

High-Order Techniques for Multi-Component Turbulent Non-Equilibrium Hypersonic Flows

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This work focuses on the development and application of high-order discretization techniques for multi-component turbulent non-equilibrium hypersonic flows. The governing equations (*i.e.*, Navier-Stokes) are discretized in space using finite differences. High-order approximation of the inviscid flux derivatives are sought within the framework of Weighted Essentially Non-Oscillatory (WENO) schemes, with particular emphasis on minimization of dissipation and dispersion errors. Central finite differences are adopted to discretize the diffusive flux derivatives. Time-integration is performed via split/un-split Strong-Stability-Preserving schemes. The proposed numerical methods are implemented in an innovative high-performance tool, HYPERCODE, described in a companion paper. Thermodynamic and transport properties, and source terms due to chemistry are evaluated using the PLATO library developed at University of Illinois. Applications consider two canonical problems: (i) Taylor-Green vortex and (ii) decay of compressible isotropic turbulence.

I. Introduction

The calculation of the flow past a vehicle flying at hypersonic speeds requires accounting for a broad family of physical phenomena such as non-equilibrium kinetic processes (*e.g.*, dissociation, excitation), transition and turbulence [1]. Currently, the solution to the above problem by Computational Fluid Dynamics (CFD) techniques is often (if not always) achieved via legacy multi-temperature models [2, 3]. The former are, however, correlation-based models and, as such, they have a limited range of accuracy. Moreover, the software tools employed for the numerical solution of the governing equations (*i.e.*, Navier-Stokes) are often designed around second-order upwind-biased finite volume upwind schemes. This is motivated by the built-in dissipation of upwind schemes which helps preventing numerical instabilities across shocks and/or regions of steep gradients [4–6]. These features may lead however to excessive smearing and extrema clipping and are therefore unacceptable when simulating turbulent flows.

The present paper is first a step towards the development of low dispersion and dissipation high-order schemes of the WENO family for turbulent non-equilibrium hypersonic flows. These schemes are currently being implemented

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in an innovative high-performance tool, HYPERCODE, described in a companion paper [7]. In order to go beyond the intrinsic limitations of multi-temperature models, both State-to-State (StS) [8–16] and reduced-order models [17–27] are considered with the purpose of a more accurate understanding of the inter-play among non-equilibrium and turbulence.

The present manuscript is structured as follows. Section II describes the physical model. The numerical method is discussed in Sec. III. Results are discussed in Sec. IV. Conclusions and future work are outlined in Sec V.

II. Physical modeling

The multi-component gases considered in this work are made of atoms and molecules. The set of species is denoted by the symbol S and their number is denoted by N_s. For the sake of generality, the set S may refer to either the chemical components when using a macroscopic model or to the bound states (*e.g.*, vibrational, electronic) of atoms and molecules in the case of a StS approach [8, 28]. In the case of a macroscopic formulation, non-equilibrium effects may be taken into account via legacy multi-temperature models or via an innovative and more accurate Maximum-Entropy (ME) reduced-order model framework[21]. In this method the *internal* energy ladder is first divided in groups/bins. The population within each group is then approximated by means of an energy polynomial subjected to a series of moment constraints (*e.g.*, mass, energy) [21]. In the linear case (*i.e.*, first-order polynomial) the whole procedure is equivalent to assume that each group follows a Maxwell-Boltzmann distribution at its own *internal* temperature T_k . These additional temperatures are stored in the set I and their number is denoted by N_i. The ME model has been applied with success to dissociating/ionizing and radiating flows [19–27]. Results discussed in the above works have shown that using 3–6 energy groups allows to retrieve StS predictions which require, in general, tracking hundreds to thousands of species.

Thermodynamics It is assumed that each component of the mixture behaves as a perfect gas. In light of this, the gas pressure readily follows from Dalton's law, $p = \sum_{s \in S} \rho_s R_s T$, where ρ_s and R_s stand, respectively, for partial densities and specific gas constants, whereas *T* is the temperature. The sensible and formation energies per unit mass are denoted by the symbols e_s and e_s^f , respectively. Following Grossman and Cinnella [29] the sensible energy e_s is conveniently split as the sum of two contributions, $e_s = \hat{e}_s(T) + \sum_{k \in I} \tilde{e}_{sk}(T_k)$, where the first term accounts for the degree(s) of freedom in thermal equilibrium with translation whereas the second includes those in lack of equilibrium. The mass density is obtained by summing the contribution from all species, $\rho = \sum_{s \in S} \rho_s e_s$ and $\rho e_k = \sum_{s \in S} \rho_s \tilde{e}_{sk}(T_k)$, respectively.

Transport The calculation of transport properties and fluxes is accomplished by means of the first-order Chapman-Enskog solution method for the Boltzmann equation [28, 30]. The application of the latter procedure allows to obtain macroscopic balance equations in closed-form and proves that, for a simple gas, the stress tensor, τ_{ij} , and the heat-flux vector, q_i , are given by Newton and Fourier's laws, respectively. The calculation of transport properties such as viscosity, η , and translational thermal conductivity, κ , is accomplished upon solution of linear symmetric transport systems stemming from the application of a Sonine-Laguerre polynomial expansion [30]. The same holds true for the mass diffusion fluxes, J^s , which are obtained by solving Stefan-Maxwell's equations [30]. The contributions of internal degrees of freedoms (*e.g.*, rotation, vibration) to the thermal conductivity, κ_k , are modeled based on the generalized Eucken correction [30].

Kinetics The mass and energy production terms (ω_s and Ω_k , respectively, in what follows) due to kinetic processes are evaluated based on the zeroth-order reaction rate theory. This corresponds to a Maxwellian reaction regime in the Champan-Enskog method [28, 30]. Kinetic data for rate coefficients of direct processes (*e.g.*, dissociation) are taken from the available literature for both multi-temperature and StS models. Rate coefficients for the reverse processes (*e.g.*, recombination) are obtained based on micro-reversibility [31].

The evaluation of the above quantities is accomplished using the PLATO library developed at University of Illinois [32]. For more details, the reader is referred to the above reference which provides an exhaustive presentation of the available physico-chemical models.

