PROGRAMMER'S MANUAL FOR OPEN3DCFD

OPEN3DCFD Group

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Contents

List of Tables

NOMENCLATURE

Symbol	
a	Speed of sound.
a_0	Reference speed of sound.
A, B, C	Flux Jacobians.
CFL	Courant-Friedrichs-Lewy.
C_v	Mixture specific heat at constant volume.
C_{vi}	Species specific heat at constant volume.
C_p	Pressure coefficient.
D	Chemistry Jacobian
$\tilde{e}$	Total internal energy.
e_{el}	Electronic contribution to internal energy.
e_i	Species internal energy.
e_{rot}	Rotational contribution to internal energy.
e_{tr}	Translational contribution to internal energy.
e_o	Total energy.
e_{vib}	Vibrational contribution to internal energy.
$\hat{\mathbf{F}}, \hat{\mathbf{G}}, \hat{\mathbf{H}}$	Cartesian flux Jacobians.
$\mathbf{F}, \mathbf{G}, \mathbf{H}$	Transformed flux vectors.
h_i^o	Reference species heat of formation.
h_o	Total enthalpy.

Symbol	
I	Identity matrix.
J	Metric Jacobian.
$k_b(T)$	Backward reaction rate.
$k_f(T)$	Forward reaction rate.
K	General Flux Jacobain Matrix of conserved variables.
L	Nonlinear flux limiter.
$\bar{l}_{ref}$	Reference length.
$\dot{m}$	Massflow.
M	Transformation matrix from conserved to non-conserved variables
M_i	Species mass.
n	Number of degrees-of-freedom for species.
NS	Number of species in fluid.
P	static pressure.
P_κ	Matrix of right eigenvectors for κ.
q^2	Magnitude of Cartesian velocity.
$\mathbf{q}$	Vector of non-conserved variables.
$\hat{\mathbf{Q}}$	Dependent variable vector in Cartesian coordinates.
$\mathbf{Q}$	Computational space dependent variable vector.
$\widehat{R}$	Ideal gas constant.
R_i	Species gas constant.
s_0	Reference entropy.
t	time in physical space.
T	Fluid temperature.
T_k	Matrix of right eigenvectors for K.

Symbol	
u, v, w	Cartesian velocity components.
$\tilde{u}, \tilde{v}, \tilde{w}$	Contravariant velocity.
$\dot{\mathbf{W}}$	Chemistry source term.
X_m	Chemical species in the fluid.
x, y, z	Cartesian coordinates.
α_j	Jump in characteristic variables.
β	Angle between the relative velocity vector and the axial direction.
δ	Central difference operator.
Δ	Upwind difference operator.
γ	Ratio of specific heats.
κ	General flux Jacobian matrix of non-conserved varaibles.
λ	Eigenvalue.
ν, ν	Stochiometric coefficients.
Ω	Control volume.
ξ, η, ζ	Curvilinear coordinates.
ρ	Density.
ρ_i	Species density.
τ	Time in computational space.
θ_d	Characteristic dissociation temperature.
θ_v	Characteristic vibrational temperature.

Subscripts

a	Internal location in computational grid.
b	External to computational grid.
i, j, k	Grid index.
o	Reference quatntites.
∞	Freestream reference condition.

Superscripts

(j)	Corresponds to j^{th} wave.
n	Time step parameter.

Chapter 1

INTRODUCTION

The development of numerical tools for the simulation of finite-rate chemistry flows has received increasing attention over the past decade. Chemically reacting flows play an important role in a wide range of scientific fields, such as combustion, hypersonic flight, missile launches aboard ships, environmental concerns, and explosion analysis. For an example, analysis of the flow encountered by a hypersonic vehicle requires the description of the behavior and chemical composition of air behind very strong shocks [1]. Rocket plumes resulting from missile launches aboard Navy ships [2] require the accurate description of heating and shipboard ablation effects in order to assure the ship's safety and optimal operation. Of growing concern are environmental hazards associated with the operation of internal combustion engines and the resultant NO_x emissions [3], [4]. Another interesting problem in the area of reacting flows is associated with explosions within a closed compartment [5].

There are various levels of approximations that can be used to model high-speed, high-temperature flow. The simplest one is the perfect gas model, which ignores the effects of chemical reactions, and is limited to lower temperatures [6]. This approximation is grossly inaccurate for problems dominated by chemical activity. A local chemical equilibrium assumption [7] offers another somewhat ideal scenario: the chemical reactions are assumed to instantaneously reach equilibrium. This assumption results in the requirement of solving only five partial differential equations for a three-dimensional flow, along with computing the equilibrium concentrations of the fluid mixture. The shortcoming of the equilibrium solution is that the chemical kinetics is inaccurate. The most general model employs a full description of finite-rate chemistry, which is desirable for many of the above applications because it is the most realistic description of the physics associated with chemical reactions. The downside of using a finite-rate model is that the numerical solution requires an additional differential equation to be added for each chemical species present in the fluid. That is, for a mixture of NS species, $NS+4$ equations must be solved for a three-dimensional, compressible, inviscid flow. The trade-off of accuracy versus computational speed is always a difficult choice.

The purpose of the programmer's manual is to describe the implementation of the governing equations necessary to develop accurate and efficient solutions for flows with finite-rate chemistry. The document will describe the governing equations, the thermodynamic system, the grid metrics calculations and the PDE solver that are to be implemented. A final section will describe the compuational flow of the model.

Two time integration models will be implemented for this project: a fully implicit, modified two-pass method and a semi-implicit method. The eigensystem was developed specifically for this project and will be described in a later section. Suffice to say that this is a well designed set of eigenvectors for higher-order upwind applications which do not contain possible indefinite mass species source terms in the eigensystem. Essentially this work is an extension of the methods developed by Whitfield and Janus [8] for a perfect gas and their later extensions [9].

The description of the eigenvalues and eigenvectors is necessary for the development of the numerical schemes. The choice of eigenvectors is somewhat arbitrary, due to the presence of repeated eigenvalues. The choice of eigenvectors used by Cinnella [13] and Slomski [14] involves additional sets of unit basis vectors to account for the repeated eigenvalues. As noted in [12], this computation is unnecessary if the eigenvectors are only used in MUSCL schemes, because the left eigenvectors are not needed in the evaluation of the MUSCL schemes.

Further, Cinnella's eigensystem, while ideally suited when used with higher-order spatially accurate MUSCL schemes, can prove inadequate when used in conjunction with non-MUSCL schemes, due to the occurrence of species mass fractions in the denominator of elements in the matrix of left eigenvectors. This can cause large values when computing trace elements (where species density is very small) and can lead to numerical convergence problems. Included in this study is the development of an eigensystem which can be applied for non-MUSCL, upwinding schemes as well as with MUSCL methodologies.

The layout of this document is the following. Chapter 3 will describe the governing equations for flows in chemical nonequilibrium and the thermodynamic models utilized. Chapter 4 will discuss the chemical kinetics equations and two chemistry models that currently reside in the chemistry database: a five-species, 17 reaction air model and a six-species, 28 reaction hydrogen/oxygen combustion model. The eigensystem for non-MUSCL upwinding scheme is presented in Chapter 5.

The fully-implicit, approximately-factored scheme and the semi-implicit scheme will be derived in Chapter 6. The schemes represent two of the more popular methods in use today.

Chapter 2

INITIALIZATION

2.1 Variable Initialization

The purpose of this section is to define the variables that initialized at start-up of the program either through user input or database initialization due to user selections. Table 3.2 lists these variables, their name used throughout this document, the program name (defined by the programmer for use throughout the program), additional functions where the variable is used or modified and a short definition of the variable. It is expected that this data will be provided in some interactive fashion or through an input file if batch execution is needed by the user.

Variable	Program Name	Function(s) U/M	Definition	type
i_{chem}			Chemistry Model Flag	int
int_{type}			Type of integration: 0 - fully implicit, 1 - semi-implicit	int

Table 2.1: Initialization Variables

2.2 Input File Data

Currently one input file file is expected for execution. This is the *grid.in* file. The *grid.in* files contains the block, structured compuatational grid. The format is expected to be in *block3d* format but additional formats will be included as user's request them or as others add to the solver.

2.3 Chemistry Data Base

The FORTRAN version of this program contained a very basic set of arrays that defined necessary chemical reactions and chemical physical definitions. It is expected that a more talented person will define a better database - either external to OPEN3DCFD or internal to facillitate growth of the database and hence, the possible number of problems that can be solved.

Chapter 3

GOVERNING EQUATIONS

3.1 Euler Equations

This chapter describes the equations which govern the three-dimensional flow of an inviscid, chemically reacting gas. The equations will be written in general curvilinear coordinates, which are used to describe problems with complicated boundaries.

As mentioned in Chapter 1, these equations are an extension of the Euler Equations for a perfect gas, the main difference being that the conservation of mass of each species must be included. That is, for a gas mixture containing NS distinct species, it it necessary to write $NS + 4$ partial differential equations. The production/disappearance of each chemical species is governed by a source term $\widehat{\mathbf{W}}$, and will be discussed in detail in the next chapter.

3.2 Curvilinear Coordinates

As stated above, in order to compute flows involving arbitrary shapes and the complex boundaries associated with these shapes, it is convenient to transform the equations to a general body-fitted curvilinear coordinate system. This is accomplished using the transformation equations listed below. (See [33] for a derivation of the transformation.):

$$\begin{aligned} \xi &= \xi(x, y, z), \\ \eta &= \eta(x, y, z), \\ \zeta &= \zeta(x, y, z), \\ \tau &= t. \end{aligned} \tag{3.1}$$

The vector form of the three-dimensional compressible Euler equations in

differential, conservative form is

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{F}}{\partial \xi} + \frac{\partial \mathbf{G}}{\partial \eta} + \frac{\partial \mathbf{H}}{\partial \zeta} = \mathbf{W}, \tag{3.2}$$

where $\mathbf{Q}$ is the dependent variable vector, and $\mathbf{F}$, $\mathbf{G}$, and $\mathbf{H}$ are the inviscid flux vectors. The dependent variable vector and flux vectors are now defined as follows:

$$\mathbf{Q} = J \begin{bmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_{NS} \\ \rho u \\ \rho v \\ \rho w \\ \rho e_0 \end{bmatrix}, \qquad \mathbf{F} = J \begin{bmatrix} \rho_1 \tilde{u} \\ \rho_2 \tilde{u} \\ \vdots \\ \rho_{NS} \tilde{u} \\ \rho u \tilde{u} + \xi_x P \\ \rho v \tilde{u} + \xi_y P \\ \rho w \tilde{u} + \xi_z P \\ \rho h_0 \tilde{u} \end{bmatrix},$$

$$\mathbf{G} = J \begin{bmatrix} \rho_1 \tilde{v} \\ \rho_2 \tilde{v} \\ \vdots \\ \rho_{NS} \tilde{v} \\ \rho u \tilde{v} + \eta_x P \\ \rho v \tilde{v} + \eta_y P \\ \rho w \tilde{v} + \eta_z P \\ \rho h_0 \tilde{v} \end{bmatrix},$$

$$\mathbf{H} = J \begin{bmatrix} \rho_1 \tilde{w} \\ \rho_2 \tilde{w} \\ \vdots \\ \rho_{NS} \tilde{w} \\ \rho u \tilde{w} + \eta_x P \\ \rho v \tilde{w} + \eta_y P \\ \rho w \tilde{w} + \eta_z P \\ \rho h_0 \tilde{w} \end{bmatrix}, \qquad \mathbf{W} = J \begin{bmatrix} \dot{w}_1 \\ \dot{w}_2 \\ \vdots \\ \dot{w}_{NS} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

In the above, $\widehat{\mathbf{W}}$ is the vector of source terms, NS represents the number of species present in the fluid, ρ_i is the ith species density, ρ is the total density of the gas, h_0 is the total enthalpy, e_0 is the total energy per unit mass, P is the pressure and u, v and w are the velocity components in the x, y, and z directions, respectively. The total energy per unit volume, ρe_0 is defined as

$$\rho e_0 = \rho e + \frac{\rho q^2}{2}, \tag{3.3}$$

where

$$q^2 = u^2 + v^2 + w^2. \tag{3.4}$$

The source terms $\dot{w}_i$ will be discussed in Chapter 4.

The system is closed by a caloric equation of state, to be discussed in more detail in Section 3.4, and by a thermal equation of state, given by

$$P = \sum_{i=1}^{NS} \rho_i R_i T. \tag{3.5}$$

where R_i is the species gas constant and T is the mixture temperature.

The contravariant velocities, $\tilde{u},\ \tilde{v},\ \tilde{w}$ in directions normal to the $\xi,\ \eta,\ \zeta$ surfaces, respectively, are:

$$\tilde{u} = \xi_x u + \xi_y v + \xi_z w, \tag{3.6}$$

$$\tilde{v} = \eta_x u + \eta_y v + \eta_z w, \tag{3.7}$$

$$\tilde{w} = \zeta_x u + \zeta_y v + \zeta_z w. \tag{3.8}$$

3.3 Grid Metrics

For a stationary grid, the grid metrics are computed only at program initialization. The Jacobian of the inverse transformation, J, and the metric quantities are given by

$$J = x_\xi \left(y_\eta z_\zeta - z_\eta y_\zeta\right) - y_\xi \left(x_\eta z_\zeta - z_\eta x_\zeta\right) + z_\xi \left(x_\eta y_\zeta - y_\eta x_\zeta\right), \tag{3.9}$$

$$\begin{aligned} \xi_x &= J^{-1}\left(y_\eta z_\zeta - z_\eta y_\zeta\right), & \eta_x &= J^{-1}\left(z_\xi y_\zeta - y_\xi z_\zeta\right), \\ \xi_y &= J^{-1}\left(z_\eta x_\zeta - x_\eta z_\zeta\right), & \eta_y &= J^{-1}\left(x_\xi z_\zeta - z_\xi x_\zeta\right), \\ \xi_z &= J^{-1}\left(x_\eta y_\zeta - y_\eta x_\zeta\right), & \eta_z &= J^{-1}\left(y_\xi x_\zeta - x_\xi y_\zeta\right), \end{aligned}$$

$$\begin{aligned} \zeta_x &= J^{-1}\left(y_\xi z_\eta - z_\xi y_\eta\right), \\ \zeta_y &= J^{-1}\left(z_\xi x_\eta - x_\xi z_\eta\right), \\ \zeta_z &= J^{-1}\left(x_\xi y_\eta - y_\xi x_\eta\right). \end{aligned}$$

3.4 Thermodynamic Models

Compressible fluid dynamic flows can be broadly categorized into four types, based on fluid temperature and molecular interactions within the fluid. The description *real gas* in many papers actually refers to flows which are not chemically reacting and are, in reality, mixtures of *perfect gases*. Anderson [36] offers the following description of categories of fluid flows:

Variable	Program Name	Function(s) U/M	Definition	type
$\mathbf{F}$			Flux vector in ξ direction	vector::real
$\mathbf{G}$			Flux vector in η direction	vector::real
$\mathbf{H}$			Flux vector in ζ direction	vector::real
h_0			Total enthalpy at cell center	vector::real
NS			Number of species in mixture	int
P			Pressure at cell center	vector::real
q^2			velocity squared at cell center	real
R_i			Ideal Gas Constant for species i	real
ρe_0			Total energy at cell center	vector::real
ρ_i			Density of species i at cell center	vector::real
ρ			Mixture density at cell center	vector::real
ρe_0			Total energy at cell center	vector::real
T			Mixture temperature at cell center	vector::real
u			Velociy in x-direction at cell enter	vector::real
$\tilde{u}$			Contravariant velociy in ξ-direction at cell enter	vector::real
v			Velociy in y-direction at cell enter	vector::real
$\tilde{v}$			Contravariant velociy in η-direction at cell enter	vector::real
w			Velociy in z-direction at cell enter	vector::real
$\tilde{w}$			Contravariant velociy in ζ-direction at cell enter	vector::real

Table 3.1: Flux Variables

1. Calorically Perfect Gas: By definition a perfect gas has constant specific heats and thus a constant ratio of specific heat (e.g., $\gamma = 1.4$ for air).

2. Thermally Perfect Gas: A thermally perfect gas is defined as one in which the specific heats are functions of temperature only.

3. Mixture of chemically reacting, thermally perfect gases: Components are thermally perfect while the mixture is thermally perfect if no chemistry is present. The mixture is *not* thermally perfect in the presence of chemical reactions.

4. Real Gas: In this case, intermolecular forces must be included. A real gas occurs in the presence of very high pressures or low temperatures. The perfect gas equation of state is no longer valid. The mixture enthalpy and energy are now functions of temperature and a second state variable (e.g. density or pressure). This program does not provide real gas solutions.

For this study, the fluids will be considered to be mixtures of thermally perfect gases. The associated equation of state will be developed in this section.

