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Abstract

Inviscid flux Jacobian matrices and their properties used in numerical solutions of conservation laws are extended to general, equilibrium gas laws. Exact and approximate generalizations of the Roe average are presented. Results are given for one-dimensional flow, and then extended to three-dimensional flow with time-varying grids.

Introduction

Most treatments of inviscid terms in the numerical solution of conservation laws utilize the properties of flux Jacobian matrices. For central difference methods, the Beam-Warming scheme [1] requires the true flux Jacobians matrices, and their eigenvalues and eigenvectors are needed for the diagonal algorithms [2]. Most upwind methods, such as the Steger-Warming flux-vector splitting [3], the van Leer flux-vector splitting [4], and the Roe approximate Riemann solver [5], all utilize the properties of the flux Jacobian matrix. Their original derivations relied on the algebraic simplicity of the perfect gas law. Many flows of current interest involve departure from a perfect gas due to vibrational excitation, dissociation, and ionization, although the assumption of thermodynamic and chemical equilibrium is still valid. The purpose of this paper is to derive the flux Jacobian matrices and their properties for a general, equilibrium gas law, and to present the generalization of the Roe average used in Roe's approximate Riemann solver. Generalizations of the flux-vector splitting methods are reported elsewhere [6–9].

The generalizations of the Roe average proposed by other investigators [10–12] are all based on an approximate flux Jacobian matrix, or utilize some other approximations. In the earlier stages of this work, whose results are reported in Refs. 7–9, it was established that a Roe-averaged state exists for an equilibrium gas, but its precise value is not uniquely defined. A particular method for obtaining a unique state was proposed. In the present paper, a new, exact definition of a unique Roe-averaged state is given. Since its exact implementation may not always be practical, several approximations to the relations are also given. For simplicity, the analysis is first presented for one-dimensional flow with a fixed grid. The results are then

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generalized to three-dimensional flow with time-varying grids.

Flux Jacobian Matrices for One-Dimensional Flow

The primitive variables defining a fluid state are the density ρ, velocity u, and the internal energy per unit mass ϵ. Note that there is an arbitrary additive constant in the definition of ϵ. Since conservation laws are expressed in terms of conserved quantities per unit volume, it is convenient to introduce the internal energy per unit volume $\tilde{\epsilon} = \rho\epsilon$. The corresponding set of conservative variables U can be represented by the algebraic column vector

$$U = \begin{bmatrix} \rho \\ m \\ e \end{bmatrix}, \tag{1}$$

where $m = \rho u$ is the momentum per unit volume, and $e = \tilde{\epsilon} + \frac{1}{2}\rho u^2$ is the total energy per unit volume.

The calculation of the flux of U plays a central role in the numerical solution of conservation laws. The set of inviscid flux components F is given by the algebraic column vector

$$F = \begin{bmatrix} M \\ P \\ E \end{bmatrix} = \begin{bmatrix} \rho u \\ mu + p \\ eu + pu \end{bmatrix}, \tag{2}$$

where M, P, and E are the flux of mass, momentum, and energy, and the pressure p is given by a general equation of state of the form

$$p = p(\rho, \tilde{\epsilon}). \tag{3}$$

The derivatives will be denoted by

$$\chi = \left(\frac{\partial p}{\partial \rho}\right)_{\tilde{\epsilon}} \quad \text{and} \quad \kappa = \left(\frac{\partial p}{\partial \tilde{\epsilon}}\right)_{\rho}. \tag{4}$$

If $h = (\tilde{\epsilon} + p)/\rho$ is the specific enthalpy, the speed of sound c can then be expressed as

$$c^2 = \chi + \kappa h. \tag{5}$$

It will also be convenient to define nondimensional parameters

$$\gamma = \frac{\rho c^2}{p} \quad \text{and} \quad \tilde{\gamma} = 1 + \frac{p}{\tilde{\epsilon}}. \tag{6}$$

Using Eq. (5) one can also express $\bar{\gamma}$ as

$$\bar{\gamma} = \frac{1}{\gamma - \kappa}(\gamma + \frac{\chi}{\epsilon}). \tag{7}$$

Note that while κ, c, and γ have well defined values, the values of χ and $\bar{\gamma}$ depend on the choice of arbitrary constant in the definition of ϵ.

An important special equation of state is that for a thermally perfect (but calorically imperfect) gas, which has the form

$$p = \rho f(\epsilon). \tag{8}$$

This law is valid for a dilute gas consisting of a single chemical species, and is also a very good approximation for air below the temperature when oxygen starts to dissociate (approximately 2000 K). Using Eqs. (4)–(7) one can readily obtain the relations

$$p = \chi(\epsilon)\rho + \kappa(\epsilon)\widetilde{\epsilon} \tag{9}$$

and

$$\gamma = \kappa + 1, \quad \bar{\gamma} = \gamma + \frac{\chi}{\epsilon}. \tag{10}$$

If one further specializes Eq. (8) by letting $f(\epsilon)$ be just a linear function of ϵ, one obtains the equation for a gas that is also calorically perfect — better known simply as a perfect gas. This law is valid for a gas consisting of structureless particles, and is also a very good approximation for air at low temperatures. The derivatives χ and κ are now constants. It follows from Eqs. (9) and (10) that a great simplification is obtained if one chooses the arbitrary constant in the definition of ϵ so that $\chi = 0$ and $\bar{\gamma} = \gamma$. In fact, this choice is tacitly made in the usual definition of a perfect gas. It is therefore also customary to choose the arbitrary energy constant for a general gas so that χ approaches zero at low temperatures.

