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Proteus Two-Dimensional Navier-Stokes Computer Code–Version 2.0

Volume 1–Analysis Description

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CONTENTS

PRINCIPAL NOTATION

SYMBOLS

Unless specified otherwise, all variables are nondimensional.

Symbol	Definition
a	Speed of sound.
$\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$	Coefficient submatrices in block tridiagonal system of equations.
$\mathbf{A'}$, $\mathbf{B'}$, $\mathbf{C'}$	Coefficient submatrices for boundary conditions.
c_p, c_v	Specific heats at constant pressure and volume.
$\mathbf{E}$, $\mathbf{F}$	Inviscid flux vectors in the Cartesian or cylindrical coordinate form of the governing equations.
$\hat{\mathbf{E}}$, $\hat{\mathbf{F}}$	Inviscid flux vectors in the computational coordinate form of the governing equations.
E_T	Total energy per unit volume.
$\mathbf{E}_V$, $\mathbf{F}_V$	Viscous flux vectors in the Cartesian or cylindrical coordinate form of the governing equations.
$\hat{\mathbf{E}}_V$, $\hat{\mathbf{F}}_V$	Viscous flux vectors in the computational coordinate form of the governing equations.
$\hat{\mathbf{E}}_{V_1}$, $\hat{\mathbf{F}}_{V_1}$	Non-cross derivative viscous flux vectors in the computational coordinate form of the governing equations.
$\hat{\mathbf{E}}_{V_2}$, $\hat{\mathbf{F}}_{V_2}$	Cross derivative viscous flux vectors in the computational coordinate form of the governing equations.
$\mathbf{F}$, $\mathbf{G}$	Flux vectors in the Cartesian or cylindrical coordinate form of the k-ε turbulence model equations.
$\hat{\mathbf{F}}$, $\hat{\mathbf{G}}$	Flux vectors in the computational coordinate form of the k-ε turbulence model equations.
h_T	Stagnation enthalpy per unit mass.
$\mathbf{H}$, $\mathbf{H}_V$	Non-derivative inviscid and viscous terms in the Cartesian coordinate form of the governing equations for axisymmetric flow.
$\hat{\mathbf{H}}$, $\hat{\mathbf{H}}_V$	Non-derivative inviscid and viscous terms in the computational coordinate form of the governing equations for axisymmetric flow.
i, j	Grid indices in the ξ and η directions.
J	Jacobian matrix of the generalized grid transformation.
k	Effective thermal conductivity coefficient.
k	Turbulent kinetic energy.
k_l, k_t	Laminar and turbulent thermal conductivity coefficient.
L_r	Dimensional reference length.
N_{eq}	Number of governing equations being solved.

Symbol	Definition
N_1, N_2	Number of grid points in the ξ and η directions.
p	Static pressure.
Pr_r	Reference Prandtl number.
Pr_l, Pr_t	Laminar and turbulent Prandtl number.
q_x, q_r	Heat fluxes in the cylindrical x and r directions.
q_x, q_y	Heat fluxes in the Cartesian x and y directions.
$\mathbf{Q}$	Vector of dependent variables in the Cartesian or cylindrical coordinate form of the governing equations.
$\hat{\mathbf{Q}}$	Vector of dependent variables in the computational coordinate form of the governing equations.
R	Gas constant.
Re_r	Reference Reynolds number.
$\mathbf{S}$	Source term subvector in block tridiagonal system of equations.
$\mathbf{S}'$	Source term subvector for boundary conditions.
$\mathbf{S}$, $\mathbf{T}$	Non-derivative terms in the Cartesian or cylindrical coordinate form of the k-ε turbulence model equations.
$\hat{\mathbf{S}}$, $\hat{\mathbf{T}}$	Non-derivative terms in the computational coordinate form of the k-ε turbulence model equations.
t	Physical time.
T	Static temperature.
u, v	Velocities in the Cartesian x and y directions.
u, v, w	Velocities in the cylindrical x, r, and swirl directions.
$\mathbf{W}$	Vector of dependent variables in the Cartesian or cylindrical coordinate form of the k-ε turbulence model equations.
$\hat{\mathbf{W}}$	Vector of dependent variables in the computational coordinate form of the k-ε turbulence model equations.
x, r	Cylindrical axial and radial coordinates.
x, y	Cartesian coordinates.
γ	Ratio of specific heats, c_p/c_v.
δ	Difference operator.
Δ, ∇	First-order forward and backward difference operators.
ε	Turbulent dissipation rate.
$\varepsilon_E^{(2)}$, $\varepsilon_E^{(4)}$	Second- and fourth-order explicit artificial viscosity coefficients in constant coefficient model.
ε_I	Implicit artificial viscosity coefficient.
$\varepsilon_\xi^{(2)}$, $\varepsilon_\xi^{(4)}$, etc.	Second- and fourth-order artificial viscosity coefficients in nonlinear coefficient model.
θ_1, θ_2, θ_3	Parameters determining type of time differencing used.
κ_2, κ_4	Constants in nonlinear coefficient artificial viscosity model.
λ	Effective second coefficient of viscosity.

Symbol	Definition
$\lambda_l,\ \lambda_t$	Laminar and turbulent second coefficient of viscosity.
μ	Effective viscosity coefficient.
$\mu_l,\ \mu_t$	Laminar and turbulent viscosity coefficient.
v	Laminar kinematic viscosity.
ξ, η	Computational coordinate directions.
ρ	Static density.
σ	Pressure gradient scaling parameter in nonlinear coefficient artificial viscosity model.
τ	Computational time.
$\tau_{xx},\ \tau_{xy},$ etc.	Elements of shear stress tensor.
ψ	Spectral radius in nonlinear coefficient artificial viscosity model.

SUBSCRIPTS

Subscript	Definition
i, j	Denotes grid location in ξ and η directions.
r	Denotes dimensional reference condition.
t	Denotes differentiation with respect to physical time.
x, r	Denotes differentiation with respect to cylindrical coordinate directions.
x, y	Denotes differentiation with respect to Cartesian coordinate directions.
ξ, η	Denotes differentiation with respect to computational coordinate directions.
τ	Denotes differentiation with respect to computational time.

SUPERSCRIPTS

Superscript	Definition
n	Denotes time level.
*	Denotes solution after first ADI sweep.

PROTEUS TWO-DIMENSIONAL
NAVIER-STOKES COMPUTER CODE - VERSION 2.0
Volume 1 - Analysis Description

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SUMMARY

A computer code called *Proteus* has been developed to solve the two-dimensional planar or axisymmetric, Reynolds-averaged, unsteady compressible Navier-Stokes equations in strong conservation law form. The objective in this effort has been to develop a code for aerospace propulsion applications that is easy to use and easy to modify. Code readability, modularity, and documentation have been emphasized.

