Application of Characteristic Boundary Conditions 홍 승규*, 이 광섭*

Abstract.

Characteristic boundary conditions are discussed in conjunction with a flux-difference splitting formulation as modified from Roe's linearization. Details of how one can implement the characteristic boundary conditions which are compatible with the discrete formulation at interior points are given for different types of boundaries including subsonic outflow and adiabatic wall. The latter conditions are demonstrated through computation of supersonic ogive-cylinder flow at high angle of attack and the computed wall pressure distribution is compared with experiment.

1. Introduction

Pioneering works on CFD developments, especially at NASA-Ames along the line of flux-vector splitting methods¹⁻⁵ elevated potential and usefulness of CFD codes both as a design tool for future airplanes and as detailed flow simulations for phenomenological study. The advances in CFD can be categorically summarized in the four areas of (i) transformation of the Navier-Stokes equations into generalized coordinate system. (ii) linearization of the governing equations and their discretizations with flux-splitting schemes. (iii) boundary condition applications and (iv) multiple block/grid approach for application to complex geometries. Lombard et al. 6-9 have also contributed their share in computing Navier-Stokes equations through elaborate approaches which enable one to switch among the primitive, conservative and characteristic variable vectors easily and to apply the characteristic boundary conditions naturally. Despite noble ideas and much achievements, there are still considerable differences in both discretization and integration methods among the leading CFD proponents; all for the sake of fast and robust simulations of compressible Navier-Stokes equations.

Having recognized this, an accurate and robust Navier-Stokes solver have been under development at ADD for engineering flow analysis and design through improvements in (i) flux-difference splitting formulations, (ii) algorithms for inverting three-dimensional (3-D) matrix equations, and (iii) boundary condition applications utilizing characteristics propagation. Present paper focuses on the last element from above and tries to illuminate the application procedure for characteristic boundary conditions.

First, a flux-difference splitting method as applied to compressible Navier-Stokes equations is described in Section 2, and details of how the characterictic boundary conditions are implemented are given in Section 3. Results of a test case are presented for a supersonic ogive-cylinder flow, followed by concluding remarks.

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2. Flux-Difference Splitting Method

Formulation for one-dimensional gasdynamics equations will be elaborated first to show its commutative nature among the conservative, primitive, and characteristic variable vectors.

One-dimensional gasdynamics equation written in conservative form reads:

$$\int_{-1}^{1} \frac{\partial q}{\partial t} + \frac{\partial F}{\partial E} = 0 \tag{1}$$

or in a difference form

$$\frac{\int_{-1}^{1} \delta q + \Delta_{\xi} F = 0}{2}$$

where the conservative variable vector q and the flux vector F are defined, respectively, as

$$\partial q = \begin{bmatrix} \partial \rho \\ \partial (\rho u) \\ \partial e \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + \rho \\ (e+p)u \end{bmatrix}$$
 (3)

J is the Jacobian of coordinate transformation from x to ξ , e is the total energy per unit volume, $\partial($) represents differential, and $\delta q = q^{n+1} - q^n$. Since Eq. (2) is nonlinear, it is rewritten in a linear form with primitive vector as

$$\frac{\int_{-1}^{1} \delta \tilde{q} + A \delta \tilde{q} = 0}{\Delta t}$$
 (4)

where \hat{q} is the primitive variable vector

$$\Delta \tilde{q} = \begin{bmatrix} \frac{\partial \rho}{\rho \partial u} \\ \frac{\partial \rho}{\partial p} \end{bmatrix} \tag{5}$$

and the primitive Jacobian matrix A is determined as

$$A = \begin{bmatrix} \overline{\hat{U}} & \overline{\xi}_x & 0 \\ 0 & \overline{\hat{U}} & (\gamma - 1) \overline{\xi}_x \\ 0 & \overline{\xi}_x \overline{\frac{\gamma P}{\rho}} & \overline{\hat{U}} \end{bmatrix}$$
 (6)

where $\overline{U} = \overline{\int_{-1}^{1} \xi_{x}} \, \overline{u} = \overline{\xi_{x}} \, \overline{u}$, $\overline{P} = \overline{p}/(\gamma - 1)$, with ξ_{x} representing the projection of cell volume $\int_{-1}^{1} \cot y - z$ plane for 3-D case. Overbar, $\overline{(\)}$, represents that the corresponding quantities are averaged over the interval, [j, j+1], and $\Delta q = q_{j+1} - q_{j}$.