The differential expression $dF = A\,dU$ defines the flux Jacobian matrix operator A. The differential

$$dp = \chi\, d\rho + \kappa\, d\widetilde{\epsilon}, \tag{11}$$

can be rewritten in terms of the differentials of the conservative variables as

$$dp = K_1\, d\rho - \kappa u\, dm + \kappa\, de, \tag{12}$$

where $K_1 = \frac{1}{2}\kappa u^2 + \chi$. The matrix A can then be written as

$$A = \begin{bmatrix} 0 & 1 & 0 \\ K_1 - u^2 & (2-\kappa)u & \kappa \\ (K_1 - H)\,u & H - \kappa u^2 & (1+\kappa)\,u \end{bmatrix}, \tag{13}$$

where $H = h + \frac{1}{2}u^2$ is the total enthalpy per unit mass. The three eigenvalues of A are readily found to be

$$\lambda_1 = u, \quad \lambda_2 = u + c, \quad \text{and} \quad \lambda_3 = u - c. \tag{14}$$

The corresponding right eigenvector matrix R is

$$R = \begin{bmatrix} 1 & 1 & 1 \\ u & u+c & u-c \\ K_2 & H+cu & H-cu \end{bmatrix}, \tag{15}$$

where $K_2 = \frac{1}{2}u^2 - \chi/\kappa = H - c^2/\kappa$, while the left eigenvector matrix R^{-1} takes the form

$$R^{-1} = \begin{bmatrix} 1 - K_1/c^2 & \kappa u/c^2 & -\kappa/c^2 \\ \frac{1}{2}\left(K_1/c^2 - u/c\right) & -\frac{1}{2}\left(\kappa u/c^2 - 1/c\right) & \frac{1}{2}\kappa/c^2 \\ \frac{1}{2}\left(K_1/c^2 + u/c\right) & -\frac{1}{2}\left(\kappa u/c^2 + 1/c\right) & \frac{1}{2}\kappa/c^2 \end{bmatrix}. \tag{16}$$

The only difference between the expressions in Eqs. (13), (15), and (16) and the corresponding expressions for a perfect gas is the presence of χ in the terms K_1 and K_2, and the fact that κ is a variable instead of a constant. By writing K_1 and K_2 in terms of H and c^2, using Eq. (5), one can obtain expressions in which the only difference with the perfect gas expressions is the presence of the variable κ.

One can define functions of the matrix A through

$$f(A) = f(\lambda_1)P_1 + f(\lambda_2)P_2 + f(\lambda_3)P_3, \tag{17}$$

where the projection operators P_i are the tensor products

$$P_i = R_i R_i^{-1}. \tag{18}$$

Examples of $f(\lambda)$ are λ, $|\lambda|$, $\text{sgn}\lambda = |\lambda|/\lambda$, and $\lambda^{\pm} = (\lambda \pm |\lambda|)/2$. The formula for P_1 is

$$P_1 = \begin{bmatrix} 1 - K_1/c^2 & \kappa u/c^2 & -\kappa/c^2 \\ (1 - K_1/c^2)u & \kappa u^2/c^2 & -\kappa u/c^2 \\ u^2 - K_1 H/c^2 & (\kappa H/c^2 - 1)u & 1 - \kappa H/c^2 \end{bmatrix}. \tag{19}$$

Using the fact that

$$P_1 + P_2 + P_3 = I, \tag{20}$$

where I is the unit matrix, one can express the other two projection matrices as

$$P_{\substack{2 \\ 3}} = \frac{1}{2}[\pm A/c + I(1 \mp u/c) - P_1]. \tag{21}$$

One can easily establish that

$$AU = F + (\gamma - 1 - \kappa)p \begin{bmatrix} 0 \\ 1 \\ u \end{bmatrix}. \tag{22}$$

It follows that the necessary and sufficient condition for the homogeneity property $F = AU$ is given by a thermally perfect gas (Eq. (8)). Using Eq. (17), one can expand F for a thermally perfect gas as

$$F = \sum_{i=1}^{3} F_i, \tag{23}$$

where each F_i is associated with λ_i. The final expressions for the F_i are

$$F_1 = \frac{\lambda_1 \rho(\gamma - 1)}{\gamma} \begin{bmatrix} 1 \\ u \\ \frac{1}{2}u^2 + \epsilon - \frac{c^2}{\gamma(\gamma-1)} \end{bmatrix}, \qquad F_{\substack{2\\3}} = \frac{\lambda_{\substack{2\\3}} \rho}{2\gamma} \begin{bmatrix} 1 \\ u \pm c \\ H \pm cu \end{bmatrix}, \tag{24}$$

where $\gamma = \gamma(\epsilon)$. Eqs. (23) and (24) form the basis for the generalized Steger-Warming flux-vector splitting [6–9].

Generalized Roe Average for One-Dimensional Flow

Among the various approximate Riemann solvers, the most common one uses the Roe average because of its simplicity and its ability to satisfy the jump conditions across discontinuities exactly. The derivation in Ref. 5 for a perfect gas employed parameter vectors. To obtain a generalization for an equilibrium gas, a different, more direct approach is used here.