A. Governing equations

The conservation law form of the multi-component Navier-Stokes equations for a non-equilibrium gas reads:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial (\mathbf{F} - \mathbf{F}_{v})}{\partial x} + \frac{\partial (\mathbf{G} - \mathbf{G}_{v})}{\partial y} + \frac{\partial (\mathbf{H} - \mathbf{H}_{v})}{\partial z} = \mathbf{S},\tag{1}$$

where *t* denotes time and (x, y, z) are the Cartesian coordinates. The vector storing the conservative variables, inviscid fluxes, diffusive fluxes and source terms are:

$$\mathbf{U} = \begin{bmatrix} \rho_s & \rho u & \rho v & \rho E & \rho e_k \end{bmatrix}^{\mathrm{T}},$$
(2)

$$\mathbf{F} = \left[\rho_s u \quad p + \rho u^2 \quad \rho u v \quad \rho u w \quad \rho u H \quad \rho u e_k \right]^1,$$
(3)

$$\mathbf{G} = \begin{bmatrix} \rho_s v & p + \rho uv & p + \rho v^2 & \rho vw & \rho vH & \rho ve_k \end{bmatrix}^{\mathrm{T}}, \tag{4}$$

$$\mathbf{H} = \left[\rho_s w \quad \rho u w \quad \rho u w \quad p + \rho w^2 \quad \rho w H \quad \rho w e_k \right]^1, \tag{5}$$

$$\mathbf{F}_{\mathbf{v}} = \begin{bmatrix} -J_x^s & \tau_{xx} & \tau_{xy} & \tau_{xz} & \tau_{xx}u + \tau_{xy}v + \tau_{xz}w - q_x & -q_x^k \end{bmatrix}_{\mathbf{T}}^{\mathbf{I}}, \tag{6}$$

$$\mathbf{G}_{\mathbf{v}} = \begin{bmatrix} -J_{y}^{s} & \tau_{yx} & \tau_{yy} & \tau_{yz} & \tau_{yx}u + \tau_{yy}v + \tau_{yz}w - q_{y} & -q_{y}^{k} \end{bmatrix}^{1},$$
(7)

$$\mathbf{H}_{\mathbf{v}} = \begin{bmatrix} -J_z^s & \tau_{zx} & \tau_{zy} & \tau_{zz} & \tau_{zx}u + \tau_{zy}v + \tau_{zz}w - q_z & -q_z^k \end{bmatrix}^{\mathbf{I}},$$
(8)

$$\mathbf{S} = \begin{bmatrix} \omega_s & 0 & 0 & \Omega & \Omega_k \end{bmatrix}^{\mathrm{T}},\tag{9}$$

for all $s \in S$ and $k \in I$. Quantities u, v and w denote, respectively, the velocity components along the x, y and z directions. The total energy and enthalpy densities are $\rho E = \rho e + \rho K$ and $\rho H = \rho E + p$, respectively, where the kinetic energy per unit mass is $K = (u^2 + v^2 + w^2)/2$. The source term, Ω , in the global energy equation accounts for energy release in kinetic processes and reads $\Omega = -\sum_{s \in S} \omega_s e_s^f$. The (symmetric) stress tensor, $\tau_{ij} = \tau_{ji}$, is given by Newton's law (using a Cartesian tensor notation):

$$\tau_{ij} = \eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \eta \frac{\partial u_l}{\partial x_l},\tag{10}$$

for all $(i, j) \in \{1, 2, 3\}$, with the correspondence $(x_1, x_2, x_3) = (x, y, z,)$ and $(u_1, u_2, u_3) = (u, v, w)$. The symbol δ_{ij} , stands for Kronecker's delta. The components of the heat-flux vectors account only for Fourier and mass diffusion contributions by disregarding, for the moment, additional terms due to thermal and baro diffusion [33]:

$$q_i = -\kappa \frac{\partial T}{\partial x_i} + \sum_{s \in \mathcal{S}} J_i^s \hat{e}_s(T) + \sum_{k \in \mathcal{I}} q_i^k, \tag{11}$$

$$q_i^k = -\kappa_k \frac{\partial T_k}{\partial x_i} + \sum_{s \in S} J_i^s \tilde{e}_{sk}(T_k), \quad \text{(no sum implied over k)}, \tag{12}$$

for all $(i, j) \in \{1, 2, 3\}$ and $k \in I$.

III. Numerical method

Numerical solutions of the governing equations (1) are sought based on the method-of-lines [4]. The spatial discretization is performed first. This is then followed by a time-integration of the resulting set of ordinary differential equations. The developed computational framework has been implemented in an innovative high-performance parallel tool, HYPERCODE, described in a companion manuscript [7].

Spatial discretization The conservation law form of the governing equations (1) is discretized in space based on finite differences assuming a uniform Cartesian grid:

$$\frac{d\mathbf{U}_{ijk}}{dt} = \mathcal{L}(\mathbf{U}_{ijk}) + \mathcal{L}_{v}(\mathbf{U}_{ijk}) + \mathcal{L}_{s}(\mathbf{U}_{ijk}).$$
(13)

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Quantity \mathbf{U}_{ijk} represents the vector of conservative variables (2) at the ijk grid node of coordinates $\mathbf{x}_{ijk} = (i \Delta x, j \Delta y, k \Delta z)$, where the Δ 's denote the grid spacings. The \mathcal{L} and \mathcal{L}_{v} represent, respectively, the discrete form of the inviscid and diffusive flux derivatives in Eq. (1), whereas $\mathcal{L}_{s}(\mathbf{U}_{ijk}) = \mathbf{S}(\mathbf{U}_{ijk})$ denotes the pointwise value of the source term (9).

The inviscid flux derivative operator, \mathcal{L} , is evaluated based on a conservative finite difference [34]:

$$\mathcal{L}(\mathbf{U}_{ijk}) = -\frac{1}{\Delta x} \left(\mathbf{\hat{F}}_{i+\frac{1}{2}jk} - \mathbf{\hat{F}}_{i-\frac{1}{2}jk} \right) - \frac{1}{\Delta y} \left(\mathbf{\hat{G}}_{ij+\frac{1}{2}k} - \mathbf{\hat{G}}_{ij-\frac{1}{2}k} \right) - \frac{1}{\Delta z} \left(\mathbf{\hat{H}}_{ijk+\frac{1}{2}} - \mathbf{\hat{H}}_{ijk-\frac{1}{2}} \right), \tag{14}$$

where the () denotes numerical fluxes at interface locations. The numerical fluxes are evaluated based on a dimensionby-dimension Weighted Essentially Non-Oscillatory (WENO) reconstruction in the characteristic space [34, 35]. The steps below detail the procedure for the i + 1/2jk interface (where the dependence on the *j* and *k* indices is omitted to lighten the notation).