Now, a transformation matrix M^{-1} is defined from

$$\Delta \tilde{q} = M^{-1} \Delta q \tag{7}$$

which is independent of metric coefficients of coordinate transformation. Then, Eqs. (4) and (7) are combined into a conservative form as

$$\frac{\int_{-\Delta t}^{1} M^{-1} \delta q + A M^{-1} \Delta q = 0$$
 (8)

or,
$$\frac{\int_{-1}^{1} \delta q + MAM^{-1} \Delta q = 0.$$
 (9)

It is known^{1,10} that (i) the Jacobian matrix A possesses an eigenvalue matrix determined from $|A-\lambda I|=0$, and (ii) A can be diagonalized by a square matrix T^{-1} via $T^{-1}AT=\Lambda$, where T^{-1} is also a transformation matrix between \tilde{q} and \tilde{q} and is consisted of left-eigenvectors of A, determined from⁸

$$T^{-1}A = \Lambda T^{-1}. {10}$$

It is noted that the choice of T^{-1} is not unique, since it satisfies the linear system of Eq. (10) with respect to T^{-1} . The characteristic variable vector \ddot{q} is now introduced in its difference form:

$$\Delta \hat{q} = T^{-1} \Delta \hat{q} = T^{-1} M^{-1} \Delta q. \tag{11}$$

The rows of characteristic variable vector $\Delta \hat{q}$ represents changes in the entropy, positive and negative running characteristic variables along the characteristic lines for one-dimensional flow. Changes in covariant velocities in tangential directions are added through second and third rows of T^{-1} for three-dimensional formulation.

Equation (9) can now be rearranged in a from

$$\frac{\int_{-1}^{1} \delta q + M T \Lambda T^{-1} M^{-1} \Delta q = 0 \qquad (12)$$

or,
$$\frac{\int_{-\Delta t}^{1} \delta q + \hat{A} \Delta q = 0.$$
 (13)

Equation (12) may be equivalently written as

$$\frac{\int_{-1}^{1} \delta q^{2} + \Lambda \Delta q^{2} = 0. \tag{14}$$

Thus, Eq. (14) provides the foundation of stable upwind difference method where either backward or forward difference is utilized based on the sign of eigenvalue components of Λ^{11} . When the same idea is applied to Eq. (13), a numerically stable system can be achieved:

$$\int_{-1}^{1} \frac{\partial q}{\partial t} + \tilde{A}^{+} \nabla q + \tilde{A}^{-} \Delta q = 0$$
 (15)

where

$$\mathcal{X} = \mathcal{A}^{+} + \mathcal{A}^{-}$$

$$= M T \Lambda^{+} T^{-1} M^{-1} + M T \Lambda^{-} T^{-1} M^{-1}$$
(16)

Comparing Eq. (13) with Eq. (2), one observes that

$$\Delta F = \widetilde{A} \, \Delta q \tag{17}$$

 \widehat{A} is thus another way of expressing Roe's property $U^{12,13}$. It may be pointed out that the splitting in Eq. (16) is not unique and that other splittings are possible which render the differenced system numerically stable. But the above splitting is consistent with the spirit of Eq. (14) and is proven to yield stable results.

The one-dimensional formulation described above can be extended to two- or three-dimensional space straightforwardly. The governing Navier-Stokes equations employed in the generalized coordinate system, (ξ, η, ϕ) , are expressed for the conservative variable vector as

$$\int_{-1}^{1} \frac{\partial q}{\partial t} + \xi_x \frac{\partial}{\partial \xi} (\hat{F} + \hat{F}_v) + \tilde{\eta}_x \frac{\partial}{\partial \eta} (\hat{G} + \hat{G}_v) + \tilde{\phi}_x \frac{\partial}{\partial \phi} (\hat{H} + \hat{H}_v) = 0 \quad (18)$$
where \hat{F} , \hat{G} , and \hat{H} are inviscid flux vectors, and \hat{F}_v , \hat{G}_v , and \hat{H}_v are viscous flux vectors. Also, $\xi_x = \xi_x \cdot f^{-1} = \xi_x / f$, etc. As before, the inviscid fluxes are linearized for upwind discretizations by