In approximate Riemann solvers based on local linearization, the flux at a point separating two states $U_L$and U_R is based on the eigenvalues and eigenvectors of some average $\overline{A}$. The optimum choice for $\overline{A}$ is one satisfying

$$\Delta F = \overline{A}\,\Delta U, \tag{25}$$

where $\Delta(\cdot) = (\cdot)_R - (\cdot)_L$. This choice of $\overline{A}$ captures discontinuities exactly. One way of obtaining $\overline{A}$ is to seek an average state $\overline{U}$, such that

$$\overline{A} = A(\overline{U}). \tag{26}$$

The notation $\overline{U}$ implies only those variables that appear explicitly in Eq. (26). Such a state is known as a Roe-averaged state, and was derived by Roe for a perfect gas.

The generalization to an equilibrium gas is obtained by substituting Eqs. (1), (2), (13), and (26) into Eq. (25). The second component of Eq. (25) results in

$$\begin{aligned}\rho_R u_R^2 - \rho_L u_L^2 + \Delta p = \left[(\frac{1}{2}\overline{\kappa} - 1)\overline{u}^2 + \overline{\chi}\right] \Delta\rho + (2-\overline{\kappa})\overline{u}(\rho_R u_R - \rho_L u_L) \\ + \overline{\kappa}\,\Delta\tilde{\epsilon} + \frac{1}{2}\overline{\kappa}(\rho_R u_R^2 - \rho_L u_L^2).\end{aligned} \tag{27}$$

The average velocity $\overline{u}$ must be some linear combination of u_L and u_R. Therefore let

$$\overline{u} = \alpha u_L + \beta u_R. \tag{28}$$

Since u_L and u_R can vary independently, the products u_L^2, u_R^2, and $u_L u_R$ are also independent. After substituting Eq. (28) into Eq. (27), the terms involving each of those products must satisfy the equation separately. From the coefficients of u_L^2 one obtains the quadratic equation

$$\alpha^2(\rho_R - \rho_L) + 2\alpha\rho_L - \rho_L = 0. \tag{29}$$

The only root that is finite when $\rho_R = \rho_L$ is

$$\alpha = \frac{\sqrt{\rho_L}}{\sqrt{\rho_L} + \sqrt{\rho_R}}. \tag{30}$$

From the coefficients of u_R^2 one can show that $\beta = 1 - \alpha$. The equation obtained from the coefficients of $u_L u_R$ is also satisfied by these expressions for α and β. Therefore Eq. (28) can be rewritten as

$$\overline{u} = \alpha u_L + (1-\alpha)u_R. \tag{31}$$

Eqs. (30) and (31) are the identical relations derived by Roe for a perfect gas. The remaining terms in Eq. (27) result in the new condition

$$\overline{\chi}\,\Delta\rho + \overline{\kappa}\,\Delta\tilde{\epsilon} = \Delta p. \tag{32}$$

This is just the discrete form of Eq. (11), averaged between the two states. This last condition is automatically satisfied for a perfect gas. In a similar manner, the third component of Eq. (25) results in the additional relation

$$\overline{H} = \alpha H_L + (1-\alpha)H_R, \tag{33}$$

which is also true for a perfect gas. From the definition of H, Eqs. (31) and (33) can be combined to define the Roe-averaged specific enthalpy as

$$\overline{h} = \alpha h_L + (1-\alpha)h_R + \frac{1}{2}\alpha(1-\alpha)(\Delta u)^2. \tag{34}$$

Note that $\bar{h}$ could lie outside the range given by h_L and h_R if the magnitude of Δu is sufficiently large. The Roe-averaged sound speed is given by Eq. (5) as

$$\bar{c}^2 = \bar{\chi} + \bar{\kappa}\bar{h}. \tag{35}$$

For a perfect gas, Eqs. (30), (31), (33), (34), and (35) are sufficient to define uniquely $\bar{\lambda}_i$, $\bar{R}$, and $\bar{R}^{-1}$, since $\bar{\chi} = 0$ and $\bar{\kappa}$ is a given constant.

For an arbitrary equilibrium gas, Eq. (32) provides only one relation for the variables $\bar{\chi}$ and $\bar{\kappa}$. We thus have the paradoxical situation that not only does a Roe-averaged state exist for an equilibrium gas, its precise value is not uniquely defined. For the special case in which state L and R are precisely those that satisfy the jump conditions across a discontinuity, Eqs. (30) through (35) are consistent with the exact Riemann solver, even though $\bar{\chi}$ and $\bar{\kappa}$ are not uniquely defined. For a stationary shock wave,

$$\Delta M = \Delta P = \Delta H = 0. \tag{36}$$

By combining the definitions of M and P with Eqs. (30), (31), and (36), one can readily show that

$$\bar{u}^2 = \frac{M^2}{\rho_L \rho_R} = u_L u_R = \frac{\Delta p}{\Delta \rho}. \tag{37}$$

The definitions of M, P, and H can be combined with Eqs. (36) and (37) to derive the relation

$$\Delta \tilde{\epsilon} = \bar{h}\, \Delta \rho. \tag{38}$$

By substituting Eqs. (32) and (38) into Eq. (35), it follows that for a stationary shock wave, if $\bar{\chi}$ and $\bar{\kappa}$ satisfy Eq. (32), then

$$\bar{c}^2 = \frac{\Delta p}{\Delta \rho}. \tag{39}$$

From Eqs. (37) and (39) it follows that for a stationary shock wave the magnitude of the Roe-averaged velocity is equal to the Roe-averaged sound speed. This could have been predicted ahead of time from Eq. (14), since one of the eigenvalues had to be equal to zero. From the definitions of M and H and Eq. (36) it follows that

$$\frac{1}{2}(\Delta u)^2 = \frac{\Delta \rho \, \Delta h}{\rho_L + \rho_R}. \tag{40}$$