- 1) Evaluate the interface average state based on a Roe average [36] between U_i and U_{i+1} .
- 2) Form the components of the positive and negative characteristic flux split vectors ($\mathcal{F}_{s}^{(+)}$ and $\mathcal{F}_{s}^{(-)}$, respectively) at all stencil locations using a Lax-Friedrichs splitting [34]:

$$\mathcal{F}_{s}^{(+)r} = \mathbf{L}_{i+\frac{1}{2}}^{r} \frac{1}{2} \left[\mathbf{F}(\mathbf{U}_{s}) + \hat{\lambda}_{i+\frac{1}{2}}^{r} \mathbf{U}_{s} \right], \quad \mathcal{F}_{s}^{(-)r} = \mathbf{L}_{i+\frac{1}{2}}^{r} \frac{1}{2} \left[\mathbf{F}(\mathbf{U}_{s}) - \hat{\lambda}_{i+\frac{1}{2}}^{r} \mathbf{U}_{s} \right], \tag{15}$$

for all $s \in \{i - 2, ..., i + 3\}$ and for all $r \in \{1, ..., N_e\}$, where N_e is the number of governing equations. The symbol $\mathbf{L}_{i+1/2}^r$ denotes the *r*-th row of the left eigenvector matrix associated to $\mathbf{A}(\mathbf{U}) = \partial \mathbf{F}/\partial \mathbf{U}$. The interface absolute eigenvalues $\hat{\lambda}_{i+1/2}^r$ are computed as [37]:

$$\hat{\lambda}_{i+\frac{1}{2}}^{r} = \alpha \max\left(|\lambda_{i+\frac{1}{2}}^{r}|, |\lambda_{i}^{r}|, |\lambda_{i+1}^{r}|\right),\tag{16}$$

for all $r \in \{1, ..., N_e\}$, where $\lambda_{i+1/2}^r$ are the Roe average eigenvalues corrected through Harten and Hymann's second entropy fix to prevent violations of the entropy condition (*e.g.*, expansion shocks) [4]. The coefficient α in Eq. (16) controls the amount of dissipation (*i.e.*, the larger α the larger the dissipation) and is currently set to 1.1. Balsara and Shu [37] suggest to replace Eq. (16) with:

$$\hat{\lambda}_{i+\frac{1}{2}}^{r} = \alpha \max\left(|\lambda_{i+\frac{1}{2}}^{r}|, |\lambda_{i-2}^{r}|, \dots, |\lambda_{i+3}^{r}|\right),$$
(17)

since the above formula shows a slightly better dependence on the stencil being used and improves the robustness of the numerical scheme at reflecting boundaries. Since in the simulations discussed in this work all boundaries are periodic, the simpler relation (16) is used.

3) Obtain the components of the positive and negative characteristic flux split vectors at the interface using a fifth-order upwind-biased WENO reconstruction (WENO5) [35]:

$$\mathcal{F}_{i+\frac{1}{2}}^{(+)r} = \text{WENO5}\left[\mathcal{F}_{i-2}^{(+)r}, \mathcal{F}_{i-1}^{(+)r}, \mathcal{F}_{i}^{(+)r}, \mathcal{F}_{i+1}^{(+)r}, \mathcal{F}_{i+2}^{(+)r}\right],\tag{18}$$

$$\mathcal{F}_{i+\frac{1}{2}}^{(-)r} = \text{WENO5}\left[\mathcal{F}_{i+3}^{(-)r}, \mathcal{F}_{i+2}^{(-)r}, \mathcal{F}_{i+1}^{(-)r}, \mathcal{F}_{i-1}^{(-)r}\right],\tag{19}$$

for all $r \in \{1, ..., N_e\}$. The stencil weights for the scalar WENO5 reconstructions (18)-(19) are computed based on the smoothness indicators proposed by Borges *et al.* [38].

4) Project the interface characteristic split fluxes onto the physical space via multiplication by the right eigenvector matrix and sum the result to finally obtain the numerical flux:

$$\hat{\mathbf{F}}_{i+\frac{1}{2}} = \mathbf{R}_{i+\frac{1}{2}} \left(\mathcal{F}_{i+\frac{1}{2}}^{(+)} + \mathcal{F}_{i+\frac{1}{2}}^{(-)} \right).$$
(20)

The expression for the eigenvalues and the eigenvector matrices are provided in App. A. The diffusive flux operator, $\mathcal{L}_{\nu}(\mathbf{U}_{ijk})$, in Eq. (13) is evaluated as explained in Ref. [39].

Time integration (operator splitting) It is well known that kinetic processes occurring in hypersonic flows are a significant source of stiffness. As a result the maximum allowable explicit time-step is generally more constrained by

chemistry than by the Courant condition [2]. Under these circumstances using an explicit time-stepper (*e.g.*, Runge-Kutta) would result in over-resolving the time-scales of interest since the time-step selection is only driven by stability and not by the physics. To avoid this issue one may move to implicit methods in light of their more favourable stability properties. However, implicit methods (*e.g.*, backward Euler) often require solving large sparse linear systems and pose more challenges in terms of scaling than explicit methods. In this situation operator splitting methods may be selected as they represent a good compromise between the efficiency of explicit methods and stability of implicit ones.

Motivated by the above discussion, operator splitting methods are employed in this work by adopting the symmetric formulation proposed by Strang (*i.e.*, Strang splitting) [40]. In Strang splitting the evolution in time of the semi-discrete system (13) from t^n to $t^{n+1} = t^n + \Delta t$ (where Δt is the imposed time-step), goes as follows.

1) Advance of half time-step, $\Delta t/2$, the solution at t^n by solving the advection-diffusion sub-system:

$$\frac{d\mathbf{U}_{ijk}}{dt} = \mathcal{L}(\mathbf{U}_{ijk}) + \mathcal{L}_{\nu}(\mathbf{U}_{ijk}).$$
(21)

This will lead to an intermediate solution \mathbf{U}^* .

2) Evolve U^{*} from step 1 of a full time-step, Δt , by solving the kinetic sub-system:

$$\frac{d\mathbf{U}_{ijk}}{dt} = \mathbf{S}(\mathbf{U}_{ijk}). \tag{22}$$

This will lead to an intermediate solution $\mathbf{U}^{n+1/2}$.

3) Repeat step 1 using $U^{n+1/2}$ as initial solution to obtain U^{n+1} .



Fig. 1 Calling scheme for the application operator splitting methods (e.g., Strang) within HYPERCODE.

The order of accuracy of operator splitting depends on the type of splitting under use. Strang splitting can be made second-order accurate in time provided that both the advection-diffusion and kinetics sub-steps are performed using a second-order (or higher) time-accurate integrator [40, 41]. In this work the evolution of the advection-diffusion sub-system (21) is accomplished based on the second-order Strong-Stability-Preserving (SSP) Runge-Kutta scheme by Shu, Gottlieb and Osher [42, 43], whereas a second-order Backward Differentiation Formula (BDF2) linear multi-step method [44]* is used for the kinetic sub-system (22). Strang splitting is well suited for un-steady problems. However it may fail to preserve a steady solution for steady-state problems. This issue may be cured using balance splitting [41]. This option, which is currently not available in HYPERCODE, may be considered in future developments.

