CHAPTER III

THE NUMERICAL METHOD

III.1 Introduction

In this chapter the numerical method that was used to solve the governing differential equations is derived and discussed. The numerical method is based on that proposed by MacCormack (1985). It is fully implicit and uses Gauss-Seidel line-relaxation. It has been shown to yield steady-state results efficiently for perfect gas hypersonic flows[1] and for this reason, it was used for this work. The method itself is discussed for the specific equation set derived in the previous chapter, however the generalization to other equation sets of the same class is straight-forward.

III.2 The Conservation-Law Form of the Governing Equations

The governing equations for the nonequilibrium flow that were presented in the previous chapter may be written in a form that is more suitable for the derivation of the numerical method. This is the conservation-law form of the differential equations where the time rate of change of the vector of conserved quantities is balanced by the gradients in the flux vectors and the source vector. In two-dimensions the governing equations written in this form are

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = W, \tag{3.2.1}$$

where the vector of conserved quantities, U, is given by

$$U = \big(\rho_1,\ \rho_2,\ \ldots,\ \rho_n,\ \rho u,\ \rho v,\ E_{v1},\ \ldots,\ E_{vm},\ E_e,\ E\big)^T. \tag{3.2.2}$$

The quantities u and v are the mass-averaged velocity components in the x and y directions respectively. The x direction flux is written as

[1] See MacCormack (1985) and Candler and MacCormack (1987a)

$$F = \begin{pmatrix} \rho_1(u + \mathrm{u}_1) \\ \rho_2(u + \mathrm{u}_2) \\ \vdots \\ \rho_n(u + \mathrm{u}_n) \\ \rho u^2 + p + \tau_{xx} \\ \rho uv + \tau_{xy} \\ E_{v1}(u + \mathrm{u}_1) + q_{v1x} \\ \vdots \\ E_{vm}(u + \mathrm{u}_m) + q_{vmx} \\ E_e(u + \mathrm{u}_e) + q_{ex} \\ (E + p + \tau_{xx})u + \tau_{xy}v + q_x + q_{vx} + q_{ex} + \sum_{s=1}^{n} \rho_s h_s \mathrm{u}_s \end{pmatrix}. \tag{3.2.3}$$

And the y direction flux is

$$G = \begin{pmatrix} \rho_1(v + \mathrm{v}_1) \\ \rho_2(v + \mathrm{v}_2) \\ \vdots \\ \rho_n(v + \mathrm{v}_n) \\ \rho uv + \tau_{yx} \\ \rho v^2 + p + \tau_{yy} \\ E_{v1}(v + \mathrm{v}_1) + q_{v1y} \\ \vdots \\ E_{vm}(v + \mathrm{v}_m) + q_{vmy} \\ E_e(v + \mathrm{v}_e) + q_{ey} \\ (E + p + \tau_{yy})v + \tau_{yx}u + q_y + q_{vy} + q_{ey} + \sum_{s=1}^{n} \rho_s h_s \mathrm{v}_s \end{pmatrix}. \tag{3.2.4}$$

where the quantities u_s and v_s are the x and y components of the diffusion velocity of species s. The source vector that is made up of terms that represent the mass, momentum, and energy transfer rates may be written as

$$
W = \begin{pmatrix}
w_1 \\
w_2 \\
\vdots \\
w_n \\
-\sum_{s=1}^{n} Z_s \frac{N_s}{N_e} \frac{\partial p_e}{\partial x} \\
-\sum_{s=1}^{n} Z_s \frac{N_s}{N_e} \frac{\partial p_e}{\partial y} \\
Q_{T-v\,1} + Q_{v-v\,1} + Q_{e-v\,1} + w_1 e_{v1} \\
\vdots \\
Q_{T-v\,m} + Q_{v-v\,m} + Q_{e-v\,m} + w_m e_{vm} \\
-p_e\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + Q_{T-e} - \sum_{s=1}^{m} Q_{e-v\,s} + w_e e_e \\
-\sum_{s=1}^{n} Z_s \frac{N_s}{N_e}\left(u\frac{\partial p_e}{\partial x} + v\frac{\partial p_e}{\partial y}\right)
\end{pmatrix}. \tag{3.2.5}
$$

Equation (3.2.1) is written in Cartesian coordinates, however we are interested in applying the numerical method to a general grid and thus we must make a transformation to a general coordinate system, ξ and η. Using the chain rule of differentials, we can write

$$
\begin{aligned}
\frac{\partial}{\partial x} &= \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta}, \\
\frac{\partial}{\partial y} &= \frac{\partial \xi}{\partial y}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial y}\frac{\partial}{\partial \eta}.
\end{aligned} \tag{3.2.6}
$$