Substituting Eq. (40) into Eq. (34) one obtains

$$\bar{h} = \frac{\rho_L h_L + \rho_R h_R}{\rho_L + \rho_R} = \frac{(1-\alpha)^2 h_L + \alpha^2 h_R}{(1-\alpha)^2 + \alpha^2}. \tag{41}$$

It is easy to show that Eqs. (39) and (41) are also valid for a non-stationary shock wave.The values of $\overline{h}$ and $\overline{c}^2$ as given by Eqs. (39) and (41) will in general not be consistent with a thermally perfect gas law, except for the special case of a perfect gas.

It is clear that unique values of $\overline{\chi}$ and $\overline{\kappa}$ must be defined in terms of the thermodynamic states L and R. Accurate numerical calculations for air [13] show that $\overline{\chi}$ and $\overline{\kappa}$ can have a non-convex behavior if the states L and R are far apart. A clue to a simple definition for the two derivatives can be obtained by considering the special case $\widetilde{\epsilon}_L = \widetilde{\epsilon}_R$, i.e., $\Delta\widetilde{\epsilon} = 0$. Integrating Eq. (11) and substituting into Eq. (32) yields

$$\overline{\chi} = \frac{\Delta p}{\Delta \rho} = \frac{1}{\Delta \rho} \int_{\rho_L}^{\rho_R} \chi(\rho, \widetilde{\epsilon}_L)\, d\rho. \tag{42}$$

Thus $\overline{\chi}$ is the integrated average of χ along the straight-line path between states L and R in the ρ-$\widetilde{\epsilon}$ plane for this special case. Actually, there is an infinite set of paths that can be used to define $\overline{\chi}$, but the straight-line path is the simplest one that can be defined for an arbitrary function. Similarly, for $\Delta\rho = 0$ one obtains

$$\overline{\kappa} = \frac{\Delta p}{\Delta \widetilde{\epsilon}} = \frac{1}{\Delta \widetilde{\epsilon}} \int_{\widetilde{\epsilon}_L}^{\widetilde{\epsilon}_R} \kappa(\rho_L, \widetilde{\epsilon})\, d\widetilde{\epsilon}. \tag{43}$$

Let an arbitrary path between any two states L and R be defined parametrically by the functions $\rho(t)$ and $\widetilde{\epsilon}(t)$, where the parameter t is normalized so that $t_L = 0$ and $t_R = 1$. Integrating Eq. (11) along this path, one obtains

$$\Delta p = \int_0^1 \chi[\rho(t), \widetilde{\epsilon}(t)]\rho'(t)\, dt + \int_0^1 \kappa[\rho(t), \widetilde{\epsilon}(t)]\widetilde{\epsilon}\,'(t)\, dt. \tag{44}$$

The simplest choice is the straight-line path

$$\rho(t) = \rho_L + t\,\Delta\rho, \tag{45a}$$
$$\widetilde{\epsilon}(t) = \widetilde{\epsilon}_L + t\,\Delta\widetilde{\epsilon}. \tag{45b}$$

Substituting Eqs. (45) into Eq. (44), and comparing with Eq. (32), yields the general relations

$$\overline{\chi} = \int_0^1 \chi[\rho(t), \widetilde{\epsilon}(t)]\, dt, \tag{46a}$$
$$\overline{\kappa} = \int_0^1 \kappa[\rho(t), \widetilde{\epsilon}(t)]\, dt. \tag{46b}$$

Eqs. (45) and (46) give unique definitions of $\bar{\chi}$ and $\bar{\kappa}$ satisfying condition (32) for arbitrary values of $\Delta\rho$ and $\Delta\tilde{\epsilon}$, including the limiting case $\Delta\rho = \Delta\tilde{\epsilon} = 0$. From Eqs. (34) and (35) one sees that even if $\Delta u = 0$, $\bar{c}^2$ is not equal to the integrated average of c^2. Since h is a smoothly varying function (compared to χ and κ), it is reasonable to expect that $\bar{c}^2$ will always be positive. For a thermally perfect gas law obeying Eq. (8), and $\Delta\epsilon \neq 0$, Eqs. (46a) and (46b) become

$$\bar{\chi} = \rho_L \rho_R \, \Delta\epsilon \int_{\epsilon_L}^{\epsilon_R} \frac{(f - \epsilon f')\, d\epsilon}{(\Delta\tilde{\epsilon} - \epsilon\, \Delta\rho)^2}, \tag{47a}$$

$$\bar{\kappa} = \rho_L \rho_R \, \Delta\epsilon \int_{\epsilon_L}^{\epsilon_R} \frac{f'\, d\epsilon}{(\Delta\tilde{\epsilon} - \epsilon\, \Delta\rho)^2}. \tag{47b}$$