The equations described in Section 3.1 describe a flow in chemical nonequilibrium. The equations are valid for flows where high temperatures exist, but it becomes necessary to modify the traditional caloric equation of state. In many cases, the high temperatures cause the onset of chemical reactions, which lead to the dissociation of molecules and the ionization of neutral species. Also, the internal vibrational state of molecules can become excited and the de-excitation typically requires a time scale that might be of the same order as the flow time scale. The description of this process would then require a finite-rate model.

3.4.1 Internal Energy Calculation

A description for the internal energy for species i in the mixture can be written as a summation of the separate contributions of the internal energy states

$$e_i = e_{tr} + e_{rot} + e_{vib} + e_{el} + h_i^o, \tag{3.10}$$

where e_{tr} is the translational contribution, e_{rot} is the rotational contribution, e_{vib} is vibrational contribution, e_{el} is the contribution from electronic excitation, and h_i^o is the heat of formation for the ith species at a reference temperature of zero. The additivity assumption of the internal energy contributions is a simplification of the more general statistical mechanics result that describes the internal structure contributions. As shown below, this simplification allows for a straightforward description of species internal energy and can be found in [37].

The assumption of thermal equilibrium means that enough collisions have occurred to allow the rotational and translational components of internal energy to reach an equilibrium state. This simplification can be accepted for most flows because equilibration of translational and rotational contributions is a very fast process (i.e., it requires on the order of ten molecular collisions). These contributions can now be written as

$$e_{rot+tr_i} = n_i R_i T \tag{3.11}$$

where n_i is defined as

$$n_i = \begin{cases} \frac{3}{2} & \text{for atoms,} \\ \frac{5}{2} & \text{for diatomic and linear polyatomic molecules,} \\ \frac{6}{2} & \text{for nonlinear polyatomic molecules.} \end{cases} \tag{3.12}$$

The vibrational equilibrium contribution is included through a harmonic oscillator assumption. For a diatomic species i, it is given as

$$e_{vib,i} = \frac{R_i \theta_{v,i}}{e^{\theta_{v,i}/T} - 1} \tag{3.13}$$

where $\theta_{v,i}$ is the characteristic vibrational temperature and R_i is the species gas constant. More than one characteristic temperature are needed to describe

the vibrational contribution for polyatomic molecules. Table 3.4.5 lists the characteristic temperatures for the species used in the chemical models described in Chapter 4. The characteristic temperatures were obtained from the JANAF tables [38].

Finally, electronic contributions are ignored because the are usually very small. Using the approximations described above, the final equation for internal energy per unit mass of a mixture can now be obtained by summing equations 3.11 and 3.13 over all species (using a standard mixture "rule"):

$$\tilde{e} = \sum_{i=1}^{NS} \left(\frac{\rho_i}{\rho}\right) \left(n_i R_i T + \frac{R_i \theta_{v,i}}{e^{\theta_{v,i}/T} - 1} + h_i^o\right) \tag{3.14}$$

The total energy of the system, per unit volume, as given by the *conserved variable* ρe_0 is

$$\rho e_0 = \rho \tilde{e} + \rho \frac{q^2}{2} = \sum_{i=1}^{NS} \rho_i \left(n_i R_i T + \frac{R_i \theta_{v,i}}{e^{\theta_{v,i}/T} - 1} + h_i^o\right) + \rho \frac{q^2}{2} \tag{3.15}$$

Note, with correct input, this above equations are valid for perfect gas air.

Variable	Program Name	Function(s) U/M	Definition	type
NS			Number of species in mixture	int
q^2			velocity squared at cell center	real
h_i^o		Chem DB	Reference species specific enthalpy	real
n_i		Chem DB	Species degree of rotation	int
R_i			Ideal Gas Constant for species i	real
ρ			Chemistry Model Flag	int
ρe_0			Total energy at cell center	vector::real
ρ_i			Density of species i at cell center	vector::real
ρ			Mixture density at cell center	vector::real
ρe_0			Total energy at cell center	vector::real
T			Mixture temperature at cell center	vector::real
$\theta_{v,i}$		Chem DB	Dissociation temperature for species i	real

Table 3.2: Thermodynamic Variables

3.4.2 Temperature

Equation 3.15 is a nonlinear function of temperature and density. In particular, temperature must be found from known values of $\tilde{e}$, ρ_i and q. Newton's method is used to compute temperatures, and provided solutions within three to four iterations.

3.4.3 Enthalpy

Total enthalpy, h_0, is computed as

$$h_0 = e_0 + \frac{P}{\rho}. \tag{3.16}$$

3.4.4 Specific Heat

The specific heat at constant volume for species i, C_{v_i} is

$$C_{vi} = n_i R_i + R\left(\frac{\theta_v}{T}\right)^2 \frac{e^{\theta_v/T}}{\left[e^{\theta_v/T} - 1\right]^2}. \tag{3.17}$$

3.4.5 Frozen Speed of Sound

The frozen speed of sound can be easily found for a mixture of thermally perfect gases. The final results reads

$$a = \sqrt{\frac{\hat{\gamma} P}{\rho}}, \tag{3.18}$$

where $\hat{\gamma}$ is the mixture ratio of frozen specific heats. A detailed derivation of the speed of sound for a mixture of thermally perfect gases can be found in [13].

Name	$\theta_v(1)$	$\theta_v(2)$	$\theta_v(3)$
N_2	3392.0		
O_2	2273.0		
NO	2739.0		
H_2	6338.3		
H_2O	2294.3	5261.7	5403.8
OH	5374.2		

Table 3.3: Vibrational Characteristic Temperatures

Chapter 4

CHEMICAL SOURCE TERMS

4.1 Source Term Description

The right-hand-side of equation 3.2 describes the production and consumption of each of the chemical species in a particular fluid, due to the occurrence of chemical reactions. The general equation for a chemical reaction (assuming that NR reactions are occurring simultaneously) is given by

$$\sum_{i=1}^{NS} \nu_{m,r}^{'} X_m \rightleftharpoons \sum_{i=1}^{NS} \nu_{m,r}^{''} X_m, \qquad \text{r=1,2,...,NR,} \tag{4.1}$$

where X_m is a chemical species in the fluid, $\nu_{m,r}^{'}$ are the stoichiometric coefficients for the reactants (related to species m in reaction r) and $\nu_{m,r}^{''}$ are the stoichiometric coefficients for the product (related to species m in reaction r). From this mass balance the rate of change for a given species, i, is defined as [37]:

$$\dot{w}_i = \widehat{M}_i \sum_{r=1}^{NR} \left(\nu_{i,r}^{''} - \nu_{i,r}^{'}\right) K_{f,r} \left[\prod_{m=1}^{NS} \left(\frac{\rho_m}{\widehat{M}_m}\right)^{\nu_{m,r}^{'}} - \frac{1}{K_{c,r}} \prod_{m=1}^{NS} \left(\frac{\rho_m}{\widehat{M}_m}\right)^{\nu_{m,r}^{''}}\right]. \tag{4.2}$$

where $\widehat{M}_i$ is the molecular weight of species i, $\mathrm{K}_{f,r}$ is the forward reaction rate for reaction r, $\mathrm{K}_{c,r}$ is the equilibrium reaction rate and NS is the number of species in the fluid.

It should be noted that this equation depends on accurate experimental data in order to provide valid results.

The forward reaction rate is usually described, for a given reaction r, by an Arrhenius equation:

$$K_{f,r} = C_f T^{\eta_r} e^{\theta_d/T}. \tag{4.3}$$

The coefficients C_f, η_r and θ_d have been obtained experimentally for many different reactions over a wide range of temperatures.

The equilibrium rate equation, like the forward rate equation, can be represented in an Arrhenius form using experimental data. Another option for defining the equilibrium rate, the one used in this study, is based on the minimization of Gibbs free energy at constant pressure and energy. This method is not dependent on experimental data but on reference values which are easily obtained. The method does depend on the thermodynamic model used and will be affected by any shortcomings or assumptions included in the thermodynamic model.

Anderson [36] and Cox[7] provide a derivation of the equilibrium rate equation from the Gibb's free energy method:

$$K_{c,r} = \left(\frac{P_{ref}}{\widehat{R}T}\right)^{\sum_{i=1}^{NS}\left(\nu''_{i,r}-\nu'_{i,r}\right)} \exp\left[-\sum_{i=1}^{NS}\frac{\omega_i(T)}{R_iT}\left(\nu''_{i,r}-\nu'_{i,r}\right)\right], \tag{4.4}$$

where

$$\omega_i(T) = 1 + n_i + ln\left(1 - e^{-\theta_{v,i}/T}\right) - (1+n_i)\,lnT + \frac{h_i^o}{R_iT} - \frac{s_i^o}{R_i}. \tag{4.5}$$

The reference values are: h_i^o, the reference species enthalpy at absolute zero and s_i^o, the species entropy at absolute zero.

4.2 Chemical Derivatives

Development of the numerical schemes in Chapter 6 requires the derivatives of the source term, $\mathbf{W}$ with respect to the conserved variable, $\mathbf{Q}$. This matrix of partial derivatives is usually referred to as the chemical Jacobian, and is defined as

$$D = \frac{\partial \mathbf{W}}{\partial \mathbf{Q}}. \tag{4.6}$$

Since $w_i = 0$ for $i > NS$, that is

$$\frac{\partial w_i}{\partial \mathbf{Q}} = 0 \qquad \text{for i} > \text{NS} \tag{4.7}$$

then the Jacobian can be written as

$$D = \frac{\partial w_i}{\partial Q_j} \qquad \text{for } i = 1, 2, \ldots, NS;\ j = 1, 2, \ldots, NS+4. \tag{4.8}$$

Equation 4.2 shows that the source terms are a function of density and temperature. As such, application of the chain rule is necessary to obtain the final form of the chemical Jacobian. This results in a complete description of the chemical Jacobian:

$$\frac{\partial w_i}{\partial Q_j} = \frac{\partial w_i}{\partial \rho_j} + \frac{\partial w_i}{\partial T}\left.\frac{\partial T}{\partial \rho_j}\right|_{(\rho u, \rho v, \rho w, \rho e_0)} \qquad \text{for } i, j = 1, 2, \ldots, NS, \tag{4.9}$$

Variable	Program Name	Function(s) U/M	Definition	type
C_f	chem	Chem DB		real
η_r		Chem DB		real
i_{chem}			Chemistry Model Flag	int
h_i^o		Chem DB	Reference species enthalpy at absolute zero	real
n_i		Chem DB		int
$\widehat{M_i}$		Chem DB	The molecular weight of species i	real
NS			Number of species in mixture	int
$\nu_{m,r}^{'}$		Chem DB	Stoichimetric coefficient for reactant related to species m in reaction r	int
$\nu_{m,r}^{''}$		Chem DB	Stoichimetric coefficient for product related to species m in reaction r	int
s_i^o		Chem DB	Reference species entropy at absolute zero	real
θ_d		Chem DB		real
$\theta_{v,i}$		Chem DB		real
T			Mixture Temperature	real

Table 4.1: Chemistry Variables

$$\frac{\partial w_i}{\partial Q_{N+1}} = \frac{\partial w_i}{\partial(\rho u)} = \frac{\partial w_i}{\partial T}\,\frac{\partial T}{\partial(\rho u)}\bigg|_{(\rho_i,\rho v,\rho w,\rho e_0)}, \tag{4.10}$$

$$\frac{\partial w_i}{\partial Q_{N+2}} = \frac{\partial w_i}{\partial(\rho v)} = \frac{\partial w_i}{\partial T}\,\frac{\partial T}{\partial(\rho v)}\bigg|_{(\rho_i,\rho u,\rho w,\rho e_0)}, \tag{4.11}$$

$$\frac{\partial w_i}{\partial Q_{N+3}} = \frac{\partial w_i}{\partial(\rho w)} = \frac{\partial w_i}{\partial T}\,\frac{\partial T}{\partial(\rho w)}\bigg|_{(\rho_i,\rho u,\rho v,\rho e_0)}, \tag{4.12}$$

$$\frac{\partial w_i}{\partial Q_{N+4}} = \frac{\partial w_i}{\partial(\rho e_0)} = \frac{\partial w_i}{\partial T}\,\frac{\partial T}{\partial(\rho e_0)}\bigg|_{(\rho_i,\rho u,\rho v,\rho w)}. \tag{4.13}$$

The derivatives necessary for equations 4.9 through 4.13 can be expressed as:

$$\frac{\partial w_i}{\partial \rho_j} = \widehat{M_i}\sum_{r=1}^{NR}(\nu_{i,r}^{''}-\nu_{i,r}^{'})K_{f,r}(T)\left[\prod_{m=1}^{NS}\nu_{j,r}^{'}\left(\frac{\rho_m}{\widehat{M_m}}\right)^{\bar{\nu}_{m,r}^{'}} - \frac{1}{K_{c,r}}\prod_{m=1}^{NS}\nu_{j,r}^{''}\left(\frac{\rho_m}{\widehat{M_m}}\right)^{\bar{\nu}_{m,r}^{''}}\right] \tag{4.14}$$

where

$$\bar{\nu}'_{m,r}, \bar{\nu}''_{m,r} = \begin{cases} \nu'_{m,r}, \nu''_{m,r} & : \quad m \neq j, \\ \nu'_{m,r} - 1, \nu''_{m,r} - 1 & : \quad m = j, \nu'_{m,r} \neq 0, \nu''_{m,r} \neq 0, \\ 0 & : \quad m = j, \nu'_{j,r} = 0, \nu''_{m,r} = 0, \end{cases} \tag{4.15}$$

and

$$\frac{\partial w_i}{\partial T} = \widehat{M}_i \sum_{r=1}^{NR} \left(\nu''_{i,r} - \nu'_{i,r} \right) \left[\frac{dK_{f,r}}{dT} \prod_{m=1}^{NS} \left(\frac{\rho_m}{\widehat{M}_m} \right)^{\nu'_{m,r}} - \frac{dK_b}{dT} \prod_{m=1}^{NS} \left(\frac{\rho_m}{\widehat{M}_m} \right)^{\nu''_{m,r}} \right], \tag{4.16}$$

and the derivatives of the thermodynamic variables (T, P and γ) with respect to conserved variables are presented in Appendix A.

The derivatives of the rate equations with respect to temperature are given by the following equations:

$$\frac{dK_f}{dT} = K_f \left(\frac{\eta T + \theta_d}{T^2} \right), \tag{4.17}$$

$$\frac{dK_c}{dT} = \frac{-a_r K_{c,r}}{T^2} \left[T + \sum_{s=1}^{NS} \left(\frac{-\theta_{v,s}}{1 - e^{\frac{\theta_{v,s}}{T}}} + (1 + n_s)T + \frac{h_s^o}{R_s} \right) \right], \tag{4.18}$$

where

$$a_r = \sum_{s=1}^{NS} \left(\nu''_{s,r} - \nu'_{s,r} \right), \tag{4.19}$$

and finally

$$\frac{dK_b}{dT} = \frac{K_c dK_f - dK_c K_f}{K_c^2}. \tag{4.20}$$

4.3 Chemical Models - Examples

Two chemical models are described in this section. The first one is a five species air model with 17 reactions. The five species are N_2, N, O_2, O and NO. The seventeen reactions can be represented as five basic reactions: three dissociation-recombination reactions for N_2, O_2 and NO (each one representing five reactions) and two rearrangement (shuffle) reactions:

$$N_2 + M \rightleftharpoons 2N + M, \tag{4.21}$$

$$O_2 + M \rightleftharpoons 2O + M, \tag{4.22}$$

$$NO + M \rightleftharpoons N + O + M, \tag{4.23}$$

$$N_2 + O \rightleftharpoons NO + N, \tag{4.24}$$

$$NO + O \rightleftharpoons O_2 + N, \tag{4.25}$$

where M is a catalytic particle (any of the species present). Reaction rates are given in Kang and Dunn [39].

The second model is a hydrogen-oxygen combustion model with six species and 28 reactions. The species are H_2, O_2, H_2O, OH, H and O. The reactions are given as:

$$O_2 + M \rightleftharpoons 2O + M, \tag{4.26}$$
$$H_2 + M \rightleftharpoons 2H + M, \tag{4.27}$$
$$OH + M \rightleftharpoons H + O + M, \tag{4.28}$$
$$H_2O + M \rightleftharpoons OH + H + M, \tag{4.29}$$
$$O_2 + H \rightleftharpoons OH + O, \tag{4.30}$$
$$H_2 + O \rightleftharpoons OH + H, \tag{4.31}$$
$$H_2O + O \rightleftharpoons OH + OH, \tag{4.32}$$
$$H_2O + H \rightleftharpoons OH + H_2. \tag{4.33}$$

Reaction rates for this model are given in [29].

