these can be damped with improvements to the artificial-viscosity formulation (e.g., smooth artificial viscosity [20]) or more complex limiting strategies (outside the scope of this paper). Furthermore, the small-scale instabilities do not impede the temporal advancement of the solution or cause solver divergence.

Fig. 6.12 displays X_{OH} and temperature distributions along various x_1x_2 -planes at $t = 176$ μ s, shortly before the detonation front collides with the wall. The distributions along the corresponding x_1x_3 -planes are qualitatively very similar and therefore omitted for brevity. In the post-shock region, X_{OH} and temperature generally decrease with distance from the shock front. Nevertheless, small pockets of low OH mole fraction, surrounded by regions of higher OH mole fraction, can be observed. These results highlight the multidimensional nature of this flow and further illustrate that the complex flow topology is well-captured using the proposed formulation.

Fig. 6.13 presents several instantaneous pressure isosurfaces colored by the quantity $x_1 - \bar{x}_1$, where \bar{x}_1 is the mean x_1 -coordinate of the given isosurface, in order to illustrate the structure of the detonation front, which is characterized by two orthogonal, two-dimensional waves. Two vertical triple-point lines and two horizontal triple-point lines move in-phase with each other in the horizontal and vertical directions, respectively, indicating an in-phase rectangular mode [47]. Each pair of triple-point lines propagates outwards, collides with the boundary walls, and then reflects inwards. Subsequently, they collide with each other and then reflect outwards, continuing in a periodic manner.

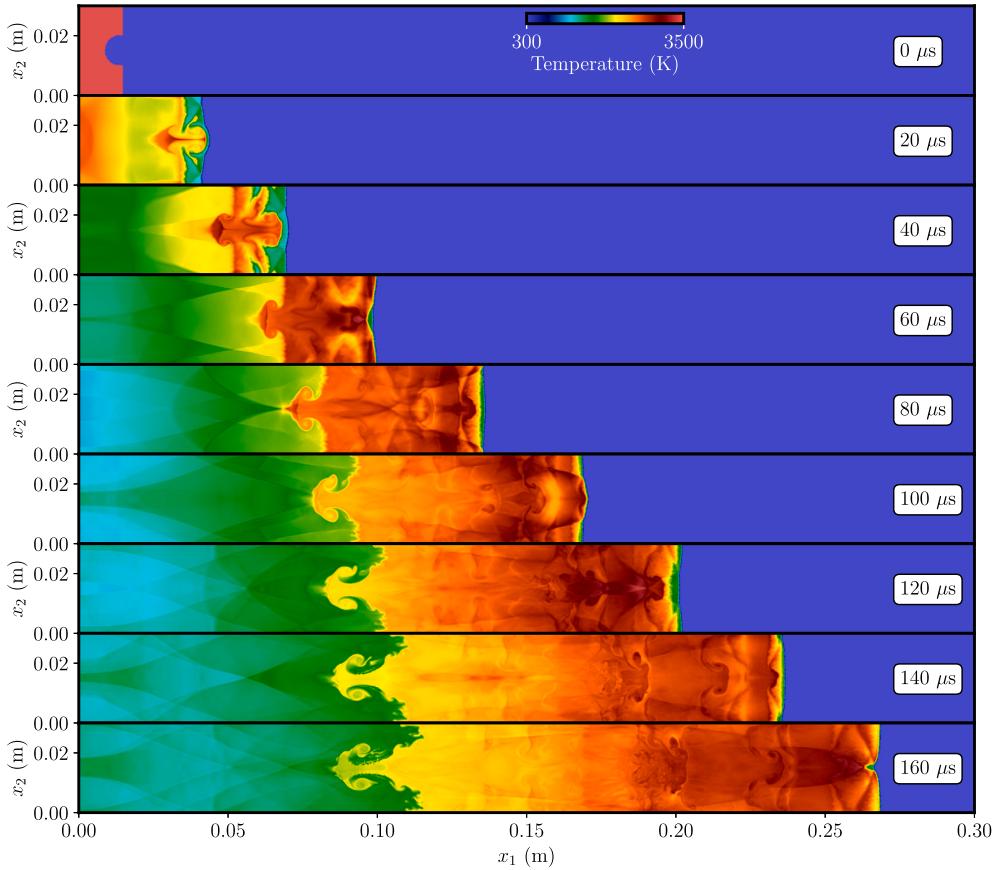


Fig. 6.11. Temperature distributions along the center $x_3 = 0.015$ mm plane for a three-dimensional moving detonation wave computed with $p = 2$ and $4.8h$, where $h = 9 \times 10^{-5}$ m. The initial conditions are given in Equation (6.3).

Distributions of maximum-pressure history along various x_1x_2 -planes and x_1x_3 -planes at $t = 176$ μ s are given in Fig. 6.14. Approximately two and a half cells are observed in the region $x_1 > 0.15$ mm. High-pressure explosions occur when the triple-point lines collide with each other and with the corners. “Slapping” waves result from reflections of the triple-point lines, indicated with the white arrow in Fig. 6.14a (top) [47]. The x_1x_2 -distributions are nearly identical to the corresponding x_1x_3 -distributions. Fig. 6.15 shows isosurfaces of maximum-pressure history for $x_1 \in [0.236, 0.292]$ m, which illustrate, from a three-dimensional perspective, not only the temporal evolution of triple-point-line intersections, but also the slapping waves along the walls and the strong, high-pressure explosions. Overall symmetry in the x_2 - and x_3 -directions is observed. Figs. 6.14 and 6.15 further confirm that the detonation front is characterized by an in-phase rectangular mode.

7. Concluding remarks

In this second part of our two-part paper, we introduced a positivity-preserving, entropy-bounded, multidimensional DG methodology for the chemically reacting, compressible Euler equations, extending the one-dimensional version presented in Part I [1]. Compared to current multidimensional positivity-preserving and/or entropy-bounded DG schemes in the literature, restrictions on the quadrature rules, numerical flux function, polynomial order of the geometric approximation, and physical modeling are relaxed. In particular, the formulation is compatible with arbitrary, curved elements, any invariant-region-preserving flux, and mixtures of thermally perfect gases. A simple linear-scaling limiter enforces nonnegative species concentrations, positive density, positive pressure, and bounded entropy. Artificial viscosity aids in suppressing small-scale instabilities not eliminated by the linear scaling. We discussed how to maintain compatibility with the strategies introduced in [2] to maintain pressure equilibrium and avoid generating spurious pressure oscillations.

