

A SYMMETRIZING VARIABLES FORMULATION FOR HYPERSONIC THERMO-CHEMICAL NON-EQUILIBRIUM FLOW, WITH APPLICATION TO RESIDUAL DISTRIBUTION SCHEMES

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Key words: Symmetrizing variables, Residual distribution schemes, Hypersonic flow, Thermal and chemical non-equilibrium

Abstract. *Simulation of hypersonic flows in thermo-chemical non-equilibrium is very challenging in terms of computational efficiency, due to the potentially large number of species conservation equations and the extra energy equations for the additional energetic modes that have to be solved together with the momentum and total energy equations. A strong reduction of the computational effort can be obtained by decoupling the species and vibrational energy equations in the convective terms, specially in upwinding methods when a characteristic decomposition is used for stabilization and monotone shock capturing based on positive or local extremum diminishing discretizations.*

*In this paper an innovative decoupling method for the inviscid terms is proposed for thermal and chemical non-equilibrium based on a symmetrizing variable transformation. The derivation of the new symmetrizing variables is presented for a two-temperatures model considering a translational-rotational and a vibrational-electronic mode, applied to different mixtures like N_2 -N, **air5** or **air11**.*

1 INTRODUCTION

Any space vehicle intended to survive an atmospheric entry process must be protected by a thermal protection system (**TPS**). Optimized design of these **TPS** requires an accurate prediction of the flowfield around the vehicle, since this one defines the aerothermal loads to be endured. Given the high velocities involved, aerodynamics has to be coupled with additional physical phenomena, such as chemistry and high temperature effects. This makes simulation of hypersonic flows in thermo-chemical non-equilibrium a challenging application, not the least in terms of computational cost, since a potentially large number of species conservation equations and the additional energy equations for various energetic modes have to be solved together with the momentum and energy equations.

In this paper an innovative decoupling method for the inviscid terms is proposed for thermal and chemical non-equilibrium based on a symmetrizing variable transformation, thus extending the work presented in¹ -which considers only chemical non-equilibrium. The derivation of the new symmetrizing variables is presented for a two-temperatures model considering a translational-rotational and a vibrational-electronic mode, applied to different mixtures like $N-N_2$ or **air5**. The transformation is such that mass species and electronic-vibrational energy related terms get completely decoupled from the momentum and the total energy variables. The resulting advection Jacobian matrix presents a block diagonal structure. Moreover, the mass conservation related block is fully diagonal and the contribution from the only vibrational energy related term boils down to a single scalar.

This transformation has been applied in a Residual Distribution (**RD**) context to alleviate the computational expense connected to the non-equilibrium effects. The improvement in efficiency with respect to a solver formulated in conserved variables has been evaluated for an Euler testcase. Influence of the cost of the source term evaluation in the computational gains obtained has also been analysed. Finally, the modified code has been used to simulate a well documented test case for hypersonic flows, finding good matching between the results obtained and those in literature.

2 PHYSICAL MODEL

The Navier-Stokes equations governing a N -species gas mixture in thermal and chemical non-equilibrium (**TCNEq**) conditions are expressed in compact, vector form (reference⁵) as:

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}_j^c}{\partial x_j} = \frac{\partial \vec{F}_j^d}{\partial x_j} + \vec{S}^v \quad (1)$$

where \vec{U} stands for the vector of conservative variables. If a two-temperature model (as described in¹²) is employed, it is given by:

$$\vec{U} = [\rho_s, \quad \rho u_j, \quad \rho E, \quad \rho e_v]^t \quad (2)$$

where $s = 1, \dots, N$ and $j = 1, \dots, 3$. On the one hand, the unknowns are the N species partial densities, the 3 components of the momentum vector (2 for a $2D$ or axisymmetric case), the total energy per unit volume and the vibrational energy per unit volume¹. On the other hand, there are N mass continuity equations, 3 momentum conservation equations (or 2 for $2D$ /axisymmetric problem), one total energy conservation and one electronic-vibrational energy conservation equation.

The convective and diffusive fluxes are respectively defined by:

$$\vec{F}_j^c = (\rho_s u_j, \quad \rho u_i u_j + p \delta_{i,j}, \quad \rho H u_j, \quad \rho e_v u_j)^t \quad (3)$$

and

$$\vec{F}_j^d = (-\rho_s u_{s,j}, \quad \tau_{i,j}, \quad \tau_{i,j} u_j - q_i, \quad -q_{v,i})^t \quad (4)$$

Diffusive velocities \vec{u}_s are formulated as:

$$u_{s,j} = D_s \frac{\partial y_s}{\partial x_j} \quad (5)$$

where D_s and y_s are the s -th species diffusivity and mass fraction respectively.

Viscous stress tensor components are given, under the hypothesis of negligible bulk viscosity effects, by:

$$\tau_{i,j} = \mu \left[\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) - \frac{2}{3} \frac{\partial u_j}{\partial x_j} \right] \quad (6)$$

Roto-translational heat flux components are defined as:

$$q_i = -\lambda \frac{\partial T}{\partial x_i} - \lambda_v \frac{\partial T_v}{\partial x_i} - \sum_s \rho_s h_s u_i \quad (7)$$

while for the vibrational heat flux, one has:

$$q_{v,i} = -\lambda_v \frac{\partial T_v}{\partial x_i} - \sum_s \rho_s h_s^v u_i \quad (8)$$

The source term \vec{S}^U is given by:

$$\vec{S}^U = (\dot{\omega}_s, \quad \vec{0}_{3 \times 1}, \quad 0, \quad \Omega_v)^t \quad (9)$$

and the mass production term for a given species s is by:

$$\frac{\dot{\omega}_s}{M_s} = \sum_{\text{reactions}} (\nu''_{s,r} - \nu'_{s,r}) \left\{ k_{r,f} \prod_{\text{species}} \left(\frac{\rho_k}{M_k} \right)^{\nu'_{k,r}} - k_{r,b} \prod_{\text{species}} \left(\frac{\rho_k}{M_k} \right)^{\nu''_{k,r}} \right\} \quad (10)$$

¹In the two-temperatures model, translational and rotational modes are treated as a single joint mode, characterized by the temperature T , while the vibrational and electronic modes are also considered together, being T_v the corresponding descriptive temperature.