Given an equation of state, or some interpolation representation (such as Ref. 13), the integrals in Eqs. (46) can be evaluated for any two end states L and R. Since the exact evaluation may not be practical, some approximate quadratures may be required. Let $\widehat{\chi}$ and $\widehat{\kappa}$ be approximations to Eqs. (46a) and (46b). They will not satisfy Eq. (32) exactly. One therefore requires values of $\bar{\chi}$ and $\bar{\kappa}$ satisfying Eq. (32) which are closest to $\widehat{\chi}$ and $\widehat{\kappa}$. This can be formulated geometrically as projecting the point $\widehat{\chi}$, $\widehat{\kappa}$ onto the straight line defined by Eq. (32). But in order for the Roe-averaged state to be independent of the arbitrary constant in the definition of ϵ, one must first recast the problem so that geometric relationships will not be affected by the choice of this constant. This can be accomplished if one first divides Eq. (32) by $\bar{\kappa}$. The slope of the straight line for the variables $1/\bar{\kappa}$ and $\bar{\chi}/\bar{\kappa}$ is now given by Δp and $\Delta\rho$, both of which are uniquely defined by states L and R. A further scale factor $\widehat{s}$ with the dimension of $\bar{\chi}$ must be introduced, since $\bar{\chi}$ is not dimensionless. The projection on to the straight line is then defined by the relation

$$\frac{\widehat{s}^2}{\bar{\kappa}}\, \Delta\rho + \frac{\bar{\chi}}{\bar{\kappa}}\, \Delta p = \frac{\widehat{s}^2}{\widehat{\kappa}}\, \Delta\rho + \frac{\widehat{\chi}}{\widehat{\kappa}}\, \Delta p. \tag{48}$$

If one introduces the error

$$\delta p = \Delta p - \widehat{\chi}\, \Delta\rho - \widehat{\kappa}\, \Delta\tilde{\epsilon} \tag{49}$$

and the quantity

$$D = (\widehat{s}\, \Delta\rho)^2 + (\Delta p)^2, \tag{50}$$

one can solve Eqs. (32) and (48) to obtain the final relations

$$\bar{\chi} = \frac{D\widehat{\chi} + \widehat{s}^2\, \Delta\rho\, \delta p}{D - \Delta p\, \delta p}, \tag{51a}$$

$$\bar{\kappa} = \frac{D\widehat{\kappa}}{D - \Delta p\, \delta p}. \tag{51b}$$

A natural choice for the scale factor $\widehat{s}$ is

$$\widehat{s} = \widehat{c^2} = \widehat{\chi} + \widehat{\kappa h}, \tag{52}$$

where the same quadrature approximation that was used to calculate $\widehat{\chi}$ and $\widehat{\kappa}$ is assumed. Note that the $\widehat{s}$ given by Eq. (52) is guaranteed to be positive. This is not necessarily true if one defined $\widehat{s} = \widehat{\chi} + \widehat{\kappa}\overline{h}$.

Let $\rho_M = (\rho_L + \rho_R)/2$ and $\widetilde{\epsilon}_M = (\widetilde{\epsilon}_L + \widetilde{\epsilon}_R)/2$ define the midpoint state M. Then possible quadrature rules for $\widehat{\chi}$ are the midpoint rule

$$\widehat{\chi} = \chi_M, \tag{53}$$

the trapezoidal rule

$$\widehat{\chi} = (\chi_L + \chi_R)/2, \tag{54}$$

and Simpson's rule

$$\widehat{\chi} = (\chi_L + 4\chi_M + \chi_R)/6, \tag{55}$$

with analogous formulas for $\widehat{\kappa}$ and $\widehat{c^2}$. Eqs. (53) and (54) are exact if p is a quadratic polynomial in ρ and $\widetilde{\epsilon}$, while Eq. (55) is exact if p is a cubic polynomial. While the expressions for $\overline{\chi}$ and $\overline{\kappa}$ given in Refs. 7–9 used approximation (54), they differ from the present results since Eq. (48) was written in terms of $\widehat{1/\kappa}$ and $\widehat{\chi/\kappa}$. If the states L and R are reasonably close, approximations (53) or (54) should be adequate. For large separation of the two states, Simpson's rule (55) may be required. The quantity D/p_L^2 is a useful nondimensional parameter measuring the separation of the two states.

While the above relations are all that are required to construct a Riemann solver using Roe's linearization, an additional algebraic simplicity can be achieved by expressing differences in conservative variables in terms of differences in primitive variables. If one *formally* defines

$$\overline{\rho} = \sqrt{\rho_L \rho_R}, \tag{56}$$

one obtains the identities

$$\Delta(\rho u) = \overline{\rho}\,\Delta u + \overline{u}\,\Delta\rho \tag{57}$$

and

$$\Delta(\rho u^2) = 2\overline{\rho}\,\overline{u}\,\Delta u + \overline{u}^2\,\Delta\rho. \tag{58}$$

An important quantity in the approximate Riemann solver is the column vector $R^{-1}\Delta U$. Its components are the jumps in the characteristic variables. Using Eqs. (32), (57), and (58), it can be expressed simply in term of Δp, $\Delta\rho$ and Δu as

$$R^{-1}\Delta U = \begin{bmatrix} \Delta\rho - \Delta p/\overline{c}^2 \\ \frac{1}{2}(\Delta p/\overline{c}^2 + \overline{\rho}\,\Delta u/\overline{c}) \\ \frac{1}{2}(\Delta p/\overline{c}^2 - \overline{\rho}\,\Delta u/\overline{c}) \end{bmatrix}. \tag{59}$$

These expressions have the same form as for the perfect gas case. The quantities $\overline{\chi}$ and $\overline{\kappa}$ do not appear explicitly.