$$\Delta_{\varepsilon}F = \mathcal{A}\Delta q = (\mathcal{A}^+ + \mathcal{A}^-)\Delta q$$

and
$$\widehat{A}^{\pm} = M T \Lambda^{\pm} T^{-1} M^{-1}$$
, (19) yielding

$$\int_{-1}^{-1} \delta q + \widehat{A}^{+} \nabla_{\xi} q + \widehat{A}^{-} \Delta_{\xi} q + \widehat{B}^{+} \nabla_{\eta} q + \widehat{B}^{-} \Delta_{\eta} q
+ \widehat{C}^{+} \nabla_{\phi} q + \widehat{C}^{-} \Delta_{\phi} q + \text{(viscous terms)} = 0$$
(20)

Upwind flux-difference splitting for the inviscid fluxes and second-order central differencing for the viscous fluxes are applied for discretizations. Presently, solutions are updated from q^n to q^{n+1} via implicit approximate factorization in (η, ϕ) -plane and symmetric Gauss-Seidel relaxation for ξ -direction.

3. Characteristic Boundary Conditions

Choice of proper boundary conditions is crucial for fast convergence. In real flow applications, often times the boundary values are not fully available so that one may have to either extrapolate the flow variables or introduce some hypothetical assumptions. Characteristic boundary procedure is a way to provide the missing boundary information without having to specify the boundary value; for example, static pressure at the subsonic exit plane. Application of characteristic boundary procedure is based upon a realization that there are five characteristics associated with the convective part of the Navier-Stokes equations. The basic idea is that one retains the characteristic equation(s) which transport(s) information from interior domain to the boundary. The characteristic equations whose corresponding waves travel from outside of the computational domain to the boundary are replaced by suitable auxiliary equations which represent the physical nature of the incoming characteristics as best as possible. As shown earlier in Section 2, the Navier-Stokes equations, without the viscous fluxes, can be put into a characteristic form

$$\frac{\dot{f}}{At}\delta\dot{q} + \Lambda\Delta\dot{q} = 0 \tag{21}$$

which become at the boundary

$$\frac{f}{At}MTT^{-1}M^{-1}\delta q + MT\Lambda T^{-1}M^{-1}\Delta q = 0$$
 (22)

where $\Lambda = \Lambda^-$ on the left boundary and $\Lambda = \Lambda^+$ on the right.

Recall that $\Delta \tilde{q} = T^{-1}\Delta \tilde{q} = T^{-1}M^{-1}\Delta q$. Since $\Delta \tilde{q}$ being a primitive variable vector is already fixed by definition, it is sufficient to modify certain rows of T^{-1} if one wishes to change the pertinent row of characteristic variable \tilde{q} . For the interior points, the transformation matrix T^{-1} becomes

$$T^{-1} = \begin{bmatrix} -\frac{1}{\overline{\rho}} & 0 & 0 & 0 & \frac{1}{\gamma \overline{P}} \\ 0 & \overline{x_{\eta'}} & \overline{y_{\eta'}} & \overline{z_{\eta'}} & 0 \\ 0 & \overline{x_{\phi'}} & \overline{y_{\phi'}} & \overline{z_{\phi'}} & 0 \\ 0 & \frac{\overline{\xi_x}}{\overline{\rho} c_4} & \frac{\overline{\xi_y}}{\overline{\rho} c_4} & \frac{\overline{\xi_z}}{\overline{\rho} c_4} & \frac{1}{\gamma \overline{P}} \\ 0 & -\frac{\overline{\xi_x}}{\overline{\rho} c_5} & -\frac{\overline{\xi_y}}{\overline{\rho} c_5} & -\frac{\overline{\xi_z}}{\overline{\rho} c_5} & \frac{1}{\gamma \overline{P}} \end{bmatrix}$$

$$(23)$$

with $\overline{c}_4 \cong \overline{c}_5 \cong \overline{\xi} \cdot \overline{c}$