Here $k_{r,f}$ and $k_{r,b}$ stand for the forward and backward reaction rates for the r -th reaction; $\nu'_{k,r}$ and $\nu''_{k,r}$ are the stoichiometric coefficients and M_k is the molar weight for the k -th species.

Finally the term Ω_v accounts both for the energy exchange (relaxation) between translational and vibrational modes and the energy gained through dissociation or recombination:

$$\Omega_v = \sum_{species} \rho_s \frac{e_{v,s}^* - e_{v,s}}{\tau_s} + \sum_{species} \hat{D}_s \dot{\omega}_s \quad (11)$$

Details on the definition of the parameters D_s , μ , λ , λ_v , $k_{r,f}$, $k_{b,f}$, τ_s ... can be found in report¹² and further references therein.

3 RESIDUAL DISTRIBUTION METHODS

Consider an unstructured simplicial mesh of the computational domain of interest Ξ . Assigning the unknowns at the simplices vertices and making use of $P1$ linear elements (see figure 1), a standard Finite Element (**FE**) representation with linear nodal shape functions $N_l(\vec{x})$ is obtained.

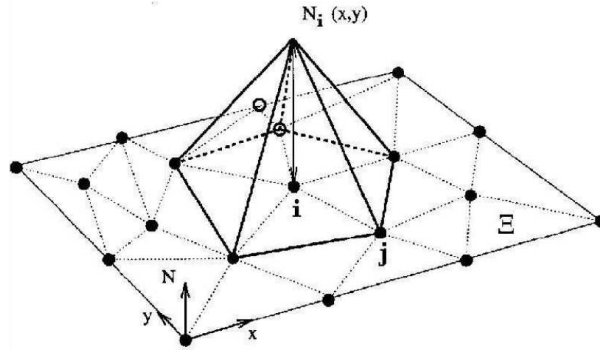


Figure 1: Linear shape function associated to a generic 2D-simplicx.

$$\vec{U}^h(\vec{x}, t) = \sum_{l=1}^{nodes} \vec{U}_l(t) N_l(\vec{x}) \quad (12)$$

Remember that relation $N_l(\vec{x}_k) = \delta_{kl}$ holds.

To construct upwind discretizations equation (1) is expressed in quasilinear form:

$$\frac{\partial \vec{U}}{\partial t} + A_j^U \cdot \frac{\partial \vec{U}}{\partial x_j} = \frac{\partial \vec{F}_j^d}{\partial x_j} + \vec{S}^U \quad (13)$$

through the advective term Jacobian matrices A_j^U :

$$A_j^U|_{m,n} = \frac{\partial \vec{F}_j^c|_m}{\partial \vec{U}|_n} \quad (14)$$

where $\vec{F}_j^c|_m$ refers to the m -th component of the convective flux vector in the j -th direction and $\vec{U}|_n$ refers to n -th component of the conservative variables vector. The superscript U denotes that the Jacobian has been obtained with respect to the conservative variables.

Central for the method is the concept of residual. The (steady state) cell residual for an element Ω is defined as the volume integral:

$$\vec{\Phi}^\Omega = \int_V \left(A_j^U \cdot \frac{\partial \vec{U}}{\partial x_j} - \frac{\partial \vec{F}_j^d}{\partial x_j} - \vec{S}^U \right) dV = \vec{\Phi}^{c,U} - \vec{\Phi}^{d,U} - \vec{\Phi}^{S,U} \quad (15)$$

Equations for the nodal unknowns are obtained by distributing fractions of the cell residuals to the nodes forming the cell. So, for the l -th node:

$$\Xi_l \frac{d\vec{U}_l}{dt} + \vec{\Phi}_l^{c,U} - \vec{\Phi}_l^{d,U} - \vec{\Phi}_l^{S,U} = \vec{0} \quad (16)$$

where Ξ_l is volume of the median dual cell for node l (see fig. 2).

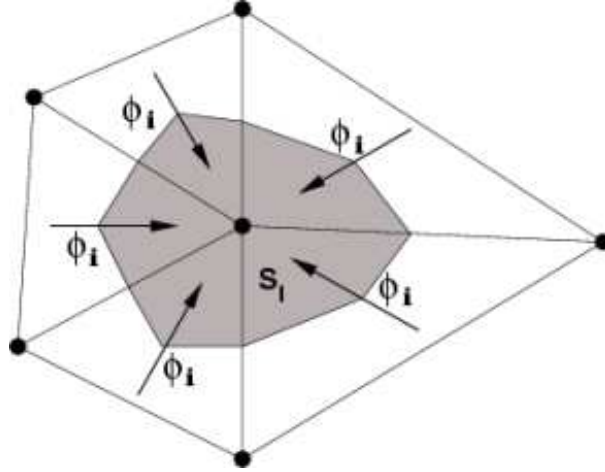


Figure 2: Median dual cell for the l -th node.

The formulation stays at this moment in open form, as no decision on how the cell residuals are to be distributed among its neighbouring nodes has been taken. Also notice that convective, diffusive and source term contributions to the residuals can be treated differently if needed. In this work we will be concerned only with distribution of residuals from the convective term; treatment of diffusive terms is based on a standard Galerkin **FE** discretization, more details including also source terms residuals are found in⁵ and thoroughly detailed in⁶.

