# Boundary Conditions and Uniqueness in Internal Gas Dynamic Flows

ANTHONY A. GANZ* AND RAYMOND A. SERRA†
*Pratt & Whitney Aircraft, East Hartford, Conn.*

## Theme

THE importance of correct boundary conditions for establishing uniqueness in the numerical computation of internal gas dynamic flows is stressed. A procedure based on the general theory of Linear Symmetric Positive Systems is shown which generates proper boundary conditions. In particular, boundary conditions are developed for subsonic, transonic, and supersonic internal flows in steady-state and transient formulations.

## Contents

The theoretical analysis of the numerical solution of large equation systems in multidimensional internal gas dynamic flows has traditionally been restricted to the consideration of difference representations of derivatives, linear stability analysis, and solution algorithms. One area which has received little attention is the proper establishment of boundary conditions which insure the uniqueness of the computed result, i.e., the problem must not be either overspecified or underspecified with some "ad hoc uniqueness" ultimately arising from the solution algorithm selected. For example, the subsonic channel flow problem cannot be solved by specifying a priori all the inlet conditions; physically, the downstream properties must determine some of the upstream conditions. The correct selection of boundary conditions is more critical if the numerical procedure utilizes a difference scheme of higher order than the basic differential system. Furthermore, the situation is complicated when the equations change type (transonic flow) within the domain. Examples of this have arisen in the recent work of one of the authors[1] as well as in the work of others.[2,3] It is the purpose of this paper to show how the general theory of Linear Symmetric Positive Systems[4] can be applied as a practical method in engineering applications to generate various types and combinations of boundary data which insure uniqueness in gas dynamic flows.

The single issue of uniqueness for large systems of linear partial differential equations can be obtained by a generalization of the concept of "energy integrals" and is briefly summarized below. (Note that this summarizes in classical fashion only a small portion of Ref. 4). The general equation system in a bounded domain $R$ (with boundary $\partial R$) is

$$A_1 \frac{\partial U}{\partial x_1} + \cdots + A_m \frac{\partial U}{\partial x_m} + CU = 0 \tag{1}$$

where $A_i(x)$, $C(x)$ are matrices and $U$ is a vector of dependent variables. The system is symmetric positive when $A_i$ are symmetric, and $\kappa = 2C - (\partial A_1/\partial x_1) \cdots - (\partial A_m/\partial x_m)$ is positive in the sense $(U, \kappa U) \geqq 0$ where $(U, V) = u_1 v_1 + \cdots + u_J v_J$. Let $U$ be a solution of Eq. (1). On left multiplying by $U^T$ integrating throughout $R$ and using the $m$-dimensional divergence theorem, there is obtained

$$\int \cdots \int_{\partial R} (U, \beta U)\, dx_{m-1} + \int \cdots \int_R (U, \kappa U)\, dx = 0 \tag{2}$$

where $\beta$ is defined as $A_1 n_1 + \cdots + A_m n_m$ and $n_1, \ldots, n_m$ are components of the outward normal. This is written as

$$\int \cdots \int_{\partial R} (U, \mu U)\, dx_{m-1} + 2 \int \cdots \int_{\partial R} (U, \beta_- U)\, dx_{m-1} + \int \cdots \int_R (U, \kappa U)\, dx = 0 \tag{3}$$

where $\beta$ has been decomposed into two matrices $\beta_+, \beta_-$ at each boundary point such that $\beta = \beta_+ + \beta_-$ and the symmetric part of $\mu = \beta_+ - \beta_-$ is non-negative. If the components of $U$ are linearly constrained at each point of the boundary by the condition $\beta_- U = 0$, it follows from Eq. (3) that $U = 0$ everywhere in the interior since, as defined, $(U, \mu U)$ and $(U, \kappa U) \geqq 0$. Thus uniqueness is obtained when boundary conditions on $u_1, \ldots, u_J$ are selected such that $\beta_- U = 0$. Alternately uniqueness can be determined directly from Eq. (2) by selecting $l$ linear relations

$$\begin{aligned} L_1(u_1, \ldots, u_J) &= 0 \\ &\vdots \\ L_l(u_1, \ldots, u_J) &= 0 \end{aligned} \tag{4}$$

among $u_1, \ldots, u_J$ such that when substituted into the quadratic form $(U, \beta U)$ there results an expression which is zero or positive. This indirectly defines the split which results in the symmetric part of $\mu$ being positive. The relations (4) are equivalent to $\beta_- U = 0$ for establishing uniqueness.