Comparisons with Other Formulations

The formulas for Roe's approximate Riemann solver described by Grossman and Walters [10] involve three approximations. They assume that 1) $\Delta\bar{\gamma}$ and $\Delta\gamma$ are small, 2) $\Delta\bar{\gamma}$ can be related to Δp via an isentropic formula, and 3) $\bar{\gamma}$ is nearly equal to γ. All these approximations can be poor if the two states are far apart. If one notes that

$$c^2 = \frac{(\bar{\gamma}-1)}{\bar{\gamma}}\gamma h, \tag{60}$$

their final expressions are equivalent to setting $\chi = 0$, with $\bar{\gamma}$ and γ replaced by their arithmetic averages. The calculations of Ref. 13 show that setting $\chi = 0$ in the first eigenvector of Eq. (15) may not be justified.

Glaister [11] follows an analysis similar to the present one, except that he employs ϵ instead of $\tilde{\epsilon}$ in Eqs. (3), (4), and (11). As a result it is necessary to introduce $\bar{\rho}$ via Eq. (56), as well as to define

$$\bar{\epsilon} = \alpha\epsilon_L + (1-\alpha)\epsilon_R \tag{61}$$

in order to obtain Eq. (32) in terms of $\Delta\epsilon$. In the limit of a perfect gas, note the inconsistency between Eqs. (34) and (61). He suggests a different integration path in order to define his $\overline{\chi}$ and $\overline{\kappa}$. Let ρ_L, ϵ_R define the fictitious state T, and ρ_R, ϵ_L define state B. Then $\overline{\chi}$ and $\overline{\kappa}$ are defined as the arithmetic averages of the values resulting from integrating Eq. (32) via paths *L-T-R* and *L-B-R*, respectively. This results in

$$\overline{\chi} = \frac{1}{2}(\Delta p + p_B - p_T)/\Delta\rho, \tag{62a}$$

$$\overline{\kappa} = \frac{1}{2}(\Delta p + p_T - p_B)/\Delta\epsilon. \tag{62b}$$

These are replaced by $\overline{\chi} = \frac{1}{2}(\chi_L + \chi_R)$ if $\Delta\rho = 0$, and $\overline{\kappa} = \frac{1}{2}(\kappa_L + \kappa_R)$ if $\Delta\epsilon = 0$. If the states L and R are far apart, and the equation of state is non-convex, the introduction of the fictitious states T and B could give poor results.

Liou et al [12] also follow Glaister's analysis, employing ϵ instead of $\tilde{\epsilon}$, but suggest using the state $\overline{M}$ defined by Eqs. (56) and (61) instead of M to calculate their approximate $\widehat{\chi}$ and $\widehat{\kappa}$ by the midpoint rule (53). From the interpretation of $\widehat{\chi}$ and $\widehat{\kappa}$ as quadrature approximations to integrals, it would appear that evaluating at the average state M would give a better approximation in general. Their formulas for the values of $\overline{\chi}$ and $\overline{\kappa}$ satisfying Eq. (32) which are closest to $\widehat{\chi}$ and $\widehat{\kappa}$ also break down when either $\Delta\rho$ or $\Delta\epsilon$ approaches zero.

Generalization to Three-Dimensional Flow

The generalization of the above results to three-dimensional flow can be accomplished in a compact manner by employing the vector approach of the author [14]. Here the word vector refers to a physical vector such as velocity or momentum, as distinguished from an algebraic *vector* representing a set of variables. If $\mathbf{u}$ is the fluid velocity vector, then U can be represented by the column *vector*

$$U = \begin{bmatrix} \rho \\ \mathbf{m} \\ e \end{bmatrix}, \tag{63}$$

where $\mathbf{m} = \rho\mathbf{u}$ is the momentum vector per unit volume, and $e = \tilde{\epsilon} + \frac{1}{2}\rho\mathbf{u}\cdot\mathbf{u}$ is the total energy per unit volume. Let $\mathbf{n}$ be the unit normal vector in a positive direction to a cell surface in a finite-volume grid, or a coordinate surface in a finite-difference grid. If v_n is the normal component of the velocity of a time-varying surface, and $u_n = \mathbf{u}\cdot\mathbf{n}$, one can define the normal relative velocity component $u' = u_n - v_n$. The set of inviscid normal flux components F_n is given by the column *vector*

$$F_n = \begin{bmatrix} M \\ \mathbf{P} \\ E \end{bmatrix} = \begin{bmatrix} \rho u' \\ \mathbf{m}u' + p\mathbf{n} \\ eu' + pu_n \end{bmatrix}, \tag{64}$$

where M, $\mathbf{P}$, and E are the normal flux of mass, momentum, and energy.

