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Time-Dependent Boundary Conditions for Hyperbolic Systems, II

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A previous paper introduced the concept of nonreflecting boundary conditions for hyperbolic equations in more than one dimension. This paper develops a general boundary condition formalism for all types of boundary conditions to which hyperbolic systems are subject (including the nonreflecting conditions). The formalism is described in detail, and many examples are provided for common problems in hydrodynamics, including solid wall and nonreflecting boundaries.

1. INTRODUCTION

This paper presents a unified formalism for the treatment of boundary conditions for systems of hyperbolic equations. This treatment is intended to encompass all possible boundary conditions for first-order hyperbolic systems in any number of dimensions. A general theory of boundary conditions is given first, which is then followed by a more detailed exposition for common problems in computational fluid dynamics.

This paper differs from earlier work in that it attempts to unify all types of physically reasonable boundary conditions into a single formalism. The resulting formalism makes possible a "cookbook" approach to boundary conditions, in which new boundary "recipes" may be derived from the formalism, and old ones are simply looked up as needed. The latter portion of this paper (Section 3.2) begins a compendium of boundary conditions for problems in fluid dynamics.

The central concept of this paper is that hyperbolic systems of equations represent the propagation of waves and that at any boundary some of the waves are propagating into the computational volume while others are propagating out of it. The outward propagating waves have their behavior defined entirely by the solution at and within the boundary, and no boundary conditions can be specified for them. The inward propagating waves depend on the solution exterior to the model volume and therefore require boundary conditions to complete the specification of their behavior. This paper describes how to decompose hyperbolic equations into

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wave modes of definite velocity and then how to specify boundary conditions for those modes which require them.

The paper begins with theory and ends with practice. Section 2 looks at the problem of boundary conditions for general hyperbolic systems. Section 3 represents several common boundary conditions for fluid dynamics problems. Finally, Section 4 describes the complete numerical solution of the fluid equations with boundary conditions.

2. Initial Boundary Value Problems for Hyperbolic Systems

Let $\mathbf{U}(\mathbf{x}, t)$ be a vector of m components U_i, each of which is a time varying field defined in a finite n dimensional volume $\mathcal{V}$. The general behavior of $\mathbf{U}$ is described by a hyperbolic set of m first-order differential equations in the n spatial coordinates x_k and time t. The time dependent solution for $\mathbf{U}$ is completely determined by (i) the governing differential equations; (ii) the initial values for $\mathbf{U}$ in $\mathcal{V}$; and (iii) the time dependent boundary conditions on the boundary of $\mathcal{V}$.

Some ambiguity exists as to what exactly constitutes a boundary condition. This paper presents the following conceptual model: a boundary condition consists of a single mathematical expression of information which (i) is external to the calculation, i.e., cannot be obtained solely from knowledge of $\mathbf{U}$ within $\mathcal{V}$; and (ii) contributes to, but does not by itself define, the values of $\partial\mathbf{U}/\partial t$ along the boundary. In other words, the boundary conditions contain whatever information is needed to completely specify $\partial\mathbf{U}/\partial t$, and which cannot be obtained from information within $\mathcal{V}$.

It is important to separate the concept of boundary conditions from that of the boundary treatment. The boundary treatment is the complete algorithm for determining the values of $\partial\mathbf{U}/\partial t$ along the boundary of $\mathcal{V}$, and incorporates information from within $\mathcal{V}$ as well as the boundary conditions. One must have a boundary treatment at all boundaries of the computational domain when obtaining a solution for $\mathbf{U}$ within $\mathcal{V}$. However, in the case of hyperbolic equations, the number of boundary conditions required at a given point on the boundary ranges from 0 to m and may vary with time and position as the solution evolves (e.g., an initially subsonic and outward-directed flow may become supersonic at some later time, reducing the number of boundary conditions from one to zero).

Another important point is that at any time t the boundary conditions contribute only to the determination of $\partial\mathbf{U}/\partial t$ at the boundary, and never define $\mathbf{U}$ itself. For example, a boundary treatment which explicitly sets the normal velocity of a fluid to zero at a wall boundary is not allowed in this model. Instead one would set the normal velocity to zero in the initial data and then specify boundary conditions which would force the time derivative of the normal velocity to be zero at all times. One advantage of this approach is that it decouples the boundary treatment from the time integration of the differential equations, so that the integration may be performed without reference to any special behavior at the boundaries.

2.1. *Conservation Laws*

The analysis performed here follows that of references [1, 2]. The starting point is a first-order hyperbolic system of m equations in m unknowns, in a space of n dimensions. The case where $n = 3$ is considered below.

The unknowns we wish to solve for comprise a solution vector of m components. It is usually the case that the choice of unknown variables is not unique; for example, in fluid dynamics we might choose the conservative variables (denoted by $\tilde{\mathbf{U}}$) or the primitive variables (denoted by $\mathbf{U}$), as in Section 3. While the definition of conservative variables is unique (e.g., momentum is conserved, while velocity is not), the primitive variables are selected for convenience, as many formulations are possible.

The choice of conservative variables is often made to preserve exactly the conservation properties of the system in the interior of $\mathscr{V}$. However, the boundary condition analysis is greatly simplified when the primitive variables are used, so I will begin with the conservative variables and describe the transformation which connects the two representations. The reader who is interested only in the primitive forms may skip the initial and final steps of this analysis, which describe the transformation from conservative variables to primitive variables and back.

Let $\tilde{\mathbf{U}}$ be the vector of m conserved quantities $\tilde{U}_i$, which obey the equation

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} + \frac{\partial \mathbf{F}^1}{\partial x_1} + \frac{\partial \mathbf{F}^2}{\partial x_2} + \frac{\partial \mathbf{F}^3}{\partial x_3} + \tilde{\mathbf{D}} = 0, \tag{1}$$

where $\mathbf{F}^k$ is the vector of fluxes in the kth coordinate direction and $\tilde{\mathbf{D}}$ is a vector of inhomogeneous terms which do not involve derivatives of any of the components of $\mathbf{U}$.[1]

Other equations may be required to close the system, such as algebraic relations between the variables (including equations of state), constraint equations (such as $\nabla \cdot \mathbf{B} = 0$ in magnetohydrodynamics [5]), or other differential equations (such as $\nabla^2 \Phi = 4\pi G\rho$ for the gravitational potential in self gravitating systems). However, such auxiliary equations do not alter the boundary condition analysis, although they are required by the solution process as a whole.

2.2. *Characteristic Analysis*

The conservation laws of the previous section may be converted to an equivalent set of wave equations, which represent nonlinear waves propagating at charac-

[1] For example, $\mathbf{D}$ may contain source terms, such as heating, cooling, or gravitational forces; or it may contain inhomogeneous terms from the breakup of divergence terms, such as

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \rho u_r) \to \frac{\partial}{\partial r}(\rho u_r) + \frac{2}{r}\rho u_r,$$

which is required by the form of Eq. (1) at the boundaries.

teristic velocities, which in turn are functions of the local solution and generally vary in space and time. These characteristic velocities are given as the solutions to an eigenvalue problem below.

The equations of one-dimensional fluid dynamics may be put into a characteristic form in which the waves propagate in a single well-defined direction because only one direction is available. However, no unique direction of propagation exists in multidimensional problems [3, 4], because the coefficient matrices involved are not simultaneously diagonalizable. Fortunately, the boundary condition analysis only requires that any one coordinate direction be diagonalizable at a time, and this may always be done.