The residual of the convective term at the l -th node can be related to the residuals of those elements (triangles/tetrahedra for our particular application) that are its neighbours (those contained in the set Ξ_l) through the distribution matrices $B_l^{\Omega_i,U}$, as follows:

$$\vec{\Phi}_l^{c,U} = \sum_{\Omega_i \in \Xi_l} B_l^{\Omega_i,U} (K^\pm) \cdot \vec{\Phi}_{\Omega_i}^{c,U} \quad (17)$$

Upwinding schemes are obtained by downwind distribution of the cell residuals, which requires the splitting of the Jacobians normal to the cell faces:

$$\begin{aligned} K_l &= \frac{1}{d} \bar{A}_j^U n_{lj} \\ &= \frac{1}{d} R_l^U \cdot \Lambda_l \cdot L_l^U \end{aligned} \quad (18)$$

where d is the dimension of the problem studied (either 2 or 3), and \bar{A}_j^U are the Jacobians evaluated in a conservative linearised state and n_{lj} is the j -th component of the inward normal opposite to node l (see figure 3). Given the hyperbolic nature of the system (1), the Jacobian matrices have a complete set of real eigenvalues and eigenvectors (reference¹²) and the second equality in (18) also holds, with Λ_l^U the diagonal eigenvalue matrix of A_j^U , and R_l^U and L_l^U the matrices of the associated right and left eigenvectors.

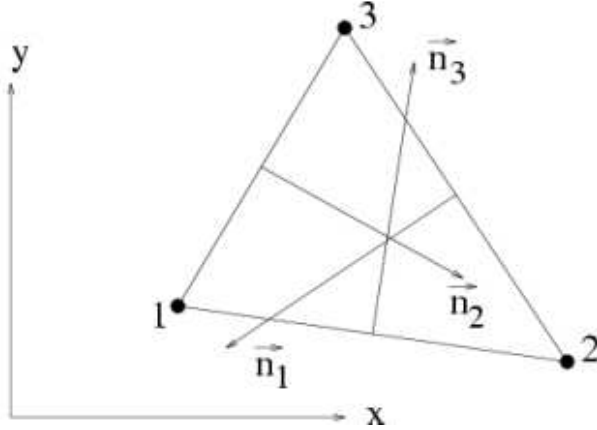


Figure 3: Scaled inward normals in a generic 2D-simplex.

Efficient upwinding is obtained if positive and negative eigenvalues are separated as:

$$K_l^\pm = \frac{1}{d} R_l^U \cdot \Lambda_l^\pm \cdot R_l^U \quad (19)$$

Here, Λ^+ is obtained substituting negative eigenvalues by zeros (and the other way around for Λ^-).

Particular choices for the distribution matrices $B_l^{\Omega_i,U}$ (that is, a specific dependence on the upwind matrices K_l^\pm) define different schemes, see *e.g.* references^{9,14}.

The method as formulated up to now is known as linearisation based residual distribution (**LRD**) method. As explained in references^{5,13}, it presents the drawback of requiring

a conservative linearisation (based on a Roe-like average state vector) for computing the convective Jacobians, such that equation (15) is equivalent to a contour integral of the fluxes over the cell faces. However, there is not such a linearisation available for the **TCNEq** Navier-Stokes equations. This problem can nevertheless be overcome using a modified version of the method, called contour-integration based residual distribution (**CRD**). Details on this technique are given in what follows.

3.1 The CRD method and the Nc scheme

CRD schemes retain conservation at the discrete level no matter the variables chosen for the linearisation of the cell advective Jacobian, at the price of an additional contour integration of the fluxes in each element. Extensive information on this class of schemes can be found in references^{7,8,13}. In this work, only the Nc scheme will be presented.

The Nc system scheme is the **CRD** counterpart of the linear, positive, multidimensional upwind N system scheme (reference⁹). In fact, it is defined as the **LRD** N scheme applied to a non-conservative linearisation plus a conservation correction defined in terms of the upwinded linearisation error:

$$\vec{\Phi}_l^{Nc} = \vec{\Phi}_{l,*}^N - B_{l,*}^{LDA} \delta \vec{\Phi}^c = \vec{\Phi}_{l,*}^N - B_{l,*}^{LDA} \left(\vec{\Phi}_{\Omega,*}^c - \vec{\Phi}_{\Omega}^c \right) \quad (20)$$

In the expression above, subscript $*$ refers to magnitudes computed using an arbitrary non conservative average \bar{Z} and the cell convective residual is computed as the surface integral:

$$\vec{\Phi}_{\Omega}^c = \oint_{\delta\Omega} \vec{F}_j^c n_j dS \quad (21)$$

where Gauss theorem has been applied.

The **LRD** N scheme (reference⁹) is given then by the standard form:

$$\vec{\Phi}_{l,*}^N = K_{l,*}^+ \left(\vec{W}_l^c - \vec{W}_{in} \right) \quad (22)$$

with the inflow parameter \vec{W}_{in} defined as:

$$\vec{W}_{in} = \left(\sum_{j=1}^{d+1} K_{j,*}^- \right)^{-1} \left(\sum_{j=1}^{d+1} K_{j,*}^- \vec{W}_j^c \right) \quad (23)$$

in terms of the consistent distribution variables \vec{W}^c , as a function of the arbitrary linearisation variables \bar{Z} :

$$\vec{W}_j^c = \frac{\partial \vec{W}}{\partial \bar{Z}} (\bar{Z}) \bar{Z}_j \quad (24)$$

Finally, the distribution matrix $B_{l,*}^{LDA}$, corresponding to the **LRD** linear second order *LDA* scheme, is defined as:

$$B_{l,*}^{LDA} = K_{l,*}^+ \left(\sum_{j=1}^{d+1} K_{j,*}^+ \right)^{-1} \quad (25)$$