Chapter 5

EIGENVALUES AND EIGENVECTORS FOR THE FLUX JACOBIANS

5.1 Introduction

The system of equations developed in Chapter 3 is non-linear, coupled, and can be written in various equivalent forms. Section 3.1 presented the equations in terms of conserved variables in differential form and Section **??** presented the integral form of the equations. Again, this form of the equations is also conservative. As previously discussed, the conservation form of the equations is necessary in order to correctly compute propagation and intensity of discontinuities (weak solutions), such as shocks, which occur in the flow.

A set of variables that is *primitive* or *non-conservative* is also available. The variables, given as

$$\mathbf{q} = [\rho_1, \rho_2, \ldots, u, v, w, p]^T , \tag{5.1}$$

yield equivalent results when used in the Euler equations for smooth flows. These variables are often used to develop physical boundary conditions necessary for the numerical solution of the Euler equations [40].

In a hyperbolic system of equations the quantities that propagate along characteristic lines can be defined and the system can be cast in terms of its *characteristic* form. A set of characteristic variable boundary conditions can then be developed, which will contribute to a well-posed boundary-value problem.

The development of the eigensystem of the flux Jacobians will be discussed in this section. The intent is to develop the eigensystem for the flux Jacobians for mixtures of thermally perfect gases. The description will include the relationship between the conservative, quasi-linear, and non-conservative form of the Euler equations. The resulting eigensystem will also be used to develop the

set of characteristic equations and the resulting characteristic variable boundary conditions.

5.2 Eigenvalues

With reference to equation 3.2 the flux Jacobians for the Euler equations are defined to be:

$$K = \frac{\partial \mathbf{S}}{\partial \mathbf{Q}}, \tag{5.2}$$

where $\mathbf{S}$ represents the flux vector $\mathbf{F}$, $\mathbf{G}$, or $\mathbf{H}$. Of importance here is the fact that $\mathbf{S}$ can be written in terms of the conserved variables, that is,

$$\mathbf{S} = \mathbf{S}\left(Q_1, Q_2, \ldots, Q_{NS+4}\right). \tag{5.3}$$

The three-dimensional Euler equations are cast in quasi-linear form as follows:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial \mathbf{Q}}\frac{\partial \mathbf{Q}}{\partial \xi} + \frac{\partial \mathbf{G}}{\partial \mathbf{Q}}\frac{\partial \mathbf{Q}}{\partial \eta} + \frac{\partial \mathbf{H}}{\partial \mathbf{Q}}\frac{\partial \mathbf{Q}}{\partial \zeta} = \mathbf{W}, \tag{5.4}$$

or

$$\frac{\partial \mathbf{Q}}{\partial t} + A\frac{\partial \mathbf{Q}}{\partial \xi} + B\frac{\partial \mathbf{Q}}{\partial \eta} + C\frac{\partial \mathbf{Q}}{\partial \zeta} = \mathbf{W}. \tag{5.5}$$

In the above, A, B and C are called the flux Jacobian matrices. The general expression for a flux Jacobian matrix, K, is derived in Appendix B.

From Appendix B, it is evident that the flux Jacobian is a dense matrix and solving for the eigenvalues directly would not be an easy task. The application of the non-conservative equations can be introduced in order to simplify this problem. The quasi-linear, *non-conservative* form for the Euler equations, in vector form, is [40]:

$$\frac{\partial \mathbf{q}}{\partial t} + a\frac{\partial \mathbf{q}}{\partial \xi} + b\frac{\partial \mathbf{q}}{\partial \eta} + c\frac{\partial \mathbf{q}}{\partial \zeta} = \mathbf{W}, \tag{5.6}$$

where

$$\kappa = \frac{\partial \mathbf{s}}{\partial \mathbf{q}} \tag{5.7}$$

and κ is the Jacobian matrix of the flux $\mathbf{s}$. A transformation between the conserved and non-conserved variables is defined by

$$M = \frac{\partial \mathbf{Q}}{\partial \mathbf{q}} \tag{5.8}$$

This mapping is unique, therefore the inverse mapping exists and is given by

$$M^{-1} = \frac{\partial \mathbf{q}}{\partial \mathbf{Q}} \tag{5.9}$$

The matrix, M, can easily be computed:

$$M = \begin{bmatrix} 1 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 & 0 & 0 & 0 \\ 0 & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 & 0 & 0 \\ u & u & \dots & u & \rho & 0 & 0 & 0 \\ v & v & \dots & v & 0 & \rho & 0 & 0 \\ w & w & \dots & w & 0 & 0 & \rho & 0 \\ T_1 & T_2 & \dots & T_N & \rho u & \rho v & \rho w & \frac{1}{\gamma-1} \end{bmatrix}, \tag{5.10}$$

where

$$T_i = \frac{q^2}{2} + e_i - \frac{R_i T}{\gamma - 1}. \tag{5.11}$$

Also, its inverse M^{-1} can be computed directly will little difficulty:

$$M^{-1} = \begin{bmatrix} 1 & \dots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & 0 & 0 & 0 & 0 \\ 0 & \dots & 1 & 0 & 0 & 0 & 0 \\ -\frac{u}{\rho} & \dots & -\frac{u}{\rho} & \frac{1}{\rho} & 0 & 0 & 0 \\ -\frac{v}{\rho} & \dots & -\frac{v}{\rho} & 0 & \frac{1}{\rho} & 0 & 0 \\ -\frac{w}{\rho} & \dots & -\frac{w}{\rho} & 0 & 0 & \frac{1}{\rho} & 0 \\ \phi + \psi_1 & \dots & \phi + \psi_N & -u(\gamma-1) & -v(\gamma-1) & -w(\gamma-1) & \gamma - 1 \end{bmatrix}, \tag{5.12}$$

where

$$\phi = (\gamma - 1)\frac{q^2}{2}, \tag{5.13}$$

and

$$\psi_i = -(\gamma - 1)\tilde{e}_i + R_i T. \tag{5.14}$$

The mapping M also provides a similarity transformation to describe the relation between the conservative Jacobians, K, and the non-conservative Jacobians, κ. The quasi-linear, conservative equations, 5.4, can be written as

$$\frac{\partial \mathbf{Q}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial t} + A\frac{\partial \mathbf{Q}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial \xi} + B\frac{\partial \mathbf{Q}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial \eta} + C\frac{\partial \mathbf{Q}}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial \zeta} = \frac{\partial \mathbf{Q}}{\partial \mathbf{q}}\mathbf{W}. \tag{5.15}$$

Multiplication by M^{-1} and use of equation 5.8 yields:

$$\frac{\partial \mathbf{q}}{\partial t} + M^{-1}AM\frac{\partial \mathbf{q}}{\partial \xi} + M^{-1}BM\frac{\partial \mathbf{q}}{\partial \eta} + M^{-1}CM\frac{\partial \mathbf{q}}{\partial \zeta} = \mathbf{W}. \tag{5.16}$$

From equations 5.16 and 5.6 the similarity relation for the Jacobians is:

$$\kappa = M^{-1}KM \qquad \text{and} \qquad K = M\kappa M^{-1}. \tag{5.17}$$

Thus, κ is given as:

$$\kappa = \begin{bmatrix} \tilde{u} & \dots & 0 & \rho_1 k_x & \rho_1 k_y & \rho_1 k_z & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \tilde{u} & \rho_{NS} k_x & \rho_{NS} k_y & \rho_{NS} k_z & 0 \\ 0 & \dots & 0 & \tilde{u} & 0 & 0 & \frac{k_x}{\rho} \\ 0 & \dots & 0 & 0 & \tilde{u} & 0 & \frac{k_y}{\rho} \\ 0 & \dots & 0 & 0 & 0 & \tilde{u} & \frac{k_z}{\rho} \\ 0 & \dots & 0 & \rho k_x a^2 & \rho k_y a^2 & \rho k_z a^2 & \tilde{u} \end{bmatrix}, \tag{5.18}$$

where a is the frozen sound speed, and $\tilde{u}$ is given as

$$\tilde{u} = k_x u + k_y v + k_z w. \tag{5.19}$$

Due to the simple structure of κ it is easier to develop the eigenstructure of the Euler equations using the nonconserved form of the equations. The eigenvalues of κ can be found by solving:

$$|\kappa - \lambda I| = \mathbf{0}, \tag{5.20}$$

resulting in the following eigenvalues:

$$\begin{aligned} &\lambda_1 = \lambda_2 = \ldots = \lambda_{N+2} = \tilde{u} \\ &\lambda_{N+3} = \tilde{u} + a \\ &\lambda_{N+4} = \tilde{u} - a. \end{aligned} \tag{5.21}$$

Matrices K and κ are similar so the eigenvalues for K are the same as those for κ.

5.3 Eigenvectors

A set of linearly independent eigenvectors can be developed for the Jacobians, κ. This set must be chosen carefully due to the presence of repeated eigenvalues associated with the Euler equations. The development will be similar to that followed by Whitfield and Janus [8]. The right eigenvectors can be found by solving the equation:

$$(\kappa - \lambda_i I)\,\bar{\mathbf{x}} = \mathbf{0}. \tag{5.22}$$

For the repeated eigenvalue, $\lambda_1 = \tilde{u}$ the system of equations is given by

$$\begin{bmatrix} \tilde{u} & \dots & 0 & \rho_1 k_x & \rho_1 k_y & \rho_1 k_z & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \tilde{u} & \rho_{NS} k_x & \rho_{NS} k_y & \rho_{NS} k_z & 0 \\ 0 & \dots & 0 & \tilde{u} & 0 & 0 & \frac{k_x}{\rho} \\ 0 & \dots & 0 & 0 & \tilde{u} & 0 & \frac{k_y}{\rho} \\ 0 & \dots & 0 & 0 & 0 & \tilde{u} & \frac{k_z}{\rho} \\ 0 & \dots & 0 & \rho k_x a^2 & \rho k_y a^2 & \rho k_z a^2 & \tilde{u} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_{NS} \\ x_{N+1} \\ x_{NS+2} \\ x_{NS+3} \\ x_{NS+4} \end{bmatrix} = \mathbf{0}. \tag{5.23}$$

A linearly independent set of N+2 eigenvectors can be found from this equation:

$$r_1 \dots r_{NS+2} = \left\{ \begin{array}{ccccc} \alpha & \dots & 0 & \alpha_1 k_y & \alpha_1 k_z \\ \vdots & \ddots & \vdots & \alpha_2 k_y & \alpha_2 k_z \\ 0 & \dots & \alpha & \alpha_{NS} k_y & \alpha_{NS} k_z \\ 0 & \dots & 0 & -k_z & k_y \\ k_z & \dots & k_z & 0 & -k_x \\ -k_y & \dots & -k_y & k_x & 0 \\ 0 & \dots & 0 & 0 & 0 \end{array} \right\}, \tag{5.24}$$

where

$$\alpha_i = \frac{\rho_i}{\sqrt{2}a} \tag{5.25}$$

and

$$\alpha = \frac{\rho}{\sqrt{2}a}. \tag{5.26}$$

For the second eigenvalue, $\lambda_2 = \tilde{u} + a$ a similar set of equations can be solved for the related eigenvector:

$$r_{NS+3} = \left\{ \begin{array}{c} \frac{\rho_1}{\sqrt{2}c} \\ \vdots \\ \frac{\rho_{NS}}{\sqrt{2}c} \\ \frac{k_x}{\sqrt{2}} \\ \frac{k_y}{\sqrt{2}} \\ \frac{k_z}{\sqrt{2}} \\ \alpha a^2 \end{array} \right\}. \tag{5.27}$$

Finally for $\lambda_3 = \tilde{u} - a$ the associated eigenvector is

$$r_{NS+4} = \left\{ \begin{array}{c} \frac{\rho_1}{\sqrt{2}c} \\ \vdots \\ \frac{\rho_{NS}}{\sqrt{2}c} \\ -\frac{k_x}{\sqrt{2}} \\ -\frac{k_y}{\sqrt{2}} \\ -\frac{k_z}{\sqrt{2}} \\ \alpha a^2 \end{array} \right\}. \tag{5.28}$$

The matrix of right eigenvectors for the matrix κ can be written as the combination of equations 5.24, 5.27 and 5.28:

$$P_k = \begin{bmatrix} \alpha & \dots & 0 & \alpha_1 k_y & \alpha_1 k_z & \frac{\rho_1}{\sqrt{2}a} & \frac{\rho_1}{\sqrt{2}a} \\ \vdots & \ddots & \vdots & \dots & \dots & \dots & \dots \\ 0 & \dots & \alpha & \alpha_N k_y & \frac{\rho_{NS}}{\sqrt{2}a} & \frac{\rho_{NS}}{\sqrt{2}a} & \\ 0 & \dots & 0 & -k_z & k_y & \frac{k_x}{\sqrt{2}} & \frac{-k_x}{\sqrt{2}} \\ k_z & \dots & k_z & 0 & -k_x & \frac{k_y}{\sqrt{2}} & \frac{-k_y}{\sqrt{2}} \\ -k_y & \dots & -k_y & k_x & 0 & \frac{k_z}{\sqrt{2}} & \frac{-k_z}{\sqrt{2}} \\ 0 & \dots & 0 & 0 & 0 & \alpha a^2 & \alpha a^2 \end{bmatrix}. \tag{5.29}$$

The set of left eigenvectors can be found in a similar manner by solving

$$\mathbf{x}^T (\kappa - \lambda I) = \mathbf{0} \tag{5.30}$$

The set of left eigenvectors is:

$$P_k{}^{-1} = \begin{bmatrix} \frac{\alpha\beta - \alpha_1\left(1-k_x^2\right)}{\alpha^2\beta} & \dots & \frac{-\alpha_1\left(1-k_x^2\right)}{\alpha^2\beta} & 0 & \frac{\alpha_1 k_z}{\alpha\beta} & \frac{-\alpha_1 k_y}{\sqrt{2}} & \frac{-\alpha_1 k_x}{\alpha^2\beta a^2} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{-\alpha_{NS}\left(1-k_x^2\right)}{\alpha^2\beta} & \dots & \frac{\alpha\beta - \alpha_{NS}\left(1-k_x^2\right)}{\alpha^2\beta} & 0 & \frac{\alpha_{NS} k_z}{\alpha\beta} & \frac{-\alpha_{NS} k_y}{\sqrt{2}} & \frac{-\alpha_{NS} k_x}{\alpha^2\beta a^2} \\ \frac{k_y}{\alpha\beta} & \dots & \frac{k_y}{\alpha\beta} & -k_z & \frac{-k_y k_z(1-k_x)}{\beta} & \frac{1-k_z^2(1-k_x)}{\beta} & \frac{-k_y}{\alpha\beta a^2} \\ \frac{k_z}{\alpha\beta} & \dots & \frac{k_z}{\alpha\beta} & k_y & \frac{-1+k_y^2(1-k_x)}{\beta} & \frac{k_y k_z(1-k_x)}{\beta} & \frac{-k_z}{\alpha\beta a^2} \\ 0 & \dots & 0 & \frac{k_x}{\sqrt{2}} & \frac{k_y}{\sqrt{2}} & \frac{k_z}{\sqrt{2}} & \frac{1}{2\alpha a^2} \\ 0 & \dots & 0 & \frac{-k_x}{\sqrt{2}} & \frac{-k_y}{\sqrt{2}} & \frac{-k_z}{\sqrt{2}} & \frac{1}{2\alpha a^2} \end{bmatrix} \tag{5.31}$$

From McCann [41] a square $N \times N$ matrix which has N linearly independent eigenvectors is diagonalizable, so that

$$P_k^{-1} k P_k = \Lambda_k, \tag{5.32}$$

where Λ_κ is the matrix which contains the eigenvalues of κ on the main diagonal. Now, since the eigenvalues of κ and K are the same, equation 5.32 can be used to provide the eigenvectors for K. A series of matrix multiplications starting from equation 5.32 yields:

$$k = P_k \lambda_k P_k^{-1}, \tag{5.33}$$

which then can used to obtain:

$$K = MkM^{-1} = MP_k \lambda_k P_k^{-1} M^{-1}, \tag{5.34}$$

and finally,

$$(MP_k)^{-1} K (MP_k) = \lambda_k. \tag{5.35}$$

The set of right eigenvectors for K can now be computed by:

$$T_k = MP_k, \tag{5.36}$$

and the left eigenvectors are:

$$T_k^{-1} = P_k^{-1} M^{-1}. \tag{5.37}$$

The final matrices for the right and left eigenvectors are listed in Appendix C.

5.4 Characteristic Variable Boundary Conditions

The extension of characteristic variable boundary conditions to reacting flows is based on the derivation described in [8]. The assumption, that the characteristic variables can be developed independently in each coordinate direction, is applied. Additionally, the source term $\mathbf{W}$ is not considered in the development of the characteristics: only the homogeneous (frozen) problem is addressed.