The evolution of the kinetic sub-system (22) is completely local to each grid node and, in light of this, does not require any information exchange among processors. In order to hide as many details as possible to a non-expert user, the integration of Eq. (22) is entirely delegated to the PLATO library where the time-advancement is accomplished via the legacy LSODE package [45] or the more modern CVODE library contained in the SUNDIALS suite [46] (see Fig. 1). In the latter case, the user may employ the multi-threaded OPENBLAS library for matrix/vector operations which leads to a substantial speed-up for large kinetic mechanisms.

^{*}The BDF2 method is equivalent to the three-point backward formula.

For the sake of efficiency, the kinetics sub-system (22) is re-written by adopting mass fraction and temperatures as solution variables since both mass and momentum densities remain constant within the chemistry sub-step (see Eq. (22)). This has the advantage of avoiding non-linear solves needed to retrieve temperatures from energy densities.

The data structure needed to implement operator splitting in HYPERCODE (*e.g.*, call to an external ODE time-stepper) has been used to add the capability of solving pure initial value kinetic problems relevant to hypersonics such as: (i) adiabatic/isothermal isochoric chemical reactor and (ii) flow behind a normal shock wave. This feature can be quite useful as it allows for quick testing of newly developed models. Figures 2-5 show some application examples.



Fig. 2 Isochoric adiabatic relaxation of Air (N, O, N₂, NO, O₂, two-temperature Park model [3]): left mole fractions, right temperatures. Initial conditions are $p_0 = 10\,000$ Pa and $T_0 = 300$ K. At t = 0 the translational temperature is suddenly raised to 15 000 K to emulate shock-induced heating whereas the density is kept constant.



Fig. 3 Isochoric isothermal relaxation of Oxygen (O, $O_2(v)$, vibrational State-to-State model [47]): left mole fractions, right vibrational distribution. Initial conditions are $p_0 = 1000$ Pa, $T_0 = 1000$ K and 5 % of O. At t = 0 the translational temperature is suddenly raised to 10 000 K to emulate shock-induced heating. Both density and temperature are kept constant during the simulation.

6



Fig. 4 Isochoric isothermal relaxation of Oxygen (O, $O_2(g)$, coarse-grained reduced-order model [47]): left mole fractions, right temperatures. Initial conditions are $p_0 = 1000$ Pa, $T_0 = 1000$ K and 5 % of O. At t = 0 the translational temperature is suddenly raised to 10 000 K to emulate shock-induced heating. Both density and temperature are kept constant during the simulation.



Fig. 5 Isochoric isothermal relaxation of Oxygen (O, $O_2(v, J)$, rovibrational State-to-State model [48]): left mole fractions, right rivibrational distribution. Initial conditions are $p_0 = 1000$ Pa, $T_0 = 300$ K and 5 % of O. At t = 0 the translational temperature is suddenly raised to 12 000 K to emulate shock-induced heating. Both density and temperature are kept constant during the simulation.

IV. Applications

The computational framework discussed in Sec. III has been tested on two popular fluid problems: (i) Taylor-Green vortex and (ii) decay of compressible isotropic turbulence.

Taylor-Green vortex Direct numerical simulations of compressible Taylor-Green vortex flow are performed using the conditions from Peng and Yang [49]. The computational domain is a three-dimensional cube with side lengths equal to L = 0.01 m and is discretized using a uniform grid along all three Cartesian directions. All boundaries are periodic.

The working fluid is air modeled as a calorically perfect gas with specific heat ratio and gas constant equal to $\gamma = 1.4$ and R = 287.06 J/kgK, respectively. The reference (∞) Reynolds and Mach numbers are, respectively, Re $_{\infty} = 400$ and $M_{\infty} = 2$. The reference temperature is $T_{\infty} = 273.15 \text{ K}$. The dynamics viscosity, $\mu = \mu(T)$, is modeled using Surtherland's law. The thermal conductivity is obtained from the viscosity assuming a constant Prandtl number (Pr = 0.72). The reference velocity, density and pressure are computed based on the above parameters and the reference length which is set to $L_{\infty} = L/2\pi$ to match the conditions in Ref. [49]:

$$U_{\infty} = M_{\infty} \sqrt{\gamma R T_{\infty}},\tag{23}$$

$$\rho_{\infty} = \frac{\operatorname{Re}_{\infty} \mu_{\infty}}{U_{\infty} L_{\infty}},\tag{24}$$

$$p_{\infty} = \rho_{\infty} R T_{\infty}, \tag{25}$$

where $\mu_{\infty} = \mu(T_{\infty})$ denotes the reference viscosity. The reference time is $t_{\infty} = L_{\infty}/U_{\infty}$.

The solution is initialized as follows. Density and pressure are uniform and equal to their reference values (*i.e.*, constant initial conditions). The velocity field is sinusoidal with Cartesian components given by:

$$u = U_{\infty} \sin\left(\frac{x}{L_{\infty}}\right) \cos\left(\frac{y}{L_{\infty}}\right) \cos\left(\frac{z}{L_{\infty}}\right), \quad v = -U_{\infty} \cos\left(\frac{x}{L_{\infty}}\right) \sin\left(\frac{y}{L_{\infty}}\right) \cos\left(\frac{z}{L_{\infty}}\right), \quad w = 0.$$
(26)

Figure 6 shows the decay of kinetic energy with time as a function of the grid resolution together with the vorticity magnitude colored by Mach number at $t/t_{\infty} = 10$.



Fig. 6 Compressible Taylor-Green vortex ($\text{Re}_{\infty} = 400$, $M_{\infty} = 2$): left decay of volume-averaged kinetic energy, right vorticity magnitude colored by Mach number at $t/t_{\infty} = 10$.

Decay of compressible isotropic turbulence The second test considered is the decay of compressible isotropic turbulence. The fluid model, grid, geometry and boundary conditions are the same as those for the compressible Taylor-Green vortex above. The reference Reynolds and Mach number are $\text{Re}_{\infty} = 333.33$ and $M_{\infty} = 0.3$, respectively. The reference values for velocity, density and pressure are obtained based on Eqs. (23)-(23) where the reference temperature is always set to 273.15 K.