The governing equations are written in Cartesian coordinates and transformed into generalized nonorthogonal body-fitted coordinates. They are solved by marching in time using a fully-coupled alternating-direction-implicit solution procedure with generalized first- or second-order time differencing. The boundary conditions are also treated implicitly,-and may be steady or unsteady. Spatially periodic boundary conditions are also available. All terms, including the diffusion terms, are linearized using second-order Taylor series expansions. Turbulence is modeled using either an algebraic or two-equation eddy viscosity model.

The program contains many operating options. The governing equations may be solved for two-dimensional planar flow, or axisymmetric flow with or without swirl. The thin-layer or Euler equations may be solved as subsets of the Navier-Stokes equations. The energy equation may be eliminated by the assumption of constant total enthalpy. Explicit and implicit artificial viscosity may be used to damp pre- and post-shock oscillations in supersonic flow and to minimize odd-even decoupling caused by central spatial differencing of the convective terms in high Reynolds number flow. Several time step options are available for convergence acceleration, including a locally variable time step and global time step cycling. Simple Cartesian or polar grids may be generated internally by the program. More complex geometries require an externally generated computational coordinate system.

The documentation is divided into three volumes. Volume 1, the current volume, is the Analysis Description, and presents the equations and solution procedure used in *Proteus*. It describes in detail the governing equations, the turbulence model, the linearization of the equations and boundary conditions, the time and space differencing formulas, the ADI solution procedure, and the artificial viscosity models. Volume 2 is the User's Guide, and contains information needed to run the program. It describes the program's general features, the input and output, the procedure for setting up initial conditions, the computer resource requirements, the diagnostic messages that may be generated, the job control language used to run the program, and several test cases. Volume 3 is the Programmer's Reference, and contains detailed information useful when modifying the program. It describes the program structure, the Fortran variables stored in common blocks, and the details of each subprogram.

Version 1.0 of the two-dimensional *Proteus* code was released in late 1989. The current documentation covers Version 2.0, released in early 1992.

1.0 INTRODUCTION

Much of the effort in applied computational fluid dynamics consists of modifying an existing program for whatever geometries and flow regimes are of current interest to the researcher. Unfortunately, nearly all of the available non-proprietary programs were started as research projects with the emphasis on demonstrating the numerical algorithm rather than ease of use or ease of modification. The developers usually intend to clean up and formally document the program, but the immediate need to extend it to new geometries and flow regimes takes precedence.

The result is often a haphazard collection of poorly written code without any consistent structure. An extensively modified program may not even perform as expected under certain combinations of operating options. Each new user must invest considerable time and effort in attempting to understand the underlying structure of the program if intending to do anything more than run standard test cases with it. The user's subsequent modifications further obscure the program structure and therefore make it even more difficult for others to understand.

The *Proteus* two-dimensional Navier-Stokes computer program is a user-oriented and easily-modifiable flow analysis program for aerospace propulsion applications. Readability, modularity, and documentation were primary objectives during its development. The entire program was specified, designed, and implemented in a controlled, systematic manner. Strict programming standards were enforced by immediate peer review of code modules; Kernighan and Plauger (1978) provided many useful ideas about consistent programming style. Every subroutine contains an extensive comment section describing the purpose, input variables, output variables, and calling sequence of the subroutine. With just three clearly-defined exceptions, the entire program is written in ANSI standard Fortran 77 to enhance portability. A master version of the program is maintained and periodically updated with corrections, as well as extensions of general interest (e.g., turbulence models.)

The *Proteus* program solves the unsteady, compressible, Reynolds-averaged Navier-Stokes equations in strong conservation law form. The governing equations are written in Cartesian coordinates and transformed into generalized nonorthogonal body-fitted coordinates. They are solved by marching in time using a fully-coupled alternating-direction-implicit (ADI) scheme with generalized time and space differencing (Briley and McDonald, 1977; Beam and Warming, 1978). Turbulence is modeled using either the Baldwin and Lomax (1978) algebraic eddy-viscosity model or the Chien (1982) two-equation model. All terms, including the diffusion terms, are linearized using second-order Taylor series expansions. The boundary conditions are treated implicitly, and may be steady or unsteady. Spatially periodic boundary conditions are also available.

The program contains many operating options. The governing equations may be solved for two-dimensional planar flow, or axisymmetric flow with or without swirl. The thin-layer or Euler equations may be solved as subsets of the Navier-Stokes equations. The energy equation may be eliminated by the assumption of constant total enthalpy. Explicit and implicit artificial viscosity may be used to damp pre- and post-shock oscillations in supersonic flow and to minimize odd-even decoupling caused by central spatial differencing of the convective terms in high Reynolds number flow. Several time step options are available for convergence acceleration, including a locally variable time step and global time step cycling. Simple grids may be generated internally by the program; more complex geometries require external grid generation, such as that developed by Chen and Schwab (1988).

The documentation is divided into three volumes. Volume 1, the current volume, is the Analysis Description, and presents the equations and solution procedure used in *Proteus*. It describes in detail the governing equations, the turbulence model, the linearization of the equations and boundary conditions, the time and space differencing formulas, the ADI solution procedure, and the artificial viscosity models. Volume 2 is the User's Guide, and contains information needed to run the program. It describes the program's general features, the input and output, the procedure for setting up initial conditions, the computer resource

requirements, the diagnostic messages that may be generated, the job control language used to run the program, and several test cases. Volume 3 is the Programmer's Reference, and contains detailed information useful when modifying the program. It describes the program structure, the Fortran variables stored in common blocks, and the details of each subprogram.

Version 1.0 of the two-dimensional *Proteus* code was released in late 1989 (Towne, Schwab, Benson, and Suresh, 1990). The current documentation covers Version 2.0, released in early 1992.

The authors would like to acknowledge the significant contributions made by their co-workers. Tom Benson provided part of the original impetus for the development of *Proteus*, and did the original coding of the block tri-diagonal inversion routines. Simon Chen did the original coding of the Baldwin-Lomax turbulence model, and consulted in the implementation of the nonlinear coefficient artificial viscosity model. William Kunik developed the original code for computing the metrics of the generalized nonorthogonal grid transformation. Frank Molls has created separate diagonalized and patched-grid versions of the code. Ambady Suresh did the original coding for the second-order time differencing and for the nonlinear coefficient artificial viscosity model. These people, along with Dick Cavicchi, Julie Conley, Jason Solbeck, and Pat Zeman, have also run many debugging and verification cases.