The linearized, homogeneous Euler equation can be derived from equation 5.6 and equation 5.33 to form:

$$\frac{\partial \mathbf{q}}{\partial t} + P_\xi \Lambda_A P_\xi^{-1} \frac{\partial \mathbf{q}}{\partial \xi} + P_\eta \Lambda_B P_\eta^{-1} \frac{\partial \mathbf{q}}{\partial \eta} + P_\zeta \Lambda_C P_\zeta^{-1} \frac{\partial \mathbf{q}}{\partial \zeta} = 0. \tag{5.38}$$

Multiply equation 5.38 by P_k^{-1} and rewriting in terms of a normal direction, k, and tangential direction, m [43], [8]: to obtain:

$$P_k^{-1} \frac{\partial \mathbf{q}}{\partial t} + \Lambda_k P_k^{-1} \frac{\partial \mathbf{q}}{\partial k} + S_{k,m} = 0, \tag{5.39}$$

where k can be ξ, η or ζ and $S_{k,m}$ represents a summation over the other two coordinates. From [42], it is necessary for P_k^{-1} to be constant everywhere in order to define the characteristic variables. Setting

$$P_k^{-1} = P_{k,o}^{-1}, \tag{5.40}$$

then the characteristic variables can be defined as

$$\mathbf{V}_\kappa = P_{k,o}^{-1} \mathbf{q}, \tag{5.41}$$

and equation 5.39 becomes:

$$\frac{\partial \mathbf{V}_\kappa}{\partial t} + \Lambda_k \frac{\partial \mathbf{V}_\kappa}{\partial \kappa} + S_{\kappa,m} = 0. \tag{5.42}$$

$P_{\kappa,o}^{-1}$ is defined in Appendix C where the variables, ρ, ρ_i and a (the speed of sound), are defined at a reference condition, ρ_o, $(\rho_i)_o$ and a_o.

The characteristic variables can now be written as:

$$\mathbf{V}_\kappa = \begin{bmatrix} \frac{1}{\alpha_0 \beta}\left[\beta \rho_1 - \frac{\alpha_{10}}{\alpha_0}\left(\left(1-k_x^2\right)\rho + \frac{k_x P}{c_0^2}\right) + \alpha_{10}\left(k_z v - k_y w\right)\right] \\ \frac{1}{\alpha_0 \beta}\left[\beta \rho_2 - \frac{\alpha_{20}}{\alpha_0}\left(\left(1-k_x^2\right)\rho + \frac{k_x P}{c_0^2}\right) + \alpha_{20}\left(k_z v - k_y w\right)\right] \\ \vdots \\ \frac{1}{\alpha_0 \beta}\left[\beta \rho_N - \frac{\alpha_{N0}}{\alpha_0}\left(\left(1-k_x^2\right)\rho + \frac{k_x P}{c_0^2}\right) + \alpha_{N0}\left(k_z v - k_y w\right)\right] \\ \frac{k_y}{\alpha_0 \beta}\left(\rho - \frac{P}{c_0^2}\right) - \frac{k_z}{\beta}\left[\left(1-k_x\right)\tilde{u} + u\right] - \frac{w}{\beta} \\ \frac{k_z}{\alpha_0 \beta}\left(\rho - \frac{P}{c_0^2}\right) + \frac{k_y}{\beta}\left[\left(1-k_x\right)\tilde{u} + u\right] - \frac{v}{\beta} \\ \frac{1}{\sqrt{2}}\tilde{u} + \frac{P}{2\alpha_0 c_0^2} \\ \frac{-1}{\sqrt{2}}\tilde{u} + \frac{P}{2\alpha_0 c_0^2} \end{bmatrix}. \tag{5.43}$$

The boundary conditions derived in this section only include locally one-dimensional flow in the normal direction. Neglecting the tangential directions in equation 5.42 yields

$$\frac{\partial \mathbf{V}_\kappa}{\partial t} + \Lambda_k \frac{\partial \mathbf{V}_\kappa}{\partial \kappa} = 0. \tag{5.44}$$

The eigenvalues in Λ_κ represent a characteristic direction

$$\Lambda_\kappa = \frac{d\kappa}{dt}, \tag{5.45}$$

along which the characteristic variables are strictly conserved [40]. That is, each characteristic direction transports given information defined by the characteristic variable. The characteristic directions define the number of *physical* boundary conditions that can be defined for a given boundary. Variables which are transported from the boundaries towards the interior can be imposed at a given boundary as physical boundary conditions. The remaining variables depend on the computation flow solution and are referred to as numerical boundary conditions [40].

Characteristic variable boundary conditions will now be developed for multi-species flows for an impermeable surface and subsonic outflow. The boundary conditions for supersonic inflow and supersonic outflow will also be discussed.

5.4.1 Subsonic Outflow

At a subsonic outlet, the first four eigenvalues are positive and are numerical boundary conditions which must be computed. The final eigenvalue, $\tilde{u} - a$, is negative and represents a physical boundary. Typically downstream static pressure is imposed as the physical boundary condition. To be consistent with Whitfield's nomenclature, the subscript a represents an interior point of the computational domain and the subscript l represents a point outside the domain.

Equation 5.43 can now be applied to obtain the set of $NS + 4$ equations (with the exit pressure P_b imposed):

$$\begin{aligned}\frac{1}{\alpha_o\beta}\left[\beta(\rho_i)_a - \left(\frac{\alpha_i}{\alpha}\right)_o \left(\left(1-k_x^2\right)\rho_a + \frac{k_x P_a}{c_o^2}\right)\alpha_{io}\left(k_z v_a - k_y w_a\right)\right] = \\ \frac{1}{\alpha_o\beta}\left[\beta(\rho_i)_b - \left(\frac{\alpha_i}{\alpha}\right)_o \left(\left(1-k_x^2\right)\rho_b + \frac{k_x P_b}{c_o^2}\right)\alpha_{io}\left(k_z v_b - k_y w_b\right)\right]\end{aligned} \tag{5.46}$$

$$\begin{aligned}\frac{k_y}{\alpha_o\beta}\left(\rho_a - \frac{P_a}{c_o^2}\right) - \frac{k_z}{\beta}\left[\left(1-k_x\right)\tilde{u}_a + u_a\right] + \frac{w_a}{\beta} = \\ \frac{k_y}{\alpha_o\beta}\left(\rho_b - \frac{P_b}{c_o^2}\right) - \frac{k_z}{\beta}\left[\left(1-k_x\right)\tilde{u}_b + u_b\right] + \frac{w_b}{\beta}\end{aligned} \tag{5.47}$$

$$\begin{aligned}\frac{k_z}{\alpha_o\beta}\left(\rho_a - \frac{P_a}{c_o^2}\right) + \frac{k_y}{\beta}\left[\left(1-k_x\right)\tilde{u}_a + u_a\right] - \frac{v_a}{\beta} = \\ \frac{k_z}{\alpha_o\beta}\left(\rho_b - \frac{P_b}{c_o^2}\right) + \frac{k_y}{\beta}\left[\left(1-k_x\right)\tilde{u}_b + u_b\right] - \frac{v_b}{\beta}\end{aligned} \tag{5.48}$$

$$\frac{1}{\sqrt{2}}\tilde{u}_a + \frac{P_a}{2\alpha_o c_o^2} = \frac{1}{\sqrt{2}}\tilde{u}_b + \frac{P_b}{2\alpha_o c_o^2} \tag{5.49}$$

The above set of equations can now be solved to determine the characteristic boundary conditions:

$$\begin{aligned}
&(\rho_i)_b = (\rho_i)_a + \left(\tfrac{\alpha_i}{\alpha}\right)_o \tfrac{(P_b - P_a)}{c_o^2} \qquad i = 1, 2, \ldots, NS \\
&u_b = u_a + \tfrac{\sqrt{2}k_x}{2\alpha_o c_o^2}(P_a - P_b) \\
&v_b = v_a + \tfrac{\sqrt{2}k_y}{2\alpha_o c_o^2}(P_a - P_b) \\
&w_b = w_a + \tfrac{\sqrt{2}k_z}{2\alpha_o c_o^2}(P_a - P_b) \\
&P_b = P_l
\end{aligned} \tag{5.50}$$

5.4.2 Impermeable Surface

For an impermeable surface there is no flow across the boundary so the first $NS + 2$ eigenvalues are zero. One of the remaining eigenvalues is positive and the other is negative, so one condition must be specified. The condition in this case is that no flow across the boundary can occur. All other information must be obtained from the interior of the domain, which is denoted by the subscript r. The equations that must be solved for boundary equations are:

$$\begin{aligned}
&\frac{1}{\alpha_o\beta}\left[k_x\rho_{ib} - \frac{k_x P_b}{c_o^2}\right] + \frac{1}{\beta}(k_z v_b - k_y w_b) = \\
&\qquad \frac{1}{\alpha_o\beta}\left[k_x\rho_{ir} - \frac{k_x P_r}{c_o^2}\right] + \frac{1}{\beta}(k_z v_r - k_y w_r)
\end{aligned} \tag{5.51}$$

$$\begin{aligned}
&\frac{k_y}{\alpha_o\beta}\left(\rho_{ib} - \frac{P_b}{c_o^2}\right) - \frac{k_z}{\beta}\left[(1-k_x)\tilde{u}_b + u_b\right] + \frac{w_b}{\beta} = \\
&\qquad \frac{k_y}{\alpha_o\beta}\left(\rho_{ir} - \frac{P_r}{c_o^2}\right) - \frac{k_z}{\beta}\left[(1-k_x)\tilde{u}_r + u_r\right] + \frac{w_r}{\beta}
\end{aligned} \tag{5.52}$$

$$\begin{aligned}
&\frac{k_z}{\alpha_o\beta}\left(\rho_{ib} - \frac{P_b}{c_o^2}\right) + \frac{k_y}{\beta}\left[(1-k_x)\tilde{u}_b + u_b\right] - \frac{v_b}{\beta} = \\
&\qquad \tfrac{k_z}{\alpha_o\beta}\left(\rho_{ir} - \tfrac{P_r}{c_o^2}\right) + \tfrac{k_y}{\beta}\left[(1-k_x)\tilde{u}_r + u_r\right] - \tfrac{v_r}{\beta}
\end{aligned} \tag{5.53}$$

$$\frac{1}{\sqrt{2}}\tilde{u}_b + \frac{P_b}{2\alpha_o c_o^2} = \frac{1}{\sqrt{2}}\tilde{u}_r + \frac{P_r}{2\alpha_o c_o^2} \tag{5.54}$$

$$\tilde{u}_b = 0 \tag{5.55}$$

yielding the following boundary conditions for an impermeable surface:

$$\begin{aligned}
&(\rho_i)_b = (\rho_i)_r + \left(\tfrac{\rho_i}{\rho}\right)_o \left(\tfrac{P_b - P_r}{c_o^2}\right) \\
&u_b = u_r - k_x\tilde{u}_r \\
&v_b = v_r - k_y\tilde{v}_r \\
&w_b = w_r - k_z\tilde{w}_r \\
&P_b = P_r - \rho_o c_o \tilde{u}_r
\end{aligned} \tag{5.56}$$

5.4.3 Supersonic Inflow and Outflow

For supersonic inflow all eigenvalues have the same sign so all flows values will need to be specified. For this study, all variables were specified at the freestream inflow conditions. For supersonic outflow, all of the characteristics need to be computed from the solution. That is, none of the variables need to be specified. For this boundary condition, the variables at the boundary were computed using a first order extrapolation of the interior cell-centered values.

5.4.4 Phantom Points and Conserved Variables

In each of the above derivations, the value for the characteristic variables were found from the boundary of the computational domain. Finite-volume schemes, such as the ones which will be developed in Chapter 6, require at least one phantom cell outside of the computational domain. The values for the characteristic variables in these cells are computed as a first-order extrapolation from the boundary:

$$\psi_p = 2\psi_b - \psi_{in} \tag{5.57}$$

where ψ is a dependent variable, ρ_i, u, v, w or P. In the above, p is the phantom cell, b is the boundary and in is the center of the first interior cell.

The values of the dependent variables are used to compute the remaining conserved and thermodynamic variables necessary in the computation. From the primitive dependent variables, values can be obtained for total density, temperature and species internal energy.

Chapter 6

NUMERICS

6.1 Introduction

In Section 3.1, the system of partial differential equations that describes compressible, inviscid, chemically reacting flows was introduced. As discussed in Section **??**, the integral form of the equations is valid across discontinuities such as slip lines or shock waves. In order to solve either set of equations numerically, they must be discretized to form a set of algebraic equations that can be solved computationally. The discretization of the equations will be an extension of the methods used by Whitfield et al. [9] and examined in detail for viscous flows by Simpson [44]. The general methods used have also been discussed for chemically reacting flows by Cinnella [13].

A very useful method of discretization is the finite-volume technique, whereby the integral form of the conserved governing equations is discretized over a control volume (cell). The conservative property of the integral form of the equations is retained in the finite-volume approach.

A fully implicit, linerized, three-dimensional finite-volume discretization will be used in this chapter as a baseline for development of the computational schemes for modeling flows with finite-rate chemistry. The basic discretization is a combination of a flux-vector-split scheme based on Steger-Warming splitting [45] and developed for reacting flows by Cinnella [13], and the flux difference method of Roe [46] used in the evaluation of the fluxes of the Euler equations. Finally, two time integration procedures: a fully-implicit (modified two-pass) algorithm, and a semi-implicit scheme, will be implemented.

6.2 Implicit Finite-Volume Discretization

The discretization is defined as:

$$\Delta\mathbf{Q}^n + \Delta\tau\left[\delta_i\left(\mathbf{F}^n + A\frac{\Delta\mathbf{Q}}{\Delta\tau}\right) + \delta_j\left(\mathbf{G}^n + B\frac{\Delta\mathbf{Q}}{\Delta\tau}\right) + \delta_k\left(\mathbf{H}^n + C\frac{\Delta\mathbf{Q}}{\Delta\tau}\right)\right] =$$

$$\Delta\mathbf{W} + D\Delta\mathbf{Q}, \tag{6.1}$$

where A, B and C are the flux Jacobians associated with **F**, **G**, and **H**, respectively and D is the chemical Jacobian (see Chapter 4).

Rearranging 6.1 yields:

$$\left[\frac{I}{\Delta\tau} + \delta_i A^n + \delta_j B^n + \delta_k C^n - D^n\right]\Delta\mathbf{Q} = \\ -\left(\delta_i \mathbf{F}^n + \delta_j \mathbf{G}^n + \delta_k \mathbf{H}^n - \mathbf{W}^n\right). \tag{6.2}$$

6.3 Temporal Discretization

As discussed in Chapter 1, the Euler equations are advanced in time using one of two methods, a fully implicit (modified two-pass) scheme as described by Vanden[55], or a semi-implicit scheme. In the following sections they will be presented in some detail.

6.3.1 Modifed Two-Pass

The fully implicit scheme given in equation 6.2 can now be written to include, in three dimensions, the Steger-Warming flux vector splitting (equation **??**) and the flux difference scheme of Roe (equation 6.26). The result is:

$$\left[\frac{I}{\Delta\tau} + \delta_i A^+ \cdot + \delta_i A^- \cdot + \delta_i B^+ \cdot + \delta_i B^- \cdot + \delta_i C^+ \cdot + \delta_i C^- \cdot\right]\Delta\mathbf{Q} = \\ -\left(\mathbf{f}^n + \mathbf{g}^n + \mathbf{h}^n - \mathbf{w}^n\right) \tag{6.3}$$

Equation 6.3 can be expanded to obtain:

$$\left[\frac{I}{\Delta\tau} + A^+_{i,j,k} + B^+_{i,j,k} + C^+_{i,j,k} - A^-_{i,j,k} - B^-_{i,j,k} - C^-_{i,j,k} - D_{i,j,k}\right]\Delta\mathbf{Q}_{i,j,k} \\ + \left(-A^+_{i-1,j,k}\Delta\mathbf{Q}_{i-1,j,k} - B^+_{i,j-1,k}\Delta\mathbf{Q}_{i,j-1,k} - C^+_{i,j,k-1}\Delta\mathbf{Q}_{i,j,k-1}\right) \\ \left(A^-_{i+1,j,k}\Delta\mathbf{Q}_{i+1,j,k} + B^-_{i,j+1,k}\Delta\mathbf{Q}_{i,j+1,k} + C^-_{i,j,k+1}\Delta\mathbf{Q}_{i,j,k+1}\right) = -\mathbf{r}_{i,j,k}, \tag{6.4}$$

where

$$\mathbf{r}_{i,j,k} = \mathbf{f_i} + \mathbf{g_j} + \mathbf{h_k} - \mathbf{w}. \tag{6.5}$$

Now, following Vanden, equation 6.4 can be approximately factoring into a two-pass numerical scheme as:

$$\left[I - E^{-1}_{i,j,k} M^+_{\ell-1}\cdot\right]\left[I + E^{-1}_{i,j,k} M^-_{\ell+1}\cdot\right]\Delta\mathbf{Q} = -E^{-1}_{i,j,k}\mathbf{r}_{i,j,k}, \tag{6.6}$$

where

$$E_{i,j,k} = \frac{I}{\Delta\tau} + A^+_{i,j,k} + B^+_{i,j,k} + C^+_{i,j,k} - A^-_{i,j,k} - B^-_{i,j,k} - C^-_{i,j,k} - D_{i,j,k}, \tag{6.7}$$

$$M^-_{\ell+1} = A^-_{i+1,j,k} + B^-_{i,j+1,k} + C^-_{i,j,k+1}, \tag{6.8}$$

$$M^+_{\ell-1} = A^+_{i-1,j,k} + B^+_{i,j-1,k} + C^+_{i,j,k-1}. \tag{6.9}$$

The subscript ℓ represents the off-diagonal elements in the i, j, and k computational directions.