Thus the Cartesian derivatives in equation (3.2.1) may be replaced to yield

$$
\frac{\partial U}{\partial t} + \frac{\partial}{\partial \xi}\left(\frac{\partial \xi}{\partial x}F + \frac{\partial \xi}{\partial y}G\right) + \frac{\partial}{\partial \eta}\left(\frac{\partial \eta}{\partial x}F + \frac{\partial \eta}{\partial y}G\right) = W. \tag{3.2.7}
$$

If we define

$$
\begin{aligned}
F' &= \frac{\partial \xi}{\partial x}F + \frac{\partial \xi}{\partial y}G, \\
G' &= \frac{\partial \eta}{\partial x}F + \frac{\partial \eta}{\partial y}G,
\end{aligned} \tag{3.2.8}
$$

our set of governing equations becomes

$$
\frac{\partial U}{\partial t} + \frac{\partial F'}{\partial \xi} + \frac{\partial G'}{\partial \eta} = W. \tag{3.2.9}
$$

This is the basic equation that will be used in the derivation of the numerical method. The means for computing the metrics, $\frac{\partial\xi}{\partial x}$, $\frac{\partial\xi}{\partial y}$, $\frac{\partial\eta}{\partial x}$, and $\frac{\partial\eta}{\partial y}$, is discussed in Appendix B.

III.3 The Numerical Method

The finite-volume approximation to the governing equations will be derived in this section. The finite-volume approach discretizes the flowfield into a grid of quadrilateral finite volumes. The x and y locations of the volume corners are stored. And the state of the gas is represented with volume-averaged quantities stored at the centroids of the volumes. Figure 3.1 gives a graphical representation of this scheme.

The basic equation set written in conservation-law form, equation (3.2.9), may be first-order finite differenced in space and time to yield the implicit difference equation

$$U^{n+1} - U^n + \Delta t\Big[\frac{D}{\Delta\xi}F'^{n+1} + \frac{D}{\Delta\eta}G'^{n+1}\Big] = \Delta t\, W^{n+1}, \tag{3.3.1}$$

where we have assumed that the solution is known at time level n. The equation is expressed entirely at the future time level, $n+1$ where the solution is unknown. The spatial difference operators are generic; the direction of the differencing will become apparent later. Both of the flux vectors may be broken into two parts, the flux due to the inviscid terms and that due to the viscous terms. For example

$$F' = F'_{\mathrm{I}} + F'_{\mathrm{v}}, \tag{3.3.2}$$

where the subscripts denote the inviscid and viscous terms of F' respectively. The inviscid part of the flux may then be linearized to yield the expression

$$F'^{n+1}_{\mathrm{I}} = F'^{n}_{\mathrm{I}} + A'^{n}\big(U^{n+1} - U^n\big) + O(\Delta t^2), \tag{3.3.3}$$

where A' is the Jacobian of F'_{I} with respect to U. Due to the homogeneity of F'_{I}, we can also express the flux at time level n in terms of the Jacobian A' as

$$F'^{n}_{\mathrm{I}} = A'^{n} U^{n} = \left(A'^{n}_{+} + A'^{n}_{-}\right) U^{n}, \tag{3.3.4}$$

where A' has been broken into the elements of the fluxes moving in the positive ξ direction, A'_{+}, and those moving in the negative ξ direction, A'_{-}. This partitioning is performed by diagonalizing A'. We can do this by writing

$$A' = \frac{\partial F'_{\mathrm{I}}}{\partial U} = \frac{\partial U}{\partial V} \cdot \frac{\partial V}{\partial U} \frac{\partial F'_{\mathrm{I}}}{\partial V} \cdot \frac{\partial V}{\partial U}, \tag{3.3.5}$$

where V is a vector of non-conserved flow variables introduced for convenience. The choice of V is not unique, but in this case we have used

$$V = \left(\rho_1,\ \rho_2,\ \ldots,\ \rho_n,\ u,\ v,\ e_{v1},\ \ldots,\ e_{vm},\ e_e,\ p\right)^{T}. \tag{3.3.6}$$

With this choice of V the diagonalization of $\frac{\partial V}{\partial U} \frac{\partial F'_{\mathrm{I}}}{\partial V}$ is straight-forward and the result may be written as

$$\frac{\partial V}{\partial U} \frac{\partial F'_{\mathrm{I}}}{\partial V} = C_{A'}^{-1}\, \Lambda_{A'}\, C_{A'}, \tag{3.3.7}$$

where $\Lambda_{A'}$ is a diagonal matrix. A discussion of the diagonalization procedure and the resulting matrices are given in Appendix C.