2.0 GOVERNING EQUATIONS

2.1 GOVERNING EQUATIONS IN CARTESIAN COORDINATES

The basic governing equations are the two-dimensional compressible Navier-Stokes equations. These equations may be found in several standard references (e.g., Hughes and Gaylord, 1964; Schlichting, 1968; White, 1974; Anderson, Tannehill, and Pletcher, 1984). In Cartesian coordinates, the two-dimensional planar equations[1] can be written in strong conservation law form using vector notation as

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = \frac{\partial E_V}{\partial x} + \frac{\partial F_V}{\partial y} \qquad (2.1)$$

where

$$Q = [\rho \quad \rho u \quad \rho v \quad E_T]^T \qquad (2.2a)$$

$$E = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (E_T + p)u \end{bmatrix} \qquad (2.2b)$$

$$F = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (E_T + p)v \end{bmatrix} \qquad (2.2c)$$

$$E_V = \frac{1}{Re_r} \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ u\tau_{xx} + v\tau_{xy} - \frac{1}{Pr_r} q_x \end{bmatrix} \qquad (2.2d)$$

$$F_V = \frac{1}{Re_r} \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ u\tau_{xy} + v\tau_{yy} - \frac{1}{Pr_r} q_y \end{bmatrix} \qquad (2.2e)$$

Equation (2.1) thus represents, in order, the continuity, x-momentum, y-momentum, and energy equations, with dependent variables ρ, ρu, ρv, and E_T.

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[1] *Proteus* can be used for both two-dimensional planar or axisymmetric flow. However, the axisymmetric equations have some additional terms that complicate the analysis somewhat. For the sake of clarity, the main body of this report describes the two-dimensional planar analysis, and the axisymmetric analysis is described in Appendix B.

The shear stresses and heat fluxes are given by

$$\tau_{xx} = 2\mu \frac{\partial u}{\partial x} + \lambda \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)$$

$$\tau_{yy} = 2\mu \frac{\partial v}{\partial y} + \lambda \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)$$

$$\tau_{xy} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \tag{2.3}$$

$$q_x = -k \frac{\partial T}{\partial x}$$

$$q_y = -k \frac{\partial T}{\partial y}$$

In these equations, t represents time; x and y represent the Cartesian coordinate directions; u and v are the velocities in the x and y directions; ρ, p, and T are the static density, pressure, and temperature; E_T is the total energy per unit volume; and μ, λ, and k are the coefficient of viscosity, second coefficient of viscosity, and coefficient of thermal conductivity.

All of the above equations have been nondimensionalized using appropriate normalizing conditions. Lengths have been nondimensionalized by L_r, velocities by u_r, density by ρ_r, temperature by T_r, viscosity by μ_r, thermal conductivity by k_r, pressure and total energy by $\rho_r u_r^2$, and time by L_r/u_r. The reference Reynolds and Prandtl numbers are thus defined as $Re_r = \rho_r u_r L_r/\mu_r$ and $Pr_r = \mu_r u_r^2/k_r T_r$.[2]

Turbulence is modeled using the Boussinesq approach (Schlichting, 1968). The equations presented in this section are thus used for both laminar and turbulent flow. For turbulent flow they represent the Reynolds time-averaged form of the Navier-Stokes equations, with density fluctuations neglected. They may also be interpreted as the Favre or mass-weighted time-averaged form of the equations. With Favre time averaging, however, the velocities and thermal variables represent mass-averaged quantities defined by $\tilde{u} = \overline{\rho u}/\bar{\rho}$, etc., where the overbar represents a conventional Reynolds time-averaged quantity. Details on Reynolds and Favre time-averaging procedures may be found in Cebeci and Smith (1974), and in Anderson, Tannehill, and Pletcher (1984). In either case, μ, λ, and k represent *effective* coefficients. For example, in turbulent flow $\mu = \mu_l + \mu_t$, where μ_l and μ_t are the laminar and turbulent viscosity coefficients, and μ_t comes from some appropriate turbulence model. The models currently available in the *Proteus* code are the algebraic eddy viscosity model of Baldwin and Lomax (1978) and the two-equation model of Chien (1982), implemented as described in Section 9.0.

2.2 EQUATION OF STATE

In addition to the equations presented above, an equation of state is required to relate pressure to the dependent variables. Any appropriate equation, or even table, could be used. The equation currently built into the *Proteus* code is the equation of state for thermally perfect gases, $p = \rho RT$, where R is the gas constant. For calorically perfect gases, this can be rewritten as

$$p = (\gamma - 1)\left[E_T - \frac{1}{2}\rho(u^2 + v^2) \right] \tag{2.4}$$

where γ is the ratio of specific heats, c_p/c_v. Here the gas constant and specific heats have been nondimensionalized by u_r^2/T_r.

If the flow is such that we can assume a perfect gas with constant stagnation enthalpy, the energy equation may be eliminated. This assumption is reasonable, for example, in inviscid regions, and in

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[2] Note that this Prandtl number does not have a physically meaningful value, but is merely defined by a combination of the normalizing conditions for c_p, μ, and k that appear when the equations are nondimensionalized.

adiabatic wall boundary layers if the Prandtl number is near 1 (Briley and McDonald, 1977). The stagnation enthalpy is defined as

$$h_T = c_p T + \frac{1}{2} (u^2 + v^2)$$

(2.5)

Here the stagnation enthalpy is nondimensionalized by u_r^2. The temperature is thus

$$T = \frac{1}{c_p} \left[h_T - \frac{1}{2} (u^2 + v^2) \right]$$

(2.6)

and the equation of state becomes

$$p = \frac{\gamma - 1}{\gamma} \rho \left[h_T - \frac{1}{2} (u^2 + v^2) \right]$$

(2.7)

This equation of state does not require the total energy E_T, and the energy equation need not be solved. The total energy may be computed from

$$E_T = \rho h_T - p$$

(2.8)

2.3 GENERALIZED GRID TRANSFORMATION

Because the governing equations in the previous section are written in Cartesian coordinates, they are not well suited for general geometric configurations. For most applications a body-fitted coordinate system is desired. This greatly simplifies the application of boundary conditions and the bookkeeping in the numerical method used to solve the equations. The following generalized grid transformation, which can be orthogonal or nonorthogonal, is therefore used to transform the governing equations from physical (x, y, t) coordinates to rectangular orthogonal computational (ξ, η, τ) coordinates.

$$\begin{aligned} \xi &= \xi(x, y, t) \\ \eta &= \eta(x, y, t) \\ \tau &= t \end{aligned}$$

(2.9)

In *Proteus*, the spatial computational domain is square, with ξ and η each running from 0 to 1. Using the chain rule for partial differentiation, the derivatives in the Cartesian form of the governing equations can be replaced using the following expressions.

$$\begin{aligned} \frac{\partial}{\partial x} &= \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial y} &= \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial t} &= \xi_t \frac{\partial}{\partial \xi} + \eta_t \frac{\partial}{\partial \eta} + \frac{\partial}{\partial \tau} \end{aligned}$$

(2.10)