The modified two-pass scheme forms a block triangular system which can be solved in two sweeps defined as:

$$\left(E_\ell - M^+_{\ell-1}\right) \Delta\mathbf{Q}^* = -\mathbf{r}^n \tag{6.10}$$

$$\left(E_\ell + M^-_{\ell+1}\right) \Delta\mathbf{Q}^n = E_\ell \Delta\mathbf{Q}^*. \tag{6.11}$$

6.3.2 Semi-Implicit Scheme

The chemical reactions occurring in the flows are usually responsible for *stiffness* in the resulting discretized system of equations. The use of semi-implicit time integration schemes can be implemented in order to address the stiffness of the system in a computationally efficient manner. The chemistry source terms, are directly responsible for the computational stiffness [17]: the semi-implicit method treats them implicitly, while the fluxes remain explicit. The advantage of the semi-implicit scheme over the fully-implicit scheme is that it avoids solving the large block matrices associated with the fully-implicit scheme described above.

The implicit treatment of the chemical source terms in the semi-implicit method allows chemistry phenomena to evolve at comparable pseudo-time scales, retaining this feature from the fully-implicit method. However, due to the lack of implicit treatment of the flux Jacobians, the CFL number is limited to an upper value of one [31]. The discretization of the Euler equations for the semi-implicit scheme is:

$$\left[\frac{I}{\Delta\tau} - D^n_{i,j,k}\right] \Delta\mathbf{Q}_{i,j,k} = \mathbf{r}^n, \tag{6.12}$$

where $\mathbf{r}^n$ is defined in equation 6.5. Equation 6.12 can be solved directly for the conserved variables. The next chapter will compare the above two schemes in an effort to determine which method is more efficient in the computation of reacting flows.

6.4 Steger-Warming Flux Splitting

The flux Jacobians (on the left hand side of equation 6.2) are evaluated by using the flux-split algorithm of Steger-Warming [45]. This method was developed for perfect gases, extended to flows in chemical equilibrium by Vinokur and Montagné [47] and for flows in chemical nonequilibrium by Grossman and Cinnella [48]. The split-flux Jacobians are presented in Appendix D.

6.5 Flux-Difference Splitting

6.5.1 Flux Evaluation

The flux vectors appearing on the right hand side of the discretized equation 6.2 are obtained using the flux differencing scheme developed by Roe for perfect gases [46] and extended to reacting flows by Cinnella [13]. The Roe scheme involves solving local Riemann problems at each cell interface using the left state, $(\cdot)_l$, and right state, $(\cdot)_r$, at the cell centers.

Roe's derivation of the numerical fluxes assumes a one-dimensional problem. The extension to three-dimensional problems is accomplished by considering each direction as locally one-dimensional [49]. As a result, the fluxes for the ξ direction will be presented with the understanding that they are applied in the same fashion for the η and ζ directions.

The first-order numerical flux at cell face $i + 1/2$ resulting from Roe's approximate Riemann solver can be written in any one of the following equivalent forms [50]:

$$f_{i+1/2} = [f(q_i)]_{i+1/2} + \sum_{j=1}^{n} \alpha_{j,i+1/2}\, \lambda^{-(j)}_{i+1/2}\, r^{(j)}_{i+1/2}, \tag{6.13}$$

$$f_{i+1/2} = [f(q_{i+1})]_{i+1/2} - \sum_{j=1}^{n} \alpha_{j,i+1/2}\, \lambda^{+(j)}_{i+1/2}\, r^{(j)}_{i+1/2}, \tag{6.14}$$

$$f_{i+1/2} = \frac{1}{2}\left[f(q_i) + f(q_{i+1})\right]_{i+1/2} - \frac{1}{2}\sum_{j=1}^{n} \alpha_{j,i+1/2}\, \left|\lambda^{(j)}_{i+1/2}\right|\, r^{(j)}_{i+1/2}, \tag{6.15}$$

where

$$\left|\lambda^{(j)}_{i+1/2}\right| = \lambda^{+(j)}_{i+1/2} - \lambda^{-(j)}_{i+1/2}, \tag{6.16}$$

r is the set of right eigenvectors, α contains the left eigenvectors ℓ and n is the number of distinct eigenvalues:

$$\alpha_j = \ell_j \cdot \delta\mathbf{Q}. \tag{6.17}$$

The flux is represented by a lower case $\mathbf{f}$ in order to highlight the fact that it is a numerical approximation. Similar results apply in the η direction for the numerical flux $\mathbf{g}$, and in the ζ direction for $\mathbf{h}$. The first element in equations 6.13-6.15 is evaluated using the conserved variables computed at cell centers. The terms in the summation are evaluated with Roe-averaged variables (except for $\delta\mathbf{Q}$ in equation 6.17) computed at the cell faces $(i + 1/2)$. Finally, the subscript $i+1/2$ indicates that the metrics are also evaluated at the cell face at $i + 1/2$.

6.5.2 Roe-Averaged Variables

The Roe scheme requires the development of averaged values for elements of the eigenvalues, $\widehat{\lambda}_i$, right eigenvectors, $\widehat{r}_i$, and wave strengths which satisfy the jump conditions for the conserved values:

$$[\![\mathbf{Q}]\!] = \sum_{i=1}^{NS+4} \widehat{\alpha}_i \widehat{r}_i, \tag{6.18}$$

and for the fluxes:

$$[\![\mathbf{S}]\!] = \sum_{i=1}^{NS+4} \widehat{\alpha}_i \widehat{\lambda}_i \widehat{r}_i, \tag{6.19}$$

where the symbol, $\widehat{\ }$, implies that the variables are Roe-averaged. A derivation of the Roe-averaged variables is presented in [13]. In summary, species density, $\hat{\rho}_i$, velocity components, $\hat{u}, \hat{v}, \hat{w}$, total enthalpy, mixture gas constant, $\widehat{R}$, temperature, $\widehat{T}$, and species internal energy are computed with the general formula:

$$\widehat{(\cdot)} = \frac{<(\cdot)\sqrt{\rho}>}{<\sqrt{\rho}>} \tag{6.20}$$

where:

$$<\widehat{x}>= \frac{1}{2}\left[(x)_r + (x)_l\right]. \tag{6.21}$$

The Roe-averaged specific heat is computed as

$$\hat{c_v} = \sum_{i=1}^{NS} \hat{\rho}_i c^*_{v_i}, \tag{6.22}$$

where

$$c^*_{v_i} = \frac{1}{[\![T]\!]} \int_{T_\ell}^{T_r} C_{v_i} dT. \tag{6.23}$$

The Roe-averaged ratio of specific heats is:

$$\hat{\gamma} = \frac{\hat{R}}{\hat{c_v}} + 1. \tag{6.24}$$

Finally, the Roe-averaged speed of sound is:

$$\hat{a}^2 = (\hat{\gamma} - 1)\left[\hat{h_o} - \frac{\hat{q}^2}{2} + \hat{c_v}\hat{T} - \sum_{i=1}^{NS} \hat{\rho}_i \hat{e}_i\right]. \tag{6.25}$$

6.5.3 Higher-Order Spatial Accuracy

As stated in Section 6.5.1, the flux given by any of the equations 6.13-6.15 is first order accurate in space. Higher-order schemes which are total variational

diminishing (TVD), or monoticity preserving, have been shown to prevent oscillations when applied across discontinuities. Harten [51] and Van Leer [52] describe the development of TVD schemes and the fact that nonlinear limiters are necessary to ensure a monoticity preserving method.

Two techniques are available for higher order spatially accurate schemes: the variable extrapolation method or Monotone Upstream-centered Scheme for Conservation Laws (MUSCL) developed by Van Leer [53]; and flux extrapolation such as the scheme by Osher and Chakravarthy [54]. While either method can be applied using the eigensystem developed in Chapter 5, the flux extrapolation method is used. This method is a direct extension of the perfect gas model by Whitfield, Janus and Simpson [9] and the equilibrium solver of Cox [7].

The higher-order flux computation in the ξ direction, as defined in [9], is:

$$\begin{aligned}\mathbf{f}_{i+1/2} = [\mathbf{f}(Q_i)]_{i+1/2} + \sum_{j=1}^{NS+4} \hat{\sigma}^{-}_{j,i+1/2} r^{(j)}_{i+1/2} \\ + \sum_{j=1}^{NS+4} \left\{ \frac{1-\psi}{4} \left[L^{+}_{j}(-1,1) - L^{-}_{j}(3,1) \right] + \frac{1+\psi}{4} \left[L^{+}_{j}(1,-1) - L^{-}_{j}(1,3) \right] \right\} \\ r^{(j)}_{i+1/2},\end{aligned} \tag{6.26}$$

where $L^{\pm}_{j}$ is the nonlinear flux limiter which ensures the TVD condition. For this study the minmod limiter is used. Here, the limiter is defined as:

$$L^{\pm}_{j}(l,m) = minmod\left(\widehat{\sigma}^{\pm}_{j,i+l/2}, b\widehat{\sigma}^{\pm}_{j,i+n/2}\right), \tag{6.27}$$

where

$$\sigma^{\pm}_{j,i+P/2} = \lambda^{\pm(j)}_{i+1/2} \alpha_{j,i+P/2}, \tag{6.28}$$

$$minmod(x,y) = sign(x) max\left\{0, min\left[|x|, y sign(x)\right]\right\}, \tag{6.29}$$

and

$$b = \frac{3-\psi}{1-\psi}. \tag{6.30}$$

The remaining variables in equation 6.26 are defined as:

$$\alpha_{j,i-1/2} = \ell^{(j)}_{i+1/2} \cdot (Q_i - Q_{i-1}), \tag{6.31}$$

$$\alpha_{j,i+1/2} = \ell^{(j)}_{i+1/2} \cdot (Q_{i+1} - Q_i), \tag{6.32}$$

$$\alpha_{j,i+3/2} = \ell^{(j)}_{i+1/2} \cdot (Q_{i+2} - Q_{i+1}). \tag{6.33}$$

Second and third-order accuracy can be obtained by means of the parameter ψ. A second order scheme is used when $\psi = -1$. A third-order scheme corresponds to a selection of $\psi = \frac{1}{3}$.

6.5.4 Variable Step Computations

For the discretization schemes developed in the previous sections a variable time step method was implemented to control time step size. The method is a simple control used to vary the CFL number, and therefore the time step, to make the numerical scheme converge as quickly as possible. Another useful feature is the fact that the method can quickly change during the initial iterations to adjust user input that is either too small or too large. The method is an extension of the scheme used by Busby and Moore [56] for an ordinary differential solver and Slomski and Gorski [57] for an incompressible upwind flow solver. In each case, the norm of the residual variables, ΔQ^n, is used to compute a percentage change in CFL number:

$$C_{n+1} = C_n \left(\frac{||\Delta Q^{n-1}||}{||\Delta Q^n||} \right), \tag{6.34}$$

where C_{n+1} is the new CFL number and C_n is the current CFL number.

Chapter 7

OUTLINE OF MODEL

7.1 Introduction

The purpose of this chapter is to put the information from the previous chapters together to describe the compuatation flow of the program. The outline will include necessary initialization - with very little information of the user input since the overall design of the user GUI is not complete, the computations needed once, and the computations necessary for the iterative solver.

7.2 Initialization

- This user input information is covered in Chapter 2.
- The flow field - ρ, ρu, ρv, ρw, ρe_0. will be initialized to a constant, equilibrium state based on user input.
- The thermodynamic system will be computed based on user input of Pressure, temperature, densit and mass fractions.

7.3 One-Time Computations

The grid metrics described in section ?? are computed once at the start of the program.

7.4 Iterative Solver

Given the values for the thermodynamic system and flow field.

- Compute the flux Jacobians $\mathbf{F}$, $\mathbf{G}$, and $\mathbf{H}$ as described in Appendix D.
- Compute the fluxes $\mathbf{f}$, $\mathbf{g}$, and $\mathbf{h}$ based on the use of Roe's scheme and Roe-averaged variables described in section ??

- Compute the chemistry Jacobian as developed in Section ??. This will include the use of the Thermodynamic derivatives given in the same section.
- Build the maxtrices necessary to solve the linear systems of equations.
- Solve the linear system using the modified two-pass or semi-implicit solver as requested by the user.
- Update the values for the unknows: ρ, ρu, ρv, ρw, ρe_0.
- Update the thermodynamic variables.
- Iterate

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Appendix A

THERMODYNAMIC DERIVATIVES

A.1 Introduction

The derivatives of some thermodynamic quantities with respect to the conserved variables are necessary to define the flux and chemical Jacobians. This section will derive the temperature, pressure, ratio of specific heats, speed of sound, and eigenvalue derivatives with respect to the conserved variables.

A.2 Temperature Derivatives

The total energy, as defined in equation 3.15, can be written as:

$$\rho e_0 = \frac{(\rho q)^2}{2\rho} + \sum_{i=1}^{NS} \rho_i \tilde{e}_i(T). \tag{A.1}$$

The differential of equation A.1 is:

$$d(\rho e_o) = ud(\rho u) + vd(\rho v) + wd(\rho w) - \frac{q^2}{2} d\rho + \sum_{i=1}^{NS} \rho_i d\tilde{e}_i + \sum_{i=1}^{NS} \tilde{e}_i d\rho_i. \tag{A.2}$$

From Section 3.4,

$$\tilde{e}_i = \int_{T_o}^{T} C_{vi}(\tau) d\tau + h_i^o \tag{A.3}$$

and the temperature differential is:

$$d\tilde{e}_i = C_{vi}(T) dT \tag{A.4}$$

Substituting equation A.4 into equation A.2 yields:

$$d\left(\rho e_o\right) = ud\left(\rho u\right) + vd\left(\rho v\right) + wd\left(\rho w\right) - \frac{q^2}{2}d\rho + \rho\tilde{C}_v dT + \sum_{i=1}^{NS}\tilde{e}_i d\rho_i. \quad \text{(A.5)}$$

Rearranging equation A.5 yields

$$\rho\tilde{C}_v dT = d\left(\rho e_o\right) - ud\left(\rho u\right) - vd\left(\rho v\right) - wd\left(\rho w\right) + \frac{q^2}{2}d\rho - \sum_{i=1}^{NS}\tilde{e}_i d\rho_i. \quad \text{(A.6)}$$

The derivatives of temperature with respect to the conserved variables can be obtained directly from equation A.6:

$$\frac{\partial T}{\partial \rho_i} = \frac{\partial T}{\partial Q_i} = \frac{1}{\rho\tilde{C}_v}\left(\frac{q^2}{2} - e_i\right), \quad \text{(A.7)}$$

$$\frac{\partial T}{\partial\left(\rho u\right)} = \frac{\partial T}{\partial Q_{NS+1}} = \frac{-u}{\rho\tilde{C}_v}, \quad \text{(A.8)}$$

$$\frac{\partial T}{\partial\left(\rho v\right)} = \frac{\partial T}{\partial Q_{NS+2}} = \frac{-v}{\rho\tilde{C}_v}, \quad \text{(A.9)}$$

$$\frac{\partial T}{\partial\left(\rho w\right)} = \frac{\partial T}{\partial Q_{NS+3}} = \frac{-w}{\rho\tilde{C}_v}, \quad \text{(A.10)}$$

$$\frac{\partial T}{\partial\left(\rho e_o\right)} = \frac{\partial T}{\partial Q_{NS+4}} = \frac{1}{\rho\tilde{C}_v}. \quad \text{(A.11)}$$