Let the vector of primitive solution variables be $\mathbf{U}$, and let the conservative vector $\tilde{\mathbf{U}}$ depend only on fields which are contained in $\mathbf{U}$ (for example, the definition of total energy density should not depend on the gravitational potential; this requirement simplifies the analysis, as shown below for the equations of fluid dynamics.) Then we may write [1]

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} = \mathbf{P} \frac{\partial \mathbf{U}}{\partial t}, \tag{2}$$

where $\mathbf{P}$ is a Jacobian matrix of elements

$$p_{ij} \equiv \frac{\partial \tilde{U}_i}{\partial U_j}. \tag{3}$$

Similarly, we may write

$$\frac{\partial \mathbf{F}^k}{\partial x_k} = \mathbf{Q}^k \frac{\partial \mathbf{U}}{\partial x_k}, \qquad k = 1, 2, 3, \tag{4}$$

where the matrix $\mathbf{Q}^k$ has elements

$$q_{ij}^k \equiv \frac{\partial F_i^k}{\partial U_j}. \tag{5}$$

Consider now the characteristic analysis for the x_1 direction. (The other directions are similar). All terms not involving x_1 derivatives of U_i are carried along passively and do not contribute in any substantive fashion to the analysis; therefore we may lump them together and write

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} + \frac{\partial \mathbf{F}^1}{\partial x_1} + \tilde{\mathbf{C}} = 0, \qquad \tilde{\mathbf{C}} = \frac{\partial \mathbf{F}^2}{\partial x_2} + \frac{\partial \mathbf{F}^3}{\partial x_3} + \tilde{\mathbf{D}}. \tag{6}$$

Transform Eq. (6) into primitive form by multiplying it by $\mathbf{P}^{-1}$ and using (4), which gives

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}^1 \frac{\partial \mathbf{U}}{\partial x_1} + \mathbf{A}^2 \frac{\partial \mathbf{U}}{\partial x_2} + \mathbf{A}^3 \frac{\partial \mathbf{U}}{\partial x_3} + \mathbf{D} = 0, \tag{7}$$

or

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}^1 \frac{\partial \mathbf{U}}{\partial x_1} + \mathbf{C} = 0, \qquad \mathbf{C} = \mathbf{A}^2 \frac{\partial \mathbf{U}}{\partial x_2} + \mathbf{A}^3 \frac{\partial \mathbf{U}}{\partial x_3} + \mathbf{D}, \tag{8}$$

where

$$\mathbf{A}^k \equiv \mathbf{P}^{-1}\mathbf{Q}^k, \qquad \mathbf{C} \equiv \mathbf{P}^{-1}\tilde{\mathbf{C}}, \qquad \mathbf{D} \equiv \mathbf{P}^{-1}\tilde{\mathbf{D}}. \tag{9}$$

The m left and right eigenvectors of $\mathbf{A}^1$ will be taken as $\boldsymbol{l}_i$ and $\mathbf{r}_i$, and satisfy

$$\boldsymbol{l}_i^{\mathrm{T}}\mathbf{A}^1 = \lambda_i \boldsymbol{l}_i^{\mathrm{T}}, \qquad \mathbf{A}^1\mathbf{r}_i = \lambda_i \mathbf{r}_i, \qquad i = 1, ..., m, \tag{10}$$

where the eigenvalues λ_i are given by

$$\det(\mathbf{A}^1 - \lambda \mathbf{I}) = 0, \tag{11}$$

and where the left and right eigenvectors are mutually orthogonal:

$$\boldsymbol{l}_i^{\mathrm{T}} \cdot \mathbf{r}_j = \delta_{ij}. \tag{12}$$

The eigenvalues are real and are ordered so that $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_m$. (A system of equations of the form of (7) is defined to be hyperbolic if the eigenvalues of the coefficient matrices $\mathbf{A}^k$ are real.)

A diagonalizing similarity transformation may be generated for $\mathbf{A}^1$ by forming the matrix $\mathbf{S}$ such that its columns are the right eigenvectors $\mathbf{r}_j$, and its inverse $\mathbf{S}^{-1}$, whose rows are the left eigenvectors $\boldsymbol{l}_i^{\mathrm{T}}$. The similarity transformation is then

$$\mathbf{S}^{-1}\mathbf{A}^1\mathbf{S} = \boldsymbol{\Lambda}, \tag{13}$$

where $\boldsymbol{\Lambda}$ is the diagonal matrix of eigenvalues: $\Lambda_{ij} = 0$ for $i \neq j$, $\Lambda_{ij} = \lambda_i$ for $i = j$. Applying this transformation to Eq. (8) gives

$$\mathbf{S}^{-1}\frac{\partial \mathbf{U}}{\partial t} + \boldsymbol{\Lambda}\mathbf{S}^{-1}\frac{\partial \mathbf{U}}{\partial x_1} + \mathbf{S}^{-1}\mathbf{C} = 0, \tag{14}$$

whose m components are

$$\boldsymbol{l}_i^{\mathrm{T}}\frac{\partial \mathbf{U}}{\partial t} + \lambda_i \boldsymbol{l}_i^{\mathrm{T}}\frac{\partial \mathbf{U}}{\partial x_1} + \boldsymbol{l}_i^{\mathrm{T}}\mathbf{C} = 0, \qquad i = 1, ..., m. \tag{15}$$

The boundary condition analysis is made more convenient if we define a vector $\mathscr{L}$ of components $\mathscr{L}_i$ as

$$\mathscr{L}_i \equiv \lambda_i \boldsymbol{l}_i^{\mathrm{T}}\frac{\partial \mathbf{U}}{\partial x_1}. \tag{16}$$

Thus Eq. (14) may be written

$$\mathbf{S}^{-1}\frac{\partial \mathbf{U}}{\partial t}+\mathscr{L}+\mathbf{S}^{-1}\mathbf{C}=0, \tag{17}$$

or, in component form, as

$$\boldsymbol{l}_i^{\mathrm{T}}\frac{\partial \mathbf{U}}{\partial t}+\mathscr{L}_i+\boldsymbol{l}_i^{\mathrm{T}}\mathbf{C}=0, \qquad \mathbf{i}=1, \ldots, m. \tag{18}$$

The purpose of this analysis is to rewrite the original system of Eqs. (1) in a form which contains the quantities $\mathscr{L}_i$, as it is these quantities which we will use to specify boundary conditions. Equations (17) and (18) are the starting point for the boundary treatment.

2.3. *Boundary Treatment*

As in the previous papers [1, 5], the problem of implementing boundary conditions is reduced to the problem of computing the appropriate values for the $\mathscr{L}_i$ terms introduced above. The techniques for determining the $\mathscr{L}_i$ terms are shown below, but first we will consider what to do with these terms once they are known.

Given the values for $\mathscr{L}_i$, multiply Eq. (17) by $\mathbf{S}$ (i.e., solve for $\partial\mathbf{U}/\partial t$ in Eq. (17), either analytically or with a suitable numerical method), giving

$$\frac{\partial \mathbf{U}}{\partial t}+\mathbf{S}\mathscr{L}+\mathbf{C}=0. \tag{19}$$

If only the primitive time derivatives are required, then we simply put (8) for the definition of $\mathbf{C}$ back into (19) and we are done, as $\partial\mathbf{U}/\partial t$ is now completely defined. If, on the other hand, we want the conservative derivatives, then we multiply Eq. (19) by $\mathbf{P}$ to obtain

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t}+\mathbf{P}\mathbf{S}\mathscr{L}+\frac{\partial \mathbf{F}^2}{\partial x_2}+\frac{\partial \mathbf{F}^3}{\partial x_3}+\tilde{\mathbf{D}}=0 \tag{20}$$

at the x_1 boundaries.

The only terms which contain spatial derivatives in a direction normal to the boundary occur in the $\mathscr{L}$ terms, where they are taken care of by the boundary conditions described below. The remaining terms in (20) involve derivatives in directions transverse to the boundary and may be evaluated just as in the interior of $\mathscr{V}$. (The same is true for the corresponding terms in the primitive equation in (19).)

2.3.1. *Practical Solution for* $\partial \mathbf{U}/\partial t$

The boundary conditions described below define the values of $\mathscr{L}$. However, in order to solve for $\partial \mathbf{U}/\partial t$ in Eq. (19) we require the product $\mathbf{d} \equiv \mathbf{S}\mathscr{L}$, although we are given $\mathbf{S}^{-1}$ and $\mathscr{L}$. Thus we need to solve the system of equations

$$\mathbf{S}^{-1}\mathbf{d} = \mathscr{L} \tag{21}$$

for $\mathbf{d}$. Problems in fluid dynamics normally involve simple enough matrices that Eq. (21) can easily be solved by hand. More complicated problems, such as in magnetohydrodynamics (MHD), are too difficult for (21) to be solved analytically, and require numerical solutions.