In the above equations, and in those to follow, subscripts x and y, or ξ and η, denote partial differentiation in that coordinate direction. The only task remaining, then, is to develop expressions for the metric coefficients ξ_x, η_x, etc. In differential form we can write

$$\begin{aligned} d\xi &= \xi_x dx + \xi_y dy + \xi_t dt \\ d\eta &= \eta_x dx + \eta_y dy + \eta_t dt \\ d\tau &= dt \end{aligned}$$

In matrix form this becomes

$$\begin{bmatrix} d\xi \\ d\eta \\ d\tau \end{bmatrix} = \begin{bmatrix} \xi_x & \xi_y & \xi_t \\ \eta_x & \eta_y & \eta_t \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} dx \\ dy \\ dt \end{bmatrix}$$

Similarly,

$$\begin{bmatrix} dx \\ dy \\ dt \end{bmatrix} = \begin{bmatrix} x_\xi & x_\eta & x_\tau \\ y_\xi & y_\eta & y_\tau \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} d\xi \\ d\eta \\ d\tau \end{bmatrix}$$

Therefore,

$$\begin{bmatrix} \xi_x & \xi_y & \xi_t \\ \eta_x & \eta_y & \eta_t \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} x_\xi & x_\eta & x_\tau \\ y_\xi & y_\eta & y_\tau \\ 0 & 0 & 1 \end{bmatrix}^{-1}$$

After taking the inverse,

$$\begin{bmatrix} \xi_x & \xi_y & \xi_t \\ \eta_x & \eta_y & \eta_t \\ 0 & 0 & 1 \end{bmatrix} = J \begin{bmatrix} y_\eta & -x_\eta & x_\eta y_\tau - y_\eta x_\tau \\ -y_\xi & x_\xi & y_\xi x_\tau - x_\xi y_\tau \\ 0 & 0 & 1/J \end{bmatrix}$$

where J is the Jacobian of the transformation,

$$J = \frac{\partial(\xi, \eta)}{\partial(x,y)} = \begin{vmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{vmatrix}$$

$$J = \xi_x \eta_y - \xi_y \eta_x \qquad (2.11)$$

This can be evaluated from the known physical (x, y) coordinates by noting $J = 1/J^{-1}$ and

$$J^{-1} = \frac{\partial(x,y)}{\partial(\xi, \eta)} = \begin{vmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{vmatrix}$$

$$J^{-1} = x_\xi y_\eta - x_\eta y_\xi \qquad (2.12)$$

The metric coefficients themselves are

$$\xi_x = J y_\eta$$

$$\xi_y = - J x_\eta$$

$$\eta_x = - J y_\xi \qquad (2.13)$$

$$\eta_y = J x_\xi$$

$$\xi_t = - x_\tau \xi_x - y_\tau \xi_y$$

$$\eta_t = - x_\tau \eta_x - y_\tau \eta_y$$

Unless the physical coordinates (x, y) are defined analytically as functions of the computational coordinates (ξ, η), the metric coefficients must be computed numerically.

2.4 GOVERNING EQUATIONS IN COMPUTATIONAL COORDINATES

Applying the generalized grid transformation of the previous section to equation (2.1) yields

$$\mathbf{Q}_\tau + \mathbf{Q}_\xi \xi_t + \mathbf{Q}_\eta \eta_t + \mathbf{E}_\xi \xi_x + \mathbf{E}_\eta \eta_x + \mathbf{F}_\xi \xi_y + \mathbf{F}_\eta \eta_y - \mathbf{E}_{V_\xi} \xi_x - \mathbf{E}_{V_\eta} \eta_x - \mathbf{F}_{V_\xi} \xi_y - \mathbf{F}_{V_\eta} \eta_y = 0 \qquad (2.14)$$

This equation is in chain-rule, or weakly conservative form. That is, the conservation flow variables are used, but the metrics appear as coefficients of the derivatives instead of inside the derivatives. Following Vinokur (1974), the strong conservation law form can be recovered by first dividing by the Jacobian then adding and subtracting like terms. For example, the $\mathbf{E}_\xi \xi_x$ term becomes

$$\frac{\mathbf{E}_\xi \xi_x}{J} = \left[\frac{\mathbf{E}\xi_x}{J} \right]_\xi - \mathbf{E}\left(\frac{\xi_x}{J} \right)_\xi$$

Doing this for all the terms, and rearranging, results in

$$\left(\frac{\mathbf{Q}}{J} \right)_\tau + \left[\frac{\mathbf{E}\xi_x + \mathbf{F}\xi_y + \mathbf{Q}\xi_t}{J} \right]_\xi + \left[\frac{\mathbf{E}\eta_x + \mathbf{F}\eta_y + \mathbf{Q}\eta_t}{J} \right]_\eta$$

$$- \left[\frac{\mathbf{E}_V \xi_x + \mathbf{F}_V \xi_y}{J} \right]_\xi - \left[\frac{\mathbf{E}_V \eta_x + \mathbf{F}_V \eta_y}{J} \right]_\eta$$

$$- \mathbf{Q}\left\{ \left(\frac{1}{J} \right)_\tau + \left(\frac{\xi_t}{J} \right)_\xi + \left(\frac{\eta_t}{J} \right)_\eta \right\} - (\mathbf{E} - \mathbf{E}_V)\left\{ \left(\frac{\xi_x}{J} \right)_\xi + \left(\frac{\eta_x}{J} \right)_\eta \right\}$$

$$- (\mathbf{F} - \mathbf{F}_V)\left\{ \left(\frac{\xi_y}{J} \right)_\xi + \left(\frac{\eta_y}{J} \right)_\eta \right\} = 0 \qquad (2.15)$$

The last three terms, in braces, are called the metric invariant terms. By using the expressions for the metric coefficients, given by equations (2.13), one can show that the metric invariants are identically zero. In two dimensions, this is also true when derivatives are approximated by the finite difference formulas of Section 5.0.[3] With the metric invariant terms eliminated, no metrics or flow variables appear as coefficients, and the strong conservation law form of the governing equations has been recovered.