The flowfield is initialized as follows. Density and pressure are uniform and equal to their reference values. The velocity components are prescribed in Fourier space following the procedure in Ref. [50] by setting the non-dimensional energy spectrum of the velocity fluctuations to [51]:

$$\varepsilon(k) = 16\sqrt{\frac{2}{\pi}} \frac{u_0^2}{k_0^2} \left(\frac{k}{k_0}\right)^4 \exp\left[-2\left(\frac{k}{k_0}\right)^2\right],\tag{27}$$

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where k denotes the non-dimensional wave number, whereas u_0 is the non-dimensional Root-Mean-Square (RMS) of the initial turbulent intensity. The symbol k_0 denotes the most energetic wave number. In this work, $k_0 = 4$ and $u_0 = 0.3$. The corresponding Taylor microscale Reynolds number is $\text{Re}_{\lambda} = 50$. The dimensional formulation of the non-dimensional energy spectrum (27) may be obtained via multiplication by the appropriate reference quantities. Once this done, the initial velocity fluctuations in the physical space are obtained by means of an inverse Fourier transform. In this work this is accomplished using the FFTW library [52].

Figure 7 shows iso-surfaces of vorticity magnitude colored by pressure at $t/\tau = 3$, where τ is turbulent time-scale.



Fig. 7 Decay of compressible isotropic turbulence ($\text{Re}_{\lambda} = 50$, $M_{\infty} = 0.3$): iso-surfaces of vorticity magnitude colored by pressure [Pa] at $t/\tau = 3$.

V. Conclusions

The present manuscript has discussed preliminary developments of high-order computational methods for turbulent non-equilibrium hypersonic flows. The discretization of the hyperbolic part of the flow governing equations is achieved via a fifth-order accurate characteristic-based WENO reconstruction. The diffusive/parabolic part is discretized based on central finite differences. Time-integration is performed using either explicit Runge-Kutta time-steppers or Strang splitting. These numerical methods are implemented in an innovative software, HYPERCODE, aimed at going beyond conventional second-order upwind-biased finite volume solvers used by the hypersonics community. Non-equilibrium effects are modeled using either State-to-State or reduced-order coarse-grained models. The calculation of thermodynamic properties, transport properties and fluxes, and source terms due to kinetic processes is delegated to the PLATO library for the sake of a more general data structure. Preliminary results have been obtained for two canonical flow problems: (i) Taylor-Green vortex and (ii) decay of compressible isotropic turbulence.

Future work will focus on the development and implementation of schemes with reduced dissipation to avoid excessive smearing typical of upwind methods, and applications to more realistic and challenging configurations (*e.g.*, blunt body flows).

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References

- [1] Gnoffo, P. A., "Planetary-entry gas dynamics," Annu. Rev. Fluid Mech., Vol. 31, 1999, pp. 459–494.
- [2] Park, C., Nonequilibrium Hypersonic Aerothermodynamics, Wiley, New York, NY, 1990.
- [3] Park, C., "Review of chemical-kinetic problems of future NASA missions, I: Earth entries," J. Thermophys. Heat Transfer, Vol. 7, No. 3, 1993, pp. 385–398.
- [4] Hirsch, C., Numerical Computation of Internal and External Flows, John Wiley & Sons, New York, NY, 1990.
- [5] Gnoffo, P. A., Gupta, R. N., and Shinn, J. L., "Conservation equations and physical models for hypersonic air flows in thermal and chemical nonequilibrium," NASA Technical Paper 2867, 1989.
- [6] Candler, G. V., and MacCormack, R. W., "Computation of weakly ionized hypersonic flows in thermochemical nonequilibrium," J. Thermophys. Heat Transfer, Vol. 5, No. 3, 1991, pp. 266–273.
- [7] Vogiatzis, K., Munafò, A., Ghosh, D., Panesi, M., Vedula, P., and Josyula, E., "HyperCode: software for high-order turbulent nonequilibrium hypersonic flow simulations," 2020. Submitted to the AIAA Science and Technology Forum and Exposition 2020, Orlando FL, January 6-10, 2020.
- [8] Capitelli, M., Ferreira, C. M., Gordiets, B. F., and Osipov, A. I., Plasma Kinetics in Atmospheric Gases, Springer, 2000.
- [9] Esposito, F., and Capitelli, M., "Quasi-classical molecular dynamic calculations of vibrationally and rotationally state selected dissociation cross sections: $N + N_2(v, J) \rightarrow 3N$," *Chem. Phys. Lett.*, Vol. 302, No. 1, 1999, pp. 49–54.
- [10] Esposito, F., Gorse, C., and Capitelli, M., "Quasi-classical dynamics calculations and state-selected rate coefficients for $H + H_2(v, j) \rightarrow 3H$ processes: application to the global dissociation rate under thermal equilibrium conditions," *Chem. Phys. Lett.*, Vol. 303, No. 5, 1999, pp. 636–640.
- [11] Capitelli, M., Armenise, I., Bruno, D., Cacciatore, M., Celiberto, R., Colonna, G., De Pascale, O., Diomede, P., Esposito, F., Gorse, C., Hassouni, K., Laricchiuta, A., Longo, S., Pagano, D., Pietanza, L. D., and Rutigliano., M., "Non-equilibrium plasma kinetics: a state-to-state approach," *Plasma Sources Sci. Technol.*, Vol. 16, No. 1, 2007, pp. 30–44.
- [12] Panesi, M., Jaffe, R. L., Schwenke, D. W., and Magin, T. E., "Rovibrational internal energy transfer and dissociation of N(⁴S_u) + N₂(¹Σ_v⁺) system in hypersonic flows," *J. Chem. Phys*, Vol. 138, No. 4, 2013, p. 044312.
- [13] Panesi, M., Munafò, A., Magin, T. E., and Jaffe, R. L., "Study of the non-equilibrium shock heated nitrogen flows using a rovibrational state-to-state method," *Phys. Rev. E*, Vol. 90, 2014, p. 013009.
- [14] Andrienko, D. A., and Boyd, I. D., "Rovibrational energy transfer and dissociation in O₂-O collisions," J. Chem. Phys., Vol. 144, No. 10, 2016, p. 104301.
- [15] Luo, H., Kulakhmetov, M., and Alexeenko, A., "Ab initio state-specific N₂+O dissociation and exchange modeling for molecular simulations," J. Chem. Phys., Vol. 146, No. 7, 2017, p. 074303.
- [16] Andrienko, D. A., and Boyd, I. D., "Vibrational energy transfer and dissociation in O₂-N₂ collisions at hyperthermal temperatures," J. Chem. Phys., Vol. 148, No. 8, 2018, p. 084309.
- [17] Colonna, G., Armenise, I., Bruno, D., and Capitelli, M., "Reduction of state-to-state kinetic to macroscopic models in hypersonic flows," J. Thermophys. Heat Transfer, Vol. 20, No. 3, 2006, pp. 477–486.
- [18] Magin, T. E., Panesi, M., Bourdon, A., Jaffe, R. L., and Schwenke, D. W., "Coarse-grain model for internal energy excitation and dissociation of molecular nitrogen," *Chem. Phys.*, Vol. 398, No. 4, 2012, pp. 90–95.
- [19] Munafò, A., Panesi, M., and Magin, T. E., "Boltzmann rovibrational collisional coarse-grained model for internal energy excitation and dissociation in hypersonic flows," *Phys. Rev. E*, Vol. 89, No. 2, 2014, p. 023001.