We first applied the formulation to the two-dimensional advection of a thermal bubble. Pressure and velocity equilibrium were shown to be maintained across various polynomial orders on curved grids. The formulation was then applied to complex moving detonation waves in two and three dimensions. In the two-dimensional case, a variety of mesh sizes and polynomial orders was considered. In [2], a linear polynomial approximation of the solution and a very fine mesh were required to obtain a stable solution. With the developed formulation, we achieved robust and accurate solutions using high-order polynomials and a relatively coarse mesh. Increasing the polynomial order resulted in sharper predictions of the rich flow topology. Mass, total energy, and atomic

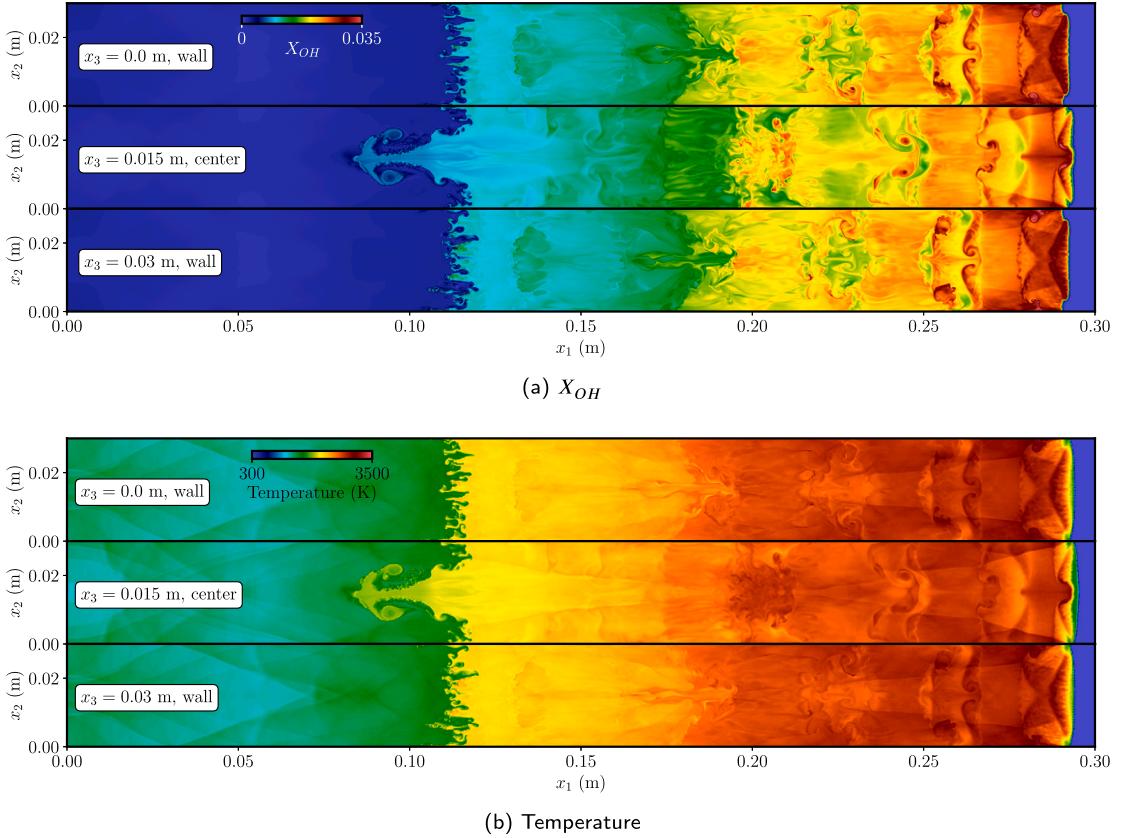


Fig. 6.12. X_{OH} and temperature distributions along various x_1x_2 -planes at $t = 176 \mu\text{s}$ for a three-dimensional moving detonation wave computed with $p = 2$ and $4.8h$, where $h = 9 \times 10^{-5} \text{ m}$. The initial conditions are given in Equation (6.3).

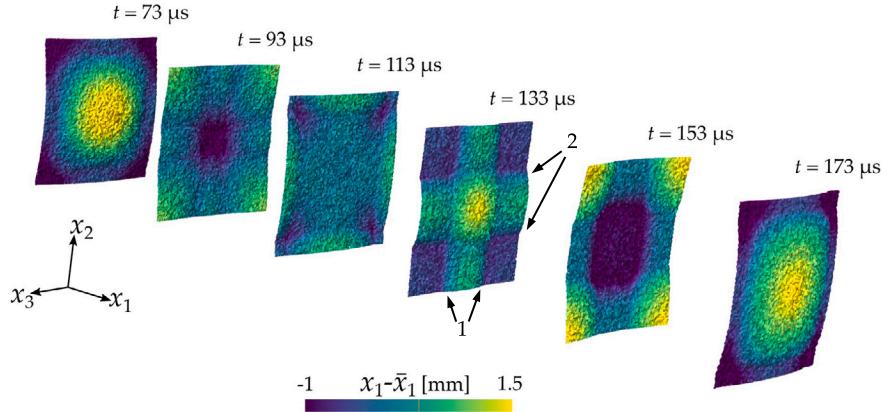


Fig. 6.13. Instantaneous pressure isosurfaces colored by the quantity $x_1 - \bar{x}_1$, where \bar{x}_1 is the mean x_1 -coordinate of the given isosurface, at various times for a three-dimensional moving detonation wave computed with $p = 2$ and $4.8h$, where $h = 9 \times 10^{-5} \text{ m}$. The “1” arrows indicate the vertical triple-point lines, and the “2” arrows indicate the horizontal triple-point lines. The initial conditions are given in Equation (6.3).

elements were shown to be conserved. An important finding is that the entropy limiter was crucial for the coarser two-dimensional detonation problems; without it (i.e., only the positivity-preserving limiter was applied), the nonlinear solver during the reaction step can slow down substantially or even stall, due to the large undershoots in temperature. In the three-dimensional detonation test case, we demonstrated that our methodology can compute accurate and robust solutions to large-scale reacting-flow problems. Future work will entail the simulation of larger-scale detonation applications involving more complex geometries.