If we define $S = \frac{\partial V}{\partial U}$ and a rotation matrix R_A, such that $C_{A'} = C_A\, R_A$, we have

$$A' = S^{-1}\, R_A^{-1}\, C_A^{-1}\, \Lambda_{A'}\, C_A\, R_A\, S, \tag{3.3.8}$$

where S, C_A, and R_A are given in Appendix C. Let the diagonal matrix $\Lambda_{A'+}$ be made up of the positive elements of $\Lambda_{A'}$ and $\Lambda_{A'-}$ be composed of its negative elements. Then we have

$$
\begin{aligned}
A'_{+} &= S^{-1}\, R_A^{-1}\, C_A^{-1}\, \Lambda_{A'+}\, C_A\, R_A\, S, \\
A'_{-} &= S^{-1}\, R_A^{-1}\, C_A^{-1}\, \Lambda_{A'-}\, C_A\, R_A\, S,
\end{aligned}
\tag{3.3.9}
$$

which represent the split-flux Jacobians of the inviscid flux vector F'_{I}.

The inviscid flux entering or leaving a volume across a surface is given in equation (3.3.4), however the grid point where each term should be evaluated is ambiguous. We do not have data stored at the surface itself, and therefore an approximation must be made. The flux traveling in the positive ξ direction originates at the point i, j and that traveling in the negative ξ direction comes from point $i{+}1, j$. Therefore the inviscid flux across surface $i{+}\frac{1}{2}, j$ is given by

$$
{F'}^{n}_{\mathrm{I}\,i+\frac{1}{2},j} = {A'}^{n}_{+i+\frac{1}{2},j} U^{n}_{i,j} + {A'}^{n}_{-i+\frac{1}{2},j} U^{n}_{i+1,j}. \tag{3.3.10}
$$

We need a scheme to determine at what grid point we should evaluate the Jacobians. Two methods have been used in this study. The primary technique used was proposed by MacCormack (1985)[2] and has been shown to have favorable characteristics for the treatment of a boundary layer. With this method, both of the Jacobians, A'_{+} and A'_{-}, are always evaluated at the same place. The point used is alternated between i, j and $i{+}1, j$. The second method was proposed by Steger and Warming (1979) and the flux-splitting is performed so that

$$
{F'}^{n}_{\mathrm{I}\,i+\frac{1}{2},j} = {A'}^{n}_{+i,j} U^{n}_{i,j} + {A'}^{n}_{-i+1,j} U^{n}_{i+1,j}. \tag{3.3.11}
$$

The second technique is very dissipative and shows poor results in a boundary layer (MacCormack and Candler (1987)), but was used in this work in strong pressure gradient regions to maintain numerical stability and to capture shock waves[3]. For simplicity, the subscript $i{+}\frac{1}{2}, j$ will be left on A' to imply that either flux-splitting method may be used.

[2] See also MacCormack and Candler (1987).

[3] At any point where the pressure changes by 25% across a surface, the Steger-Warming flux-splitting, (3.3.11), is used.

Having made these approximations, we can express the inviscid fluxes at time level $n+1$, using (3.3.3), (3.3.10), and the definition $\delta U^n \equiv U^{n+1} - U^n$, as follows

$$
\begin{aligned}
{F'}^{n+1}_{\mathrm{I}\,i+\frac{1}{2},j} &\simeq {A'}^{n}_{+i+\frac{1}{2},j} U^n_{i,j} + {A'}^{n}_{-i+\frac{1}{2},j} U^n_{i+1,j} + {A'}^{n}_{+i+\frac{1}{2},j} \delta U^n_{i,j} + {A'}^{n}_{-i+\frac{1}{2},j} \delta U^n_{i+1,j}, \\
{G'}^{n+1}_{\mathrm{I}\,i,j+\frac{1}{2}} &\simeq {B'}^{n}_{+i,j+\frac{1}{2}} U^n_{i,j} + {B'}^{n}_{-i,j+\frac{1}{2}} U^n_{i,j+1} + {B'}^{n}_{+i,j+\frac{1}{2}} \delta U^n_{i,j} + {B'}^{n}_{-i,j+\frac{1}{2}} \delta U^n_{i,j+1}.
\end{aligned}
\tag{3.3.12}
$$