Equation (2.15) can be rewritten as

$$\frac{\partial \hat{\mathbf{Q}}}{\partial \tau} + \frac{\partial \hat{\mathbf{E}}}{\partial \xi} + \frac{\partial \hat{\mathbf{F}}}{\partial \eta} = \frac{\partial \hat{\mathbf{E}}_V}{\partial \xi} + \frac{\partial \hat{\mathbf{F}}_V}{\partial \eta} \qquad (2.16)$$

where

$$\hat{\mathbf{Q}} = \frac{\mathbf{Q}}{J}$$

$$\hat{\mathbf{E}} = \frac{1}{J}(\mathbf{E}\xi_x + \mathbf{F}\xi_y + \mathbf{Q}\xi_t)$$

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[3] This is not necessarily true in three dimensions, however.

$$\hat{\mathbf{F}} = \frac{1}{J} (\mathbf{E}\eta_x + \mathbf{F}\eta_y + \mathbf{Q}\eta_t)$$

$$\hat{\mathbf{E}}_V = \frac{1}{J} (\mathbf{E}_V \xi_x + \mathbf{F}_V \xi_y)$$

$$\hat{\mathbf{F}}_V = \frac{1}{J} (\mathbf{E}_V \eta_x + \mathbf{F}_V \eta_y)$$

Using equations (2.2a) through (2.2e) these can be expanded as

$$\hat{\mathbf{Q}} = \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad E_T]^T \tag{2.17a}$$

$$\hat{\mathbf{E}} = \frac{1}{J} \begin{bmatrix} \rho u \xi_x + \rho v \xi_y + \rho \xi_t \\ (\rho u^2 + p)\xi_x + \rho uv\xi_y + \rho u\xi_t \\ \rho uv\xi_x + (\rho v^2 + p)\xi_y + \rho v\xi_t \\ (E_T + p)u\xi_x + (E_T + p)v\xi_y + E_T \xi_t \end{bmatrix} \tag{2.17b}$$

$$\hat{\mathbf{F}} = \frac{1}{J} \begin{bmatrix} \rho u \eta_x + \rho v \eta_y + \rho \eta_t \\ (\rho u^2 + p)\eta_x + \rho uv\eta_y + \rho u\eta_t \\ \rho uv\eta_x + (\rho v^2 + p)\eta_y + \rho v\eta_t \\ (E_T + p)u\eta_x + (E_T + p)v\eta_y + E_T \eta_t \end{bmatrix} \tag{2.17c}$$

$$\hat{\mathbf{E}}_V = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} 0 \\ \tau_{xx}\xi_x + \tau_{xy}\xi_y \\ \tau_{xy}\xi_x + \tau_{yy}\xi_y \\ \beta_x\xi_x + \beta_y\xi_y \end{bmatrix} \tag{2.17d}$$

$$\hat{\mathbf{F}}_V = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} 0 \\ \tau_{xx}\eta_x + \tau_{xy}\eta_y \\ \tau_{xy}\eta_x + \tau_{yy}\eta_y \\ \beta_x\eta_x + \beta_y\eta_y \end{bmatrix} \tag{2.17e}$$

where

$$\beta_x = u\tau_{xx} + v\tau_{xy} - \frac{1}{Pr_r} q_x$$

$$\beta_y = u\tau_{xy} + v\tau_{yy} - \frac{1}{Pr_r} q_y$$

In the viscous terms, the shear stresses and heat fluxes are defined exactly as in equations (2.3), except the derivatives in the Cartesian coordinate directions must be evaluated using the chain rule. For example,

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \xi} \xi_x + \frac{\partial u}{\partial \eta} \eta_x$$

Note that $\hat{\mathbf{F}}$ and $\hat{\mathbf{F}}_V$ have exactly the same form as $\hat{\mathbf{E}}$ and $\hat{\mathbf{E}}_V$, but with ξ replaced by η.

3.0 TIME DIFFERENCING

The governing equations are solved by marching in time from some known set of initial conditions using a finite difference technique. The time differencing scheme currently used in *Proteus* is the generalized scheme of Beam and Warming (1978). The time derivative term in equation (2.16) is written as

$$\frac{\partial \hat{Q}}{\partial \tau} \simeq \frac{\Delta \hat{Q}^n}{\Delta \tau} = \frac{\theta_1}{1+\theta_2} \frac{\partial(\Delta \hat{Q}^n)}{\partial \tau} + \frac{1}{1+\theta_2} \frac{\partial \hat{Q}^n}{\partial \tau} + \frac{\theta_2}{1+\theta_2} \frac{\Delta \hat{Q}^{n-1}}{\Delta \tau}$$
$$+ O\left[\left(\theta_1 - \frac{1}{2} - \theta_2\right)\Delta\tau, (\Delta\tau)^2\right]$$

or,

$$\Delta \hat{Q}^n = \frac{\theta_1 \Delta\tau}{1+\theta_2} \frac{\partial(\Delta \hat{Q}^n)}{\partial \tau} + \frac{\Delta\tau}{1+\theta_2} \frac{\partial \hat{Q}^n}{\partial \tau} + \frac{\theta_2}{1+\theta_2} \Delta \hat{Q}^{n-1} + O\left[\left(\theta_1 - \frac{1}{2} - \theta_2\right)(\Delta\tau)^2, (\Delta\tau)^3\right] \qquad (3.1)$$

where $\Delta \hat{Q}^n = \hat{Q}^{n+1} - \hat{Q}^n$. The superscripts n and $n+1$ denote the known and unknown time levels, respectively.

The parameters θ_1 and θ_2 determine the type of time differencing scheme used. Some of the methods available with the above formula are given in the following table.

θ_1	θ_2	Method	Truncation Error
0	0	Euler explicit	$O(\Delta\tau)^2$
0	$-1/2$	Leapfrog explicit	$O(\Delta\tau)^3$
1	0	Euler implicit	$O(\Delta\tau)^2$
1/2	0	Trapezoidal implicit	$O(\Delta\tau)^3$
1	1/2	3-point backward implicit	$O(\Delta\tau)^3$

Note that even though the generalized time differencing formula includes explicit methods, the *Proteus* code assumes an implicit method is being used. Note also that the truncation error listed in the table is the error in the expression for $\Delta \hat{Q}^n$. The overall numerical method used in modelling the differential equations requires $\Delta \hat{Q}^n/\Delta\tau$, so the order of the overall method is this truncation error divided by $\Delta\tau$.

Solving equation (2.16) for $\partial \hat{Q}/\partial \tau$ and substituting the result into equation (3.1) for $\partial(\Delta \hat{Q}^n)/\partial \tau$ and $\partial \hat{Q}^n/\partial \tau$ yields

$$\Delta \hat{Q}^n = -\frac{\theta_1 \Delta\tau}{1+\theta_2}\left(\frac{\partial(\Delta \hat{E}^n)}{\partial \xi} + \frac{\partial(\Delta \hat{F}^n)}{\partial \eta}\right) - \frac{\Delta\tau}{1+\theta_2}\left(\frac{\partial \hat{E}^n}{\partial \xi} + \frac{\partial \hat{F}^n}{\partial \eta}\right)$$
$$+ \frac{\theta_1 \Delta\tau}{1+\theta_2}\left(\frac{\partial(\Delta \hat{E}_V^n)}{\partial \xi} + \frac{\partial(\Delta \hat{F}_V^n)}{\partial \eta}\right) + \frac{\Delta\tau}{1+\theta_2}\left(\frac{\partial \hat{E}_V^n}{\partial \xi} + \frac{\partial \hat{F}_V^n}{\partial \eta}\right)$$
$$+ \frac{\theta_2}{1+\theta_2} \Delta \hat{Q}^{n-1} + O\left[\left(\theta_1 - \frac{1}{2} - \theta_2\right)(\Delta\tau)^2, (\Delta\tau)^3\right] \qquad (3.2)$$