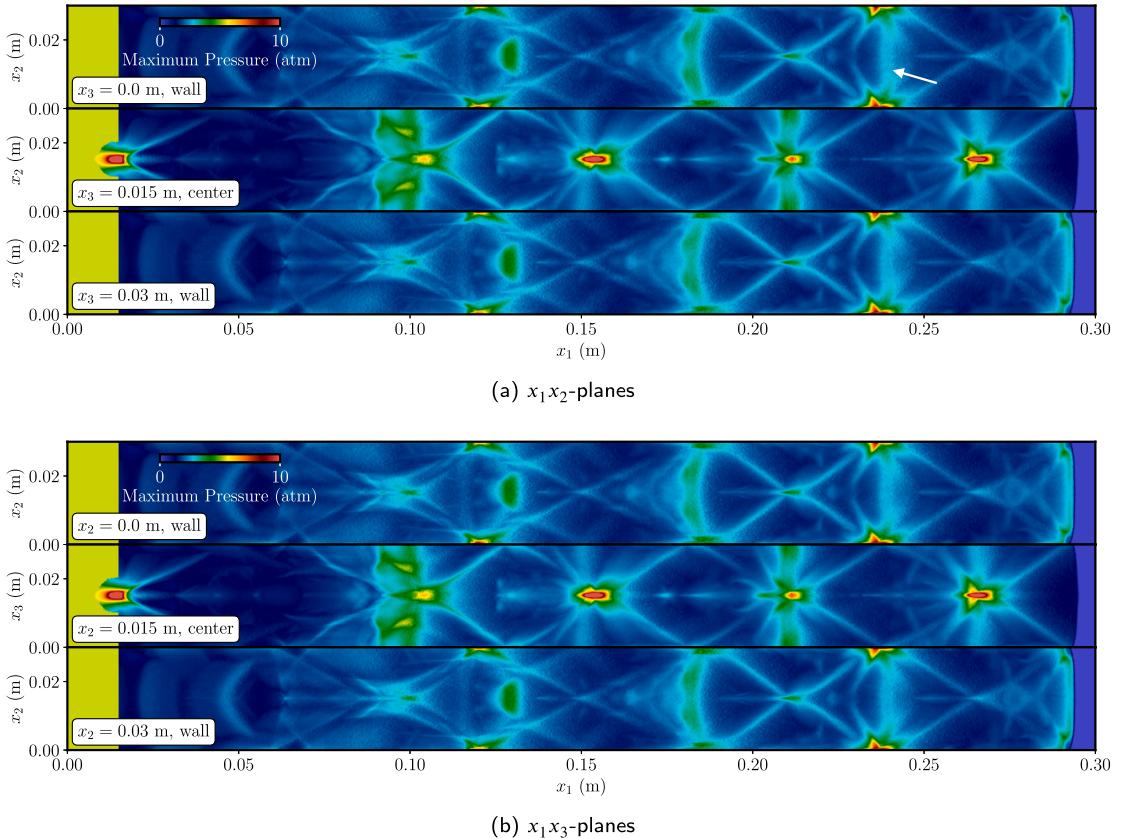


Fig. 6.14. Distributions of maximum-pressure history along various x_1x_2 -planes and x_1x_3 -planes at $t = 176 \mu\text{s}$ for a three-dimensional moving detonation wave computed with $p = 2$ and $4.8h$, where $h = 9 \times 10^{-5} \text{ m}$. The white arrow in Fig. 6.14a (top) indicates a “slapping” wave. The initial conditions are given in Equation (6.3).



Fig. 6.15. Isosurfaces of maximum-pressure history at $t = 176 \mu\text{s}$ for $x_1 \in [0.236, 0.292] \text{ m}$ for a three-dimensional moving detonation wave computed with $p = 2$ and $4.8h$, where $h = 9 \times 10^{-5} \text{ m}$. The isosurfaces are colored by x_1 -position. Each of the “1” arrows indicates a slapping wave, while the “2” arrow indicates the high-pressure explosion resulting from triple-point-line collisions. The initial conditions are given in Equation (6.3).

CRediT authorship contribution statement

Eric J. Ching: Conceptualization, Investigation, Methodology, Software, Writing – original draft. **Ryan F. Johnson:** Conceptualization, Investigation, Methodology, Software, Writing – review & editing. **Andrew D. Kercher:** Conceptualization, Methodology, Software, Writing – review & editing.

Table 1

Percentage of RK stages in which the positivity-preserving limiter and entropy limiter are activated without over-integration. Here, the positivity-preserving limiter corresponds to Steps 1 to 3 in Section 4.2.1, and the entropy limiter corresponds to Step 4.

	h	$h/2$	$h/4$	$h/8$	$h/16$
Positivity-preserving limiter	40.8%	51.9%	38.8%	0.014%	0.0034%
Entropy limiter	18.3%	36.9%	0.61%	0%	0%

Table 2

Percentage of RK stages in which the positivity-preserving limiter and entropy limiter are activated with over-integration. Here, the positivity-preserving limiter corresponds to Steps 1 to 3 in Section 4.2.1, and the entropy limiter corresponds to Step 4.

	h	$h/2$	$h/4$	$h/8$	$h/16$
Positivity-preserving limiter	35.2%	51.0%	64.3%	0.012%	0.0026%
Entropy limiter	13.8%	24.7%	0.22%	0%	0%

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 will be made available on request.