The source vector may be linearized in a similar fashion so that we have

$$
W^{n+1}_{ij} = W^n_{ij} + C^n_{ij} \delta U^n_{ij} + O(\Delta t^2), \tag{3.3.13}
$$

where C is the Jacobian of W with respect to U. The difference equation (3.3.1) becomes

$$
\begin{aligned}
\Big\{ I + \Delta t \Big[\frac{D_-}{\Delta\xi} \cdot {A'}^{n}_{+i+\frac{1}{2},j} + \frac{D_+}{\Delta\xi} \cdot {A'}^{n}_{-i-\frac{1}{2},j} + \frac{D_-}{\Delta\eta} \cdot {B'}^{n}_{+i,j+\frac{1}{2}} + \frac{D_+}{\Delta\eta} \cdot {B'}^{n}_{-i,j-\frac{1}{2}} \Big] \Big\} \delta U^n_{i,j} \\
+ \Delta t \Big[\frac{D}{\Delta\xi} {F'}^{n+1}_{\mathrm{v}i,j} + \frac{D}{\Delta\eta} {G'}^{n+1}_{\mathrm{v}i,j} \Big] - \Delta t\, C^n_{i,j} \delta U^n_{i,j} = \Delta t\, W^n_{i,j} \\
- \Delta t \Big[\frac{D_-}{\Delta\xi} \cdot {A'}^{n}_{+i+\frac{1}{2},j} + \frac{D_+}{\Delta\xi} \cdot {A'}^{n}_{-i-\frac{1}{2},j} + \frac{D_-}{\Delta\eta} \cdot {B'}^{n}_{+i,j+\frac{1}{2}} + \frac{D_+}{\Delta\eta} \cdot {B'}^{n}_{-i,j-\frac{1}{2}} \Big] U^n_{i,j}.
\end{aligned}
\tag{3.3.14}
$$

The viscous fluxes that appear in equation (3.3.14) must be expressed at time level n. To do this, define $\delta {F'}^n$ and $\delta {G'}^n$, such that

$$
\begin{aligned}
{F'}^{n+1}_{\mathrm{v}} &= {F'}^{n}_{\mathrm{v}} + \delta {F'}^{n}_{\mathrm{v}}, \\
{G'}^{n+1}_{\mathrm{v}} &= {G'}^{n}_{\mathrm{v}} + \delta {G'}^{n}_{\mathrm{v}},
\end{aligned}
\tag{3.3.15}
$$

where

$$
\begin{aligned}
F'_{\mathrm{v}} &= \frac{\partial\xi}{\partial x} F_{\mathrm{v}} + \frac{\partial\xi}{\partial y} G_{\mathrm{v}}, \\
G'_{\mathrm{v}} &= \frac{\partial\eta}{\partial x} F_{\mathrm{v}} + \frac{\partial\eta}{\partial y} G_{\mathrm{v}},
\end{aligned}
\tag{3.3.16}
$$

The viscous flux vector may be written in terms of first-order derivatives of the flow variables as discussed in the previous chapter. In the x direction it is given by

$$F_{\mathrm{v}} = -\left(\begin{array}{c} \rho\mathcal{D}_1 \frac{\partial c_1}{\partial x} \\ \vdots \\ \rho\mathcal{D}_n \frac{\partial c_n}{\partial x} \\ 2\mu\frac{\partial u}{\partial x} + \lambda\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) \\ \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \\ \rho e_{v1}\mathcal{D}_1 \frac{\partial c_1}{\partial x} + \kappa_{v1}\frac{\partial T_{vs}}{\partial x} \\ \vdots \\ \rho e_{vm}\mathcal{D}_m \frac{\partial c_m}{\partial x} + \kappa_{vm}\frac{\partial T_{vs}}{\partial x} \\ \rho e_e\mathcal{D}_e \frac{\partial c_e}{\partial x} + \kappa_e\frac{\partial T_e}{\partial x} \\ u\Big(2\mu\frac{\partial u}{\partial x} + \lambda\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)\Big) + v\mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \kappa\frac{\partial T}{\partial x} \\ + \sum_s \kappa_{vs}\frac{\partial T_{vs}}{\partial x} + \kappa_e\frac{\partial T_e}{\partial x} + \sum_s \rho h_s\mathcal{D}_s\frac{\partial c_s}{\partial x} \end{array} \right), \tag{3.3.17}$$

with a similar expression for G_{v}. The derivatives in the Cartesian coordinates may be converted to the general coordinate system through the use of equation (3.2.6).