4.0 LINEARIZATION PROCEDURE

4.1 INVISCID TERMS

Equation (3.2) is nonlinear, since, for example, $\Delta\hat{E}^n = \hat{E}^{n+1} - \hat{E}^n$ and the unknown $\hat{E}^{n+1}$ is a nonlinear function of the dependent variables and of the metric coefficients resulting from the generalized grid transformation. The equations must therefore be linearized to be solved by the finite difference procedure used in *Proteus*. This is done by expanding each nonlinear expression in a Taylor series in time about the known time level n. Letting G represent any nonlinear expression,

$$G^{n+1} = G^n + \left(\frac{\partial G}{\partial \tau} \right)^n \Delta\tau + O(\Delta\tau)^2 \tag{4.1}$$

where

$$\frac{\partial G}{\partial \tau} = \frac{\partial G}{\partial \rho}\frac{\partial \rho}{\partial \tau} + \frac{\partial G}{\partial(\rho u)}\frac{\partial(\rho u)}{\partial \tau} + \frac{\partial G}{\partial(\rho v)}\frac{\partial(\rho v)}{\partial \tau} + \frac{\partial G}{\partial E_T}\frac{\partial E_T}{\partial \tau}$$

Note that *for linearization purposes only* the metric scale coefficients have been assumed to be locally independent of time. Note also that for this linearization procedure to be second-order accurate, $\partial G/\partial \tau$ (and therefore $\partial \rho/\partial \tau$, $\partial(\rho u)/\partial \tau$, etc.) need only be first-order accurate. Using forward differences, then, so that

$$\left(\frac{\partial \rho}{\partial \tau} \right)^n = \frac{\rho^{n+1} - \rho^n}{\Delta\tau} + O(\Delta\tau)$$

$$= \frac{\Delta\rho^n}{\Delta\tau} + O(\Delta\tau)$$

etc., equation (4.1) becomes

$$G^{n+1} = G^n + \left(\frac{\partial G}{\partial \rho} \right)^n \Delta\rho^n + \left(\frac{\partial G}{\partial(\rho u)} \right)^n \Delta(\rho u)^n + \left(\frac{\partial G}{\partial(\rho v)} \right)^n \Delta(\rho v)^n + \left(\frac{\partial G}{\partial E_T} \right)^n \Delta E_T^n + O(\Delta\tau)^2 \tag{4.2}$$

As an example the $\partial(\rho u v \xi_y)/\partial \xi$ term from the x-momentum equation (part of the second element of $\partial\hat{E}/\partial\xi$) will be used. The nonlinear part of this term is $(\rho u v)^{n+1}$. Rewriting this in terms of the dependent variables,

$$(\rho u v)^{n+1} = \left[\frac{(\rho u)(\rho v)}{\rho} \right]^{n+1}$$

Using equation (4.2), this is linearized as

$$(\rho u v)^{n+1} = (\rho u v)^n - (u v)^n(\rho^{n+1} - \rho^n) + v^n[(\rho u)^{n+1} - (\rho u)^n] + u^n[(\rho v)^{n+1} - (\rho v)^n] + O(\Delta\tau)^2$$

which can be rewritten as

$$\Delta(\rho u v)^n = -(u v)^n \Delta\rho^n + v^n \Delta(\rho u)^n + u^n \Delta(\rho v)^n + O(\Delta\tau)^2$$

This linearization procedure, when applied to the entire $\Delta\hat{E}^n$ term in the vector equation (3.2), can be written as

$$\Delta \hat{E}^n = \left(\frac{\partial \hat{E}}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n + O(\Delta \tau)^2 \tag{4.3}$$

where $(\partial \hat{E}/\partial \hat{Q})^n$ is a Jacobian coefficient matrix (not to be confused with the Jacobian J of the generalized grid transformation.) A similar equation can be written for $\Delta \hat{F}^n$.

Each term in each element of $\hat{E}$ and $\hat{F}$, given by equations (2.17b) and (2.17c), is linearized using the above procedure to generate the elements of the Jacobian coefficient matrices $\partial \hat{E}/\partial \hat{Q}$ and $\partial \hat{F}/\partial \hat{Q}$. (Note that $\partial \hat{E}/\partial \hat{Q} = J \partial \hat{E}/\partial Q$.) When this is done $\partial \hat{E}/\partial \hat{Q}$ can be written as

$$\frac{\partial \hat{E}}{\partial \hat{Q}} = \begin{bmatrix} \xi_t & \xi_x & \xi_y & 0 \\[2ex] \frac{\partial p}{\partial \rho} \xi_x - u f_1 & \xi_t + f_1 + u\xi_x + \frac{\partial p}{\partial(\rho u)} \xi_x & u\xi_y + \frac{\partial p}{\partial(\rho v)} \xi_x & \frac{\partial p}{\partial E_T} \xi_x \\[2ex] \frac{\partial p}{\partial \rho} \xi_y - v f_1 & v\xi_x + \frac{\partial p}{\partial(\rho u)} \xi_y & \xi_t + f_1 + v\xi_y + \frac{\partial p}{\partial(\rho v)} \xi_y & \frac{\partial p}{\partial E_T} \xi_y \\[2ex] -f_1\left(f_2 - \frac{\partial p}{\partial \rho}\right) & f_2\xi_x + f_1 \frac{\partial p}{\partial(\rho u)} & f_2\xi_y + f_1 \frac{\partial p}{\partial(\rho v)} & \xi_t + f_1\left(1 + \frac{\partial p}{\partial E_T}\right) \end{bmatrix} \tag{4.4}$$

where $f_1 = u\xi_x + v\xi_y$ and $f_2 = (E_T + p)/\rho$. The Jacobian matrix $\partial \hat{F}/\partial \hat{Q}$ has the same form as $\partial \hat{E}/\partial \hat{Q}$, but with ξ replaced by η.

The linearized pressure terms have deliberately been left in terms of $\partial p/\partial \rho$, $\partial p/\partial(\rho u)$, etc. The expressions to be used for these derivatives depend on the equation of state. Those currently built into the *Proteus* code, for a perfect gas, are presented in Section 4.3.