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Appendix A. Effect of over-integration on limiting frequency

We investigate the effect of over-integration on the frequency of limiter activation in a one-dimensional test case involving the advection of a low-density Gaussian wave. This test case was originally introduced by Trojak and Dzanic [48] and computed in Part I [1], where optimal convergence was observed. For brevity, only $p = 2$ is considered. A periodic domain $\Omega = [-0.5, 0.5]$ m is initialized in nondimensional form as

$$\begin{aligned} v &= 1, \\ Y_1 &= \frac{1}{2} [\sin(2\pi x) + 1], \\ Y_2 &= 1 - Y_1, \\ \rho &= \exp(-\sigma x^2) + 4\epsilon, \\ P &= 2\epsilon, \end{aligned} \tag{A.1}$$

where $\sigma = 500$ and $\epsilon = 10^{-12}$. The thermodynamic relations for the two fictitious species considered here are given by

$$\begin{aligned} \frac{W_1 c_{p,1}(T)}{R^0} &= 3.5, \quad \frac{W_1 h_1(T)}{R^0} = 3.5 T_r \hat{T}, \quad \frac{W_1 s_1^o}{R^0} = 3.5 \ln \hat{T}, \\ \frac{W_2 c_{p,2}(T)}{R^0} &= 2.491, \quad \frac{W_2 h_2(T)}{R^0} = 2.491 T_r \hat{T}, \quad \frac{W_2 s_2^o}{R^0} = 2.491 \ln \hat{T}. \end{aligned}$$

Five element sizes are considered: h , $h/2$, $h/4$, $h/8$, and $h/16$, where $h = 0.04$. The solution is integrated in time using the SSPRK3 time stepping scheme. The L^2 error after one advection period is calculated in terms of the following normalized state variables:

$$\widehat{\rho v}_k = \frac{1}{\sqrt{\rho_r P_r}} \rho v_k, \quad \widehat{\rho e}_t = \frac{1}{P_r} \rho e_t, \quad \widehat{C}_i = \frac{R^0 T_r}{P_r} C_i,$$

where $\rho_r = 1 \text{ kg} \cdot \text{m}^{-3}$, $P_r = 101325 \text{ Pa}$, and $T_r = 1000 \text{ K}$. Tables 1 and 2 provide the percentage of RK stages in which the positivity-preserving limiter and the entropy limiter are activated without and with over-integration, respectively. Note that the L^2 errors obtained with and without over-integration are nearly identical (not shown for brevity). In general, the percentage of limiting

decreases with over-integration, apart from the activation of the positivity-preserving limiter in the $h/4$ case. One likely reason for this higher frequency of limiter activation is that the number of points in \mathcal{D}_k increases in the case of over-integration.

Appendix B. Supporting lemma

In the following, let $\Delta\mathcal{F} \in \mathbb{R}^m$ denote the quantity

$$\Delta\mathcal{F} = (\Delta\mathcal{F}_{\rho v}, \Delta\mathcal{F}_{\rho e_t}, \Delta\mathcal{F}_{C_1}, \dots, \Delta\mathcal{F}_{C_{n_s}})^T,$$

where $\Delta\mathcal{F}_{\rho v} \in \mathbb{R}^d$ and the remaining entries are in \mathbb{R} . The proof below is similar to that in [34, Lemma 6].

Lemma 6. Assume that $y = (\rho v, \rho e_t, C_1, \dots, C_{n_s})^T$ is in \mathcal{G} . Then $\check{y} = y - \alpha^{-1}\Delta\mathcal{F}$, where $\alpha > 0$, is also in \mathcal{G} under the following conditions:

$$\alpha > \alpha^*(y, \Delta\mathcal{F}) = \max \left\{ \max_{i=1, \dots, n_s} \frac{\mathcal{F}_{C_i} \cdot n}{C_i}, \alpha_T|_{(y, \Delta\mathcal{F})}, 0 \right\}, \quad (\text{B.1})$$

where

$$\alpha_T = \begin{cases} \frac{-b + \sqrt{b^2 - 4\rho^2 u g}}{2\rho^2 u}, & b^2 - 4\rho^2 u g \geq 0 \\ 0, & \text{otherwise} \end{cases}, \quad (\text{B.2})$$

$$b = -\rho e_t \mathbf{M} - \rho \Delta\mathcal{F}_{\rho e_t} + \rho v \cdot \Delta\mathcal{F}_{\rho v} + 2\rho u_0 \mathbf{M}, \text{ and } g = \mathbf{M} \Delta\mathcal{F}_{\rho e_t} - \frac{1}{2} |\Delta\mathcal{F}_{\rho v}|^2 - u_0 \mathbf{M}^2, \text{ and } \mathbf{M} = \sum_{i=1}^{n_s} W_i \Delta\mathcal{F}_{C_i}.$$

Proof. $\check{y} = y - \alpha^{-1}\Delta\mathcal{F}$ can be expanded as

$$\begin{aligned} \check{y} &= (\check{\rho}v, \check{\rho}e_t, \check{C}_1, \dots, \check{C}_{n_s})^T \\ &= (\rho v - \alpha^{-1}\Delta\mathcal{F}_{\rho v}, \rho e_t - \alpha^{-1}\Delta\mathcal{F}_{\rho e_t}, C_1 - \alpha^{-1}\Delta\mathcal{F}_{C_1}, \dots, C_{n_s} - \alpha^{-1}\Delta\mathcal{F}_{C_{n_s}})^T. \end{aligned}$$

First, we focus on positivity of density and species concentrations. For the i th species, $C_i - \alpha^{-1}\mathcal{F}_{C_i} \cdot n > 0$ if $\alpha > \max \left\{ \left(\mathcal{F}_{C_i} \cdot n \right) / C_i, 0 \right\}$. Accounting for all species yields

$$\alpha > \max \left\{ \max_{i=1, \dots, n_s} \frac{\mathcal{F}_{C_i} \cdot n}{C_i}, 0 \right\}.$$

Density is then also positive.