The flux Jacobian requires expressing dF_n in terms of dU. For a fixed v_n and $\mathbf{n}$, the first component of dF_n can be written as

$$d(\rho u') = -v_n\, d\rho + \mathbf{n}\cdot d\mathbf{m}. \tag{65}$$

This can be rewritten in the form of a matrix multiplication as

$$d(\rho u') = \begin{bmatrix} -v_n & \mathbf{n} & 0 \end{bmatrix} \begin{bmatrix} d\rho \\ d\mathbf{m} \\ de \end{bmatrix}, \tag{66}$$

where the dot product is implied in multiplying the second element of the row *vector* by the second element of the column *vector*. Applying the same procedure to the other components of dF_n, one can define the flux Jacobian matrix operator A satisfying $dF_n = A\, dU$, using the convention that in forming the product of a matrix element with a *vector* element, a dot product is implied if each element is either a physical vector (e.g. $\mathbf{u}$ or $\mathbf{n}$) or a tensor (e.g. $\mathbf{un}$ or $\mathbf{nu}$). The matrix A can then be written as

$$A = \begin{bmatrix} -v_n & \mathbf{n} & 0 \\ K_1\mathbf{n} - u_n\mathbf{u} & \mathbf{un} - \kappa\mathbf{nu} + u'\mathbf{I} & \kappa\mathbf{n} \\ (K_1 - H)u_n & H\mathbf{n} - \kappa u_n\mathbf{u} & u' + \kappa u_n \end{bmatrix}, \tag{67}$$

where $K_1 = \frac{1}{2}\kappa\mathbf{u}\cdot\mathbf{u} + \chi$, $H = h + \frac{1}{2}\mathbf{u}\cdot\mathbf{u}$ is the total enthalpy per unit mass, and $\mathbf{I}$ is the identity tensor. The three eigenvalues of A are

$$\lambda_1 = u', \quad \lambda_2 = u' + c, \quad \text{and} \quad \lambda_3 = u' - c. \tag{68}$$

λ_1 is a repeated eigenvalue, requiring a set of linearly independent eigenvectors, which can be defined with full generality in term of an arbitrary set of spatial basis vectors $\mathbf{a}_i$, and a set of reciprocal basis vectors $\mathbf{a}^j$ satisfying $\mathbf{a}_i \cdot \mathbf{a}^j = \delta_i^j$, where δ_i^j is the Kronecker delta. One can then define $a_{ni} = \mathbf{n}\cdot\mathbf{a}_i$, $\mathbf{b}_i = \mathbf{n}\times\mathbf{a}_i$, $a_n^j = \mathbf{n}\cdot\mathbf{a}^j$, and $\mathbf{b}^j = \mathbf{n}\times\mathbf{a}^j$. If β is an arbitrary scalar, the right eigenvector matrix R can be written in the most general form as

$$R = \begin{bmatrix} a_{ni} & 1 & 1 \\ a_{ni}\mathbf{u} + \beta\mathbf{b}_i & \mathbf{u} + c\mathbf{n} & \mathbf{u} - c\mathbf{n} \\ a_{ni}K_2 + \beta\mathbf{b}_i\cdot\mathbf{u} & H + cu_n & H - cu_n \end{bmatrix}, \tag{69}$$

where $K_2 = \frac{1}{2}\mathbf{u}\cdot\mathbf{u} - \chi/\kappa$, while the left eigenvector matrix R^{-1} takes the form

$$R^{-1} = \begin{bmatrix} a_n^j\left(1 - K_1/c^2\right) - \mathbf{b}^j\cdot\mathbf{u}/\beta & a_n^j\kappa\mathbf{u}/c^2 + \mathbf{b}^j/\beta & -a_n^j\kappa/c^2 \\ \frac{1}{2}\left(K_1/c^2 - u_n/c\right) & -\frac{1}{2}\left(\kappa\mathbf{u}/c^2 - \mathbf{n}/c\right) & \frac{1}{2}\kappa/c^2 \\ \frac{1}{2}\left(K_1/c^2 + u_n/c\right) & -\frac{1}{2}\left(\kappa\mathbf{u}/c^2 + \mathbf{n}/c\right) & \frac{1}{2}\kappa/c^2 \end{bmatrix}. \tag{70}$$

Note that i and j take on values from 1 to 3, so that R has five columns and R^{-1} has five rows. A useful choice for the basis vectors is to let one of the $\mathbf{a}_i$ be parallel to $\mathbf{n}$, so that the corresponding $\mathbf{b}_i = 0$. The remaining $\mathbf{a}_i$ are then chosen to lie in the plane perpendicular to $\mathbf{n}$, so that their corresponding $a_{ni} = 0$.

Eq. (17) which defines a function of A is still valid, with P_1 given by

$$P_1 = \begin{bmatrix} 1 - K_1/c^2 & \kappa\mathbf{u}/c^2 & -\kappa/c^2 \\ u_n\mathbf{n} - K_1\mathbf{u}/c^2 & \kappa\mathbf{uu}/c^2 - \mathbf{nn} + \mathbf{I} & -\kappa\mathbf{u}/c^2 \\ u_n{}^2 - K_1H/c^2 & \kappa H\mathbf{u}/c^2 - u_n\mathbf{n} & 1 - \kappa H/c^2 \end{bmatrix}, \tag{71}$$