For problems of interest, the viscous fluxes in the ξ direction are much smaller than those in the η direction. In this case we can apply the thin-layer assumption to the derivatives of the implicit viscous terms, which implies that the differences with respect to η are much larger than those with respect to ξ,

$$\frac{D}{\Delta\eta}\delta G'_{\mathrm{v}} \gg \frac{D}{\Delta\xi}\delta F'_{\mathrm{v}} \simeq 0. \tag{3.3.18}$$

It should be noted that all of the viscous derivatives will be retained in F'_{v} and G'_{v}, thus all of the viscous terms influence the converged solution. Therefore we need only find an expression for $\delta G'_{\mathrm{v}}$, which is given by

$$\delta G'_{\mathrm{v}} = \frac{\partial\eta}{\partial x}\delta F_{\mathrm{v}} + \frac{\partial\eta}{\partial y}\delta G_{\mathrm{v}}. \tag{3.3.19}$$

Applying the thin-layer assumption to equation (3.2.6) we have

$$\frac{\partial}{\partial x} \simeq \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta} \qquad \frac{\partial}{\partial y} \simeq \frac{\partial \eta}{\partial y}\frac{\partial}{\partial \eta}, \tag{3.3.20}$$

and thus we can write $\delta G'_{\mathrm{v}}$ as a function of the derivatives of the flow variables with respect to η only. Therefore

$$\delta G'_{\mathrm{v}} = -M_\eta \frac{\partial}{\partial \eta}\big(\delta \mathbf{V}\big). \tag{3.3.21}$$

The expression for the matrix M_η is given in Appendix D and the vector of non-conserved variables, $\mathbf{V}$, is introduced for convenience. In this case we let

$$\mathbf{V} = \Big(c_1,\ c_2,\ \ldots,\ c_n\ u,\ v,\ e_{v1},\ \ldots,\ e_{vm},\ e_e,\ T\Big)^T. \tag{3.3.22}$$

We can change variables from $\delta\mathbf{V}$ to δU by defining the Jacobian, N, to be $N = \frac{\partial \mathbf{V}}{\partial U}$, so that $\delta\mathbf{V} = N\delta U$. The details of these block matrices are given in Appendix D. Thus if we central difference[4] $\delta {G'}^n_{\mathrm{v}}$, we have

$$\frac{D}{\Delta\eta}\delta {G'}^n_{\mathrm{v}i,j+\frac{1}{2}} = -\frac{D_-}{\Delta\eta}\cdot M_\eta\Big(\frac{D_+}{\Delta\eta}N\delta U_{i,j}\Big). \tag{3.3.23}$$

Combining equations (3.3.14) and (3.3.23), we have the final form of the finite-volume difference equation which approximates the governing equations.

$$\begin{aligned}\Big\{I + \Delta t\Big[\frac{D_-}{\Delta\xi}\cdot {A'}^n_{+i+\frac{1}{2},j} + \frac{D_+}{\Delta\xi}\cdot {A'}^n_{-i-\frac{1}{2},j} + \frac{D_-}{\Delta\eta}\cdot {B'}^n_{+i,j+\frac{1}{2}} + \frac{D_+}{\Delta\eta}\cdot {B'}^n_{-i,j-\frac{1}{2}} \\ - \frac{D_-}{\Delta\eta}\cdot M^n_{\eta i,j+\frac{1}{2}}\Big(\frac{D_+}{\Delta\eta}N^n_{i,j}\Big) - C^n_{i,j}\Big]\Big\}\delta U^n_{i,j} = \Delta U^n_{i,j},\end{aligned} \tag{3.3.24}$$

where the right-hand side, $\Delta U^n_{i,j}$, is given by

[4] The viscous fluxes need not be flux-split because they are parabolic in nature.

$$\Delta U_{i,j}^n = \Delta t\, W_{i,j}^n - \Delta t\Big[\frac{D_-}{\Delta\xi}\cdot {A'}^n_{+i+\frac{1}{2},j} + \frac{D_+}{\Delta\xi}\cdot {A'}^n_{-i-\frac{1}{2},j} + \frac{D_-}{\Delta\eta}\cdot {B'}^n_{+i,j+\frac{1}{2}} + \frac{D_+}{\Delta\eta}\cdot {B'}^n_{+i,j-\frac{1}{2}}\Big]U_{i,j}^n - \Delta t\Big[\frac{D}{\Delta\xi}{F'}^n_{\mathrm{v}i,j} + \frac{D}{\Delta\eta}{G'}^n_{\mathrm{v}i,j}\Big]. \tag{3.3.25}$$

This completes the derivation of the difference equation used to solve the governing equations.

III.4 The Solution Procedure

Equation (3.3.24) represents the finite-volume approximation to the governing equations discussed in Chapter II. The technique for solving the difference equation is discussed in this section.