Next, we focus on positivity of temperature. For a given $y = (\rho v, \rho e_t, C_1, \dots, C_{n_s})^T$, let $Z(y)$ be defined as

$$Z(y) = \rho^2 u^*(y) = \rho(y) \rho e_t - |\rho v|^2 / 2 - \rho^2 u_0(y). \quad (\text{B.3})$$

Note that if $Z(y) > 0$, then $T(y) > 0$. $Z(\check{y})$ can be expressed as

$$\begin{aligned} Z(y - \alpha^{-1}\Delta\mathcal{F}) &= \sum_{i=1}^{n_s} W_i \left(C_i - \alpha^{-1}\Delta\mathcal{F}_{C_i} \right) \left(\rho e_t - \alpha^{-1}\Delta\mathcal{F}_{\rho e_t} \right) \\ &\quad - \frac{1}{2} \left| \rho v - \alpha^{-1}\Delta\mathcal{F}_{\rho v} \right|^2 - \left[\sum_{i=1}^{n_s} W_i \left(C_i - \alpha^{-1}\Delta\mathcal{F}_{C_i} \right) \right]^2 u_0, \end{aligned}$$

which, after multiplying both sides by α^2 , can be rewritten as

$$\alpha^2 Z(y - \alpha^{-1}\Delta\mathcal{F}) = \rho^2 u \alpha^2 - b \alpha + g, \quad (\text{B.4})$$

where $b = -\rho e_t \mathbf{M} - \rho \Delta\mathcal{F}_{\rho e_t} + \rho v \cdot \Delta\mathcal{F}_{\rho v} + 2\rho u_0 \mathbf{M}$, $g = \mathbf{M} \Delta\mathcal{F}_{\rho e_t} - \frac{1}{2} |\Delta\mathcal{F}_{\rho v}|^2 - u_0 \mathbf{M}^2$, and $\mathbf{M} = \sum_{i=1}^{n_s} W_i \Delta\mathcal{F}_{C_i}$. Setting the RHS of Equation (B.4) equal to zero yields a quadratic equation with α as the unknown. Since $\rho^2 u$ is positive, the quadratic equation is convex. As such, if $b^2 - 4\rho^2 u g < 0$, then no real roots exist, and $Z(y - \alpha^{-1}\Delta\mathcal{F}) > 0$ for all $\alpha \neq 0$; otherwise, at least one real root exists, in which case a sufficient condition to ensure $Z(y - \alpha^{-1}\Delta\mathcal{F}) > 0$ is $\alpha > \alpha_0$, where α_0 is given by

$$\alpha_0 = \max \left\{ \frac{-b + \sqrt{b^2 - 4\rho^2 u g}}{2\rho^2 u}, 0 \right\}. \quad \square$$

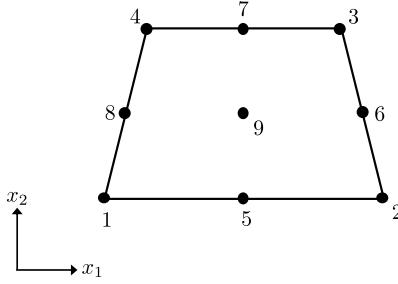


Fig. C.1. Illustrative nodal set for \check{y}_κ on two-dimensional quadrilateral elements.

Remark 7. If $\Delta\mathcal{F}_{C_i} = 0$, for all i , then α^* in (B.1) can be simplified to

$$\alpha^*(y, \Delta\mathcal{F}) = \max \left\{ \alpha_T|_{(y, \Delta\mathcal{F})}, 0 \right\}.$$

Appendix C. Alternative approach with over-integration

Here, we present an alternative approach to guarantee $\bar{y}_\kappa^{j+1} \in \mathcal{G}_{s_b}$, even when over-integration with the modified flux interpolation (3.8) for preserving pressure equilibrium is employed. The main idea is to construct a separate polynomial, denoted \check{y}_κ , that satisfies the following:

$$\begin{aligned} \bar{y}_\kappa &= \bar{y}_\kappa, \\ \check{y}_\kappa \left(\xi \left(\zeta_l^{(f)} \right) \right) &= \tilde{y}_\kappa \left(\xi \left(\zeta_l^{(f)} \right) \right), \quad f = 1, \dots, n_f, \quad l = 1, \dots, n_{q,f}^\partial, \end{aligned}$$

such that the scheme satisfied by the element averages becomes

$$\begin{aligned} \bar{y}_\kappa^{j+1} &= \bar{y}_\kappa^j - \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \frac{\Delta t v_{f,l}^\partial}{|\kappa|} \mathcal{F}^+ \left(\tilde{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \tilde{y}_{\kappa^{(f)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \\ &= \bar{y}_\kappa^j - \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \frac{\Delta t v_{f,l}^\partial}{|\kappa|} \mathcal{F}^+ \left(\check{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \tilde{y}_{\kappa^{(f)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \\ &= \sum_{v=1}^{n_q} \theta_v \check{y}_\kappa^j \left(\xi_v \right) + \sum_{f=1}^{n_f} \sum_{l=1}^{n_{q,f}^\partial} \left[\theta_{f,l} \check{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right) - \frac{\Delta t v_{f,l}^\partial}{|\kappa|} \mathcal{F}^+ \left(\tilde{y}_\kappa^j \left(\xi \left(\zeta_l^{(f)} \right) \right), \tilde{y}_{\kappa^{(f)}}^j \left(\xi \left(\zeta_l^{(f)} \right) \right), n \left(\zeta_l^{(f)} \right) \right) \right] \\ &= \sum_{v=1}^{n_q} \theta_v \check{y}_\kappa^j \left(\xi_v \right) + \sum_{f=1}^{n_f-1} \sum_{l=1}^{n_{q,f}^\partial} \theta_{f,l} \check{A}_{f,l} + \sum_{l=1}^{N-1} \theta_{n_f,l} \check{B}_l + \theta_{n_f,N} \check{C}, \end{aligned} \tag{C.1}$$