Since it will have an impact on the numerical results to be shown, a last remark on the Nc scheme as used in this work has to be made, namely that the source term residual is upwinded with the LDA scheme. So, the definitive expression of the scheme is:

$$\vec{\Phi}_l^{Nc} = \vec{\Phi}_{l,*}^N - B_{l,*}^{LDA} \left(\vec{\Phi}_{\Omega,*}^c - \vec{\Phi}_{\Omega}^c \right) - B_{l,*}^{LDA} \vec{\Phi}_{\Omega}^S \quad (26)$$

4 SYMMETRIZING VARIABLES

As seen previously, the two-temperatures model yields a systems of $N + 5$ equations per node for a $3D$ case, where N is the number of species considered. Common mixtures used for air modelling in Earth's atmospheric entry applications are:

- the N_2 - N mixture, that considers only dissociation/recombination of molecular/atomic nitrogen
- the so-called **air5** mixture, that only accounts for electrically neutral species (N , O , N_2 , NO , and O_2)
- the **air11** mixture, containing all the previous species and also the ions N^+ , O^+ , N_2^+ , NO^+ and O_2^+ and electrons e^-

The more detailed is the chemistry model, the more costly it becomes to achieve a flow solution. Moreover, other sources of complexity are inherently present when simulating hypersonic non-equilibrium flows: complex geometries, three-dimensional effects, strong shock-waves, surface effects (ablation, radiation, catalysis, ...) and others. And though faster, more efficient computers are an asset for the numerical simulation of this atmospheric entry flows, algorithmic improvements can be as important to increase efficiency of the computations. In this section an attempt is made to obtain more easily tractable equations for the two-temperatures model while retaining a general N -species chemistry model.

4.1 Symmetrization of conservation laws

For inviscid flows, it is possible to decouple one of the equations (namely, the entropy equation) from the system of the Euler equations if an adequate change of variables is performed. In this process the part of the equations that remains coupled can also be symmetrized (reference¹¹).

Degrez and van der Weide extended this idea to inviscid flows in chemical non-equilibrium (**CNEq**) in¹. They defined the set of symmetrizing variables given by:

$$\partial \vec{Q} = \left[y_s \partial p - a^2 \partial \rho_s, \quad \partial u_j, \quad \frac{1}{\rho a} \partial p \right]^t \quad (27)$$

that can be shown to be linked to the species partial entropies. When applied to the Euler equations, *all* the mass conservation equations get decoupled from the momentum and energy conservation ones. This allows to apply scalar **RD** schemes independently to each of the mass equations while matrix counterparts of the schemes are needed only for the reduced momentum-energy subsystem. In this way, inviscid flows in **CNEq** can be treated at relatively moderate numerical cost.

As stated in references ^{2,3}, symmetrizability of general conservation laws is assured if an entropy function S exists. In those cases, the linear transformation $\frac{\partial \vec{Q}}{\partial \vec{U}}$ with entropy variables \vec{Q} defined as:

$$\vec{Q}|_m = -\frac{\partial S}{\partial \vec{U}|_m} \quad (28)$$

is guaranteed to recast the complete system of equations in symmetric form.

The symmetric structure obtained through no matter what approach (either that in² or in³) offers already some numerical advantages. However, since in both cases the matrices retrieved are dense, the perspective of obtaining a block structure with scalar independent mass equations suggests the extension of Degrez and van der Weide's approach to the **TCNEq** case. The way this is done is described in the next section.

4.2 The set of symmetrizing variables

The governing equations for hypersonic, thermochemical non-equilibrium flows were presented in section 2. It is convenient to work with a sole advective matrix. Such a matrix is obtained as the sum of the advective Jacobian for each of the reference directions weighted by the components of a generic unit vector \vec{n} . The resulting matrix, as presented in¹² in terms of the set of conservative variables:

$$\vec{U} = [\rho_s, \quad \rho u_j, \quad \rho E, \quad \rho e_v]^t \quad (29)$$

has the form:

$$A^U = \begin{bmatrix} U(I_N - \vec{Y}_{N \times 1} \cdot \vec{1}_{1 \times N}) & \vec{Y}_{N \times 1} \cdot \vec{n}^t & 0_{N \times 1} & 0_{N \times 1} \\ \vec{n} \cdot \vec{\Gamma}_{1 \times N} - U \vec{u} \cdot \vec{1}_{1 \times N} & U I_3 + \vec{u} \cdot \vec{n}^t - \beta \vec{n} \cdot \vec{u}^t & \beta \vec{n} & \phi \vec{n} \\ U(\vec{\Gamma}_{1 \times N} - H \cdot \vec{1}_{1 \times N}) & H \vec{n}^t - \beta U \vec{u}^t & (1 + \beta)U & \phi U \\ -U e_v \vec{1}_{1 \times N} & e_v \vec{n}^t & 0 & U \end{bmatrix} \quad (30)$$

where $\vec{Y}_{N \times 1}$ contains the N species partial densities:

$$\vec{Y}_{N \times 1} = [y_1, \dots, y_N]^t \quad (31)$$

Parameters β , ϕ and $\vec{\Gamma}_{1 \times N}$ stand for partial derivatives of the pressure with respect to the different variables, as:

$$\beta = \frac{\partial p}{\partial \rho E}, \quad \phi = \frac{\partial p}{\partial \rho e_v}, \quad \vec{\Gamma}_{1 \times N} = \left[\frac{\partial p}{\partial \rho_1}, \dots, \frac{\partial p}{\partial \rho_N} \right] \quad (32)$$

Finally I_K , stands for a K -th order identity matrix and U is the projection of the velocity vector \vec{u} along the direction \vec{n} .