2.4. *Boundary Conditions*

The purpose of boundary conditions is to supply whatever information is needed at the boundaries of the computational volume in order to complete the definition of the behavior of the system. The number of boundary conditions which may be imposed depends on the physics of the problem and may not be specified arbitrarily. This sometimes frustrating fact is a consequence of the wave nature of hyperbolic equations. Detailed discussions of this property are given in [2], [1], and [3]. This paper simply states the appropriate rules.

Each eigenvalue λ_i obtained above represents the characteristic velocity at which a particular wave mode propagates (such as advection waves, sound waves, and Alfvén waves). At a point on (say) the x_1 boundary, some number of the characteristic velocities describe outgoing waves, while some of them describe incoming waves. The behaviour of the outgoing waves is completely determined by data contained within and on the boundary of $\mathscr{V}$, while the behavior of the incoming waves is specified by data external to and on the boundary of $\mathscr{V}$. *The number of boundary conditions which must be specified at a point on the boundary is equal to the number of incoming waves at that point.* We specify boundary conditions which determine the values of $\mathscr{L}_i$ for incoming waves, and compute from definition (16) the values of $\mathscr{L}_i$ for outgoing waves.

Let the volume $\mathscr{V}$ be defined by $a_i \leqslant x_i \leqslant b_i$. Then at all points with coordinates (a_1, x_2, x_3), compute $\mathscr{L}_i$ from definition (16) for all cases where $\lambda_i < 0$ and specify from the boundary conditions the values of those $\mathscr{L}_i$ for which $\lambda_i > 0$. Similarly, at all points with coordinates (b_1, x_2, x_3), compute $\mathscr{L}_i$ from definition (16) for all cases where $\lambda_i > 0$, and specify from the boundary conditions the values of those $\mathscr{L}_i$ for which $\lambda_i < 0$. Note that the determination of $\mathscr{L}_i$ from (16) will require one-sided derivative approximations.

If the problem under study is sufficiently complicated, the number of boundary conditions required at any point on the x_1 boundary may change with time, and the number required at any time may vary with position on the boundary. Thus a boundary treatment may have to respond to spatial and temporal changes in the solution and adjust the number and type of boundary conditions as appropriate.

Some problems, however, are sufficiently simple that one set of boundary conditions may be specified for all time. (The flow of a fluid next to a solid wall is such a case.)

While the number of boundary conditions required is rigidly governed by the interior solution, the type of each condition is not. The researcher has considerable freedom to impose physically appropriate boundary conditions. The following sections provide several examples of useful boundary conditions for common problems in fluid dynamics.

3. Fluid Dynamics

The choice of conservative versus nonconservative forms of the fluid equations depends on the problem to be solved. I will not discuss the relative merits of the two approaches here, but will describe how to construct boundary conditions for either case. The definitions of the $\mathscr{L}_i$ are independent of the choice of approach; the choice of approach determines what to do with the $\mathscr{L}_i$ once they are computed.

3.1. *Conservative Equations*

The fluid dynamics equations, in conservative form and rectangular coordinates, are

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_1}(\rho u_1)+\frac{\partial}{\partial x_2}(\rho u_2)+\frac{\partial}{\partial x_3}(\rho u_3)=0, \quad (22)$$

$$\frac{\partial e}{\partial t}+\frac{\partial}{\partial x_1}[(e+p)u_1]+\frac{\partial}{\partial x_2}[(e+p)u_2]+\frac{\partial}{\partial x_3}[(e+p)u_3]-\rho\sum_{k=1}^{3}u_k g_k=0, \quad (23)$$

$$\frac{\partial m_1}{\partial t}+\frac{\partial}{\partial x_1}(m_1 u_1)+\frac{\partial}{\partial x_2}(m_1 u_2)+\frac{\partial}{\partial x_3}(m_1 u_3)+\frac{\partial p}{\partial x_1}-\rho g_1=0, \quad (24)$$

$$\frac{\partial m_2}{\partial t}+\frac{\partial}{\partial x_1}(m_2 u_1)+\frac{\partial}{\partial x_2}(m_2 u_2)+\frac{\partial}{\partial x_3}(m_2 u_3)+\frac{\partial p}{\partial x_2}-\rho g_2=0, \quad (25)$$

$$\frac{\partial m_3}{\partial t}+\frac{\partial}{\partial x_1}(m_3 u_1)+\frac{\partial}{\partial x_2}(m_3 u_2)+\frac{\partial}{\partial x_3}(m_3 u_3)+\frac{\partial p}{\partial x_3}-\rho g_3=0, \quad (26)$$

where

$$e\equiv\frac{1}{2}\rho\sum_{k=1}^{3}u_k^2+\varepsilon, \quad (27)$$

$$p\equiv(\gamma-1)\varepsilon, \quad (28)$$

$$m_k\equiv\rho u_k, \quad (29)$$

$$g_k\equiv-\frac{\partial \Phi}{\partial x_k}, \quad (30)$$

and where ρ is the mass density, p is the thermodynamic pressure, ε is the thermal energy density, γ is the (assumed constant) ratio of specific heats, m_k is the x_k direction momentum density, e is the total energy density (kinetic + thermal), Φ is the gravitational potential field, and g_k is the gravitational acceleration. For many problems Φ and g_k are specified functions of position, usually time independent. For problems involving self-gravitating fluids, Φ is obtained by solving Poisson's equation:

$$\nabla^2 \Phi = 4\pi G\rho, \tag{31}$$

where G is the gravitational constant.

The inclusion of gravitational fields introduces some ambiguity in the definition of the total energy density, depending on whether one includes the gravitational potential energy term $\rho\Phi$ in the definition of e in (27). The gravitational potential is omitted from the total energy for the following reasons:

1. Adding $\rho\Phi$ to (27) requires putting $\rho\, \partial\Phi/\partial t$ on the right side of Eq. (23), which is difficult to evaluate for time varying gravitational fields.

2. The inclusion of a spatially varying field (Φ) in the definition of the conservative variable vector $\tilde{\mathbf{U}}$ (in the e component), when that field does not appear as a component of the primitive vector $\mathbf{U}$, invalidates Eqs. (2) and (4). We would have to replace these equations by

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} = \mathbf{P}\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \tilde{\mathbf{U}}}{\partial \Phi}\frac{\partial \Phi}{\partial t}, \tag{32}$$

and

$$\frac{\partial \mathbf{F}^k}{\partial x_k} = \mathbf{Q}^k \frac{\partial \mathbf{U}}{\partial x_k} + \frac{\partial \mathbf{F}^k}{\partial \Phi}\frac{\partial \Phi}{\partial x_k}, \qquad k = 1, 2, 3. \tag{33}$$

While this substitution can be made, it seems more trouble than it is worth and will not be done here.