A.3 Pressure Derivatives

Recall that the thermal equation of state is defined as:

$$P = \sum_{i=1}^{NS}\rho_i R_i T. \quad \text{(A.12)}$$

The differential is:

$$dP = \rho\tilde{R}dT + \sum_{i=1}^{NS}R_i T d\rho_i. \quad \text{(A.13)}$$

Solving equation A.13 for dT and substituting this value into equation A.6 yields:

$$\frac{1}{\gamma - 1} = d\rho e_o - ud\left(\rho u\right) - vd\left(\rho v\right) - wd\left(\rho w\right) + \sum_{i=1}^{NS}\left(\frac{q^2}{2} - \tilde{e}_i\frac{R_i T}{\gamma - 1}\right)d\rho_i. \quad \text{(A.14)}$$

Consequently, the pressure derivatives with respect to the conserved variables are:

$$\frac{\partial P}{\partial Q_i} = \left(\gamma - 1\right)\left(\frac{q^2}{2} + \frac{R_i T}{\gamma - 1} - e_i\right), \quad \text{(A.15)}$$

$$\frac{\partial P}{\partial Q_{NS+1}} = -u\left(\gamma - 1\right), \tag{A.16}$$

$$\frac{\partial P}{\partial Q_{NS+2}} = -v\left(\gamma - 1\right), \tag{A.17}$$

$$\frac{\partial P}{\partial Q_{NS+3}} = -w\left(\gamma - 1\right), \tag{A.18}$$

$$\frac{\partial T}{\partial Q_{NS+4}} = \left(\gamma - 1\right). \tag{A.19}$$

A.4 Ratio of Specific Heats Derivatives

The ratio of specific heats, γ, for a mixture of chemically reacting thermally perfect gases is defined as:

$$\gamma = \frac{\sum_{j=1}^{NS} \rho_j C_{p_j}\left(T\right)}{\sum_{j=1}^{NS} \rho_j C_{v_j}\left(T\right)}. \tag{A.20}$$

The general derivative of A.20, with respect to the conserved variables, is:

$$\frac{\partial \gamma}{\partial Q_i} = \frac{\sum_{j=1}^{NS} C_{p_j} \frac{\partial \rho_j}{\partial Q_i} + \rho_j \frac{\partial C_{p_j}}{\partial Q_i}}{\rho C_v} - \frac{\rho C_p \left[\sum_{j=1}^{NS} \left(C_{v_j} \frac{\partial \rho_j}{\partial Q_i} + \rho_j \frac{\partial C_{v_j}}{\partial Q_i}\right)\right]}{\left(\rho C_v\right)^2}. \tag{A.21}$$

For species densities, $i = 1, 2, \ldots, NS$; equation A.21 becomes

$$\begin{aligned} \frac{\partial \gamma}{\partial Q_i} = & \\ & \frac{1}{\rho C_v}\left[C_{p_i} - \frac{\rho C_p C_{v_i}}{\rho C_v}\right] + \frac{1}{\rho C_v}\sum_{j=1}^{NS}\left(\rho_j \frac{\partial C_{p_i}}{\partial T}\frac{\partial T}{\partial Q_i}\right) - \\ & \frac{\rho C_p}{\left(\rho C_v\right)^2}\sum_{j=1}^{NS}\rho_j \frac{\partial C_{v_j}}{\partial T}\frac{\partial T}{\partial Q_i} \end{aligned} \tag{A.22}$$

The mixture relations are:

$$\gamma = \frac{C_p}{C_v}, \tag{A.23}$$

and

$$C_v = C_p - R. \tag{A.24}$$

Applying these properties yields, for species densities ($i = 1, 2, \ldots, NS$):

$$\frac{\partial \gamma}{\partial Q_i} = \frac{\gamma - 1}{\rho C_v}\left[\frac{\gamma R_i}{\gamma = 1} - C_{v_i} - R_i - \frac{\partial T}{\partial Q_i}\left(\sum_{j=1}^{NS}\rho_j \frac{dC_{v_j}}{dT}\right)\right]. \tag{A.25}$$

For $i = NS+1, \ldots, NS+4$, the derivatives are:

$$\frac{\partial \gamma}{\partial Q_i} = \frac{-(\gamma-1)}{\rho C_v} \sum_{j=1}^{NS} \left(\rho_j \frac{dC_{vj}}{dT} \right) \frac{\partial T}{\partial Q_i}. \tag{A.26}$$

The computation of $\frac{dC_{vi}}{dT}$ is dependent on the thermodynamic model used to evaluate the thermodynamic properties. For this study, equation 3.17 defines the species specific heat equation. The derivative is:

$$\frac{dC_{vi}}{dT} = R_i \frac{d}{dT} \left[\left(\frac{\theta_{v,i}}{T} \right)^2 \frac{e^{\theta_{v,i}/T}}{\left(e^{\theta_{v,i}/T} - 1\right)^2} \right]. \tag{A.27}$$

The final result for this thermodynamic model is:

$$\frac{dC_{vi}}{dT} = \frac{-e^{\theta_{v,i}/T} \left[e^{\theta_{v,i}/T} \left(2T - \theta_{v,i}\right) - \left(2T + \theta_{v,i}\right) \right]}{T^4 \left(e^{\theta_{v,i}/T} - 1\right)^3} \tag{A.28}$$

A.5 Speed of Sound Derivatives

From Section 3.4, the speed of sound is defined as:

$$a = \sqrt{\frac{\gamma P}{\rho}}. \tag{A.29}$$

The derivative of a with respect to the conserved variables is:

$$\frac{\partial a}{\partial Q_i} = \frac{1}{2} \left(a^{-1}\right) \left[\frac{P}{\rho} \frac{\partial \gamma}{\partial Q_i} + \frac{\gamma}{\rho} \frac{\partial P}{\partial Q_i} - \frac{\gamma P}{\rho^2} \frac{\partial \rho}{\partial Q_i} \right] \tag{A.30}$$

For the species mass fractions, $i = 1, 2, \ldots, NS$, the derivatives are:

$$\frac{\partial a}{\partial Q_i} = \frac{a}{2} \left[\frac{1}{\gamma} \frac{\partial \gamma}{\partial Q_i} + \frac{1}{P} \frac{\partial P}{\partial Q_i} - \frac{1}{\rho} \right]. \tag{A.31}$$

For the remaining conserved variables $i = NS+1, NS+2, NS+3, NS+4$, the derivatives are:

$$\frac{\partial a}{\partial Q_i} = \frac{a}{2} \left[\frac{1}{\gamma} \frac{\partial \gamma}{\partial Q_i} + \frac{1}{P} \frac{\partial P}{\partial Q_i} \right]. \tag{A.32}$$

A.6 Eigenvalue Derivatives

The derivatives of the eigenvalues are necessary for the the development of flux-split Jacobians, described in Appendix D. The three distinct eigenvalues, introduced in Chapter 5, can be written in terms of the conserved variables as:

$$\lambda_1^{\pm} = \frac{1}{Q_0} \left(Q_{NS+1} k_x + Q_{NS+2} k_y + Q_{NS+3} k_z \right), \tag{A.33}$$

$$\lambda_{2,3}^{\pm} = \frac{1}{Q_0}\left(Q_{NS+1}k_x + Q_{NS+2}k_y + Q_{NS+3}k_z\right) \pm a. \tag{A.34}$$

The derivatives, with respect to the conserved variables, of the first eigenvalue are:

$$\frac{\partial \lambda_1^{\pm}}{\partial Q_i} = \frac{-u}{\rho}, \tag{A.35}$$

$$\frac{\partial \lambda_1^{\pm}}{\partial Q_{NS+1}} = \frac{k_x}{\rho}, \tag{A.36}$$

$$\frac{\partial \lambda_1^{\pm}}{\partial Q_{NS+2}} = \frac{k_y}{\rho}, \tag{A.37}$$

$$\frac{\partial \lambda_1^{\pm}}{\partial Q_{NS+3}} = \frac{k_z}{\rho}, \tag{A.38}$$

$$\frac{\partial \lambda_1^{\pm}}{\partial Q_{NS+4}} = 0. \tag{A.39}$$

The derivatives, with respect to the conserved variables, of the second and third eigenvalues are:

$$\frac{\partial \lambda_{2,3}^{\pm}}{\partial Q_i} = \frac{-u}{\rho} \pm \frac{\partial a}{\partial Q_i}, \tag{A.40}$$

$$\frac{\partial \lambda_{2,3}^{\pm}}{\partial Q_{NS+1}} = \frac{k_x}{\rho} \pm \frac{\partial a}{\partial Q_{NS+1}}, \tag{A.41}$$

$$\frac{\partial \lambda_{2,3}^{\pm}}{\partial Q_{NS+2}} = \frac{k_y}{\rho} \pm \frac{\partial a}{\partial Q_{NS+2}}, \tag{A.42}$$

$$\frac{\partial \lambda_{2,3}^{\pm}}{\partial Q_{NS+3}} = \frac{k_z}{\rho} \pm \frac{\partial a}{\partial Q_{NS+3}}, \tag{A.43}$$

$$\frac{\partial \lambda_{2,3}^{\pm}}{\partial Q_{NS+4}} = \pm\frac{\partial a}{\partial Q_{NS+4}}. \tag{A.44}$$

Appendix B

FLUX JACOBIANS

The conserved variables $\mathbf{Q}$ and the flux vector $\mathbf{S}$ were defined in Section 3.1. The flux vector can be written in terms of $\mathbf{Q}$. In this case, the primitive variable pressure, P, was also included since necessary derivatives are defined in Appendix A.

$$\mathbf{S} = \begin{bmatrix} Q_1\left(\frac{Q_1}{Q_0}Q_{N+1}k_x + \frac{Q_1}{Q_0}Q_{N+2}k_y + \frac{Q_1}{Q_0}Q_{N+3}k_z\right) \\ Q_2\left(\frac{Q_2}{Q_0}Q_{N+1}k_x + \frac{Q_2}{Q_0}Q_{N+2}k_y + \frac{Q_2}{Q_0}Q_{N+3}k_z\right) \\ \cdots \\ Q_{NS}\left(\frac{Q_{NS}}{Q_0}Q_{N+1}k_x + \frac{Q_{NS}}{Q_0}Q_{N+2}k_y + \frac{Q_{NS}}{Q_0}Q_{N+3}k_z\right) \\ Q_{NS+1}\left(\frac{Q_{NS+1}}{Q_0}k_x + \frac{Q_{NS+2}}{Q_0}k_y + \frac{Q_{NS+3}}{Q_0}k_z\right) + k_xP \\ Q_{NS+2}\left(\frac{Q_{NS+1}}{Q_0}k_x + \frac{Q_{NS+2}}{Q_0}k_y + \frac{Q_{NS+3}}{Q_0}k_z\right) + k_yP \\ Q_{NS+3}\left(\frac{Q_{NS+1}}{Q_0}k_x + \frac{Q_{NS+2}}{Q_0}k_y + \frac{Q_{NS+3}}{Q_0}k_z\right) + k_zP \\ (Q_{NS+4} + P)\left(\frac{Q_{NS+1}}{Q_0}k_x + \frac{Q_{NS+2}}{Q_0}k_y + \frac{Q_{NS+3}}{Q_0}k_z\right) \end{bmatrix}, \tag{B.1}$$

where

$$Q_0 = \sum_{i=1}^{NS} \rho_i. \tag{B.2}$$

The flux Jacobian, $K = \frac{\partial \mathbf{S}}{\partial \mathbf{Q}}$ is given by rows as:
Rows: $i = 1, 2, \ldots, NS$;

$$\begin{aligned} &K(i,j) = \delta_{i,j}\tilde{u}_k - \tfrac{\rho_i}{\rho_0} \qquad \text{for } j = 1, 2, \ldots, NS \\ &K(i, NS+1) = \tfrac{\rho_i}{\rho_0}k_x \\ &K(i, NS+2) = \tfrac{\rho_1}{\rho_0}k_y \\ &K(i, NS+3) = \tfrac{\rho_1}{\rho_0}k_z \\ &K(i, NS+4) = 0 \end{aligned} \tag{B.3}$$

Row: $NS+1$

$$\begin{aligned}
&K(NS+1,j) = -u\tilde{u}_k + \tfrac{\partial P}{\partial \rho_j} k_x \qquad \text{for } j = 1,2,\ldots,NS \\
&K(NS+1,NS+1) = \tilde{u}_k + uk_x + k_x \tfrac{\partial P}{\partial Q_{NS+1}} \\
&K(NS+1,NS+2) = k_y u + k_x \tfrac{\partial P}{\partial Q_{NS+2}} \\
&K(NS+1,NS+3) = k_z u + k_x \tfrac{\partial P}{\partial Q_{NS+3}} \\
&K(NS+1,NS+4) = k_x \tfrac{\partial P}{\partial Q_{NS+4}}
\end{aligned} \tag{B.4}$$

Row: $NS+2$

$$\begin{aligned}
&K(NS+2,j) = -v\tilde{u}_k + \tfrac{\partial P}{\partial \rho_j} k_y \qquad \text{for } j = 1,2,\ldots,NS \\
&K(NS+2,NS+1) = vk_x + k_y \tfrac{\partial P}{\partial Q_{NS+1}} \\
&K(NS+2,NS+2) = \tilde{u}_k + vk_y + k_y \tfrac{\partial P}{\partial Q_{NS+2}} \\
&K(NS+2,NS+3) = k_z v + k_y \tfrac{\partial P}{\partial Q_{NS+3}} \\
&K(NS+2,NS+4) = k_y \tfrac{\partial P}{\partial Q_{NS+4}}
\end{aligned} \tag{B.5}$$

Row: $NS+3$

$$\begin{aligned}
&K(NS+3,j) = -w\tilde{u}_k + \tfrac{\partial P}{\partial \rho_j} k_z \qquad \text{for } j = 1,2,\ldots,NS \\
&K(NS+3,NS+1) = k_x w + k_z \tfrac{\partial P}{\partial Q_{NS+1}} \\
&K(NS+3,NS+2) = k_y w + k_z \tfrac{\partial P}{\partial Q_{NS+2}} \\
&K(NS+3,NS+3) = \tilde{u}_k + k_z w + k_z \tfrac{\partial P}{\partial Q_{NS+3}} \\
&K(NS+3,NS+4) = k_z \tfrac{\partial P}{\partial Q_{NS+4}}
\end{aligned} \tag{B.6}$$

Row: $NS+4$

$$\begin{aligned}
&K(NS+4,j) = \left(\tfrac{\partial P}{\partial \rho_j} - h_0\right) \tilde{u}_k \qquad \text{for } j = 1,2,\ldots,NS \\
&K(NS+4,NS+1) = \tfrac{\partial P}{\partial \rho_{NS+1}} \tilde{u}_k + h_0 k_x \\
&K(NS+4,NS+2) = \tfrac{\partial P}{\partial \rho_{NS+2}} \tilde{u}_k + h_0 k_y \\
&K(NS+4,NS+3) = \tfrac{\partial P}{\partial \rho_{NS+3}} \tilde{u}_k + h_0 k_z \\
&K(NS+4,NS+4) = \tilde{u}_k \left(1 + \tfrac{\partial P}{\partial Q_{NS+4}}\right)
\end{aligned} \tag{B.7}$$

where

$$\begin{aligned}
K = A \qquad &\text{for} \qquad k = \xi \\
K = B \qquad &\text{for} \qquad k = \eta \\
K = C \qquad &\text{for} \qquad k = \zeta
\end{aligned}$$

Appendix C

EIGENVECTOR MATRICES

The final matrix of right eigenvectors (T_k), as derived in Chapter 5, is given by rows as:

Rows: $i = 1, 2, \ldots, NS$;

$$\begin{aligned}
&T_k(i,j) = \delta_{i,j}\alpha \qquad \text{for } j = 1, 2, \ldots, NS \\
&T_k(i, NS+1) = \alpha_i k_y \\
&T_k(i, NS+2) = \alpha_i k_z \\
&T_k(i, NS+3) = \alpha \\
&T_k(i, NS+4) = \alpha
\end{aligned} \tag{C.1}$$

Row: $NS + 1$

$$\begin{aligned}
&T_k(NS+1, j) = \alpha u \qquad \text{for } j = 1, 2, \ldots, NS \\
&T_k(NS+1, NS+1) = \alpha u k_y - \beta k_z \\
&T_k(NS+1, NS+2) = \alpha u k_z + \beta k_y \\
&T_k(NS+1, NS+3) = \alpha u + \tfrac{\rho}{\sqrt{2}} k_x \\
&T_k(NS+1, NS+4) = \alpha u - \tfrac{\rho}{\sqrt{2}} k_x
\end{aligned} \tag{C.2}$$

Row: $NS + 2$

$$\begin{aligned}
&T_k(NS+2, j) = \alpha v + \beta k_z \qquad \text{for } j = 1, 2, \ldots, NS \\
&T_k(NS+2, NS+1) = \alpha v k_y \\
&T_k(NS+2, NS+2) = \alpha v k_z - \rho k_x \\
&T_k(NS+2, NS+3) = \alpha v + \tfrac{\rho}{\sqrt{2}} k_y \\
&T_k(NS+2, NS+4) = \alpha v - \tfrac{\rho}{\sqrt{2}} k_y
\end{aligned} \tag{C.3}$$