and the other two projection matrices given by

$$P_{\substack{2\\3}} = \frac{1}{2}[\pm A/c + I(1 \mp u'/c) - P_1]. \tag{72}$$

In the diagonal algorithms [2] one encounters the product of two eigenvector matrices, each of which is associated with a different surface. Let the surface with the unit normal vector $\mathbf{n}_k$ have associated with it the set of basis vectors $\mathbf{a}_{ik}$ with reciprocal basis vectors $\mathbf{a}^j_k$, and an arbitrary scalar β_k. One can then define $a_{nik} = \mathbf{n}_k \cdot \mathbf{a}_{ik}$, $\mathbf{b}_{ik} = \mathbf{n}_k \times \mathbf{a}_{ik}$, $a^j_{nk} = \mathbf{n}_k \cdot \mathbf{a}^j_k$, and $\mathbf{b}^j_k = \mathbf{n}_k \times \mathbf{a}^j_k$. Similarly, let the surface with the unit normal vector $\mathbf{n}_l$ have associated with it the set of basis vectors $\mathbf{a}_{il}$ with reciprocal basis vectors $\mathbf{a}^j_l$, and an arbitrary scalar β_l. One can then define $a_{nil} = \mathbf{n}_l \cdot \mathbf{a}_{il}$, $\mathbf{b}_{il} = \mathbf{n}_l \times \mathbf{a}_{il}$, $a^j_{nl} = \mathbf{n}_l \cdot \mathbf{a}^j_l$, and $\mathbf{b}^j_l = \mathbf{n}_l \times \mathbf{a}^j_l$. Then the five by five matrix $R_k^{-1} R_l$ can be written as

$$R_k^{-1} R_l = \begin{bmatrix} a_{nil} a^j_{nk} + \mathbf{b}_{il} \cdot \mathbf{b}^j_k \beta_l / \beta_k & c\mathbf{b}^j_k \cdot \mathbf{n}_l / \beta_k & -c\mathbf{b}^j_k \cdot \mathbf{n}_l / \beta_k \\ \frac{1}{2}\beta_l \mathbf{b}_{li} \cdot \mathbf{n}_k / c & \frac{1}{2}(1 + \mathbf{n}_k \cdot \mathbf{n}_l) & \frac{1}{2}(1 - \mathbf{n}_k \cdot \mathbf{n}_l) \\ -\frac{1}{2}\beta_l \mathbf{b}_{li} \cdot \mathbf{n}_k / c & \frac{1}{2}(1 - \mathbf{n}_k \cdot \mathbf{n}_l) & \frac{1}{2}(1 + \mathbf{n}_k \cdot \mathbf{n}_l) \end{bmatrix} . \tag{73}$$

From the form of (73) it follows that the matrix only depends on geometric factors if both β_k and β_l are chosen to be proportional to the sound speed c.

For a thermally perfect gas one can expand F_n as

$$F_n = \sum_{i=1}^{3} F_{ni}, \tag{74}$$

where the F_{ni} are given by

$$F_{n1} = \frac{\lambda_1 \rho (\gamma - 1)}{\gamma} \begin{bmatrix} 1 \\ \mathbf{u} \\ \frac{1}{2}\mathbf{u} \cdot \mathbf{u} + \epsilon - \frac{c^2}{\gamma(\gamma - 1)} \end{bmatrix}, \qquad F_{n{}^2_3} = \frac{\lambda_{{}^2_3} \rho}{2\gamma} \begin{bmatrix} 1 \\ \mathbf{u} \pm c\mathbf{n} \\ H \pm c u_n \end{bmatrix} . \tag{75}$$

The generalization of the Roe average for a surface separating U_L and U_R is obtained by substituting Eqs. (63), (64), (67), and (26) into $\Delta F_n = \overline{A} \Delta U$, with $\mathbf{n}$ and v_n fixed at the surface. In the momentum equation, $\overline{\mathbf{u}}$ must be some linear combination of the vectors $\mathbf{u}_L$, $\mathbf{u}_R$, and $\mathbf{n}$. Since these three vectors can vary independently, the dot products $\mathbf{u}_L \cdot \mathbf{u}_L$, $\mathbf{u}_L \cdot \mathbf{u}_R$, $\mathbf{u}_R \cdot \mathbf{u}_R$, $\mathbf{u}_L \cdot \mathbf{n}$, and $\mathbf{u}_R \cdot \mathbf{n}$ are also independent. In a manner similar to the one outlined for the one-dimensional case, one can easily show that

$$\overline{\mathbf{u}} = \alpha \mathbf{u}_L + (1 - \alpha) \mathbf{u}_R, \tag{76}$$

where α is still given by Eq. (30). Eqs. (32), (33), and (35) are still valid, with $\overline{h}$ given by

$$\overline{h} = \alpha h_L + (1 - \alpha) h_R + \frac{1}{2} \alpha (1 - \alpha) \Delta \mathbf{u} \cdot \Delta \mathbf{u}. \tag{77}$$

The previously derived expressions for $\overline{\chi}$ and $\overline{\kappa}$ remain unchanged. The expression for $R^{-1}\Delta U$ becomes

$$R^{-1}\Delta U = \begin{bmatrix} a_n^j(\Delta\rho - \Delta p/\overline{c}^2) + \overline{\rho}(\mathbf{b}^j \cdot \Delta\mathbf{u})/\beta \\ \frac{1}{2}(\Delta p/\overline{c}^2 + \overline{\rho}\mathbf{n} \cdot \Delta\mathbf{u}/\overline{c}) \\ \frac{1}{2}(\Delta p/\overline{c}^2 - \overline{\rho}\mathbf{n} \cdot \Delta\mathbf{u}/\overline{c}) \end{bmatrix}. \tag{78}$$

Conclusions

Inviscid flux Jacobian matrices and their properties which are useful in CFD techniques have been derived for an arbitrary, equilibrium gas. Both exact and approximate generalizations of the Roe average have been presented.

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