The primary purpose of the paper is not to use Eq. (3) to prove uniqueness for a specific problem; rather the general equation is studied to find what types of boundary conditions are correct when the geometric contours have already been given. In most applications the technique for determining the decomposition of $\beta$ is neither straightforward nor unique, and constitutes the major obstacle to the direct use of Ref. 4.

One technique is to examine various factorizations of the quadratic form $(U, \beta U)$ which reduce the expression to a sum of squares of the $u_1, \ldots, u_J$. The squared expressions which have negative coefficients correspond exactly to Eqs. (4). An alternate guideline can be obtained by noting that $(U, \beta U)$ is positive when all eigenvalues are positive. Hence in the general case a positive form can be obtained by zeroing out the factors associated with negative eigenvalues. (The ideas and concepts underlying this matrix split can be rigorously expressed[5] in terms of projection operators and the spectral decomposition theorem.) The decomposition of $\beta$ is further complicated by the fact that, provided the remaining terms are positive, any number of linear relations may be set to zero assuring uniqueness. This may still overspecify the problem. For example, in the case of distinct nonzero eigenvalues, this occurs when the number of relations set to zero is greater than the number of negative eigenvalues—in general, existence of the solutions is lost in such cases. It is necessary to define a split which will yield a "smallest number" of linear relations, but still satisfies the general conditions. [The equivalent statement[6] is that the complement to the subspace

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* Research Engineer, Scientific Analysis Group. Associate Member AIAA

† Chief, Scientific Analysis Group. Member AIAA.

defined by Eqs. (4) should be "maximal."] If the given problem is not symmetric or positive, transformations to equivalent systems may often be found by left multiplying the system by a nonsingular matrix $Z$, or alternately enlarging the system by introducing a variety of identity relations with arbitrary multiplicative coefficients. Finally, the boundary conditions derived from the theory may not be those wanted on physical grounds, thus requiring the aforementioned transformations.

Although the gas dynamic equations are quasi-linear, it is proposed to use the abovementioned linear theory to generate boundary conditions for these equations under an appropriate linearization. Provided that the linear equation type models the global behavior of the nonlinear problem, experience has shown that the derived boundary conditions provide a valuable and useful guide for the full quasi-linear problem. In practical applications, moreover, it has been found that a linearization about a constant local state usually carries all the pertinent information.

The question of proper boundary conditions for steady internal gas dynamic flows has only been answered theoretically for some simple classical forms. For complex systems with transonic flow, it is not a priori evident how many inflow and outflow properties are required to pose a consistent problem. For illustration, boundary conditions for a specific 2-D mixed flow (choked) nozzle are developed below. In this, an axial Mach number distribution is assumed for the zero order solution about which the linearization is taken. The analysis shows clearly how the downstream boundary condition can be set in subsonic flow, "disappears" in transonic flow, and "reappears" as an upstream boundary condition in supersonic flow. This loss of a boundary condition in the transonic flow problem is emphasized for application in numerical solutions.

The nozzle contour is taken as $y_c = \pm\frac{4}{3}(1+\frac{3}{8}x^2)$. On linearizing the 2-D isentropic, potential flow equation about the 1-D Mach number distribution $M_0 = 1+\frac{3}{4}x$, there is obtained

$$\begin{bmatrix} \frac{3}{2}x & 0 \\ 0 & 1 \end{bmatrix}\frac{\partial U}{\partial x} + \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}\frac{\partial U}{\partial y} + \begin{bmatrix} \frac{3}{2}(1+\frac{1}{2}x) & 0 \\ 0 & 0 \end{bmatrix} U = 0 \tag{5}$$

where $U$ is the vector of velocity components. The abovementioned coefficient matrices are denoted by $A$, $B$, and $C$, respectively. This is a mixed flow problem, with the sonic line fixed by the linearity of the equation. Applying the theory directly, does not yield the side boundary condition $u \cdot n = 0$ correctly. To provide a more general system, Eq. (5) is left multiplied by