4.2 VISCOUS TERMS

The nonlinear viscous terms in equation (3.2), involving $\Delta \hat{E}_V^n$ and $\Delta \hat{F}_V^n$, must also be linearized. To do this, the elements of $\hat{E}_V$ and $\hat{F}_V$, given in equations (2.17d) and (2.17e), must first be rewritten in terms of the dependent variables, and with derivatives in the Cartesian directions transformed to derivatives in the computational directions using the chain rule. When the resulting expressions are substituted into equation (3.2), mixed second derivatives appear as well as second derivatives in a single coordinate direction. The mixed, or cross, derivative terms would lead to considerable complications in the implicit numerical solution algorithm if they were linearized using the procedure presented in Section 4.1. The two types of second derivatives are thus treated differently, and $\hat{E}_V$ and $\hat{F}_V$ are written as

$$\hat{E}_V = \hat{E}_{V_1} + \hat{E}_{V_2}$$
$$\hat{F}_V = \hat{F}_{V_1} + \hat{F}_{V_2} \tag{4.5}$$

where $\hat{E}_{V_1}$ and $\hat{F}_{V_1}$ only contain derivatives in the ξ and η directions, respectively, and $\hat{E}_{V_2}$ and $\hat{F}_{V_2}$ contain derivatives in the other direction. The fully expanded expressions for $\hat{E}_{V_1}$, $\hat{E}_{V_2}$, etc., are fairly long, and therefore are presented in Appendix A.

4.2.1 Non-Cross Derivatives

Examination of the elements of $\hat{E}_{V_1}$ in equations (A.2a) through (A.2c), and (A.2e), shows that every term has the form fg_ξ, where g is a function of the dependent variables, and f is a function of μ, λ, k, and/or the metric coefficients. Expanding in a Taylor series about time level n gives

$$(fg_\xi)^{n+1} = (fg_\xi)^n + \left[\frac{\partial(fg_\xi)}{\partial\tau} \right]^n \Delta\tau + O(\Delta\tau)^2$$

For linearization purposes only, we will assume f is locally independent of time. We can thus write

$$(fg_\xi)^{n+1} = (fg_\xi)^n + f^n \frac{\partial}{\partial\xi} \left[\frac{\partial g}{\partial\tau} \right]^n \Delta\tau + O(\Delta\tau)^2$$

where

$$\frac{\partial g}{\partial\tau} = \frac{\partial g}{\partial\rho}\frac{\partial\rho}{\partial\tau} + \frac{\partial g}{\partial(\rho u)}\frac{\partial(\rho u)}{\partial\tau} + \cdots$$

Therefore

$$(fg_\xi)^{n+1} = (fg_\xi)^n + f^n \frac{\partial}{\partial\xi} \left[\frac{\partial g}{\partial\rho}\Delta\rho + \frac{\partial g}{\partial(\rho u)}\Delta(\rho u) + \cdots \right]^n + O(\Delta\tau)^2$$

As with the inviscid terms, the linearization procedure for the entire $\Delta\hat{E}_{V_1}^n$ viscous term in equation (3.2) can be written as

$$\Delta\hat{E}_{V_1}^n = \left(\frac{\partial\hat{E}_{V_1}}{\partial\hat{Q}} \right)^n \Delta\hat{Q}^n + O(\Delta\tau)^2 \tag{4.6}$$

A similar equation may be written for $\Delta\hat{F}_{V_1}^n$. The Jacobian coefficient matrix $\partial\hat{E}_{V_1}/\partial\hat{Q}$ is

$$\frac{\partial\hat{E}_{V_1}}{\partial\hat{Q}} = \frac{1}{Re_r}\begin{bmatrix} 0 & 0 & 0 & 0 \\[2ex] \left(\dfrac{\partial\hat{E}_{V_1}}{\partial\hat{Q}}\right)_{21} & \alpha_{xx}\dfrac{\partial}{\partial\xi}\left(\dfrac{1}{\rho}\right) & \alpha_{xy}\dfrac{\partial}{\partial\xi}\left(\dfrac{1}{\rho}\right) & 0 \\[3ex] \left(\dfrac{\partial\hat{E}_{V_1}}{\partial\hat{Q}}\right)_{31} & \alpha_{xy}\dfrac{\partial}{\partial\xi}\left(\dfrac{1}{\rho}\right) & \alpha_{yy}\dfrac{\partial}{\partial\xi}\left(\dfrac{1}{\rho}\right) & 0 \\[3ex] \left(\dfrac{\partial\hat{E}_{V_1}}{\partial\hat{Q}}\right)_{41} & \left(\dfrac{\partial\hat{E}_{V_1}}{\partial\hat{Q}}\right)_{42} & \left(\dfrac{\partial\hat{E}_{V_1}}{\partial\hat{Q}}\right)_{43} & \alpha_0\dfrac{\partial}{\partial\xi}\left(\dfrac{\partial T}{\partial E_T}\right) \end{bmatrix} \tag{4.7}$$

where

$$\alpha_{xx} = (2\mu + \lambda)\xi_x^2 + \mu\xi_y^2$$

$$\alpha_{yy} = \mu \xi_x^2 + (2\mu + \lambda)\xi_y^2$$

$$\alpha_{xy} = (\mu + \lambda)\xi_x \xi_y$$

$$\alpha_0 = \frac{k}{Pr_r}(\xi_x^2 + \xi_y^2)$$

$$\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}}\right)_{21} = -\alpha_{xx}\frac{\partial}{\partial \xi}\left(\frac{u}{\rho}\right) - \alpha_{xy}\frac{\partial}{\partial \xi}\left(\frac{v}{\rho}\right)$$

$$\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}}\right)_{31} = -\alpha_{xy}\frac{\partial}{\partial \xi}\left(\frac{u}{\rho}\right) - \alpha_{yy}\frac{\partial}{\partial \xi}\left(\frac{v}{\rho}\right)$$

$$\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}}\right)_{41} = -\alpha_{xx}\frac{\partial}{\partial \xi}\left(\frac{u^2}{\rho}\right) - \alpha_{yy}\frac{\partial}{\partial \xi}\left(\frac{v^2}{\rho}\right) - 2\alpha_{xy}\frac{\partial}{\partial \xi}\left(\frac{uv}{\rho}\right) + \alpha_0\frac{\partial}{\partial \xi}\left(\frac{\partial T}{\partial \rho}\right)$$

$$\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}}\right)_{42} = -\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}}\right)_{21} + \alpha_0\frac{\partial}{\partial \xi}\left(\frac{\partial T}{\partial(\rho u)}\right)$$

$$\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}}\right)_{43} = -\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}}\right)_{31} + \alpha_0\frac{\partial}{\partial \xi}\left(\frac{\partial T}{\partial(\rho v)}\right)$$

Like the pressure terms discussed earlier, the form of the temperature terms will depend on the equation of state being used. Those currently built into the *Proteus* code, for a perfect gas, are presented in Section 4.3.