Row: $NS+3$

$$\begin{aligned}
&T_k(NS+3,j) = \alpha w - \rho k_y \qquad \text{for } j = 1,2,\ldots,NS \\
&T_k(NS+3,NS+1) = \alpha w k_y + \rho k_x \\
&T_k(NS+3,NS+2) = \alpha w k_z \\
&T_k(NS+3,NS+3) = \alpha w + \tfrac{\rho}{\sqrt{2}} k_z \\
&T_k(NS+3,NS+4) = \alpha w - \tfrac{\rho}{sqrt2} k_z
\end{aligned} \tag{C.4}$$

Row: $NS+4$

$$\begin{aligned}
&T_k(NS+4,j) = \alpha T_j + \rho c_1 \qquad \text{for } j = 1,2,\ldots,NS \\
&T_k(NS+4,NS+1) = \tfrac{k_y}{[\sqrt{2}c} c_2 + \rho\left(-u k_z + w K_x\right) \\
&T_k(NS+4,NS+2) = \tfrac{k_z}{[\sqrt{2}c} c_2 + \rho\left(-u k_y - v K_x\right) \\
&T_k(NS+4,NS+3) = \tfrac{k_z}{[\sqrt{2}c} c_2 + \tfrac{\rho}{\sqrt{2}} \tilde{U} + \tfrac{\alpha c^2}{\gamma-1} \\
&T_k(NS+4,NS+4) = \tfrac{k_z}{[\sqrt{2}c} c_2 - \tfrac{\rho}{\sqrt{2}} \tilde{U} + \tfrac{\alpha c^2}{\gamma-1}
\end{aligned} \tag{C.5}$$

The matrix of left eigenvectors, T_k^{-1} can be written by row as:
Rows: $i = 1,2,\ldots,NS$;

$$\begin{aligned}
&T_k^{-1}(i,j) = \tfrac{\alpha\beta - \alpha_i A}{\alpha^2\beta}\delta_{i,j} + \tfrac{\alpha_i D}{\alpha\beta\rho_0} - \alpha_i c_i \qquad \text{for } j = 1,2,\ldots,NS \\
&T_k^{-1}(i,NS+1) = \tfrac{\alpha_i k_x u(\gamma-1)}{\alpha^2 c^2 \beta} \\
&T_k^{-1}(i,NS+2) = \tfrac{\alpha_i k_z}{\alpha\beta\rho} + \tfrac{\alpha_i k_x v(\gamma-1)}{\alpha^2 c^2 \beta} \\
&T_k^{-`}(i,NS+3) = \tfrac{-\alpha_i k_y}{\alpha\beta\rho} + \tfrac{\alpha_i k_x w(\gamma-1)}{\alpha^2 c^2 \beta} \\
&T_k^{-1}(i,NS+4) = \tfrac{-\alpha_i k_x(\gamma-1)}{\alpha^2 c^2 \beta}
\end{aligned} \tag{C.6}$$

Row: $NS+1$

$$\begin{aligned}
&T_k^{-1}(NS+1,j) = \tfrac{k_y}{\alpha\beta} + \tfrac{E}{\rho\beta} - \tfrac{k_y(\phi+\psi_j)}{\alpha c^2 \beta} \qquad \text{for } j = 1,2,\ldots,NS \\
&T_k^{-1}(NS+1,NS+1) = \tfrac{k_y}{\alpha\beta} + \tfrac{E}{\rho\beta} - \tfrac{k_y(\phi+\psi_{NS})}{\alpha c^2 \beta} \\
&T_k^{-1}(NS+1,NS+2) = \tfrac{-k_z}{\rho} + \tfrac{(\gamma-1)u k_y}{\alpha c^2 \beta} \\
&T_k^{-1}(NS+1,NS+3) = \tfrac{-k_y k_z(1-k_x)}{\rho\beta} + \tfrac{v k_y(\gamma-1)}{\alpha c^2 \beta} \\
&T_k^{-1}(NS+1,NS+4) = \tfrac{1-k_z^2(1-k_x)}{\rho\beta} + \tfrac{w k_y(\gamma-1)}{\alpha c^2 \beta} \\
&\tfrac{-k_y(\gamma-1)}{\alpha c^2 \beta}
\end{aligned} \tag{C.7}$$

Row: $NS+2$

$$\begin{aligned}
&T_k^{-1}(NS+2,j) = \tfrac{k_z}{\alpha\beta} + \tfrac{F}{\rho\beta} - \tfrac{k_z(\phi+\psi_j)}{\alpha c^2 \beta} \qquad \text{for } j = 1,2,\ldots,NS \\
&T_k^{-1}(NS+2,NS+1) = \tfrac{k_y}{\rho} + \tfrac{(\gamma-1)u k_z}{\alpha c^2 \beta} \\
&T_k^{-1}(NS+2,NS+2) = \tfrac{-1+k_y^2(1-k_x)}{\rho\beta} + \tfrac{v k_z(\gamma-1)}{\alpha c^2 \beta} \\
&T_k^{-1}(NS+2,NS+3) = \tfrac{k_y k_z(1-k_x)}{\rho\beta} + \tfrac{w k_z(\gamma-1)}{\alpha c^2 \beta} \\
&T_k^{-1}(NS+2,NS+4) = \tfrac{-k_z(\gamma-1)}{\alpha c^2 \beta}
\end{aligned} \tag{C.8}$$

Row: $NS+3$

$$\begin{aligned}
&T_k^{-1}(NS+3,j) = \tfrac{-\tilde{u}}{\sqrt{2}\rho}\tfrac{\phi+\psi_j}{2\alpha c^2} \qquad \text{for } j=1,2,\ldots,NS\\
&T_k^{-1}(NS+3,NS+1) = \tfrac{k_x}{\sqrt{2}\rho} - \tfrac{u(\gamma-1)}{2\alpha c^2}\\
&T_k^{-1}(NS+3,NS+2) = \tfrac{k_y}{\sqrt{2}\rho} - \tfrac{v(\gamma-1)}{2\alpha c^2}\\
&T_k^{-1}(NS+3,NS+3) = \tfrac{k_z}{\sqrt{2}\rho} - \tfrac{w(\gamma-1)}{2\alpha c^2}\\
&T_k^{-1}(NS+3,NS+4) = \tfrac{\gamma-1}{2\alpha c^2}
\end{aligned} \tag{C.9}$$

Row: $NS+4$

$$\begin{aligned}
&T_k^{-1}(NS+4,j) = \tfrac{\tilde{u}}{\sqrt{2}\rho}\tfrac{\phi+\psi_j}{2\alpha c^2} \qquad \text{for } j=1,2,\ldots,NS\\
&T_k^{-1}(NS+4,NS+1) = \tfrac{-k_x}{\sqrt{2}\rho} - \tfrac{u(\gamma-1)}{2\alpha c^2}\\
&T_k^{-1}(NS+4,NS+2) = \tfrac{-k_y}{\sqrt{2}\rho} - \tfrac{v(\gamma-1)}{2\alpha c^2}\\
&T_k^{-1}(NS+4,NS+3) = \tfrac{-k_z}{\sqrt{2}\rho} - \tfrac{w(\gamma-1)}{2\alpha c^2}\\
&T_k^{-1}(NS+4,NS+4) = \tfrac{\gamma-1}{2\alpha c^2}
\end{aligned} \tag{C.10}$$

where:

$$\begin{aligned}
&\alpha = \tfrac{\rho}{\sqrt{2}a}, && \alpha_i = \tfrac{\rho_i}{\sqrt{2}a},\\
&T_i = \tfrac{q^2}{2} + e_i - \tfrac{R_iT}{\gamma-1}, && c_1 = vk_z - wk_y,\\
&c_2 = \rho e_0 - \tfrac{P}{\gamma-1}, && \phi = (\gamma-1)\,\tfrac{\tilde{u}}{2},\\
&\psi_i = -(\gamma-1)\,e_i + R_iT, && A = 1-k_x^2,\\
&D = k_yw - vk_z, && \beta = k_x + k_y^2 + k_z^2,\\
&F = k_yu\beta + v\left[-1+k_y^2(1-k_x)\right] + wk_yk_z(1-k_x), && c_i = \tfrac{(\phi+\psi_i)k_x}{\alpha^2c^2\beta},\\
&E = k_z\beta u + k_yk_z(1-k_x)\,v - w\left[1-k_z^2(1-k_x)\right].
\end{aligned} \tag{C.11}$$

Appendix D

Split Flux Jacobians

The Steger-Warming split flux vectors for a finite-rate flow can be written as [13]:

$$\mathbf{S}_k^{\pm} = \frac{\gamma-1}{\gamma}\lambda_1^{\pm}\begin{pmatrix}\rho_1\\ \vdots\\ \rho_{NS}\\ \rho u\\ \rho v\\ \rho w\\ \rho h_0 - \frac{\rho a^2}{\gamma-1}\end{pmatrix} + \frac{\lambda_2^{\pm}}{2\gamma}\begin{pmatrix}\rho_1\\ \vdots\\ \rho_{NS}\\ \rho\left(u+k_x a\right)\\ \rho\left(v+k_y a\right)\\ \rho\left(w+k_z a\right)\\ \rho\left(h_0+\tilde{u}a\right)\end{pmatrix} + \frac{\lambda_3^{\pm}}{2\gamma}\begin{pmatrix}\rho_1\\ \vdots\\ \rho_{NS}\\ \rho\left(u-k_x a\right)\\ \rho\left(v-k_y a\right)\\ \rho\left(w-k_z a\right)\\ \rho\left(h_0-\tilde{u}a\right)\end{pmatrix} \tag{D.1}$$

or

$$\mathbf{S}_k^{\pm} = \frac{\gamma-1}{\gamma}\lambda_1^{\pm}\mathbf{S}_1^{\pm} + \frac{\lambda_2^{\pm}}{2\gamma}\mathbf{S}_2^{\pm} + \frac{\lambda_3^{\pm}}{2\gamma}\mathbf{S}_3^{\pm} \tag{D.2}$$

where

$$\lambda_1^{\pm} = J|\nabla k|\frac{\tilde{u}_k \pm |\tilde{u}_k|}{2} \tag{D.3}$$

$$\lambda_2^{\pm} = J|\nabla k|\frac{(\tilde{u}_k + a) \pm |\tilde{u}_k + a|}{2} \tag{D.4}$$

$$\lambda_3^{\pm} = J|\nabla k|\frac{(\tilde{u}_k - a) \pm |\tilde{u}_k - a|}{2} \tag{D.5}$$

From section 6.4, the split-flux Jacobian is defined as:

$$K^{\pm} = \frac{\partial \mathbf{S}^{\pm}}{\partial \mathbf{Q}}. \tag{D.6}$$

The general form of the split-flux Jacobian, with respect to a conserved variable, Q_j, is:

$$\frac{\partial \mathbf{S}^{\pm}}{\partial Q_j} = \frac{\partial}{\partial Q_j}\left[\frac{\gamma-1}{\gamma}\right]\lambda_1^{\pm}\mathbf{S}_1 + \frac{\gamma-1}{\gamma}\frac{\partial \lambda_1^{\pm}}{\partial Q_j}\mathbf{S}_1 + \frac{\gamma-1}{\gamma}\lambda_1^{\pm}\frac{\partial \mathbf{S}_1}{\partial Q_j}$$

$$
\begin{aligned}
&+\frac{\partial}{\partial Q_j}\left[\frac{1}{2\gamma}\right]\lambda_2^{\pm}\mathbf{S}_2+\frac{1}{2\gamma}\frac{\partial\lambda_2^{\pm}}{\partial Q_j}\mathbf{S}_2+\frac{1}{2\gamma}\lambda_2^{\pm}\frac{\partial\mathbf{S}_2}{\partial Q_j}\\
&+\frac{\partial}{\partial Q_j}\left[\frac{1}{2\gamma}\right]\lambda_3^{\pm}\mathbf{S}_3+\frac{1}{2\gamma}\frac{\partial\lambda_3^{\pm}}{\partial Q_j}\mathbf{S}_3+\frac{1}{2\gamma}\lambda_3^{\pm}\frac{\partial\mathbf{S}_3}{\partial Q_j}
\end{aligned}
$$

The eigenvalue derivatives are listed in Appendix A. The derivatives for specific heats in equation D.7 can be written as:

$$\frac{\partial}{\partial Q_j}\left(\frac{\gamma-1}{\gamma}\right)=\frac{1}{\gamma^2}\frac{\partial\gamma}{\partial Q_j} \tag{D.7}$$

$$\frac{\partial}{\partial Q_j}\left(\frac{1}{2\gamma}\right)=\frac{-1}{2\gamma^2}\frac{\partial\gamma}{\partial Q_j}. \tag{D.8}$$

The specific heat derivatives are listed in Appendix A.

The elements of the split-flux Jacobians are listed can now be listed by rows. Rows: $i=1,2,\ldots,NS$; Columns: $j=1,2,\ldots,NS$

$$
\begin{aligned}
\frac{\partial S_i^{\pm}}{\partial Q_j}=&\\
&\frac{\gamma-1}{\gamma}\left[\rho_i\frac{\partial\lambda_1^{\pm}}{\partial\rho_j}+\delta_{ij}\lambda_1^{\pm}\right]+\frac{\rho_i}{\gamma^2}\lambda_1^{\pm}\frac{\partial\gamma}{\partial\rho_j}\\
&+\frac{1}{2\gamma}\left[\rho_i\frac{\partial\lambda_2^{\pm}}{\partial\rho_j}+\delta_{ij}\lambda_2^{\pm}\right]-\frac{\rho_i}{2\gamma^2}\lambda_2^{\pm}\frac{\partial\gamma}{\partial\rho_j}\\
&+\frac{1}{2\gamma}\left[\rho_i\frac{\partial\lambda_3^{\pm}}{\partial\rho_j}+\delta_{ij}\lambda_3^{\pm}\right]-\frac{\rho_i}{2\gamma^2}\lambda_3^{\pm}\frac{\partial\gamma}{\partial\rho_j}
\end{aligned}
\tag{D.9}
$$

Row: $i=1,2,\ldots,NS$; Columns: $j=NS+1,\ldots,NS+4$

$$
\begin{aligned}
\frac{\partial S_i^{\pm}}{\partial Q_j}=&\\
&\frac{1}{2\gamma}\left[2\rho_i\left(\gamma-1\right)\frac{\partial\lambda_1^{\pm}}{\partial Q_j}+\frac{2\rho_i}{\gamma}\lambda_1^{\pm}\frac{\partial\gamma}{\partial Q_j}\right]\\
&+\frac{1}{2\gamma}\left[\rho_i\frac{\partial\lambda_2^{\pm}}{\partial Q_j}-\frac{\rho_i}{\gamma}\lambda_2^{\pm}\frac{\partial\gamma}{\partial Q_j}\right]\\
&+\frac{1}{2\gamma}\left[\rho_i\frac{\partial\lambda_3^{\pm}}{\partial Q_j}-\frac{\rho_i}{\gamma}\lambda_3^{\pm}\frac{\partial\gamma}{\partial Q_j}\right]
\end{aligned}
\tag{D.10}
$$

Row $NS+1$; Columns: $j=1,2,\ldots,NS$

$$
\begin{aligned}
\frac{\partial S_{NS+1}^{\pm}}{\partial Q_j}=&\\
&\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+1}\frac{\partial\lambda_1^{\pm}}{\partial\rho_j}+2Q_{NS+1}\frac{\lambda_1^{\pm}}{\gamma}\frac{\partial\gamma}{\partial Q_j}\right]
\end{aligned}
\tag{D.11}
$$

$$+\frac{1}{2\gamma}\left[\left(Q_{NS+1}+k_x\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial\rho_j}+k_x\left(a+\rho\frac{\partial a}{\partial Q_j}\right)\lambda_2^{\pm}-\frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+1}+k_x\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]$$
$$+\frac{1}{2\gamma}\left[\left(Q_{NS+1}-k_x\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial\rho_j}-k_x\left(a+\rho\frac{\partial a}{\partial Q_j}\right)\lambda_3^{\pm}-\frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+1}-k_x\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]$$