In the discussion to follow, matrix (30) will have to be reexpressed in different sets of variables. The Jacobian matrix A^U , in terms of the conservative variables \vec{U} , can be recast in the new set of variables \vec{V} by means of the classical linear algebra relation:

$$A_j^V = \frac{\partial \vec{V}}{\partial \vec{U}} \cdot A_j^U \cdot \frac{\partial \vec{U}}{\partial \vec{V}} \quad (33)$$

where expression $\frac{\partial \vec{U}}{\partial \vec{V}}$ should be interpreted as the matrix whose components are defined as:

$$\frac{\partial \vec{U}}{\partial \vec{V}}|_{m,n} = \frac{\partial \vec{U}|_m}{\partial \vec{V}|_n} \quad (34)$$

A first step in the extension of the principles shown in reference¹ is to transform the left eigenvectors of matrix (30) to the set of primitive variables \vec{P} , defined as:

$$\vec{P} = [\rho_s, \quad u_j, \quad p, \quad e_v]^t \quad (35)$$

The matrix containing the left eigenvectors of (30) is given in reference¹² (the definition used here is inverse of the one used in¹²). The matrix L^U in primitive variables is obtained from:

$$L^U = \begin{bmatrix} a^2 I_N - \vec{Y}_{N \times 1} \cdot \vec{\Gamma}_{1 \times N} & \beta \vec{Y}_{N \times 1} \cdot \vec{u}^t & -\beta \vec{Y}_{N \times 1} & -\phi \vec{Y}_{N \times 1} \\ -V \vec{\Gamma}_{1 \times N} & \vec{l}^t & 0 & 0 \\ -W \vec{\Gamma}_{1 \times N} & \vec{m}^t & 0 & 0 \\ \vec{\Gamma}_{1 \times N} - aU \vec{\Gamma}_{1 \times N} & a\vec{n}^t - \beta \vec{u}^t & \beta & \phi \\ \vec{\Gamma}_{1 \times N} + aU \vec{\Gamma}_{1 \times N} & -a\vec{n}^t - \beta \vec{u}^t & \beta & \phi \\ -e_v \vec{\Gamma}_{1 \times N} & \beta e_v \vec{u}^t & -\beta e_v & a^2 - \phi e_v \end{bmatrix} \quad (36)$$

through the relationship:

$$L^P = L^U \cdot \frac{\partial \vec{U}}{\partial \vec{P}} \quad (37)$$

resulting in:

$$L^P = \begin{bmatrix} a^2 I_N & 0_{N \times 3} & -\vec{Y}_{N \times 1} & \vec{0}_{N \times 1} \\ \vec{0}_{1 \times N} & \rho \vec{l}^t & 0 & 0 \\ \vec{0}_{1 \times N} & \rho \vec{m}^t & 0 & 0 \\ \vec{0}_{1 \times N} & a\vec{n}^t & 1 & 0 \\ \vec{0}_{1 \times N} & -a\vec{n}^t & 1 & 0 \\ a^2 e_v \vec{\Gamma}_{1 \times N} & \vec{0}_{1 \times 3} & -e_v & \rho a^2 \end{bmatrix} \quad (38)$$

Inspecting the first (block) row of the matrix, one recognises the combination of variables that decouples the mass related terms from the rest: it is the same as for the **CNEq** case (compare with eq. (27)). Further inspection suggests the possibility of decoupling also the terms related with the vibrational energy. Both properties are achieved through the following definition for the symmetrizing variables:

$$\partial \vec{Q} = \left[y_s \partial p - a^2 \partial \rho_s, \quad \partial u_i, \quad \frac{\partial p}{\rho a}, \quad \frac{e_v}{\rho} \partial p - \frac{a^2 e_v}{\rho} \sum_s \partial \rho_s - a^2 \partial e_v \right]^t \quad (39)$$

The transformation matrices between the conservative and the symmetrizing sets of variables for thermal and chemical non-equilibrium (**TCNEq**) are:

$$\frac{\partial \vec{Q}}{\partial \vec{U}} = \begin{bmatrix} \vec{Y}_{N \times 1} \cdot \vec{\Gamma}_{1 \times N} - a^2 I_N & -\beta \vec{Y}_{N \times 1} \vec{u}^t & \beta \vec{Y}_{N \times 1} & \phi \vec{Y}_{N \times 1} \\ -\frac{\vec{u}}{\rho} \cdot \vec{1}_{1 \times N} & \frac{1}{\rho} I_3 & \vec{0}_{3 \times 1} & \vec{0}_{3 \times 1} \\ \frac{\vec{\Gamma}_{1 \times N}}{\rho a} & -\frac{\beta \vec{u}^t}{\rho a} & \frac{\beta}{\rho a} & \frac{\phi}{\rho a} \\ \frac{e_v}{\rho} \vec{\Gamma}_{1 \times N} & -\frac{\beta e_v}{\rho} \vec{u}^t & \frac{\beta e_v}{\rho} & \frac{1}{\rho} (\phi e_v - a^2) \end{bmatrix} \quad (40)$$

and:

$$\frac{\partial \vec{U}}{\partial \vec{Q}} = \begin{bmatrix} -\frac{1}{a^2} I_N & 0_{N \times 3} & \frac{\rho}{a} \vec{Y}_{N \times 1} & \vec{0}_{N \times 1} \\ -\frac{1}{a^2} \vec{u} \cdot \vec{1}_{1 \times N} & \rho I_3 & \frac{\rho}{a} \vec{u} & \vec{0}_{3 \times 1} \\ \frac{\vec{\Gamma}_{1 \times N}}{\beta a^2} - \frac{V^2}{a^2} \vec{1}_{1 \times N} & \rho \vec{u}^t & \rho \frac{H}{a} & \frac{\phi \rho}{\beta a^2} \\ \vec{0}_{1 \times N} & \vec{0}_{1 \times 3} & \frac{\rho e_v}{a} & -\frac{\rho}{a^2} \end{bmatrix} \quad (41)$$

With these matrices, the advective Jacobian in terms of symmetrizing variables is calculated simply as:

$$A^Q = \frac{\partial \vec{Q}}{\partial \vec{U}} \cdot A^U \cdot \frac{\partial \vec{U}}{\partial \vec{Q}} = \left[\begin{array}{c|c|c|c} UI_N & 0_{N \times 3} & \vec{0}_{N \times 1} & \vec{0}_{N \times 1} \\ \hline 0_{3 \times N} & UI_3 & a \vec{n} & \vec{0}_{3 \times 1} \\ \hline \vec{0}_{1 \times N} & a \vec{n}^t & U & 0 \\ \hline \vec{0}_{1 \times N} & \vec{0}_{1 \times 3} & 0 & U \end{array} \right] \quad (42)$$

where decoupling of mass terms and vibrational energy is evident. However, to take advantage of this result, eigenvectors in the new symmetrizing variables Q are needed (recall how upwind matrices are defined in eq. (19). They are computed in the next section.