The difference equation (3.3.24) may be written at the point i, j as

$$\hat{A}_{i,j}\delta U_{i,j}^n + \hat{B}_{i,j}\delta U_{i,j+1}^n + \hat{C}_{i,j}\delta U_{i,j-1}^n = -\hat{D}_{i,j}\delta U_{i+1,j}^n - \hat{E}_{i,j}\delta U_{i-1,j}^n + \Delta U_{i,j}^n, \tag{3.4.1}$$

where the matrices with tildes are defined implicitly from equation (3.3.24) as

$$\begin{aligned}
\hat{A}_{i,j} &= I + \Delta t\left[{A'}^n_{+i+\frac{1}{2},j} - {A'}^n_{-i-\frac{1}{2},j} + {B'}^n_{+i,j+\frac{1}{2}} - {B'}^n_{-i,j-\frac{1}{2}} - C_{i,j}^n \right.\\
&\qquad\left. + M^n_{\eta i,j+\frac{1}{2}}N_{i,j}^n + M^n_{\eta i,j-\frac{1}{2}}N_{i,j}^n\right],\\
\hat{B}_{i,j} &= \Delta t\left[{B'}^n_{-i,j+\frac{1}{2}} - M^n_{\eta i,j+\frac{1}{2}}N^n_{i,j+1}\right],\\
\hat{C}_{i,j} &= \Delta t\left[-{B'}^n_{+i,j-\frac{1}{2}} - M^n_{\eta i,j-\frac{1}{2}}N^n_{i,j-1}\right],\\
\hat{D}_{i,j} &= \Delta t\, {A'}^n_{-i+\frac{1}{2},j}, \qquad \hat{E}_{i,j} = -\Delta t\, {A'}^n_{+i-\frac{1}{2},j}.
\end{aligned} \tag{3.4.2}$$

Equation (3.4.1) may be solved by a block-tridiagonal matrix inversion using Gauss-Seidel line-relaxation with alternating sweeps in the backward and forward ξ directions. The backward sweeps consist of the solution of

$$
\begin{aligned}
\hat{B}\delta U_{i,j+1}^{(k)} + \hat{A}\delta U_{i,j}^{(k)} + \hat{C}\delta U_{i,j-1}^{(k)} = \\
- \hat{D}\delta U_{i+1,j}^{(k)} - \hat{E}\delta U_{i-1,j}^{(k-1)} + \Delta U_{i,j}^{n}, \quad \text{for } k = 1,\ 3,\ \ldots
\end{aligned}
\tag{3.4.3}
$$

and the forward sweeps

$$
\begin{aligned}
\hat{B}\delta U_{i,j+1}^{(k)} + \hat{A}\delta U_{i,j}^{(k)} + \hat{C}\delta U_{i,j-1}^{(k)} = \\
- \hat{D}\delta U_{i+1,j}^{(k-1)} - \hat{E}\delta U_{i-1,j}^{(k)} + \Delta U_{i,j}^{n}, \quad \text{for } k = 2,\ 4,\ \ldots
\end{aligned}
\tag{3.4.4}
$$

During the first sweep, $k=1$, we set $\delta U_{i,j}^{(0)} = 0$. For the solutions that were obtained in the current work, only two sweeps were performed per time step.

The time advancement of the solution proceeds as follows. The explicit change in the solution at time level n is computed at all i, j locations and is stored. Then the first sweep is performed form the last i line of data to the first. Equation (3.4.3) is solved using a block-tridiagonal matrix inversion technique at each constant i line. The results for $\delta U_{i,j}^{n}$ are used as they become available. Next the backward sweep for $k=2$ is performed from the first i location to the last. Again this involves the solution of a series of block-tridiagonal equations during which, the most recently available data for $\delta U_{i,j}^{n}$ is used.

In this fashion an approximation to $\delta U_{i,j}^{n}$ is obtained and the solution may be advanced to time level $n+1$ using

$$
U_{i,j}^{n+1} = U_{i,j}^{n} + \delta U_{i,j}^{n}. \tag{3.4.5}
$$

III.5 The Treatment of the Boundary Conditions

The solution of equations (3.4.3) and (3.4.4) using a block-tridiagonal matrix inversion routine is straight-forward except for the treatment of the boundaries at the first and last j volumes. As we see from Figure 3.1, the boundary at surface $j=1\frac{1}{2}$ is represented by setting the values of the flow variables in the $j=1$ volume.

The following discussion concerns the treatment of the boundaries in the calculation of $\Delta U_{i,j}^{n}$ and in the implicit matrix inversion. The boundaries must be represented differently in each case.