$$Z = \begin{bmatrix} a(x,y) & \frac{3}{2}xc(x,y) \\ c(x,y) & a(x,y) \end{bmatrix} \quad a, c \text{ arbitrary} \tag{6}$$

which is the most general combination which results in a symmetric system. The resulting equation is

$$ZA\,\partial U/\partial x + ZB\,\partial U/\partial y + ZCU = 0 \tag{7}$$

The functions $a$, $c$ are selected such that $Z$ is nonsingular, $\kappa$ is positive, and physically meaningful boundary conditions are obtained. One choice is $a = 1-10x$, $c = -y$ with the domain restricted to $-0.05 \leqq x \leqq 0.05$. This particular choice restricts the solution region to a narrow strip about the sonic line, but is retained for the simplicity of illustration. A more general definition of $a$, $c$ with subsequent recalculation of $\beta_+$, $\beta_-$ yields extensions to larger or more general domains.

From Eq. (7), the matrix $\beta$ is now given by $2ZC-(\partial/\partial x)ZA-(\partial/\partial y)ZB$. The proper outflow boundary conditions are obtained from $\beta$ evaluated at $x = 0.05$ with $n_x = 1.0$, $n_y = 0$. On this boundary the flow is supersonic. The matrix has two distinct positive eigenvalues, which shows that $(U, \beta U)_{\text{out}} \geqq 0$ for all $u, v$. Hence *no* boundary condition is to be applied. Similarly, the inflow boundary conditions are found with $\beta$ evaluated at $x = -0.05$, $n_x = -1.0$, $n_y = 0$. The flow here is subsonic. The matrix has one positive and one negative eigenvalue which shows that one linear combination of $u, v$ must be set to zero for positivity. Similar calculations can be shown for the purely subsonic and supersonic problems. The matrix decompositions corresponding to these boundaries as well as the side boundaries are algebraically complicated and are shown in Ref. 5. These uniqueness proofs developed rigorously, can be reinterpreted in terms of practical data specification for specific problems: a) if the inflow boundary is supersonic, both $u, v$ must be specified, whereas only a single combination of them can be specified for subsonic inflow, and b) if the exit flow boundary is supersonic, both $u, v$ must be left unspecified, while only one linear combination is to be specified if the boundary is subsonic.

Similar results can be obtained for transient flow problems. The equations, say, are written with $\rho$, $u$, $v$ as dependent variables. The system is linearized about an approximate solution $u_0$, $v_0$, $\rho_0$ and is then transformed into a positive system by defining a new vector of dependent variables $V = e^{-\lambda t}U$, where $\lambda$ is a large positive number. On the outflow boundary the quadratic form becomes

$$(V, \beta V) = \frac{M_0\rho_0}{a_0}\left(u + \frac{u_0}{\rho_0 {M_0}^2}\rho\right)^2 + \frac{M_0\rho_0}{a_0}\left(v + \frac{v_0}{\rho_0 {M_0}^2}\rho\right)^2 + \frac{a_0}{M_0\rho_0}({M_0}^2-1)\rho^2 \tag{8}$$

From this it is evident that $(V, \beta V)$ is positive for all $\rho$, $u$, $v$ if the exit flow is supersonic. If it is subsonic, the last term becomes negative and must be set to zero, i.e., the downstream density (equivalently pressure) must be specified. The situation is reversed on the inflow boundary, where $\rho$, $u$, $v$ must be specified if the flow is supersonic, but two linear combinations of them must be specified if subsonic.

In conclusion, we have shown the application of a technique to establish boundary conditions for systems of equations in gas-dynamics. It is emphasized, that when giving data on subsonic boundaries only some of the dependent variables can be set. The remaining variables on the boundary must be determined from the solution itself—the problem is overspecified, and in general does not exist, when more data than this is given. Particularly, note that in the case of transonic flow, there is less boundary data specified in total than either the wholly subsonic or wholly supersonic problem. For larger equation systems, the over-all considerations are similar. The theory also can be extended in its entirety to finite-difference formulations where, for example, $\int\cdots\int_R (U, \kappa U)\,dx$ is replaced by a sum of quadratic forms over the nodes of the grid.

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