- [20] Munafò, A., and Magin, T. E., "Modeling of stagnation-line nonequilibrium flows by means of quantum based collisional models," *Phys. Fluids*, Vol. 26, No. 9, 2014, p. 097102.
- [21] Liu, Y., Panesi, M., Sahai, A., and Vinokur, M., "General multi-group macroscopic modeling for thermo-chemical nonequilibrium gas mixtures," J. Chem. Phys., Vol. 142, No. 13, 2015, p. 134109.
- [22] Kulakhmetov, M., Gallis, M., and Alexeenko, A., "Ab initio-informed maximum entropy modeling of rovibrational relaxation and state-specific dissociation with application to the O₂+O system," J. Chem. Phys., Vol. 144, No. 17, 2016, p. 174302.
- [23] Sahai, A., Lopez, B., Johnston, C. O., and Panesi, M., "Adaptive coarse graining method for energy transfer and dissociation kinetics of polyatomic species," J. Chem. Phys., Vol. 147, No. 5, 2017, p. 054107.
- [24] Munafò, A., Mansour, N. N., and Panesi, M., "A reduced-order NLTE kinetic model for radiating plasmas of outer envelopes of stellar atmospheres," *Astrophys. J.*, Vol. 838, No. 2, 2017, p. 126.
- [25] Macdonald, R. L., Jaffe, R. L., Schwenke, D. W., and Panesi, M., "Construction of a coarse-grain quasi-classical trajectory method. I. Theory and application to N₂-N₂ system," *J. Chem. Phys.*, Vol. 148, No. 5, 2018, p. 054309.
- [26] Macdonald, R. L., Grover, M. S., Schwartzentruber, T. E., and Panesi, M., "Construction of a coarse-grain quasi-classical trajectory method. II. Comparison against the direct molecular simulation method," *J. Chem. Phys.*, Vol. 148, No. 5, 2018, p. 054310.
- [27] Sahai, A., Johnston, C. O., Lopez, B., and Panesi, M., "Flow-radiation coupling in CO₂ hypersonic wakes using reduced-order non-Boltzmann models," *Phys. Rev. Fluids*, Vol. 4, No. 9, 2019, p. 093401.
- [28] Nagnibeda, E., and Kustova, E., Non-Equilibrium Reacting Gas Flows, Springer, Berlin, 2009.
- [29] Grossman, B., and Cinnella, P., "Flux-split algorithms for flows with non-equilibrium chemistry and vibrational relaxation," J. Comput. Phys., Vol. 88, No. 1, 1990, pp. 131–168.
- [30] Giovangigli, V., Multicomponent Flow Modeling, Birkhäuser, Berlin, 1999.
- [31] Oxenius, J., Kinetic Theory of Particles and Photons, Springer Series in Electronics and Photonics, Vol. 20, Springer-Verlag Berlin Heidelberg, Berlin, 1986.
- [32] Munafò, A., Alberti, A., Pantano, C., Freund, J. B., and Panesi, M., "A computational model for nano-second pulse laser-plasma interactions," J. Comput. Phys., 2019. Under review.
- [33] Ferziger, J. H., and Kaper, H. G., Mathematical Theory of Transport Processes in Gases, North-Holland Pub. Co., 1972.
- [34] Shu, C.-W., "Essentially Non-Oscillatory and Weighted Essentially Non-Oscillatory Schemes for Hyperbolic Conservation Laws," NASA CR 97-206253, NASA Langley Research Center, 1997.
- [35] Jiang, G.-S., and Shu, C.-W., "Efficient implementation of weighted ENO schemes," J. Comput. Phys., Vol. 126, No. 1, 1996, pp. 202–228.
- [36] Roe, P. L., "Approximate Riemann solvers, parameter vectors and difference schemes," J. Comput. Phys., Vol. 43, No. 2, 1981, pp. 357–372.
- [37] Balsara, D. S., and Shu, C.-W., "Monotonicity preserving Weighted Essentially Non-oscillatory Schemes with increasingly high order of accuracy," J. Comput. Phys., Vol. 160, No. 2, 2000, pp. 405–452.
- [38] Borges, R., Carmona, M., Costa, B., and Don, W. S., "An improved weighted essentially non-oscillatory scheme for hyperbolic conservation laws," J. Comput. Phys., Vol. 227, No. 6, 2008, pp. 3191–3211.
- [39] Lele, S. K., "Compact finite difference schemes with spectral-like resolution," J. Comput. Phys., Vol. 103, No. 1, 1992, pp. 16–42.
- [40] Strang, G., "On the construction and comparison of difference schemes," SIAM J. Num. Anal., Vol. 5, No. 3, 1968, pp. 506-517.
- [41] Hundsdorfer, W. H., and Verwer, J. G., Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations, Springer Series in Computational Mathematics, Springer, 2003.
- [42] Gottlieb, S., and Shu, C.-W., "Total variation diminishing Runge-Kutta schemes," *Math. Comput.*, Vol. 67, No. 221, 1998, pp. 73–85.