where the definitions of $\check{A}_{f,l}$, \check{B}_l , and \check{C} can be deduced based on Section 4.2. Thus, \bar{y}_κ^{j+1} can be written as a convex combination of three-point systems and pointwise values, and an analogous version of Theorem 1 holds. The degree of \check{y}_κ may be different from that of y_κ , provided that the volume quadrature rule in Equation (C.1) is sufficiently accurate. First, we propose a strategy to construct \check{y}_κ on two-dimensional quadrilateral elements. As an illustrative example, consider the Gauss-Lobatto nodal set for \check{y}_κ displayed in Fig. C.1. Nodes 1 to 8 comprise the integration points used in the surface integrals in Equation (C.1), whereas Node 9 serves as a degree of freedom to ensure $\bar{y}_\kappa = \check{y}_\kappa$. The coefficients of \check{y}_κ are specified as

$$\begin{aligned} \check{y}_\kappa(x_k) &= \tilde{y}_\kappa(x_k), \quad k = 1, \dots, 8, \\ \check{y}_\kappa(x_9) &= \frac{\bar{y}_\kappa |\kappa| - \sum_{v=1}^{n_q} |J_\kappa(\xi_v)| w_v \sum_{k=1}^8 \tilde{y}_\kappa(x_k) \varphi_k(\xi_v)}{\sum_{v=1}^{n_q} |J_\kappa(\xi_v)| w_v \varphi_9(\xi_v)} \\ &= \tilde{y}_\kappa(x_9) + \frac{\sum_{v=1}^{n_q} |J_\kappa(\xi_v)| w_v \left[\sum_{i=1}^{n_b} y_\kappa(x_i) \phi_i(\xi_v) - \sum_{k=1}^9 \tilde{y}_\kappa(x_k) \varphi_k(\xi_v) \right]}{\sum_{v=1}^{n_q} |J_\kappa(\xi_v)| w_v \varphi_9(\xi_v)}. \end{aligned}$$

In general, $\check{y}_\kappa(x_9)$ is not expected to differ significantly from $\tilde{y}_\kappa(x_9)$ or $y_\kappa(x_9)$; in fact, $\check{y}_\kappa(x_9)$ reduces to $\tilde{y}_\kappa(x_9)$ as the discrepancies between $y_\kappa(x)$ and $\check{y}_\kappa(x)$ vanish. If necessary, the limiting procedure in Section 4.2.1 is applied to ensure that $\check{y}_\kappa(x) \in \mathcal{G}_{s_b}$, $\forall x \in D_\kappa$. Note that it is possible for the limiter to modify the pressure at the nodes; nevertheless, as observed in the thermal-bubble test case

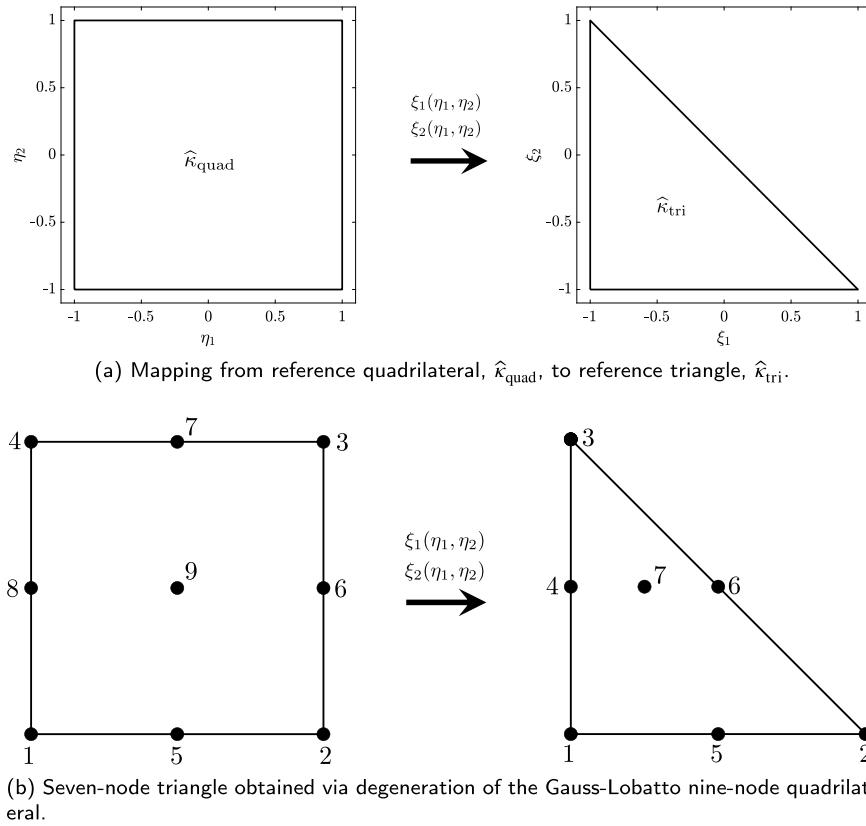


Fig. C.2. Transformation between reference quadrilateral and reference triangle, as well as an illustrative nodal set for \check{y}_k on triangular elements.

in Part I [1], the limiter typically will not destroy pressure equilibrium or cause large-scale pressure oscillations in smooth regions of the flow. This will likely remain true when limiting $\check{y}_k^j(x)$, in part because $y_k^j(x)$ will already have been limited.

Constructing \check{y}_k on two-dimensional triangular elements can be done in a similar manner, provided that the nodal set for \check{y}_k includes the surface integration points and the corresponding surface quadrature rules have positive weights. However, typical $p = 2$ nodal sets, which have six nodes, do not include any interior nodes; therefore, there are no degrees of freedom to ensure $\check{y}_k = \bar{y}_k$. Here, we propose a more general strategy that makes use of the transformation between the reference quadrilateral, $\hat{\kappa}_{\text{quad}}$, which is a bi-unit square, and the reference triangle, $\hat{\kappa}_{\text{tri}}$, which is an isosceles right triangle with side length of two, as shown in Fig. C.2a [12,13]. The bi-unit square can be mapped to the reference triangle as

$$\xi_1 = \frac{(1 + \eta_1)(1 - \eta_2)}{2} - 1,$$

$$\xi_2 = \eta_2,$$

where $\eta \in \mathbb{R}^2$ are the reference coordinates of $\hat{\kappa}_{\text{quad}}$ and $\xi \in \mathbb{R}^2$ are the reference coordinates of $\hat{\kappa}_{\text{tri}}$. The inverse mapping is given by