4.3 Eigenvectors for TCNEq in symmetrizing variables

Left and right eigenvectors matrices in symmetrizing variables are computed from those expressed in conservative variables (as taken from¹²) using the previously derived transformation matrices $\frac{\partial \vec{U}}{\partial \vec{Q}}$ and $\frac{\partial \vec{Q}}{\partial \vec{U}}$ through the relations presented in what follows.

The matrix whose rows are the left eigenvectors in Q variables is:

$$L^Q = L^U \cdot \frac{\partial \vec{U}}{\partial \vec{Q}} = \left[\begin{array}{cccc} -I_N & 0_{N \times 3} & \vec{0}_{N \times 1} & \vec{0}_{N \times 1} \\ \vec{0}_{1 \times N} & \rho \vec{l}^t & 0 & 0 \\ \vec{0}_{1 \times N} & \rho \vec{m}^t & 0 & 0 \\ \vec{0}_{1 \times N} & \rho a \vec{n}^t & \rho a & 0 \\ \vec{0}_{1 \times N} & -\rho a \vec{n}^t & \rho a & 0 \\ \vec{0}_{1 \times N} & \vec{0}_{1 \times 3} & 0 & -\rho \end{array} \right] \quad (43)$$

Conversely, the right eigenvectors matrix is:

$$R^Q = \frac{\partial \vec{Q}}{\partial \vec{U}} \cdot R^U = \begin{bmatrix} -I_N & \vec{0}_{Nx1} & \vec{0}_{Nx1} & \vec{0}_{Nx1} & \vec{0}_{Nx1} & \vec{0}_{Nx1} \\ 0_{3xN} & \frac{1}{\rho} \vec{l} & \frac{1}{\rho} \vec{m} & \frac{1}{2\rho a} \vec{n} & -\frac{1}{2\rho a} \vec{n} & \vec{0}_{3x1} \\ \vec{0}_{1xN} & 0 & 0 & \frac{1}{2\rho a} & \frac{1}{2\rho a} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{1}{\rho} \end{bmatrix} \quad (44)$$

The diagonal matrix with the eigenvalues is the same as in conservative variables U , since eigenvalues are an invariant through linear transformations. This diagonal matrix is:

$$\Lambda^Q = \Lambda^U = \begin{bmatrix} U I_N & \vec{0}_{Nx1} & \vec{0}_{Nx1} & \vec{0}_{Nx1} & \vec{0}_{Nx1} & \vec{0}_{Nx1} \\ \vec{0}_{1xN} & U & 0 & 0 & 0 & 0 \\ \vec{0}_{1xN} & 0 & U & 0 & 0 & 0 \\ \vec{0}_{1xN} & 0 & 0 & U+a & 0 & 0 \\ \vec{0}_{1xN} & 0 & 0 & 0 & U-a & 0 \\ \vec{0}_{1xN} & 0 & 0 & 0 & 0 & U \end{bmatrix} \quad (45)$$

In our new formulation, the particular structure of the transformed Jacobian allows to apply separately $N+1$ times the scalar Nc scheme to distribute the vibrational energy and all the mass related residuals and keep the system Nc scheme for the 4×4 (3×3 for the $2D$ case) momentum-total energy subsystem.

The advantage with respect using the $N+5$ system Nc can be illustrated by means of the following diagram. Let's review which algebraic operations should be performed to apply the system Nc scheme. In the following expressions, \vec{Q} substitutes \vec{W} in expressions presented in section 3.1.

The cell residual can be computed in terms of its nodes state vectors:

$$\vec{\Phi}_{\Omega,*}^c = \frac{\partial \vec{U}}{\partial \vec{Q}} \sum_{j=1}^{d+1} K_{j,*}^Q \vec{Q}_{j,*} \quad (46)$$

Since each of the $K_{j,*}$ has the structure of (42), only the matrix-vector product $K_{j,*}^Q \vec{Q}_{j,*}$ is analysed. As evident from equation (47), what would be $N+1$ vector products become $N+1$ products of scalars.

$$K_{j,*}^Q \vec{Q}_{j,*} = \left[\begin{array}{ccc|cc} \square & & & 0_{N \times 3} & \vec{0}_{N \times 1} & \vec{0}_{N \times 1} \\ & \square & & & & \\ & & \ddots & & & \\ & & & \square & & \\ \hline 0_{N \times 3} & & & M_{3 \times 3} & m_{3 \times 1} & 0_{3 \times 1} \\ 0_{N \times 1} & & & \vec{m}_{1 \times 3} & \blacksquare & 0 \\ \hline 0_{N \times 1} & & & 0_{1 \times 3} & 0 & \square \end{array} \right] \cdot \left[\begin{array}{c} \diamond \\ \diamond \\ \vdots \\ \diamond \\ \hline m_{3 \times 1} \\ \bullet \\ \hline \diamond \end{array} \right] = \left[\begin{array}{c} \square \diamond \\ \square \diamond \\ \vdots \\ \square \diamond \\ \hline m_{4 \times 1} \\ \hline \square \diamond \end{array} \right] \quad (47)$$