- [43] Gottlieb, S., Shu, C.-W., and Tadmor, E., "Strong stability-preserving high-order time discretization methods," *SIAM Rev.*, Vol. 43, No. 1, 2001, pp. 89–112.
- [44] Gear, C. W., Numerical Initial-Value Problems in Ordinary Differential Equations, Prentice-Hall, Englewood Cliffs, NJ, 1971.
- [45] Radhakrishnan, K., and Hindmarsh, A. C., "Description and use of LSODE, the Livermore solver for ordinary differential equations," NASA Report 1327, 1993.
- [46] Hindmarsh, A. C., Brown, P. N., Grant, K. E., Lee, S. L., Serban, R., Shumaker, D. E., and Woodward, C. S., "SUNDIALS: Suite of nonlinear and differential/algebraic equation solvers," *ACM Trans. Math. Softw.*, Vol. 31, No. 3, 2005, pp. 363–396.
- [47] Sharma, M. P., Munafò, A., and Panesi, M. ., "Characterization of non-equilibrium hypersonic flows using maximum entropylinear model," *Proc. of the 31st Int. Symposium on Rarefied Gas Dynamics*, AIP, 2019.
- [48] Venturi, S., Sharma, M. P., and Panesi, M., "A Machine Learning Framework for the Quantification of the Uncertainties Associated with Ab-Initio BasedModeling of Non-Equilibrium Flows," AIAA Paper 2019–0788, 2019. AIAA SciTech Meeting.
- [49] Peng, N., and Yang, Y., "Effects of the Mach number on the evolution of vortex-surface fields in compressible Taylor-Green flows," *Phys. Rev. Fluids*, Vol. 3, 2018, p. 013401.
- [50] Mansour, N. N., and Wray, A. A., "Decay of isotropic turbulence at low Reynolds number," *Phys. Fluids*, Vol. 6, No. 2, 1994, pp. 808–814.
- [51] Ghosh, D., "Compact-reconstruction weighted essentially non-oscillatory schemes for hyperbolic conservation laws," Ph.D. thesis, University of Maryland, College Park, MD, 2013.
- [52] Frigo, M., and Johnson, S. G., "The Design and Implementation of FFTW3," *Proc. IEEE*, Vol. 93, No. 2, 2005, pp. 216–231. Special issue on "Program Generation, Optimization, and Platform Adaptation".

A. Eigensystem

The evaluation of the eigensystem of the hyperbolic part of Eq. (1) is more conveniently accomplished after introducing the auxiliary variables:

$$\mathbf{V} = \left[\begin{array}{cccc} \rho_s & u & v & w & p & e_k \end{array} \right]^{\mathrm{T}}, \tag{28}$$

for all $s \in S$ and $k \in I$, with the T upper-script denoting the transpose. For the same purpose, it is convenient to evaluate pressure and energy density derivatives:

$$\frac{\partial p}{\partial \mathbf{U}} = (\gamma - 1) \left[\begin{array}{cccc} K - \hat{e}_s(T) + \frac{R_s T}{\gamma - 1} & -u & -v & -w & 1 \\ & & & \\ \end{array} \underbrace{-1, \dots, -1}_{N_i} \end{array} \right]^1,$$
(29)

$$\frac{\partial \rho E}{\partial \mathbf{V}} = \begin{bmatrix} K + \hat{e}_s(T) - \frac{R_s T}{\gamma - 1} & \rho u & \rho v & \rho w & \frac{1}{\gamma - 1} & \underbrace{\rho, \dots, \rho}_{N_i} \end{bmatrix}^{\mathrm{T}},$$
(30)

$$\frac{\partial \rho e_k}{\partial \mathbf{V}} = \left[\begin{array}{ccccc} \underline{e_k, \dots, e_k} & 0 & 0 & 0 & \rho \, \delta_{kl} \\ \underbrace{N_s} & & & \end{array}\right]^{\mathrm{T}},\tag{31}$$

for all $s \in S$ and $k, l \in I$, where the (frozen) specific heat ratio is $\gamma = 1 + R/C$, with *R* being the gas constant and *C* the constant volume heat capacity. The latter includes only for the contributions from the degrees of freedom in thermal equilibrium with translation:

$$C = \sum_{s \in \mathcal{S}} y_s \frac{\partial \hat{e}_s(T)}{\partial T}, \quad R = \sum_{s \in \mathcal{S}} y_s R_s, \tag{32}$$

where the mass fractions are $y_s = \rho_s / \rho$. The (frozen) speed of sound follows from $c = \sqrt{\gamma p / \rho}$.

The diagonalization of the conservative Jacobians (*e.g.*, $\mathbf{A}(\mathbf{U}) = \partial \mathbf{F}/\partial \mathbf{U}$) may accomplished as follows. First the above defined set of auxiliary variables (28) is used to rewrite $\mathbf{A}(\mathbf{U})$ as [29]:

$$\mathbf{A}(\mathbf{U}) = \frac{\partial \mathbf{F}}{\partial \mathbf{U}} = \frac{\partial \mathbf{U}}{\partial \mathbf{V}} \frac{\partial \mathbf{V}}{\partial \mathbf{U}} \frac{\partial \mathbf{F}}{\partial \mathbf{V}} \frac{\partial \mathbf{V}}{\partial \mathbf{U}}.$$
(33)

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Equation (33) shows that the matrices $\mathbf{A}(\mathbf{U})$ and $(\partial \mathbf{V}/\partial \mathbf{U})(\partial \mathbf{F}/\partial \mathbf{V})$ are related by a similarity transformation. Thus they share the same eigenvalues. The rearrangement in Eq. (33) is introduced since, as direct calculations show, $(\partial \mathbf{V}/\partial \mathbf{U})(\partial \mathbf{F}/\partial \mathbf{V})$ is much easier to diagonalize than $\mathbf{A}(\mathbf{U})$ [29]. The calculation of the eigensystem starts with the diagonalization of $(\partial \mathbf{V}/\partial \mathbf{U})(\partial \mathbf{F}/\partial \mathbf{V})$ which gives its eigenvalues (λ) and the related left ($\mathbf{\tilde{L}}$) and right ($\mathbf{\tilde{R}}$) eigenvector matrices. The conservative eigensystem is obtained by forming the matrix products $\mathbf{L} = \mathbf{\tilde{L}}(\partial \mathbf{V}/\partial \mathbf{U})$ and $\mathbf{R} = (\partial \mathbf{U}/\partial \mathbf{V})\mathbf{\tilde{R}}$. In what follows only the main results are quoted.