The fluid equations given here are in the conservative form of (1), with

$$\tilde{\mathbf{U}} \equiv \begin{pmatrix} \rho \\ e \\ m_1 \\ m_2 \\ m_3 \end{pmatrix}, \qquad \mathbf{F}^1 \equiv \begin{pmatrix} \rho u_1 \\ (e+p)\,u_1 \\ m_1 u_1 + p \\ m_1 u_2 \\ m_1 u_3 \end{pmatrix}, \qquad \mathbf{F}^2 \equiv \begin{pmatrix} \rho u_2 \\ (e+p)\,u_2 \\ m_2 u_1 \\ m_2 u_2 + p \\ m_2 u_3 \end{pmatrix}, \tag{34}$$

$$\mathbf{F}^3 \equiv \begin{pmatrix} \rho u_3 \\ (e+p)\,u_3 \\ m_3 u_1 \\ m_3 u_2 \\ m_3 u_3 + p \end{pmatrix}, \qquad \tilde{\mathbf{D}} \equiv \begin{pmatrix} 0 \\ -\rho \sum_{k=1}^{3} u_k g_k \\ -\rho g_1 \\ -\rho g_2 \\ -\rho g_3 \end{pmatrix}.$$

Define the primitive vector $\mathbf{U}$ as

$$\mathbf{U} \equiv \begin{pmatrix} \rho \\ p \\ u_1 \\ u_2 \\ u_3 \end{pmatrix}. \tag{35}$$

Then the Jacobian matrix $\mathbf{P} \equiv \partial \tilde{\mathbf{U}}/\partial \mathbf{U}$ of (3) is

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ \frac{1}{2}\sum_{k=1}^{3} u_k^2 & 1/(\gamma-1) & \rho u_1 & \rho u_2 & \rho u_3 \\ u_1 & 0 & \rho & 0 & 0 \\ u_2 & 0 & 0 & \rho & 0 \\ u_3 & 0 & 0 & 0 & \rho \end{pmatrix}. \tag{36}$$

The primitive equations are then found to be

$$\frac{\partial \rho}{\partial t} + u_1 \frac{\partial \rho}{\partial x_1} + u_2 \frac{\partial \rho}{\partial x_2} + u_3 \frac{\partial \rho}{\partial x_3} + \rho \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) = 0, \tag{37}$$

$$\frac{\partial p}{\partial t} + u_1 \frac{\partial p}{\partial x_1} + u_2 \frac{\partial p}{\partial x_2} + u_3 \frac{\partial p}{\partial x_3} + \gamma p \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) = 0, \tag{38}$$

$$\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_1}{\partial x_1} + u_2 \frac{\partial u_1}{\partial x_2} + u_3 \frac{\partial u_1}{\partial x_3} + \frac{1}{\rho} \frac{\partial p}{\partial x_1} - g_1 = 0, \tag{39}$$

$$\frac{\partial u_2}{\partial t} + u_1 \frac{\partial u_2}{\partial x_1} + u_2 \frac{\partial u_2}{\partial x_2} + u_3 \frac{\partial u_2}{\partial x_3} + \frac{1}{\rho} \frac{\partial p}{\partial x_2} - g_2 = 0, \tag{40}$$

$$\frac{\partial u_3}{\partial t} + u_1 \frac{\partial u_3}{\partial x_1} + u_2 \frac{\partial u_3}{\partial x_2} + u_3 \frac{\partial u_3}{\partial x_3} + \frac{1}{\rho} \frac{\partial p}{\partial x_3} - g_3 = 0. \tag{41}$$

Now we may set up the boundary condition analysis for the x_1 direction. Write Eqs. (37)–(41) as

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}^1 \frac{\partial \mathbf{U}}{\partial x_1} + \mathbf{C} = 0, \tag{42}$$

as in (8), where $\mathbf{A}^1$ is

$$\mathbf{A}^1 = \begin{pmatrix} u_1 & 0 & \rho & 0 & 0 \\ 0 & u_1 & \gamma p & 0 & 0 \\ 0 & 1/\rho & u_1 & 0 & 0 \\ 0 & 0 & 0 & u_1 & 0 \\ 0 & 0 & 0 & 0 & u_1 \end{pmatrix}, \tag{43}$$

and the **C** vector contains all remaining terms which do not involve elements of $\partial \mathbf{U}/\partial x_1$.

The eigenvalues of $\mathbf{A}^1$ are

$$\lambda_1 = u_1 - c, \qquad \lambda_2 = \lambda_3 = \lambda_4 = u_1, \qquad \lambda_5 = u_1 + c, \tag{44}$$

where c is the speed of sound:

$$c^2 = \frac{\gamma p}{\rho}. \tag{45}$$

The left eigenvectors may be written

$$\begin{aligned} \boldsymbol{l}_1^{\mathrm{T}} &= (0, 1, -\rho c, 0, 0), \\ \boldsymbol{l}_2^{\mathrm{T}} &= (c^2, -1, 0, 0, 0), \\ \boldsymbol{l}_3^{\mathrm{T}} &= (0, 0, 0, 1, 0), \\ \boldsymbol{l}_4^{\mathrm{T}} &= (0, 0, 0, 0, 1), \\ \boldsymbol{l}_5^{\mathrm{T}} &= (0, 1, \rho c, 0, 0). \end{aligned} \tag{46}$$

Eigenvalues λ_1 and λ_5 are the velocities of sound waves moving in the negative and positive x_1 directions; λ_2 is the velocity for entropy advection; while λ_3 and λ_4 are the velocities at which u_2 and u_3 are advected in the x_1 direction.

Next form the quantities $\mathscr{L}_i$ from Eq. (16), and get

$$\begin{aligned} \mathscr{L}_1 &= \lambda_1 \left(\frac{\partial p}{\partial x_1} - \rho c \frac{\partial u_1}{\partial x_1} \right), \\ \mathscr{L}_2 &= \lambda_2 \left(c^2 \frac{\partial \rho}{\partial x_1} - \frac{\partial p}{\partial x_1} \right), \\ \mathscr{L}_3 &= \lambda_3 \frac{\partial u_2}{\partial x_1}, \\ \mathscr{L}_4 &= \lambda_4 \frac{\partial u_3}{\partial x_1}, \\ \mathscr{L}_5 &= \lambda_5 \left(\frac{\partial p}{\partial x_1} + \rho c \frac{\partial u_1}{\partial x_1} \right). \end{aligned} \tag{47}$$

These definitions may be inverted to give

$$\frac{\partial \rho}{\partial x_1} = \frac{1}{c^2}\left[\frac{\mathscr{L}_2}{u_1} + \frac{1}{2}\left(\frac{\mathscr{L}_5}{u_1 + c} + \frac{\mathscr{L}_1}{u_1 - c}\right)\right],$$

$$\frac{\partial p}{\partial x_1} = \frac{1}{2}\left(\frac{\mathscr{L}_5}{u_1 + c} + \frac{\mathscr{L}_1}{u_1 - c}\right),$$

$$\frac{\partial u_1}{\partial x_1} = \frac{1}{2\rho c}\left(\frac{\mathscr{L}_5}{u_1 + c} - \frac{\mathscr{L}_1}{u_1 - c}\right), \tag{48}$$

$$\frac{\partial u_2}{\partial x_1} = \frac{\mathscr{L}_3}{u_1},$$

$$\frac{\partial u_3}{\partial x_1} = \frac{\mathscr{L}_4}{u_1}.$$

Multiplying Eq. (42) by the left eigenvectors gives Eqs. (17) and (18). The similarity transformation matrix $\mathbf{S}^{-1}$ has as its rows the left eigenvectors $\boldsymbol{l}_i^{\mathrm{T}}$ given in (46), while the vector $\mathscr{L}$ has its components given in Eq. (47). The produce $\mathbf{S}\mathscr{L}$ which is required in Eq. (19) has the components

$$\mathbf{d} \equiv \mathbf{S}\mathscr{L} = \begin{pmatrix} (1/c^2)[\mathscr{L}_2 + \frac{1}{2}(\mathscr{L}_5 + \mathscr{L}_1)] \\ (1/2)(\mathscr{L}_5 + \mathscr{L}_1) \\ (1/2\rho c)(\mathscr{L}_5 - \mathscr{L}_1) \\ \mathscr{L}_3 \\ \mathscr{L}_4 \end{pmatrix} = \begin{pmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{pmatrix}. \tag{49}$$