The product $\frac{\partial \vec{U}}{\partial \vec{Q}} \left(\sum_{j=1}^{d+1} K_{j,*}^Q \vec{Q}_{j,*} \right)$ benefits also from the structure of matrix (41):

$$\frac{\partial \vec{U}}{\partial \vec{Q}} \left(\sum_{j=1}^{d+1} K_{j,*}^Q \vec{Q}_{j,*} \right) = \quad (48)$$

$$\left[\begin{array}{ccc|cc} \square & & & & \\ & \square & & & \\ & & \ddots & & \\ & & & \square & \\ \hline M_{N \times 3} & & & & \vec{0}_{N \times 1} \\ \vec{m}_{N \times 1} & M_{3 \times 3} & m_{3 \times 1} & & \vec{0}_{3 \times 1} \\ 0_{N \times 1} & \vec{m}_{1 \times 3} & \blacksquare & \triangle & \square \end{array} \right] \cdot \left[\begin{array}{c} \diamond \\ \diamond \\ \vdots \\ \diamond \\ \hline m_{3 \times 1} \\ \bullet \\ \diamond \end{array} \right] = \left[\begin{array}{c} \square \diamond + * \bullet \\ \square \diamond + * \bullet \\ \vdots \\ \square \diamond + * \bullet \\ \hline m_{4 \times 1} \\ * \bullet + \square \diamond \end{array} \right]$$

Now, looking at the residual distribution for the N scheme, one realizes that the inlet state is computed, as in equation (23), through an expression including the factor $\left(\sum_{j=1}^{d+1} K_{j,*}^- \right)^{-1}$. This expression gets also simplified, since:

$$\left(\sum_{j=1}^{d+1} K_{j,*}^- \right)^{-1} = \left[\begin{array}{ccc|cc} 1/\square^- & & & & \\ & 1/\square^- & & & \\ & & \ddots & & \\ & & & 1/\square^- & \\ \hline 0_{N \times 4} & & & & \vec{0}_{N \times 1} \\ 0_{N \times 1} & 0_{N \times 4} & (M_{4 \times 4})^{-1} & & \vec{0}_{4 \times 1} \\ & 0_{1 \times 4} & & & 1/\square^- \end{array} \right] \quad (49)$$

The definition of the distribution matrices for the $LDAc$ scheme involves an operation similar to that in equation (49). In the end, it turns out that any quantity related with the system Nc scheme involves combinations of the types of operations detailed in equations (47), (48) or (49). With previous diagrams the potential savings tied to this formulation are clear. Results in 5.1 confirm this point.

5 NUMERICAL RESULTS

The symmetrizing variables derived before have been implemented in the `COOLFluid` code (described in references⁶) and applied to two different hypersonic flow problems. The first problem is the inviscid flow around a sharp nosed, 30° cone while the second testcase is the flow around a sharp nosed 25° - 55° double cone in particular for the conditions known in literature as `Run 42`) (see references^{6,10}).

5.1 Verification and performance evaluation: flow around a sharp cone

This first testcase has been employed to check that the solution retrieved using the new set of symmetrizing variables is exactly the same as the one obtained performing the convective residual distribution in conserved variables, and to investigate the reduction in the numerical effort associated with the particular structure of the advective Jacobians in terms of the new variables. In order to isolate as much as possible the effect of the symmetrization the flow has been assumed inviscid.

The verification of the extended code has been made by checking whether the same residuals are retrieved when computing one iteration with the different sets of variables. This must be so because the variables in which the residual is distributed (must) have not influence in the effective value of the residual. This has been the case for all the numerical experiments performed.

The improvement obtained has been measured as:

$$\eta = \frac{t_{cons} - t}{t_{cons}} \times 100.0\% \quad (50)$$

where t_{cons} and t are the times spent for an iteration if the distribution is performed in conservative or in symmetrizing variables respectively. These times have been obtained, for each case, as an average of the times needed to perform a pair of iterations in three different experiments.

The testing has been performed on an 8-core Intel(R) Xeon(R) computer with E5420 CPU at 2.50 GHz and a cache memory of 6144 kB . The mesh employed, made up of triangles, contained slightly more than 10^4 nodes.

The results obtained are presented in table 1, where two different situations are presented. In the so-called *partial decoupling* cases, mass equations have been treated with scalar **RD** schemes, applying a system **RD** scheme to the subsystem of momentum, total and vibrational energies equations. In the *full decoupling* cases, also the vibrational energy has been treated with a scalar scheme.

	N_2 - N mixture [s]	η [%]	air5 mixture [s]	η [%]
Cons. variables	9.94	0.0	32.63	0.0
Symm. variables, partial decoupling	8.38	15.7	20.57	37.0
Symm. variables, full decoupling	7.44	25.2	20.25	37.9

Table 1: Efficiency improvement, non-equilibrium case.

The improvement in the time per iteration is clear from table 1. Observe how the higher the number of species involved, the higher is the gain obtained.

As explained in section 3, the **CRD** solver employed distributes the advection and the source term residuals together. So, in order to have an idea on the impact of the source term evaluation cost in the savings obtained, an additional set of tests was performed considering a frozen flow (*switching off* the source term). Results are shown in table 2. Same tendencies as in the non-equilibrium case are observed, but yet higher improvements are obtained (since the computational demand is lower).

	N_2 - N mixture [s]	η [%]	air5 mixture [s]	η [%]
Cons. variables	6.40	0.0	21.64	0.0
Symm. variables, partial decoupling	4.47	30.2	9.09	58.0
Symm. variables, full decoupling	4.01	37.35	8.84	59.1

Table 2: Efficiency improvement, frozen case.

Results obtained show an important reduction in computational cost, which is more important if the complexity of the chemistry model is higher. It is clear also that strategies to reduce the cost of distributing the source term residual have to be sought.

5.2 Application to the flow around a double cone configuration

In this section, results obtained applying the symmetrizing variables for the well studied Run 42 (see in^{6,10}) double cone testcase are reported. These results were obtained using the Nc scheme described in 3 on a 256x512 DOF mesh.