• *x* direction. The eigenvalues and the right and left eigenvector matrices are:

$$\lambda_x = \left\{ \underbrace{u, \dots, u}_{N_s}, u - c, u, u, u + c, \underbrace{u, \dots, u}_{N_i} \right\},\tag{34}$$

$$\mathbf{R}_{x} = \begin{pmatrix} \delta_{sp} & y_{s} & 0 & 0 & y_{s} & 0 \\ u & u - c & 0 & 0 & u + c & 0 \\ v & v & \rho & 0 & v & 0 \\ w & w & 0 & \rho & w & 0 \\ \rho E_{,\rho_{p}} & H - cu & \rho v & \rho w & H + cu & 0 \\ \rho e_{k,\rho_{p}} & e_{k} & 0 & 0 & e_{k} & \rho \delta_{kl} \end{pmatrix},$$
(35)

$$\mathbf{L}_{x} = \begin{pmatrix} \delta_{sp} - y_{s} \frac{p_{,\rho p}}{c^{2}} & -y_{s} \frac{p_{,\rho u}}{c^{2}} & -y_{s} \frac{p_{,\rho v}}{c^{2}} & -y_{s} \frac{p_{,\rho E}}{c^{2}} & -y_{s} \frac{p_{,\rho e_{l}}}{c^{2}} \\ \frac{p_{,\rho p} + cu}{2c^{2}} & \frac{p_{,\rho u} - c}{2c^{2}} & \frac{p_{,\rho v}}{2c^{2}} & \frac{p_{,\rho w}}{2c^{2}} & \frac{p_{,\rho E}}{2c^{2}} & \frac{p_{,\rho e_{l}}}{2c^{2}} \\ -\frac{v}{\rho} & 0 & \frac{1}{\rho} & 0 & 0 \\ \frac{-w}{\rho} & 0 & 0 & \frac{1}{\rho} & 0 & 0 \\ \frac{p_{,\rho p} - cu}{2c^{2}} & \frac{p_{,\rho u} + c}{2c^{2}} & \frac{p_{,\rho v}}{2c^{2}} & \frac{p_{,\rho w}}{2c^{2}} & \frac{p_{,\rho E}}{2c^{2}} & \frac{p_{,\rho e_{l}}}{2c^{2}} \\ -\frac{e_{k}}{\rho} & 0 & 0 & 0 & 0 & \frac{\delta_{kl}}{\rho} \end{pmatrix},$$
(36)

for all $p, s \in S$ and $k, l \in I$. The notation $a_{,b}$ is a shorthand for the partial derivative $\partial a/\partial b$.

• *y* direction. The eigenvalues, and the right and left eigenvector matrices are:

$$\lambda_{y} = \left\{\underbrace{v, \dots, v}_{N_{s}}, v - c, v, v, v + c, \underbrace{v, \dots, v}_{N_{i}}\right\},\tag{37}$$

$$\mathbf{R}_{y} = \begin{pmatrix} \delta_{sp} & y_{s} & 0 & 0 & y_{s} & 0 \\ u & u & \rho & 0 & u & 0 \\ v & v - c & 0 & 0 & v + c & 0 \\ w & w & 0 & \rho & w & 0 \\ \rho E_{,\rho_{p}} & H - cv & \rho u & \rho w & H + cv & 0 \\ \rho e_{k,\rho_{p}} & e_{k} & 0 & 0 & e_{k} & \rho \delta_{kl} \end{pmatrix},$$
(38)

$$\mathbf{L}_{y} = \begin{pmatrix} \delta_{sp} - y_{s} \frac{p_{,\rho p}}{c^{2}} & -y_{s} \frac{p_{,\rho u}}{c^{2}} & -y_{s} \frac{p_{,\rho v}}{c^{2}} & -y_{s} \frac{p_{,\rho E}}{c^{2}} & -y_{s} \frac{p_{,\rho e_{l}}}{c^{2}} \\ \frac{p_{,\rho p} + cv}{2c^{2}} & \frac{p_{,\rho u}}{2c^{2}} & \frac{p_{,\rho v} - c}{2c^{2}} & \frac{p_{,\rho w}}{2c^{2}} & \frac{p_{,\rho E}}{2c^{2}} & \frac{p_{,\rho e_{l}}}{2c^{2}} \\ -\frac{u}{\rho} & \frac{1}{\rho} & 0 & 0 & 0 & 0 \\ & & & & & \\ -\frac{w}{\rho} & 0 & 0 & \frac{1}{\rho} & 0 & 0 \\ & & & & & \\ \frac{p_{,\rho p} - cv}{2c^{2}} & \frac{p_{,\rho u}}{2c^{2}} & \frac{p_{,\rho v} + c}{2c^{2}} & \frac{p_{,\rho w}}{2c^{2}} & \frac{p_{,\rho E}}{2c^{2}} & \frac{p_{,\rho e_{l}}}{2c^{2}} \\ & -\frac{e_{k}}{\rho} & 0 & 0 & 0 & 0 & \frac{\delta_{kl}}{\rho} \end{pmatrix},$$
(39)

for all $p, s \in S$ and $k, l \in I$.

• z direction. The eigenvalues and the right and left eigenvector matrices are:

$$\lambda_{z} = \left\{ \underbrace{w, \dots, w}_{N_{s}}, w - c, w, w, w + c, \underbrace{w, \dots, w}_{N_{i}} \right\},\tag{40}$$

$$\mathbf{R}_{z} = \begin{pmatrix} \delta_{sp} & y_{s} & 0 & 0 & y_{s} & 0 \\ u & u & \rho & 0 & u & 0 \\ v & v & 0 & \rho & v & 0 \\ w & w - c & 0 & 0 & w + c & 0 \\ \rho E_{,\rho_{p}} & H - cw & \rho u & \rho v & H + cw & 0 \\ \rho e_{k,\rho_{p}} & e_{k} & 0 & 0 & e_{k} & \rho \delta_{kl} \end{pmatrix},$$
(41)

$$\mathbf{L}_{z} = \begin{pmatrix} \delta_{sp} - y_{s} \frac{p_{,\rhop}}{c^{2}} & -y_{s} \frac{p_{,\rhou}}{c^{2}} & -y_{s} \frac{p_{,\rhov}}{c^{2}} & -y_{s} \frac{p_{,\rhoE}}{c^{2}} & -y_{s} \frac{p_{,\rhoel}}{c^{2}} \\ \frac{p_{,\rhop} + cw}{2c^{2}} & \frac{p_{,\rhou}}{2c^{2}} & \frac{p_{,\rhov}}{2c^{2}} & \frac{p_{,\rhow} - c}{2c^{2}} & \frac{p_{,\rhoE}}{2c^{2}} & \frac{p_{,\rhoel}}{2c^{2}} \\ -\frac{u}{\rho} & \frac{1}{\rho} & 0 & 0 & 0 \\ & & & & \\ -\frac{v}{\rho} & 0 & \frac{1}{\rho} & 0 & 0 & 0 \\ \frac{p_{,\rhop} - cw}{2c^{2}} & \frac{p_{,\rhou}}{2c^{2}} & \frac{p_{,\rhov}}{2c^{2}} & \frac{p_{,\rhow} + c}{2c^{2}} & \frac{p_{,\rhoE}}{2c^{2}} & \frac{p_{,\rhoel}}{2c^{2}} \\ -\frac{e_{k}}{\rho} & 0 & 0 & 0 & 0 & \frac{\delta_{kl}}{\rho} \end{pmatrix},$$
(42)

for all $p, s \in S$ and $k, l \in I$.