Because of the way that we have divided the flux vectors into the inviscid and viscous parts, we must treat each part separately. For an impermeable wall, there is no flux of mass, momentum, or energy across the surface $j = 1\frac{1}{2}$ and therefore we have the condition that

$$G'_{\mathrm{I}\,i,1\frac{1}{2}} = \big(\underbrace{0,\ 0,\ \ldots,\ 0}_{n \text{ elements}},\ 0,\ p_{i,\mathrm{wall}},\ \underbrace{0,\ \ldots,\ 0}_{m \text{ elements}},\ 0,\ 0\big)^{T}, \tag{3.5.1}$$

which is derived by setting the velocity at the wall to zero. We can assume that the normal derivative of pressure at the wall is zero (from boundary layer theory) and set $p_{i,\mathrm{wall}} = p_{i,2}$.

The boundary conditions for the explicit viscous flux across the wall are set depending on the type of wall conditions being simulated. In this work, the wall is allowed to behave so that there is either a slip or no-slip velocity condition, and either an adiabatic or fixed temperature condition. The vibrational temperatures are assumed to be equilibrated with the wall temperature for the cases where a wall temperature is prescribed. The wall is fully non-catalytic in all cases, which implies that the diffusive flux of each species is zero at the wall. Also it is assumed that the appropriate condition for electron temperature is that $\partial T_e / \partial \eta = 0$ at the wall. In this case, the viscous flux at the wall is calculated by setting the points at $i, 1$ according to the following relations. For the species densities, we set

$$\rho_{s\,i,1} = \rho_{s\,i,2}, \qquad \text{for } s = 1, n. \tag{3.5.2}$$

The velocity conditions are

$$
\begin{aligned}
u'_{i,1} &= \begin{cases} u'_{i,2}, & \text{slip condition;} \\ -u'_{i,2}, & \text{no-slip condition,} \end{cases} \\
v'_{i,1} &= -v'_{i,2},
\end{aligned}
\tag{3.5.3}
$$

where u' and v' are the velocities normal and tangential to the relevant surface, respectively. These quantities are discussed in Appendix B. The temperatures in the wall point are

$$
\begin{aligned}
T_{i,1} &= \begin{cases} T_{i,2}, & \text{adiabatic condition;} \\ 2T_{i,\text{wall}} - T_{i,2}, & \text{fixed-wall temperature condition.} \end{cases} \\
T_{vs\,i,1} &= \begin{cases} T_{vs\,i,2}, & \text{adiabatic condition;} \\ 2T_{i,\text{wall}} - T_{vs\,i,2}, & \text{fixed-wall temperature condition.} \end{cases} \\
T_{e\,i,1} &= T_{e\,i,2}.
\end{aligned}
\tag{3.5.4}
$$

The boundary conditions for the implicit part of the solution are treated in a similar fashion. However, to understand how they are implemented we must consider the form of equation (3.4.1), which may be written in block matrix form as

$$
\begin{pmatrix}
I & -\mathbf{E}_{JL} & & & & & & \\
\hat{B}_{JL-1} & \hat{A}_{JL-1} & \hat{C}_{JL-1} & & & & & \\
 & & \ddots & & & & & \\
 & & \hat{B}_j & \hat{A}_j & \hat{C}_j & & & \\
 & & & & \ddots & & & \\
 & & & & \hat{B}_2 & \hat{A}_2 & \hat{C}_2 \\
 & & & & & -\mathbf{E}_1 & I
\end{pmatrix}_i
\begin{pmatrix}
\delta U_{i,JL} \\ \delta U_{i,JL-1} \\ \vdots \\ \delta U_{i,j} \\ \vdots \\ \delta U_{i,2} \\ \delta U_{i,1}
\end{pmatrix}
=
\begin{pmatrix}
0 \\ RHS_{i,JL-1} \\ \vdots \\ RHS_{i,j} \\ \vdots \\ RHS_{i,2} \\ 0
\end{pmatrix},
\tag{3.5.5}
$$

where $RHS_{i,j} = \Delta U_{i,j} - \hat{D}_{i,j}\delta U_{i+1,j} - \hat{E}_{i,j}\delta U_{i-1,j}$, which is the right-hand side of equation (3.4.1). The top equation is used to set the conditions in the free-stream at point $j = JL$. However, the supersonic free-stream is prescribed and does not change, therefore $\delta U_{i,JL} = 0$ and we can remove this equation as trivial. The bottom equation is used to set the wall boundary condition for the inviscid flux only. We require that $\delta\rho_{s\,i,1} = \delta\rho_{s\,i,2}$, $\delta\rho u'_{i,1} = \delta\rho u'_{i,2}$, $\delta\rho v'_{i,1} = -\delta\rho v'_{i,2}$, $\delta E_{vs\,i,1} = \delta E_{vs\,i,2}$, $\delta E_{e\,i,1} = \delta E_{e\,i,2}$, and $\delta E_{i,1} = \delta E_{i,2}$ to maintain impermeability of the wall. Thus we can form the matrix $\mathbf{E}_{i,1}$, such that $\delta U_{i,1} = \mathbf{E}_{i,1}\delta U_{i,2}$, to make these conditions hold.