This result may be obtained by setting up and solving Eq. (21), or by substituting Eqs. (48) for $\partial \mathbf{U}/\partial x_1$ in terms of $\mathscr{L}$ into the terms $\mathbf{A}^1\, \partial \mathbf{U}/\partial x_1$ of Eq. (42). Either way we end up with the primitive equations in the form

$$\frac{\partial \rho}{\partial t} + \frac{1}{c^2}\left[\mathscr{L}_2 + \frac{1}{2}(\mathscr{L}_5 + \mathscr{L}_1)\right] + u_2 \frac{\partial \rho}{\partial x_2} + u_3 \frac{\partial \rho}{\partial x_3} + \rho\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right) = 0, \tag{50}$$

$$\frac{\partial p}{\partial t} + \frac{1}{2}(\mathscr{L}_5 + \mathscr{L}_1) + u_2 \frac{\partial p}{\partial x_2} + u_3 \frac{\partial p}{\partial x_3} + \gamma p\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right) = 0, \tag{51}$$

$$\frac{\partial u_1}{\partial t} + \frac{1}{2\rho c}(\mathscr{L}_5 - \mathscr{L}_1) + u_2 \frac{\partial u_1}{\partial x_2} + u_3 \frac{\partial u_1}{\partial x_3} - g_1 = 0, \tag{52}$$

$$\frac{\partial u_2}{\partial t} + \mathscr{L}_3 + u_2 \frac{\partial u_2}{\partial x_2} + u_3 \frac{\partial u_2}{\partial x_3} + \frac{1}{\rho}\frac{\partial p}{\partial x_2} - g_2 = 0, \tag{53}$$

$$\frac{\partial u_3}{\partial t} + \mathscr{L}_4 + u_2 \frac{\partial u_3}{\partial x_2} + u_3 \frac{\partial u_3}{\partial x_3} + \frac{1}{\rho}\frac{\partial p}{\partial x_3} - g_3 = 0. \tag{54}$$

multiply the vector of Eqs. (50)–(54) by T to get (28) as

$$\frac{\partial \rho}{\partial t} + d_1 + \frac{\partial}{\partial x_2}(\rho u_2) + \frac{\partial}{\partial x_3}(\rho u_3) = 0, \tag{55}$$

$$\frac{\partial e}{\partial t} + \frac{1}{2}\left(\sum_{k=1}^{3} u_k^2\right) d_1 + \frac{d_2}{\gamma - 1} + \rho u_1 d_3 + \rho u_2 d_4 + \rho u_3 d_5 + \frac{\partial}{\partial x_2}[(e+p)u_2] + \frac{\partial}{\partial x_3}[(e+p)u_3] - \rho \sum_{k=1}^{3} u_k g_k = 0, \tag{56}$$

$$\frac{\partial m_1}{\partial t} + u_1 d_1 + \rho d_3 + \frac{\partial}{\partial x_2}(m_1 u_2) + \frac{\partial}{\partial x_3}(m_1 u_3) - \rho g_1 = 0, \tag{57}$$

$$\frac{\partial m_2}{\partial t} + u_2 d_1 + \rho d_4 + \frac{\partial}{\partial x_2}(m_2 u_2) + \frac{\partial}{\partial x_3}(m_2 u_3) + \frac{\partial p}{\partial x_2} - \rho g_2 = 0, \tag{58}$$

$$\frac{\partial m_3}{\partial t} + u_3 d_1 + \rho d_5 + \frac{\partial}{\partial x_2}(m_3 u_2) + \frac{\partial}{\partial x_3}(m_3 u_3) + \frac{\partial p}{\partial x_3} - \rho g_3 = 0, \tag{59}$$

where the d_i are defined in Eq. (49).

The fluid equations are written and evaluated in the above form at the x_1 boundaries. The calculation of the $\mathscr{L}_i$ quantities depends on the boundary conditions and is described below.

3.2. *Boundary Conditions*

Now we consider boundary conditions for only the x_1 direction, as the other directions are handled similarly. Let the solution domain in the x_1 direction be $a_1 \leqslant x_1 \leqslant b_1$. For all points in $a_1 < x_1 < b_1$ (the interior), solve Eqs. (22)–(26) or (37)–(41) as written. For all points on $x_1 = a_1$ or $x_1 = b_1$ (the boundaries), solve Eqs. (55)–(59) or (50)–(54). The inhomogeneous and transverse derivative terms in the boundary equations are evaluated by the same approximation methods as in the interior.

The quantities $\mathscr{L}_i$ are determined as follows: when the characteristic velocity λ_i points out of the solution volume, compute the corresponding $\mathscr{L}_i$ from its definition in (47), using one-sided derivative approximations; when λ_i points into the solution volume, specify the value of $\mathscr{L}_i$ from the boundary conditions. Several useful boundary conditions are derived below.

3.2.1. *Slip Wall Boundary Conditions*

At a slip wall (frictionless wall), the normal velocity component is zero at all times, while the transverse velocities may be nonzero. Thus the initial data must have $u_1|_{x_1 = a_1} = u_1|_{x_1 = b_1} = 0$.

At $x_1 = b_1$, $\lambda_1 = -c$, $\lambda_2 = \lambda_3 = \lambda_4 = 0$, and $\lambda_5 = c$. Hence $\mathscr{L}_5$ must be computed from its definition in (47). Characteristic velocities 2 through 4 are zero, so the choices for $\mathscr{L}_2$ through $\mathscr{L}_4$ are ambiguous; however, setting $\mathscr{L}_2 = \mathscr{L}_3 = \mathscr{L}_4 = 0$ is consistent with the definitions in (47) and makes sense on physical grounds. Setting $\mathscr{L}_2 = 0$ means that the only entropy changes at b_1 are due to transverse advection, while setting $\mathscr{L}_3 = \mathscr{L}_4 = 0$ similarly means that the only changes to u_2 and u_3 at b_1 are due to the transverse terms in (53) and (54), which is reasonable at a frictionless wall.

$\mathscr{L}_1$ definitely represents an incoming wave, so we must specify its value. We do so by requiring that $u_1|_{x_1 = b_1} = 0$ for all time. Inspecting Eq. (52), we see that u_1 will remain zero if we set $\mathscr{L}_1 = \mathscr{L}_5 - 2\rho c g_1$. The slip wall conditions are

$$\begin{array}{ll} x_1 = a_1 \ (u_1 = 0) & x_1 = b_1 \ (u_1 = 0) \\ \hline \mathscr{L}_1 = \lambda_1 \left(\dfrac{\partial p}{\partial x_1} - \rho c \dfrac{\partial u_1}{\partial x_1} \right) & \mathscr{L}_1 = \mathscr{L}_5 - 2\rho c g_1 \\ \mathscr{L}_2 = \mathscr{L}_3 = \mathscr{L}_4 = 0 & \mathscr{L}_2 = \mathscr{L}_3 = \mathscr{L}_4 = 0 \\ \mathscr{L}_5 = \mathscr{L}_1 + 2\rho c g_1 & \mathscr{L}_5 = \lambda_5 \left(\dfrac{\partial p}{\partial x_1} + \rho c \dfrac{\partial u_1}{\partial x_1} \right) \end{array} \tag{60}$$

3.2.2. *No-Slip Wall Boundary Conditions*

At a no-slip wall, not only is the normal velocity component zero, but friction causes the transverse velocity components to be zero as well. The initial data must have all velocity components zero at the wall, and the boundary conditions are chosen to keep the velocity zero at all times.