Row: $NS+1$; Column: $NS+1$

$$\frac{\partial S_{NS+1}^{\pm}}{\partial Q_{NS+1}}=$$
$$\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+1}\frac{\partial\lambda_1^{\pm}}{\partial Q_{NS+1}}+2\lambda_1^{\pm}\left(\frac{Q_{NS+1}}{\gamma}\frac{\partial\gamma}{\partial Q_{NS+1}}+\gamma-1\right)\right] \tag{D.12}$$
$$+\frac{1}{2\gamma}\left[\left(Q_{NS+1}+k_x\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_{NS+1}}+\left(1+k_x\rho\frac{\partial a}{\partial Q_{NS+1}}\right)\lambda_2^{\pm}-\frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+1}+k_x\rho a\right)\frac{\partial\gamma}{\partial Q_{NS+1}}\right]$$
$$+\frac{1}{2\gamma}\left[\left(Q_{NS+1}-k_x\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_{NS+1}}-\left(1-k_x\rho\frac{\partial a}{\partial Q_{NS+1}}\right)\lambda_3^{\pm}-\frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+1}-k_x\rho a\right)\frac{\partial\gamma}{\partial Q_{NS+1}}\right]$$

Row: $NS+1$; Columns: $j=NS+2, NS+3, NS+4$

$$\frac{\partial S_{NS+1}^{\pm}}{\partial Q_j}=$$
$$\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+1}\frac{\partial\lambda_1^{\pm}}{\partial Q_j}+2\lambda_1^{\pm}\frac{Q_{NS+1}}{\gamma}\frac{\partial\gamma}{\partial Q_{NS+1}}\right] \tag{D.13}$$
$$+\frac{1}{2\gamma}\left[\left(Q_{NS+1}+k_x\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_j}+k_x\rho\frac{\partial a}{\partial Q_j}\lambda_2^{\pm}-\frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+1}+k_x\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]$$
$$+\frac{1}{2\gamma}\left[\left(Q_{NS+1}-k_x\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_j}-k_x\rho\frac{\partial a}{\partial Q_j}\lambda_3^{\pm}-\frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+1}-k_x\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]$$

Row: $NS+2$; Columns: $j=1,2,\ldots,NS$

$$\frac{\partial S_{NS+2}^{\pm}}{\partial Q_j}=$$
$$\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+2}\frac{\partial\lambda_1^{\pm}}{\partial Q_j}+2Q_{NS+1}\frac{\lambda_1^{\pm}}{\gamma}\frac{\partial\gamma}{\partial Q_j}\right] \tag{D.14}$$
$$+\frac{1}{2\gamma}\left[\left(Q_{NS+2}+k_y\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_j}+k_y\left(a+\rho\frac{\partial a}{\partial Q_j}\right)\lambda_2^{\pm}-\frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+2}+k_y\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]$$
$$+\frac{1}{2\gamma}\left[\left(Q_{NS+2}-k_y\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_j}-k_x\left(a+\rho\frac{\partial a}{\partial Q_j}\right)\lambda_3^{\pm}-\frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+2}-k_y\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]$$

Row: $NS+2$; Column: $j=NS+1$

$$\frac{\partial S_{NS+2}^{\pm}}{\partial Q_{NS+1}}=$$
$$\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+2}\frac{\partial\lambda_1^{\pm}}{\partial Q_{NS+1}}+2\lambda_1^{\pm}\frac{Q_{NS+2}}{\gamma}\frac{\partial\gamma}{\partial Q_{NS+1}}\right] \tag{D.15}$$
$$+\frac{1}{2\gamma}\left[\left(Q_{NS+2}+k_x\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_{NS+1}}+k_y\rho\frac{\partial a}{\partial Q_{NS+1}}\lambda_2^{\pm}-\frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+2}+k_y\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]$$
$$+\frac{1}{2\gamma}\left[\left(Q_{NS+2}-k_y\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_{NS+1}}-k_y\rho\frac{\partial a}{\partial Q_{NS+1}}\lambda_3^{\pm}-\frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+2}-k_y\rho a\right)\frac{\partial\gamma}{\partial Q_{NS+1}}\right]$$

Row: $NS+2$; Column: $j = NS+2$

$$\frac{\partial S^{\pm}_{NS+2}}{\partial Q_{NS+2}} =$$

$$\begin{aligned}
&\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+2}\frac{\partial\lambda_1^{\pm}}{\partial Q_{NS+2}} + 2\lambda_1^{\pm}\left(\frac{Q_{NS+2}}{\gamma}\frac{\partial\gamma}{\partial Q_{NS+2}} + \gamma - 1\right)\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+2} + k_y\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_{NS+2}} + \left(1 + k_y\rho\frac{\partial a}{\partial Q_{NS+2}}\right)\lambda_2^{\pm} - \frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+2} + k_y\rho a\right)\frac{\partial\gamma}{\partial Q_{NS+2}}\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+2} - k_y\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_{NS+2}} - \left(1 - k_y\rho\frac{\partial a}{\partial Q_{NS+2}}\right)\lambda_3^{\pm} - \frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+2} - k_y\rho a\right)\frac{\partial\gamma}{\partial Q_{NS+2}}\right]
\end{aligned} \tag{D.16}$$

Row: $NS+2$; Columns: $j = NS+3, NS+4$

$$\frac{\partial S^{\pm}_{NS+2}}{\partial Q_j} =$$

$$\begin{aligned}
&\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+2}\frac{\partial\lambda_1^{\pm}}{\partial Q_j} + 2\lambda_1^{\pm}\frac{Q_{NS+2}}{\gamma}\frac{\partial\gamma}{\partial Q_j}\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+2} + k_x\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_j} + k_y\rho\frac{\partial a}{\partial Q_j}\lambda_2^{\pm} - \frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+2} + k_y\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+2} - k_y\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_j} - k_y\rho\frac{\partial a}{\partial Q_j}\lambda_3^{\pm} - \frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+2} - k_y\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]
\end{aligned} \tag{D.17}$$

Row: $NS+3$; Columns: $j = 1, 2, \ldots, NS$

$$\frac{\partial S^{\pm}_{NS+3}}{\partial Q_j} =$$

$$\begin{aligned}
&\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+3}\frac{\partial\lambda_1^{\pm}}{\partial Q_j} + 2Q_{NS+3}\frac{\lambda_1^{\pm}}{\gamma}\frac{\partial\gamma}{\partial Q_j}\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+3} + k_z\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_j} + k_z\left(a + \rho\frac{\partial a}{\partial Q_j}\right)\lambda_2^{\pm} - \frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+3} + k_z\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+3} - k_z\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_j} - k_z\left(a + \rho\frac{\partial a}{\partial Q_j}\right)\lambda_3^{\pm} - \frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+3} - k_z\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]
\end{aligned} \tag{D.18}$$

Row: $NS+3$; Columns: $j = NS+1, NS+2, NS+4$

$$\frac{\partial S^{\pm}_{NS+3}}{\partial Q_j} =$$

$$\begin{aligned}
&\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+3}\frac{\partial\lambda_1^{\pm}}{\partial Q_j} + 2\lambda_1^{\pm}\frac{Q_{NS+3}}{\gamma}\frac{\partial\gamma}{\partial Q_j}\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+3} + k_z\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_j} + k_z\rho\frac{\partial a}{\partial Q_j}\lambda_2^{\pm} - \frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+3} + k_z\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+3} - k_z\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_j} - k_z\rho\frac{\partial a}{\partial Q_j}\lambda_3^{\pm} - \frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+3} - k_z\rho a\right)\frac{\partial\gamma}{\partial Q_j}\right]
\end{aligned} \tag{D.19}$$

Row: $NS+3$; Column: $NS+3$

$$\frac{\partial S^{\pm}_{NS+3}}{\partial Q_{NS+3}} =$$

$$\begin{aligned}
&\frac{1}{2\gamma}\left[2\left(\gamma-1\right)Q_{NS+3}\frac{\partial\lambda_1^{\pm}}{\partial Q_{NS+3}}+2\lambda_1^{\pm}\left(\frac{Q_{NS+3}}{\gamma}\frac{\partial\gamma}{\partial Q_{NS+3}}+\gamma-1\right)\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+3}+k_z\rho a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_{NS+3}}+\left(1+k_z\rho\frac{\partial a}{\partial Q_{NS+3}}\right)\lambda_2^{\pm}-\frac{\lambda_2^{\pm}}{\gamma}\left(Q_{NS+3}+k_z\rho a\right)\frac{\partial\gamma}{\partial Q_{NS+3}}\right] \\
&+\frac{1}{2\gamma}\left[\left(Q_{NS+3}-k_z\rho a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_{NS+3}}-\left(1-k_z\rho\frac{\partial a}{\partial Q_{NS+3}}\right)\lambda_3^{\pm}-\frac{\lambda_3^{\pm}}{\gamma}\left(Q_{NS+3}-k_z\rho a\right)\frac{\partial\gamma}{\partial Q_{NS+3}}\right]
\end{aligned} \tag{D.20}$$

Row: $NS+4$; Columns: $j=1,2,\ldots,NS$

$$\frac{\partial S^{\pm}_{NS+4}}{\partial Q_j} =$$

$$\begin{aligned}
&\frac{1}{\gamma}\left[2\left(\left(\gamma-1\right)\rho h_0-P\right)\frac{\partial\lambda_1^{\pm}}{\partial Q_j}-\frac{\lambda_1^{\pm}}{\gamma}\frac{\partial P}{\partial Q_j}+\frac{\lambda_1^{\pm}}{\gamma}\rho h_0\frac{\partial\gamma}{\partial Q_j}\right] \\
&+\frac{1}{2\gamma}\left[\left(\rho h_0+\rho\tilde{u}a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_j}+\left(\frac{\partial P}{\partial Q_j}+\rho\tilde{u}\frac{\partial a}{\partial Q_j}\right)\lambda_2^{\pm}-\frac{\lambda_2^{\pm}}{\gamma}\left(\rho h_0+\rho\tilde{u}a\right)\frac{\partial\gamma}{\partial Q_j}\right] \\
&+\frac{1}{2\gamma}\left[\left(\rho h_0-\rho\tilde{u}a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_j}+\left(\frac{\partial P}{\partial Q_j}-\rho\tilde{u}\frac{\partial a}{\partial Q_j}\right)\lambda_3^{\pm}-\frac{\lambda_3^{\pm}}{\gamma}\left(\rho h_0-\rho\tilde{u}a\right)\frac{\partial\gamma}{\partial Q_j}\right]
\end{aligned} \tag{D.21}$$

Row: $NS+4$; Columns: $j=NS+1$

$$\frac{\partial S^{\pm}_{NS+4}}{\partial Q_{NS+1}} =$$

$$\begin{aligned}
&\frac{1}{\gamma}\left[\left[\left(\gamma-1\right)\rho h_0-\gamma P\right]\frac{\partial\lambda_1^{\pm}}{\partial Q_{NS+1}}-\lambda_1^{\pm}\frac{\partial P}{\partial Q_{NS+1}}+\lambda_1^{\pm}\frac{\rho h_0}{\gamma}\frac{\partial\gamma}{\partial Q_{NS+1}}\right] \\
&+\frac{1}{2\gamma}\left[\left(\rho h_0+\rho\tilde{u}a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_{NS+1}}+\lambda_2^{\pm}\left(\frac{\partial P}{\partial Q_{NS+1}}+ak_x+\rho\tilde{u}\frac{\partial a}{\partial Q_{NS+1}}\right)-\frac{\lambda_2^{\pm}}{\gamma}\left(\rho h_0+\rho\tilde{u}a\right)\frac{\partial\gamma}{\partial Q_{NS+1}}\right] \\
&+\frac{1}{2\gamma}\left[\left(\rho h_0-\rho\tilde{u}a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_{NS+1}}+\lambda_3^{\pm}\left(\frac{\partial P}{\partial Q_{NS+1}}-ak_x-\rho\tilde{u}\frac{\partial a}{\partial Q_{NS+1}}\right)-\frac{\lambda_3^{\pm}}{\gamma}\left(\rho h_0-\rho\tilde{u}a\right)\frac{\partial\gamma}{\partial Q_{NS+1}}\right]
\end{aligned} \tag{D.22}$$

Row: $NS+4$; Columns: $j=NS+2$

$$\frac{\partial S^{\pm}_{NS+4}}{\partial Q_{NS+2}} =$$

$$\begin{aligned}
&\frac{1}{\gamma}\left[\left[\left(\gamma-1\right)\rho h_0-\gamma P\right]\frac{\partial\lambda_1^{\pm}}{\partial Q_{NS+2}}-\lambda_1^{\pm}\frac{\partial P}{\partial Q_{NS+2}}+\lambda_1^{\pm}\frac{\rho h_0}{\gamma}\frac{\partial\gamma}{\partial Q_{NS+2}}\right] \\
&+\frac{1}{2\gamma}\left[\left(\rho h_0+\rho\tilde{u}a\right)\frac{\partial\lambda_2^{\pm}}{\partial Q_{NS+2}}+\lambda_2^{\pm}\left(\frac{\partial P}{\partial Q_{NS+2}}+ak_y+\rho\tilde{u}\frac{\partial a}{\partial Q_{NS+2}}\right)-\frac{\lambda_2^{\pm}}{\gamma}\left(\rho h_0+\rho\tilde{u}a\right)\frac{\partial\gamma}{\partial Q_{NS+2}}\right] \\
&+\frac{1}{2\gamma}\left[\left(\rho h_0-\rho\tilde{u}a\right)\frac{\partial\lambda_3^{\pm}}{\partial Q_{NS+2}}+\lambda_3^{\pm}\left(\frac{\partial P}{\partial Q_{NS+2}}-ak_y-\rho\tilde{u}\frac{\partial a}{\partial Q_{NS+2}}\right)-\frac{\lambda_3^{\pm}}{\gamma}\left(\rho h_0-\rho\tilde{u}a\right)\frac{\partial\gamma}{\partial Q_{NS+2}}\right]
\end{aligned} \tag{D.23}$$

Row: $NS+4$; Columns: $j = NS+3$

$$\frac{\partial S^{\pm}_{NS+4}}{\partial Q_{NS+3}} =$$

$$\frac{1}{\gamma}\left[\left[(\gamma-1)\,\rho h_0 - \gamma P\right]\frac{\partial \lambda_1^{\pm}}{\partial Q_{NS+3}} - \lambda_1^{\pm}\frac{\partial P}{\partial Q_{NS+3}} + \lambda_1^{\pm}\frac{\rho h_0}{\gamma}\frac{\partial \gamma}{\partial Q_{NS+3}}\right] \tag{D.24}$$

$$+\frac{1}{2\gamma}\left[(\rho h_0 + \rho\tilde{u}a)\frac{\partial \lambda_2^{\pm}}{\partial Q_{NS+3}} + \lambda_2^{\pm}\left(\frac{\partial P}{\partial Q_{NS+3}} + ak_z + \rho\tilde{u}\frac{\partial a}{\partial Q_{NS+3}}\right) - \frac{\lambda_2^{\pm}}{\gamma}(\rho h_0 + \rho\tilde{u}a)\frac{\partial \gamma}{\partial Q_{NS+3}}\right]$$

$$+\frac{1}{2\gamma}\left[(\rho h_0 - \rho\tilde{u}a)\frac{\partial \lambda_3^{\pm}}{\partial Q_{NS+3}} + \lambda_3^{\pm}\left(\frac{\partial P}{\partial Q_{NS+3}} - ak_z - \rho\tilde{u}\frac{\partial a}{\partial Q_{NS+3}}\right) - \frac{\lambda_3^{\pm}}{\gamma}(\rho h_0 - \rho\tilde{u}a)\frac{\partial \gamma}{\partial Q_{NS+3}}\right]$$

Row: $NS+4$; Columns: $j = NS+4$

$$\frac{\partial S^{\pm}_{NS+4}}{\partial Q_{NS+4}} =$$

$$\frac{1}{\gamma}\left[\left(\gamma - 1 - \frac{\partial P}{\partial Q_{NS+4}}\right)\lambda_1^{\pm} + \frac{\rho h_0}{\gamma}\frac{\partial \gamma}{\partial Q_{NS+4}}\right] \tag{D.25}$$

$$+\frac{1}{2\gamma}\left[(\rho h_0 + \rho\tilde{u}a)\frac{\partial \lambda_2^{\pm}}{\partial Q_{NS+4}} + \lambda_2^{\pm}\left(1 + \frac{\partial P}{\partial Q_{NS+4}} + \rho\tilde{u}\frac{\partial a}{\partial Q_{NS+4}}\right) - \frac{\lambda_2^{\pm}}{\gamma}(\rho h_0 + \rho\tilde{u}a)\frac{\partial \gamma}{\partial Q_{NS+4}}\right]$$

$$+\frac{1}{2\gamma}\left[(\rho h_0 - \rho\tilde{u}a)\frac{\partial \lambda_3^{\pm}}{\partial Q_{NS+4}} + \lambda_3^{\pm}\left(1 + \frac{\partial P}{\partial Q_{NS+4}} - \rho\tilde{u}\frac{\partial a}{\partial Q_{NS+4}}\right) - \frac{\lambda_3^{\pm}}{\gamma}(\rho h_0 - \rho\tilde{u}a)\frac{\partial \gamma}{\partial Q_{NS+4}}\right]$$