For the implicit viscous flux at the wall we are required to enforce conditions similar to those applied to the explicit viscous flux. In this case, we have

$$\delta\rho_{s\,i,1} = \delta\rho_{s\,i,2}, \qquad \text{for } s = 1, n, \tag{3.5.6}$$

$$\begin{aligned} \delta u'_{i,1} &= \begin{cases} \delta u'_{i,2}, & \text{slip condition;} \\ -\delta u'_{i,2}, & \text{no-slip condition,} \end{cases} \\ \delta v'_{i,1} &= -\delta v'_{i,2}, \end{aligned} \tag{3.5.7}$$

and

$$\begin{aligned} \delta T_{i,1} &= \begin{cases} \delta T_{i,2}, & \text{adiabatic condition;} \\ -\delta T_{i,2}, & \text{fixed-wall temperature condition.} \end{cases} \\ \delta T_{vs\,i,1} &= \begin{cases} \delta T_{vs\,i,2}, & \text{adiabatic condition;} \\ -\delta T_{vs\,i,2}, & \text{fixed-wall temperature condition.} \end{cases} \\ \delta T_{e\,i,1} &= \delta T_{e\,i,2}. \end{aligned} \tag{3.5.8}$$

Where we have assumed that the wall temperature is not a function of time. Because we have used the bottom equation to implement the inviscid wall conditions, we must set the implicit viscous terms at the wall by altering the two block matrices $\hat{A}_{i,2}$ and $\hat{C}_{i,2}$. To do this we remove the term $-\Delta t\, M_{\eta i,1\frac{1}{2}} N_{i,1}$ from $\hat{C}_{i,2}$ to yield $\hat{C'}_{i,2}$. This prevents the viscous term from multiplying the previously altered $\delta U_{i,1}$. Secondly, the matrix $M_{\eta i,1\frac{1}{2}}$ that appears in $\hat{A}_{i,2}$ must be modified so that the conditions in equations (3.5.6) to (3.5.8) are satisfied. The resulting M_η matrix is given in Appendix D and the new $\hat{A}_{i,2}$ becomes $\hat{A'}_{i,2}$. The next to last equation in the matrix equation (3.5.5) may be modified as follows

$$\begin{aligned}
&\hat{B}_{i,2}\delta U_{i,3} + \hat{A'}_{i,2}\delta U_{i,2} + \hat{C'}_{i,2}\delta U_{i,1} = RHS_{i,2} \\
&\hat{B}_{i,2}\delta U_{i,3} + \left(\hat{A'}_{i,2} + \hat{C'}_{i,2}\mathbf{E}_{i,1}\right)\delta U_{i,2} = RHS_{i,2} \\
&\hat{B}_{i,2}\delta U_{i,3} + \hat{A''}_{i,2}\delta U_{i,2} = RHS_{i,2},
\end{aligned} \tag{3.5.9}$$

where we have defined $\hat{A''}_{i,2} = \hat{A'}_{i,2} + \hat{C'}_{i,2}\mathbf{E}_{i,1}$ The matrix equation (3.5.5) now reduces to

$$\begin{pmatrix} \hat{A}_{JL-1} & \hat{C}_{JL-1} & & & & \\ & \ddots & & & & \\ & \hat{B}_j & \hat{A}_j & \hat{C}_j & & \\ & & & \ddots & & \\ & & & \hat{B}_2 & \hat{A''}_2 \end{pmatrix}_i \begin{pmatrix} \delta U_{i,JL-1} \\ \vdots \\ \delta U_{i,j} \\ \vdots \\ \delta U_{i,2} \end{pmatrix} = \begin{pmatrix} RHS_{i,JL-1} \\ \vdots \\ RHS_{i,j} \\ \vdots \\ RHS_{i,2} \end{pmatrix}, \tag{3.5.10}$$

Using this technique of including the boundary conditions in the tridiagonal equation set we can simulate any set of boundary conditions required.

.