We still have $\mathscr{L}_1$, $\mathscr{L}_2$, and $\mathscr{L}_5$ as given in the previous section, but now choose $\mathscr{L}_3$ and $\mathscr{L}_4$ to force $u_2 = u_3 = 0$ at the wall. From Eqs. (53) and (54) we see that the necessary conditions are $\mathscr{L}_3 = g_2 - (1/\rho)\, \partial p/\partial x_2$ and $\mathscr{L}_4 = g_3 - (1/\rho)\, \partial p/\partial x_3$, where $\partial p/\partial x_2$ and $\partial p/\partial x_3$ must be computed using the interior derivative approximation methods, because they are in the transverse directions. The complete list of boundary conditions is

$$\begin{array}{ll} x_1 = a_1 \ (u_1 = u_2 = u_3 = 0) & x_1 = b_1 \ (u_1 = u_2 = u_3 = 0) \\ \hline \mathscr{L}_1 = \lambda_1 \left(\dfrac{\partial p}{\partial x_1} - \rho c \dfrac{\partial u_1}{\partial x_1} \right) & \mathscr{L}_1 = \mathscr{L}_5 - 2\rho c g_1 \\ \mathscr{L}_2 = 0 & \mathscr{L}_2 = 0 \\ \mathscr{L}_3 = g_2 - \dfrac{1}{\rho} \dfrac{\partial p}{\partial x_2} & \mathscr{L}_3 = g_2 - \dfrac{1}{\rho} \dfrac{\partial p}{\partial x_2} \\ \mathscr{L}_4 = g_3 - \dfrac{1}{\rho} \dfrac{\partial p}{\partial x_3} & \mathscr{L}_4 = g_3 - \dfrac{1}{\rho} \dfrac{\partial p}{\partial x_3} \\ \mathscr{L}_5 = \mathscr{L}_1 + 2\rho c g_1 & \mathscr{L}_5 = \lambda_5 \left(\dfrac{\partial p}{\partial x_1} + \rho c \dfrac{\partial u_1}{\partial x_1} \right) \end{array} \tag{61}$$

3.2.3. *Free Boundary Conditions*

The boundaries of a computational domain often do not coincide with walls, but are simply the edges of some finite region, across which the fluid is free to flow. I will call these free boundaries. The flow direction and velocity at a free boundary will exhibit a wide range of behavior, depending on the local solution. The number and type of boundary conditions required may vary from time to time or place to place along the boundaries, even for one particular problem. Because the appropriate boundary conditions are so problem dependent, it is not possible to provide an exhaustive list, but a few useful examples and their derivations are given below. Deriving boundary conditions is often simpler than determining which conditions one ought to impose, and experimentation is usually necessary.

3.2.4. *Supersonic Inflow*

Supersonic inflow at $x_1 = b_1$ is characterized by $u_1 < -c$, so that all $\lambda_i < 0$. Consequently we must specify all values of $\mathscr{L}_i$ from boundary conditions.

Supersonic inflow is most often implemented as a steady state or near steady state boundary condition, the latter case being one in which only the transverse derivative terms may introduce a time dependence at the inflow boundary. If we allow the transverse terms to have such an effect, then the near steady state conditions are

$x_1 = a_1 \ (u_1 > c)$	$x_1 = b_1 \ (u_1 < -c)$
$\mathscr{L}_1 = -\rho c g_1$	$\mathscr{L}_1 = -\rho c g_1$
$\mathscr{L}_2 = 0$	$\mathscr{L}_2 = 0$
$\mathscr{L}_3 = g_2$	$\mathscr{L}_3 = g_2$
$\mathscr{L}_4 = g_3$	$\mathscr{L}_4 = g_3$
$\mathscr{L}_5 = \rho c g_1$	$\mathscr{L}_5 = \rho c g_1$

(62)

The initial data must also specify supersonic inflow at the boundaries, in order to be consistent with the boundary conditions.

3.2.5. *Supersonic Outflow*

Supersonic outflow at $x_1 = b_1$ is characterized by $u_1 > c$, so that all $\lambda_i > 0$. Consequently we can specify no boundary conditions at all, and the evolution of the flow at the boundary is determined completely by interior data. In this case we simply compute all $\mathscr{L}_i$ values from their definitions in (47), using one sided approximations to the derivatives.

Supersonic outflow at $x_1 = a_1$ has $u_1 < -c$, so that all $\lambda_i < 0$, and all $\mathscr{L}_i$ values are computed from their definitions in (47).

3.2.6. *Subsonic Outflow*

Subsonic outflow at $x_1 = b_1$ is characterized by $0 < u_1 < c$, for which $\lambda_1 < 0$ and $\lambda_{2-5} > 0$. Thus we compute $\mathscr{L}_{2-5}$ from their definitions in (47) and specify $\mathscr{L}_1$ according to some boundary condition. While there is no unique choice for $\mathscr{L}_1$, the following possibilities are often useful.

3.2.6.1. *Nonreflecting boundary condition.* This condition was described in some detail in [1] and was first introduced correctly (for nonlinear equations) by Hedstrom [6]. The nonreflecting boundary condition demands that the amplitude of an incoming wave be constant in time. This condition is equivalent to stating that there is no incoming wave, as it is the variation in amplitude which constitutes wave motion.

If we drop the transverse terms, then the first component of (18) is the characteristic equation

$$\left(\frac{\partial p}{\partial t} - \rho c \frac{\partial u_1}{\partial t}\right) + \mathscr{L}_1 + \rho c g_1 = 0, \tag{63}$$

where the expression in parentheses represents the time derivative of the amplitude of the characteristic wave (see, for example, Whitham [3], or Landau and Lifshitz [7], for a discussion of characteristic waves and Riemann invariants). The wave amplitude remains constant if we set $\mathscr{L}_1 = -\rho c g_1$.

Thus the nonreflecting boundary condition for subsonic outflow is

$$\begin{array}{ll} x_1 = a_1 \ (-c < u_1 < 0) & x_1 = b_1 \ (0 < u_1 < c) \\ \hline \mathscr{L}_5 = \rho c g_1 & \mathscr{L}_1 = -\rho c g_1 \end{array} \tag{64}$$

with all other $\mathscr{L}_i$ values being computed from (47).

Nonreflecting boundary conditions are well suited for problems in which a rarefaction wave propagates out of the boundary and into a previously undisturbed medium, or in general for problems in which nothing useful is known about the external solution and the suppression of incoming waves seems like a reasonable choice of boundary condition.

3.2.6.2. *Force-free boundary condition.* For some problems the nonreflecting boundary condition is inappropriate. The "correct" solution implicitly contains an incoming wave which must not be suppressed. This situation most often arises when the real solution exterior to the model volume is changing in time and must communicate its behavior to the interior through the boundaries.

In the absence of more knowledge about the exterior solution, one approach to this case is to apply a boundary condition which sets to zero the sum of all forces acting on the fluid in the direction normal to the boundary. This choice effectively eliminates all normal terms except the advective term $u_1 \partial u_1 / \partial x_1$, so that a fluid element at the boundary is simply advected outward at the fluid velocity.

From Eq. (39) we see that imposing a zero net force in the x_1 direction requires that

$$\frac{1}{2\rho c}(\mathscr{L}_5 - \mathscr{L}_1) - g_1 = u_1 \frac{\partial u_1}{\partial x_1}, \tag{65}$$

which gives the boundary conditions

$$\begin{array}{ll} x_1 = a_1 \ (-c < u_1 < 0) & x_1 = b_1 \ (0 < u_1 < c) \\ \hline \mathscr{L}_5 = \mathscr{L}_1 + 2\rho c \left(u_1 \dfrac{\partial u_1}{\partial x_1} + g_1 \right) & \mathscr{L}_1 = \mathscr{L}_5 - 2\rho c \left(u_1 \dfrac{\partial u_1}{\partial x_1} + g_1 \right) \end{array} \tag{65}$$

A good example of when the force-free condition is useful is the case when a pressure equilibrium (or other zero net force) exists at the boundary. A pressure equilibrium is maintained by the propagation of sound waves, which serve to equalize the pressure across the boundary; therefore the exterior solution must communicate this equilibrium to the interior. In this case fluid elements follow "ballistic" trajectories. The homologous expansion of a uniform gas [1] is such a problem, for which the nonreflecting boundary conditions destroy the pressure balance.

3.2.6.3. *Constant pressure boundary condition.* There are some problems for which a particular constraint must be satisfied. This section describes the case where the pressure is known to be constant at the boundary. Other such conditions may be handled in a similar fashion (as was the case of zero normal velocity previously).