yielding

$$\Delta \tilde{q} = \begin{bmatrix}
-\frac{\Delta \rho}{\overline{\rho}} + \frac{\Delta P}{\gamma \overline{P}} \\
\overline{\rho} (\overline{x}_{\eta}' \Delta u + \overline{y}_{\eta}' \Delta v + \overline{z}_{\eta}' \Delta w) \\
\overline{\rho} (\overline{x}_{\phi}' \Delta u + \overline{y}_{\phi}' \Delta v + \overline{z}_{\phi}' \Delta w)
\end{bmatrix}$$

$$(\overline{\xi}_{x} \Delta u + \overline{\xi}_{y} \Delta v + \overline{\xi}_{z} \Delta w) / \overline{c_{4}} + \frac{\Delta P}{\gamma \overline{P}}$$

$$-(\overline{\xi}_{x} \Delta u + \overline{\xi}_{y} \Delta v + \overline{\xi}_{z} \Delta w) / \overline{c_{5}} + \frac{\Delta P}{\gamma \overline{P}}$$

representing, from the first row, the entropy change along the characteristic line associated with λ_1 , the tangential velocity difference in the η - and ϕ - directions at ξ =constant plane, and the right-running characteristics associated with $\lambda_4 \cong u+c$ for the fourth row of \hat{q} and the left-running characteristics whose corresponding eigenvalue $\lambda_5 \cong u-c$. The fourth and fifth characteristics are also known as P^+ - and P^- -compatibility equations, respectively. Application of characteristic boundary procedure is to replace certain row of T^{-1} such that the product of T^{-1} and $\Delta \hat{q}$ replace the original \hat{q} by other physical property that is suitable as boundary condition. A few examples are illustrated below.

3.1 Subsonic Outflow

At the outflow on the right boundary, the characteristics associated with $\lambda = u - c$ comes from outside to the right boundary; thus, we need to replace the 5th row of \hat{q} which is left-running characteristics. One way is to replace the δP^- -equation at the boundary with $\delta p = 0$, forcing the

pressure p to converge to a certain value as the iteration increases. The fifth characteristic equation

$$\frac{\int_{-1}^{1} \delta \widetilde{q}_{5}^{\infty} + \lambda_{5}^{-} \Delta \widetilde{q}_{5}^{\infty} = 0$$
 (25)

is displaced by
$$\frac{\int_{-\Delta t}^{1} \delta p + \lambda_{5}^{-} \Delta \delta p = -\lambda_{5}^{-} \Delta p \qquad (26)$$

The change of equation from Eq.(24) to Eq.(25) is achieved simply by the switch in the 5th row of T^{-1} in Eq. (23) by [0, 0, 0, 0, $\frac{1}{\gamma P}$] to replace the 5th δP^- -equation at the right boundary. It is noted that one needs not to specify the pressure value at the exit plane, but a stable value of p is reached as the iteration is increased. If one were to choose other variable, say the speed of sound c, than the pressure p, one may substitude the corresponding row of T^{-1} by $\left[-\frac{1}{a}, 0, 0, \frac{1}{b}\right]$ to enforce $\delta c = 0$.

3.2 Adiabatic Wall Condition

At the viscous, adiabatic wall, the five constraints are: i) zero normal temperature gradient, ii) three no-slip conditions for u, v, w and iii) retention of P^- or P^+ characteristic equation depending on whether it is left or right boundary. The adiabatic condition, $\Delta(\text{Temp}) = 0$, is enforced through the change of the first row of T^{-1} by $\left[-\frac{1}{a}, 0, 0, \frac{1}{B}\right]$, and the second and third rows of T^{-1} are kept but their corresponding eigenvalues are set to zero. The fourth row of T^{-1} is also retained if the wall boundary is on the left, but the fifth row is replaced by [0, $\overline{\hat{\xi}_x}$, $\overline{\hat{\xi}_y}$, $\overline{\hat{\xi}_z}$, 0] to warrant $\delta \overline{\widehat{W}_{\xi}} = 0$. All together, these conditions transpire the characteristic equations into a form which is still consistent with the current flux-difference formulation and its block-tridiagonal matrix equation; resulting at the wall boundary

$$\delta T = \mp \Delta T \qquad (T: \text{Temperature})$$

$$\delta(\overrightarrow{r_{\eta}} \cdot \overrightarrow{q}) = 0$$

$$\delta(\overrightarrow{r_{\phi}} \cdot \overrightarrow{q}) = 0$$

$$\delta(W_{\xi}) = 0$$

$$\delta P^{-} = -\Delta P^{-}$$
(27)

with $\vec{q} = (u, v, w)$.