The corresponding free-stream flow conditions and the wall temperature for are shown in the table 3:

M_∞	$\rho_\infty [kg/m^3]$	$U_\infty [m/s]$	$T_\infty [K]$	$T_{v,\infty} [K]$	$y_{N,\infty} [-]$	$y_{N_2,\infty} [-]$	$T_w [K]$
11.5	0.001468	3849.3	268.7	3160	0	1	294.7

Table 3: Free-stream conditions and wall temperature for run 42.

Results obtained have been compared with those presented in reference⁶. Again, and for the same reasons exposed in section 5, results obtained using the symmetrizing variables and those using the original formulation overlap exactly. In what follows, contour maps for the Mach number (fig. 4), the roto-translational (fig. 5) and electronic-vibrational (fig. 6) temperatures and atomic nitrogen mass fraction (fig. 7) are shown.

6 CONCLUSIONS

In the present work, the advective Jacobian of the Navier-Stokes equations for a two temperatures **TCNEq** model has been reformulated in terms of a set of symmetrizing variables, allowing decoupling of the mass and vibrational energy conservation terms from the momentum and total energy subsystem. The particular structure of the transformed Jacobian can be

used advantageously in a **RD** context to reduce the computational cost of distributing the cell residuals.

The symmetrizing reformulation has been implemented into **CRD** code, so that discrete conservativity has not been a concern. Indeed, it has been shown that use of these symmetrizing variables yields exactly the same results as those obtained with the baseline code (both for inviscid and viscous hypersonic flows), with the only difference of requiring less computational effort. This improvement in numerical performance comes from the fact of moving from operations involving $N + 5$ matrices (in the $3D$ case) to operations with a 4×4 submatrix and $N + 1$ scalars.

There is no conceptual incompatibility in applying these variables to other system schemes than Nc . Thus, achieving second order accuracy through non linear blending of the present system Nc and $LDAc$ schemes is straightforward, and work in this direction is ongoing.

Results obtained in this work identify the evaluation and distribution on the source term cell residuals as an important bottleneck in the code performance and further work on improving these operations is needed.

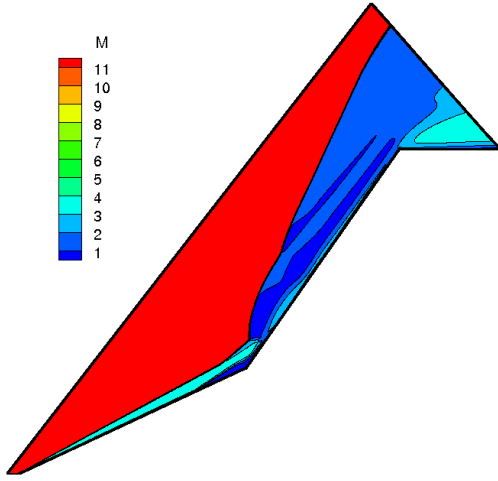


Figure 4: Mach number field for run 42, with symmetrizing variables.

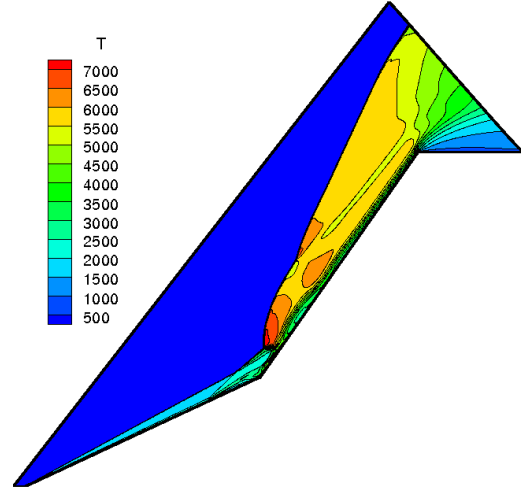


Figure 5: Roto-translational temperature field for run 42, with symmetrizing variables.

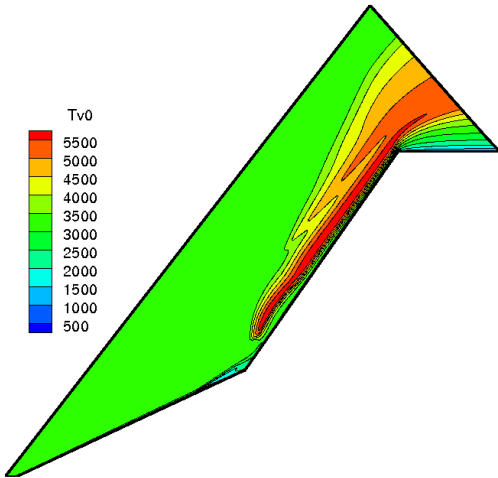


Figure 6: Vibrational temperature field for run 42, with symmetrizing variables.

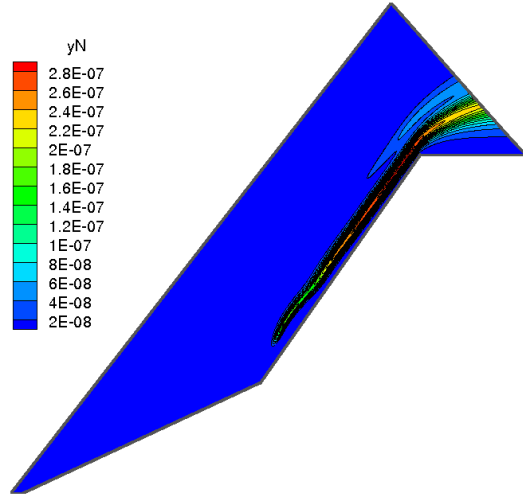


Figure 7: Atomic N mass fraction field for run 42, with symmetrizing variables.

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