$$\eta_1 = 2 \frac{1 + \xi_1}{1 - \xi_2} - 1,$$

$$\eta_2 = \xi_2.$$

Consider the seven-node triangle in Fig. C.2b, obtained by degeneration of the Gauss-Lobatto nine-node quadrilateral [49]. Specifically, Nodes 3, 4, and 7 of $\hat{\kappa}_{\text{quad}}$ are coalesced into Node 3 of $\hat{\kappa}_{\text{tri}}$, such that

$$\begin{aligned} \check{y}_k(\eta) &= \sum_{\substack{k=1 \\ k \neq 3,4,7}}^9 \check{y}_k(x_k) \varphi_k(\eta) + \check{y}_k(x_3) [\varphi_3(\eta) + \varphi_4(\eta) + \varphi_7(\eta)], \\ &= \sum_{k=1}^7 \check{y}_k(x_k) \check{\varphi}_k(\eta), \end{aligned}$$

Table 3
Coefficients for the thermodynamic fits for each species.

Species	a_{i0}	a_{i1}	a_{i2}	a_{i3}	a_{i4}	a_{i5}	a_{i6}
O	2.72	-3.61E-01	2.01E-01	-4.53E-02	3.79E-03	29.17	3.98
O ₂	3.17	1.47	-5.96E-01	1.25E-01	-9.78E-03	-1.01	6.19
H	2.50	0	0	0	0	25.47	-0.45
H ₂	3.38	9.77E-02	2.56E-01	-7.59E-02	6.63E-03	-1.02	-3.6
OH	3.58	-2.13E-01	4.84E-01	-1.44E-01	1.30E-02	3.42	1.74
HO ₂	3.41	3.22	-1.12	2.03E-01	-1.50E-02	0.33	7.24
H ₂ O	3.57	1.37	1.71E-01	-1.31E-01	1.46E-02	-30.21	1.94
H ₂ O ₂	3.70	5.62	-2.22	4.17E-01	-2.96E-02	-17.68	5.57
N ₂	3.23	8.55E-01	-1.51E-01	-6.39E-03	2.68E-03	-1.	4.42
Ar	2.50	0	0	0	0	-0.75	4.37

where $\{\varphi_1, \dots, \varphi_9\}$ is ordered according to the $\hat{\kappa}_{\text{quad}}$ node numbering and $\{\check{\varphi}_1, \dots, \check{\varphi}_7\}$ is ordered according to the $\hat{\kappa}_{\text{tri}}$ node numbering. Note that $\check{\varphi}_7$ is equal to $\varphi_3 + \varphi_4 + \varphi_7$. Nodes 1 to 6 of $\hat{\kappa}_{\text{tri}}$ make up the Gauss-Lobatto points used in the surface integrals. $\bar{\check{y}}_\kappa$ can be computed using a sufficiently accurate quadrature rule for quadrilaterals as [13]

$$\begin{aligned}\bar{\check{y}}_\kappa &= \frac{1}{|\kappa|} \int_{\kappa} \check{y}_\kappa(x) dx = \frac{1}{|\kappa|} \int_{\hat{\kappa}_{\text{tri}}} \check{y}_\kappa(\xi) |J_\kappa(\xi)| d\xi \\ &= \frac{1}{|\kappa|} \int_{\hat{\kappa}_{\text{quad}}} \check{y}_\kappa(\eta) |J_\kappa(\xi(\eta))| |J_{\hat{\kappa}}(\eta)| d\eta \\ &= \frac{1}{|\kappa|} \sum_{v=1}^{n_q} \check{y}_\kappa(\eta_v) |J_\kappa(\xi(\eta_v))| |J_{\hat{\kappa}}(\eta_v)| w_v,\end{aligned}$$

where $|J_{\hat{\kappa}}(\eta)|$ is the Jacobian determinant of the mapping from the reference quadrilateral to the reference triangle, given by

$$|J_{\hat{\kappa}}(\eta)| = \frac{1 - \eta_2}{2},$$

which is positive everywhere in $\hat{\kappa}_{\text{tri}}$ except along the collapsed face, such that the analysis in Section 4.2 holds. Using the $\hat{\kappa}_{\text{tri}}$ node numbering, the coefficients of \check{y}_κ are then prescribed as

$$\begin{aligned}\check{y}_\kappa(x_k) &= \tilde{y}_\kappa(x_k), k = 1, \dots, 6 \\ \check{y}_\kappa(x_7) &= \frac{\bar{\check{y}}_\kappa |\kappa| - \sum_{v=1}^{n_q} |J_\kappa(\xi(\eta_v))| |J_{\hat{\kappa}}(\eta_v)| w_v \sum_{k=1}^6 \tilde{y}_\kappa(x_k) \check{\varphi}_k(\eta_v)}{\sum_{v=1}^{n_q} |J_\kappa(\xi(\eta_v))| |J_{\hat{\kappa}}(\eta_v)| w_v \check{\varphi}_7(\eta_v)} \\ &= \tilde{y}_\kappa(x_7) + \frac{\sum_{v=1}^{n_q} |J_\kappa(\xi(\eta_v))| |J_{\hat{\kappa}}(\eta_v)| w_v \left[\sum_{i=1}^{n_b} y_\kappa(x_i) \phi_i(\xi(\eta_v)) - \sum_{k=1}^7 \tilde{y}_\kappa(x_k) \check{\varphi}_k(\eta_v) \right]}{\sum_{v=1}^{n_q} |J_\kappa(\xi(\eta_v))| |J_{\hat{\kappa}}(\eta_v)| w_v \check{\varphi}_7(\eta_v)}.\end{aligned}$$

This approach can be generalized to other orders and shapes as well.