It is usually the case the one wants $\partial p/\partial t = 0$ in the absence of transverse effects, but not otherwise. This condition is satisfied if $\mathscr{L}_5 + \mathscr{L}_1 = 0$, giving

$$\begin{array}{ll} x_1 = a_1 \ (-c < u_1 < 0) & x_1 = b_1 \ (0 < u_1 < c) \\ \hline \mathscr{L}_5 = -\mathscr{L}_1 & \mathscr{L}_1 = -\mathscr{L}_5 \end{array} \tag{67}$$

3.2.7. *Subsonic Inflow*

Subsonic inflow at $x_1 = b_1$ is characterized by $-c < u_1 < 0$, so that $\lambda_{1-4} < 0$ and $\lambda_5 > 0$. Thus we compute $\mathscr{L}_5$ from its definition in (47) and must specify the other $\mathscr{L}_i$ from boundary conditions. The value of $\mathscr{L}_1$ may be determined by any of the methods in the previous sections, or any other similar condition. This section will focus on the determination of $\mathscr{L}_2$, $\mathscr{L}_3$, and $\mathscr{L}_4$.

[redacted]

inflow, nonreflecting boundary conditions work well enough in the specification of $\mathscr{L}_{2-4}$. $\mathscr{L}_2$ describes the inflow entropy, so setting $\mathscr{L}_2 = 0$ states that the inflow

entropy is constant in the x_1 direction. Setting $\mathscr{L}_3 = g_2$ and $\mathscr{L}_4 = g_3$ will hold the u_2 and u_3 velocities constant in the absence of tangential effects.

$x_1 = a_1\ (0 < u_1 < c)$	$x_1 = b_1\ (-c < u_1 < 0)$
$\mathscr{L}_1 = \lambda_1 \left(\dfrac{\partial p}{\partial x_1} - \rho c \dfrac{\partial u_1}{\partial x_1} \right)$	$\mathscr{L}_1$ from Section 3.2.6
$\mathscr{L}_2 = 0$	$\mathscr{L}_2 = 0$
$\mathscr{L}_3 = g_2$	$\mathscr{L}_3 = g_2$
$\mathscr{L}_4 = g_3$	$\mathscr{L}_4 = g_3$
$\mathscr{L}_5$ from Section 3.2.6	$\mathscr{L}_5 = \lambda_5 \left(\dfrac{\partial p}{\partial x_1} + \rho c \dfrac{\partial u_1}{\partial x_1} \right)$

(68)

Note that any of these conditions may be used in conjunction with any of the conditions from the previous sections.

3.2.7.2 *Constant mass flux.* Some problems assume mass flux ρu_1 at the inflow boundary. If the correct mass flux is specified initially, then it will be maintained at later times if

$$\frac{\partial}{\partial t}(\rho u_1) = \rho \frac{\partial u_1}{\partial t} + u_1 \frac{\partial \rho}{\partial t} = 0.$$

From (50) and (52), ignoring tangential effects, we get

$$2u_1 \mathscr{L}_2 + (u_1 - c)\, \mathscr{L}_1 + (u_1 + c)\, \mathscr{L}_5 = 2\rho c^2 g_1, \tag{69}$$

which gives

$x_1 = a_1\ (0 < u_1 < c)$	$x_1 = b_1\ (-c < u_1 < 0)$
$\mathscr{L}_5 = \dfrac{1}{u_1 + c} [2\rho c^2 g_1 - 2u_1 \mathscr{L}_2 - (u_1 - c)\, \mathscr{L}_1]$	$\mathscr{L}_1 = \dfrac{1}{u_1 - c} [2\rho c^2 g_1 - 2u_1 \mathscr{L}_2 - (u_1 + c)\, \mathscr{L}_5]$

(70)

assuming that $\mathscr{L}_2$ has been specified. If $\mathscr{L}_2$ is not known, then we might specify $\mathscr{L}_1$ (or $\mathscr{L}_5$) from one of the methods of Section 3.2.6 and solve for $\mathscr{L}_2$ from (69) as

$x_1 = a_1\ (0 < u_1 < c)$	$x_1 = b_1\ (-c < u_1 < 0)$
$\mathscr{L}_2 = \dfrac{1}{2u_1} [2\rho c^2 g_1 - (u_1 - c)\, \mathscr{L}_1 - (u_1 + c)\, \mathscr{L}_5]$	$\mathscr{L}_2 = \dfrac{1}{2u_1} [2\rho c^2 g_1 - (u_1 - c)\, \mathscr{L}_1 - (u_1 + c)\, \mathscr{L}_5]$

(71)

Note that (70) could be used as an outflow boundary condition in principle, since it involves $\mathscr{L}_1$ and $\mathscr{L}_5$. In practice, however, one normally wishes to fix the mass flux at an inflow boundary, not an outflow boundary.

4. Numerical Implementation

Space limitations preclude a comprehensive set of computational examples for all the boundary conditions described in this paper. However, I will present a general numerical solution for a system of fluid dynamics equations, including the implementation of the boundary formalism. The reader is referred to the previous paper [1] for sample problems.

The complete implementation breaks down into two parts: the calculation of time derivatives based on the current solution and the integration of time derivatives to obtain a future solution.

4.1. *Computing the Time Derivatives*

Let the computational volume $\mathscr{V}$ be defined by $a_l \leqslant x_l \leqslant b_l$, $l = 1, 2, 3$. For simplicity, discretize the solution on a uniform grid with grid spacings $\Delta x_l = (b_l - a_l)/N_l$, so that $x_{li} = a_l + i\,\Delta x_l$, $i = 0, 1, ..., N_l$, with $x_{l0} = a_l$ and $x_{lN_l} = b_l$. Thus the interior points in the lth direction are denoted by $0 < i < N_l$, while the boundary points have $i = 0$ or $i = N_l$. Any function $f = f(x_1, x_2, x_3)$ is represented in discrete form as $f_{ijk} \equiv f(x_{1i}, x_{2j}, x_{3k})$.

The calculation of time derivatives in the interior consists simply of approximating the spatial derivatives in Eqs. (22)–(26) or (37)–(41) with some suitable numerical scheme, and evaluating the inhomogeneous terms, at the interior points. Of the many approximation methods available, finite difference methods are the simplest and will be used here. The accuracy of a finite difference method is described by its order of convergence, i.e., by the power of Δx at which its error vanishes in the limit as $\Delta x \to 0$. The higher the order, the more accurate the approximation.

A globally second-order accurate scheme may be achieved by using the approximations

$$\left.\frac{\partial f}{\partial x_1}\right|_{ijk} = \frac{1}{2\,\Delta x_1}(f_{i+1jk} - f_{i-1jk}), \qquad i = 1, ..., N_1 - 1; \tag{72}$$

$$\left.\frac{\partial f}{\partial x_1}\right|_{0jk} = \frac{1}{\Delta x_1}(f_{1jk} - f_{0jk}); \tag{73}$$

$$\left.\frac{\partial f}{\partial x_1}\right|_{N_1 jk} = \frac{1}{\Delta x_1}(f_{N_1 jk} - f_{N_1 - 1jk}); \tag{74}$$

and similarly for the x_2 and x_3 directions.

A globally fourth-order accurate scheme may be achieved by using the approximations

$$\left.\frac{\partial f}{\partial x_1}\right|_{ijk} = \frac{1}{12\,\Delta x_1}[8(f_{i+1\,jk} - f_{i-1\,jk}) - (f_{i+2\,jk} - f_{i-2\,jk})],$$

$$i = 2, \ldots, N_1 - 2; \tag{75}$$

$$\left.\frac{\partial f}{\partial x_1}\right|_{0jk} = \frac{1}{6\,\Delta x_1}[18(f_{1jk} - f_{0jk}) - 9(f_{2jk} - f_{0jk}) + 2(f_{3jk} - f_{0jk})]; \tag{76}$$

$$\left.\frac{\partial f}{\partial x_1}\right|_{1jk} = \frac{1}{6\,\Delta x_1}[2(f_{1jk} - f_{0jk}) + 6(f_{2jk} - f_{1jk}) - (f_{3jk} - f_{1jk})]; \tag{77}$$

$$\left.\frac{\partial f}{\partial x_1}\right|_{N_1-1\,jk} = \frac{1}{6\,\Delta x_1}[2(f_{N_1jk} - f_{N_1-1\,jk}) + 6(f_{N_1-1\,jk} - f_{N_1-2\,jk}) - (f_{N_1-1\,jk} - f_{N_1-3\,jk})]; \tag{78}$$

$$\left.\frac{\partial f}{\partial x_1}\right|_{N_1jk} = \frac{1}{6\,\Delta x_1}[18(f_{N_1jk} - f_{N_1-1\,jk}) - 9(f_{N_1jk} - f_{N_1-2\,jk}) + 2(f_{N_1jk} - f_{N_1-3\,jk})]; \tag{79}$$

and similarly for the x_2 and x_3 directions.