Other boundaries such as subsonic inflow can also be treated similarly by i) finding a suitable candidate for \hat{q} and ii) substituting the correspong row of T^{-1} .

4. Results

An example case is run for a supersonic flow past an ogive-cylinder at Mach 2 with $\alpha = 20^{\circ 14}$. The computational grid in Fig. 1 consists of 55x55x37 for (ξ, η, ϕ) . The pressue contours in symmetry plane are shown in Fig. 2, exhibiting an obliqe shock on the windward side. The vortical flow pattern in the cross plane is clearly captured and shown in Fig. 3 in terms of velocity vectors and the pressure distribution in Fig. 4 is found to compare well with experiment. Overall no difficulties have been encountered in the process of convergence and the flow pattern seems to match physical nature of the flow.

Concluding Remarks

The characteristic boundary procedure is elaborated in relation to flux-difference splitting method. The current form of characteristic procedure may also be applied to other types of boundries including subsonic inflow and viscous wall with fixed temperature, among others. However, some uncertainty still remains in the choice of replacing candidate for the characteristic variable. For this one may pose a question: Is the pressure right variabe to substitude P^- in the case, for example, of subsonic outflow?

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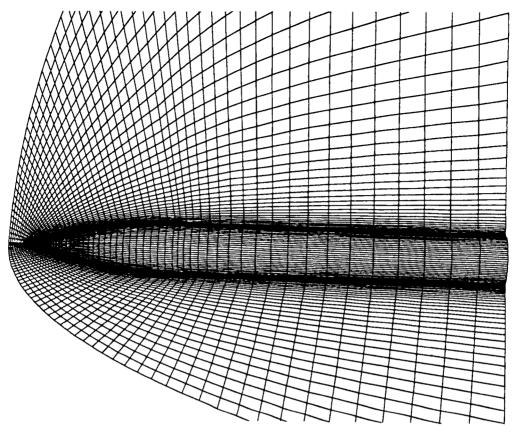


Fig. 1. Computational grid in symmetry plane.

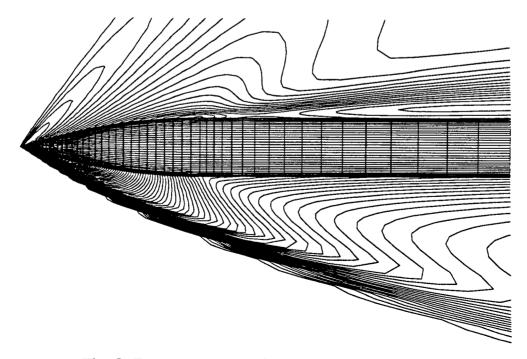


Fig. 2. Pressure contours in symmetry plane.

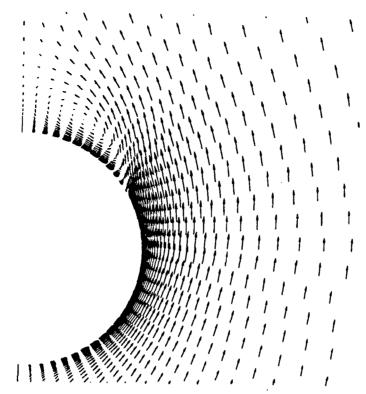


Fig. 3. Velocity vectors in a cross plane at J=45.

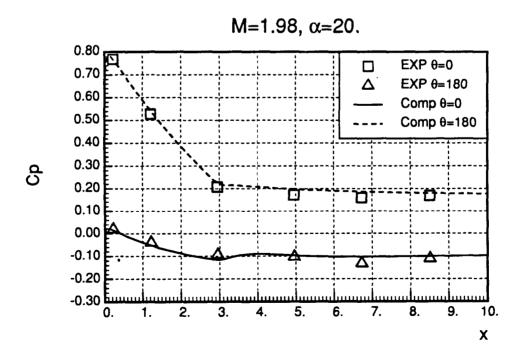


Fig. 4. Comparison of wall pressure distribution in windward and leeward symmetry plane.