Appendix D. Chemical mechanism

Here, we provide information on the thermodynamic fits and reaction-rate coefficients for the chemical mechanism used in Sections 6.2 and 6.3, which is based on the Westbrook mechanism [44]. The thermodynamic relations for the i th species are given by

$$\begin{aligned}\frac{W_i c_{p,i}(T)}{R^0} &= a_{i0} - a_{i1} \hat{T} + a_{i2} \hat{T}^2 - a_{i3} \hat{T}^3 + a_{i4} \hat{T}^4, \\ \frac{W_i h_i(T)}{R^0} &= \int \frac{W_i c_{p,i}(\tau) d\tau}{R^0} - a_{i5} T_r, \quad \frac{W_i s_i^0}{R^0} = \int \frac{W_i c_{p,i}(\tau) d\tau}{R^0 \tau} - a_{i6},\end{aligned}$$

where $T_r = 1000$ K, $\hat{T} = T/T_r$, and τ is a dummy variable for T . The coefficients are given in Table 3.

The production rate of the i th species in Equation (2.6) is computed as

$$\omega_i = \sum_{j=1}^{n_r} v_{ij} q_j,$$

Table 4

List of elementary reactions for which the forward rate constant is of the form (D.2). The units of A_j are a combination of kmol, m³, s, and K that depend on the reaction.

j , reaction #	Equation	A_j	b_j	E_j/R^0 (K)
1	H + O ₂ → O + OH	1.86E11	0	8449
2	O + OH → H + O ₂	1.48E10	0	342
3	H ₂ + O → H + OH	1.82E7	1	4479
4	H + OH → H ₂ + O	8.32E6	1	3497
5	H ₂ O + O → OH + OH	3.39E10	0	9234
6	OH + OH → H ₂ O + O	3.16E9	0	554
7	H ₂ O + H → H ₂ + OH	9.55E10	0	10215
8	H ₂ + OH → H ₂ O + H	2.19E10	0	2592
9	H ₂ O ₂ + OH → H ₂ O + HO ₂	1.00E10	0	906
10	H ₂ O + HO ₂ → H ₂ O ₂ + OH	2.82E10	0	16501
11	HO ₂ + O → OH + O ₂	5.01E10	0	503
12	OH + O ₂ → HO ₂ + O	6.46E10	0	28261
13	HO ₂ + H → OH + OH	2.51E11	0	956
14	OH + OH → HO ₂ + H	1.20E10	0	20179
15	HO ₂ + H → H ₂ + O ₂	2.51E10	0	352
16	H ₂ + O ₂ → HO ₂ + H	5.50E10	0	29086
17	HO ₂ + OH → H ₂ O + O ₂	5.01E10	0	503
18	H ₂ O + O ₂ → HO ₂ + OH	6.31E11	0	37168
19	H ₂ O ₂ + O ₂ → HO ₂ + HO ₂	3.98E10	0	21457
20	HO ₂ + HO ₂ → H ₂ O ₂ + O ₂	1.00E10	0	503
21	H ₂ O ₂ + H → HO ₂ + H ₂	1.70E9	0	1887
22	HO ₂ + H ₂ → H ₂ O ₂ + H	7.24E8	0	9410

Table 5

List of three-body reactions for which the rate of progress is of the form (D.3). The units of A_j are a combination of kmol, m³, s, and K that depend on the reaction. The third-body efficiencies are assumed to be unity, apart from $\alpha_{H_2O,j}$ and $\alpha_{O_2,j}$.

j , reaction #	Equation	A_j	b_j	E_j/R^0 (K)	$\alpha_{H_2O,j}$	$\alpha_{O_2,j}$
23	H ₂ O + M → H + OH + M	2.19E13	0	52838	6.5	0.4
24	H + OH + M → H ₂ O + M	1.41E17	-2	0	6.5	0.4
25	H + O ₂ + M → HO ₂ + M	1.66E9	0	-503	6.5	0.4
26	HO ₂ + M → H + O ₂ + M	2.29E12	0	23098	6.5	0.4
27	H ₂ O ₂ + M → OH + OH + M	1.20E14	0	22896	6.5	0.4
28	OH + OH + M → H ₂ O ₂ + M	9.12E8	0	-2551	6.5	0.4
29	O + H + M → OH + M	1.00E10	0	0	6.5	0.4
30	OH + M → O + H + M	7.94E16	-1	52194	6.5	0.4
31	O ₂ + M → O + O + M	5.13E12	0	57870	6.5	0.4
32	O + O + M → O ₃ + M	4.68E9	-0.28	0	1	1
33	H ₂ + M → H + H + M	2.19E11	0	48309	6.5	0.4
34	H + H + M → H ₂ + M	3.02E9	0	0	6.5	0.4

where n_r is the number of reactions, $v_{ij} = v_{ij}^r - v_{ij}^f$ is the difference between the reverse (v_{ij}^r) and the forward stoichiometric coefficients (v_{ij}^f), and q_j is the rate of progress of the j th reaction. The chemical mechanism here contains only irreversible reactions, such that q_j is computed as

$$q_j = k_j^f \prod_{i=1}^{n_s} C_i^{v_{ij}^f}, \quad (\text{D.1})$$

where k_j^f is the forward rate constant of the j th reaction. The units of q_j are assumed to be kmol m⁻³ s⁻¹. The forward rate constants are computed using the Arrhenius form

$$k_j^f = A_j T^{b_j} \exp\left(-\frac{E_j}{R^0 T}\right), \quad (\text{D.2})$$

where $A_j > 0$ and b_j are parameters and E_j is the activation energy [21,50]. Table 4 lists the elementary chemical reactions included in the chemical mechanism, for which the production rates are computed as above.

Table 5 lists the three-body reactions, for which the rate of progress is scaled by a prefactor as [50]

$$q_j = \left(\sum_{i=1}^{n_s} \alpha_{ij} C_i \right) \left(k_j^f \prod_{i=1}^{n_s} C_i^{v_{ij}^f} \right), \quad (\text{D.3})$$

where α_{ij} are the third-body efficiencies. Unless otherwise specified, the third-body efficiencies are taken to be unity. Only $\alpha_{\text{H}_2\text{O},j}$ and $\alpha_{\text{O}_2,j}$ assume non-unity values (although they are also taken to be unity in Reaction 32).

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