The global order of convergence may be one greater than the order of convergence of the approximations used at and near the boundary. Thus Eqs. (72)–(74) will yield a globally second-order scheme, even though Eqs. (73)–(74) are first-order accurate; similarly, Eqs. (75)–(79) will yield a globally fourth-order scheme, even though Eqs. (76)–(79) are third-order accurate. In each case the order of the scheme away from the boundaries is one higher than the order at and near the boundaries, and the global order is the same as that of the scheme away from the boundaries. It is sometimes the case that using boundary approximations which are the same order as the interior scheme (second or fourth here) will lead to an unstable solution, which is why the boundary approximations are of lower order than the interior approximations in the above formulas.

At the x_1 boundaries ($i = 0$ or $i = N_1$) the fluid equations are put in the form of (50)–(54) or (55)–(59). The transverse derivatives and inhomogeneous terms are evaluated with the same approximation methods used for the interior, as these quantities do not require information external to the model volume for their evaluation.

The normal (x_1) derivatives are subsumed into the definitions of the $\mathscr{L}_i$ quantities. Those $\mathscr{L}_i$ for which the corresponding characteristic velocities λ_i are directed out of the model volume are evaluated from their definitions in (47), using one-sided approximations (73), (74), (76), or (79) for the spatial derivatives. The remaining $\mathscr{L}_i$ values are determined from the boundary condition formulas of Section 3.2.

Complications arise at corner points, where two or three coordinate directions require boundary conditions simultaneously. In this case (supposing that all three directions are involved) we perform the characteristic analysis for each coordinate direction, and obtain quantities $\mathscr{M}_i$ and $\mathscr{N}_i$ for the x_2 and x_3 directions which are analogous to $\mathscr{L}_i$ for the x_1 direction. The x_2 and x_3 derivatives are then replaced by the appropriate linear combinations of $\mathscr{M}_i$ and $\mathscr{N}_i$ quantities. The values of $\mathscr{M}_i$ and $\mathscr{N}_i$ are then determined by one-sided derivatives or boundary conditions, depending on the values of the corresponding characteristic velocities μ_i and ν_i in the x_2 and x_3 directions. (Note that $\mu_1 = u_2 - c$, $\mu_2 = \mu_3 = \mu_4 = u_2$, $\mu_5 = u_2 + c$; $\nu_1 = u_3 - c$, $\nu_2 = \nu_3 = \nu_4 = u_3$, $\nu_5 = u_3 + c$.)

4.2. *Integrating the Time Derivatives*

The solution is discretized in time as well as space. Given the solution at the current time step n, where $t = t^n$, we wish to compute the solution at time step $n+1$, where $t^{n+1} = t^n + \Delta t$. The time step size Δt must normally be less than a certain upper limit, which is described below, and usually varies during the course of the calculation.

Having computed the time derivatives $d\tilde{\mathbf{U}}_{ijk}/dt$ (say) at all grid points, we are free to integrate the time derivatives from time t^n to time t^{n+1} with any suitable ordinary differential equation solver. The constraints on the integrator to be used are that it must be stable for reasonable time steps and must be sufficiently accurate for the purpose at hand. The accuracy of a time integration method is also described by its order of convergence, i.e., by the power of Δt at which its error vanishes in the limit as $\Delta t \to 0$. The higher the order, the more accurate the integration.

For time dependent calculations the accuracy of the numerical solution to a system such as the fluid dynamics equations is described by the global convergence rate. If we let $\Delta x_l \to 0$ and $\Delta t \to 0$ while keeping $\Delta x_l / \Delta t$ constant (i.e., at a fixed Courant number), then $\Delta x_l \propto \Delta t$ and the norm of the error in the solution at any fixed time also goes to zero as some power of Δt, that power being the global order of convergence. If the spatial derivative approximations and the time integration have different orders of convergence, then the global order of convergence is the lesser of the two. Thus it is desirable to match the orders of convergence of the spatial derivative and time integration schemes for optimum accuracy and efficiency. Otherwise some effort is wasted in the calculation of some quantities to excessively high accuracy.

An exception to the matching rule occurs when the purpose of the calculation is to achieve a steady state solution, for which the preceding time dependent solution is of no interest. In this case one should choose a simple (and consequently fast) low order time integration scheme to minimize the calculation time required. Once a steady state has been achieved, the time derivatives are zero and the order of the time integration is irrelevant, and the global order of convergence is simply the order of the spatial derivative approximation.

One of the simplest and most efficient fourth order time integrators is the classic fourth-order Runge–Kutta method, which may be written

$$\begin{aligned}
\tilde{\mathbf{U}}_{ijk}^{(1)} &= \tilde{\mathbf{U}}_{ijk}^{n} + \frac{1}{2}\Delta t \left.\frac{d\tilde{\mathbf{U}}_{ijk}}{dt}\right|^{n}, \\
\tilde{\mathbf{U}}_{ijk}^{(2)} &= \tilde{\mathbf{U}}_{ijk}^{n} + \frac{1}{2}\Delta t \left.\frac{d\tilde{\mathbf{U}}_{ijk}}{dt}\right|^{(1)}, \\
\tilde{\mathbf{U}}_{ijk}^{(3)} &= \tilde{\mathbf{U}}_{ijk}^{n} + \Delta t \left.\frac{d\tilde{\mathbf{U}}_{ijk}}{dt}\right|^{(2)}, \\
\tilde{\mathbf{U}}_{ijk}^{n+1} &= \tilde{\mathbf{U}}_{ijk}^{n} + \frac{1}{6}\Delta t \left(\left.\frac{d\tilde{\mathbf{U}}_{ijk}}{dt}\right|^{n} + 2\left.\frac{d\tilde{\mathbf{U}}_{ijk}}{dt}\right|^{(1)} + 2\left.\frac{d\tilde{\mathbf{U}}_{ijk}}{dt}\right|^{(2)} + \left.\frac{d\tilde{\mathbf{U}}_{ijk}}{dt}\right|^{(3)} \right),
\end{aligned} \tag{80}$$

(or similarly for $\mathbf{U}$, if a nonconservative (primitive) form has been chosen for the fluid equations). This scheme should be used along with the fourth-order spatial derivative approximations to achieve a globally fourth-order convergent calculation. (For a suitable second-order integrator, see [1].) Note that $d\tilde{\mathbf{U}}_{ijk}/dt|^{(m)}$ refers to the time derivative of $\tilde{\mathbf{U}}$ at the grid points (x_{1i}, x_{2j}, x_{3k}) as computed from the intermediate step solution $\tilde{\mathbf{U}}^{(m)}$.

The time step Δt is given by

$$\Delta t = \sigma \Big/ \max_{i,j,k} \left(\frac{|u_{1ijk}| + c_{ijk}}{\Delta x_1} + \frac{|u_{2ijk}| + c_{ijk}}{\Delta x_2} + \frac{|u_{3ijk}| + c_{ijk}}{\Delta x_3} \right), \tag{81}$$

where σ (the "Courant number") may be given any value $\leqslant 2.0612...$, which is the maximum stable limit [2]. Values of $\sigma = 0.5$ or $\sigma = 1$ are conservative and normally work well.

5. Conclusion

This paper has presented a unified framework for specifying boundary conditions for systems of hyperbolic equations. The framework is flexible enough to encompass virtually any type of boundary condition. Many useful conditions have been derived for common problems in computational fluid dynamics.

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