Note that in equation (4.6) the derivatives appearing in the Jacobian coefficient matrix $\partial \hat{E}_{V_1}/\partial \hat{Q}$ are also to be applied to the $\Delta \hat{Q}^n$ appearing outside the parentheses. For example, the element in the second row and second column of $\partial \hat{E}_{V_1}/\partial \hat{Q}$, which corresponds to the $\Delta(\rho u)$ term in the x-momentum equation, is $\alpha_{xx}\partial(1/\rho)/\partial \xi$. For this term, the notation used in equation (4.6) means

$$\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}}\right)_{22}^n \Delta \hat{Q}_2^n = \alpha_{xx}^n \frac{\partial}{\partial \xi}\left(\frac{1}{\rho}\right)^n \Delta(\rho u/J)^n$$

$$= \alpha_{xx}^n \frac{\partial}{\partial \xi}\left(\frac{\Delta(\rho u/J)^n}{\rho^n}\right)$$

The Jacobian coefficient matrix for the remaining non-cross derivative viscous terms, $\partial \hat{F}_{V_1}/\partial \hat{Q}$, has the same form as $\partial \hat{E}_{V_1}/\partial \hat{Q}$, but with ξ replaced by η.

4.2.2 Cross Derivatives

As stated earlier, linearizing the cross derivative viscous terms in the same way as the remaining terms is very complicated within the framework of the implicit numerical solution algorithm used in *Proteus*.

They are therefore simply lagged (i.e., evaluated at the known time level n and treated as source terms.) As noted by Beam and Warming (1978), this does not lead to a formal accuracy loss since

$$\Delta \hat{\mathbf{E}}_{V_2}^n = \Delta \hat{\mathbf{E}}_{V_2}^{n-1} + O(\Delta \tau)^2$$
$$\Delta \hat{\mathbf{F}}_{V_2}^n = \Delta \hat{\mathbf{F}}_{V_2}^{n-1} + O(\Delta \tau)^2 \tag{4.8}$$

4.3 EQUATION OF STATE

The expressions to be used for $\partial p/\partial \rho$, $\partial T/\partial \rho$, etc., which arise from the linearization procedure, depend on the equation of state. The equation currently built into *Proteus* is for perfect gases, and can be written as

$$p = (\gamma - 1)\left[E_T - \frac{1}{2}\rho(u^2 + v^2) \right] \tag{4.9}$$

or, in terms of temperature, as

$$T = \frac{1}{c_v}\left[\frac{E_T}{\rho} - \frac{1}{2}(u^2 + v^2) \right] \tag{4.10}$$

With this equation of state, then, the appropriate derivatives are

$$\frac{\partial p}{\partial \rho} = \frac{\gamma - 1}{2}(u^2 + v^2) \tag{4.11a}$$

$$\frac{\partial p}{\partial(\rho u)} = -(\gamma - 1)u \tag{4.11b}$$

$$\frac{\partial p}{\partial(\rho v)} = -(\gamma - 1)v \tag{4.11c}$$

$$\frac{\partial p}{\partial E_T} = \gamma - 1 \tag{4.11d}$$

$$\frac{\partial T}{\partial \rho} = -\frac{1}{c_v}\left[\frac{E_T}{\rho^2} - \frac{1}{\rho}(u^2 + v^2) \right] \tag{4.12a}$$

$$\frac{\partial T}{\partial(\rho u)} = -\frac{u}{c_v \rho} \tag{4.12b}$$

$$\frac{\partial T}{\partial(\rho v)} = -\frac{v}{c_v \rho} \tag{4.12c}$$

$$\frac{\partial T}{\partial E_T} = \frac{1}{c_v \rho} \tag{4.12d}$$

If constant stagnation enthalpy is assumed, as discussed in Section 2.2, the appropriate equation of state is

$$p = \frac{\gamma - 1}{\gamma}\rho\left[h_T - \frac{1}{2}(u^2 + v^2) \right] \tag{4.13}$$

and the temperature becomes

$$T = \frac{1}{c_p}\left[h_T - \frac{1}{2}(u^2 + v^2) \right] \tag{4.14}$$

With these equations, the derivatives of p and T with respect to the dependent variables are

$$\frac{\partial p}{\partial \rho} = \frac{\gamma - 1}{\gamma}\left[h_T + \frac{1}{2}(u^2 + v^2)\right] \tag{4.15a}$$

$$\frac{\partial p}{\partial(\rho u)} = -\frac{\gamma - 1}{\gamma}u \tag{4.15b}$$

$$\frac{\partial p}{\partial(\rho v)} = -\frac{\gamma - 1}{\gamma}v \tag{4.15c}$$

$$\frac{\partial T}{\partial \rho} = \frac{1}{c_p \rho}(u^2 + v^2) \tag{4.16a}$$

$$\frac{\partial T}{\partial(\rho u)} = -\frac{u}{c_p \rho} \tag{4.16b}$$

$$\frac{\partial T}{\partial(\rho v)} = -\frac{v}{c_p \rho} \tag{4.16c}$$

4.4 LINEARIZED GOVERNING EQUATION

The linearized form of equation (3.2) can now be written as

$$
\begin{aligned}
\Delta\hat{Q}^n + \frac{\theta_1 \Delta\tau}{1+\theta_2}&\left\{\frac{\partial}{\partial\xi}\left[\left(\frac{\partial\hat{E}}{\partial\hat{Q}}\right)^n \Delta\hat{Q}^n\right] + \frac{\partial}{\partial\eta}\left[\left(\frac{\partial\hat{F}}{\partial\hat{Q}}\right)^n \Delta\hat{Q}^n\right]\right\} \\
-\frac{\theta_1 \Delta\tau}{1+\theta_2}&\left\{\frac{\partial}{\partial\xi}\left[\left(\frac{\partial\hat{E}_{V_1}}{\partial\hat{Q}}\right)^n \Delta\hat{Q}^n\right] + \frac{\partial}{\partial\eta}\left[\left(\frac{\partial\hat{F}_{V_1}}{\partial\hat{Q}}\right)^n \Delta\hat{Q}^n\right]\right\} = \\
&-\frac{\Delta\tau}{1+\theta_2}\left(\frac{\partial\hat{E}}{\partial\xi} + \frac{\partial\hat{F}}{\partial\eta}\right)^n + \frac{\Delta\tau}{1+\theta_2}\left(\frac{\partial\hat{E}_{V_1}}{\partial\xi} + \frac{\partial\hat{F}_{V_1}}{\partial\eta}\right)^n \\
&+\frac{(1+\theta_3)\Delta\tau}{1+\theta_2}\left(\frac{\partial\hat{E}_{V_2}}{\partial\xi} + \frac{\partial\hat{F}_{V_2}}{\partial\eta}\right)^n - \frac{\theta_3\Delta\tau}{1+\theta_2}\left(\frac{\partial\hat{E}_{V_2}}{\partial\xi} + \frac{\partial\hat{F}_{V_2}}{\partial\eta}\right)^{n-1} \\
&+\frac{\theta_2}{1+\theta_2}\Delta\hat{Q}^{n-1} + O\left[\left(\theta_1 - \frac{1}{2} - \theta_2\right)(\Delta\tau)^2, (\theta_3 - \theta_1)(\Delta\tau)^2, (\Delta\tau)^3\right]
\end{aligned} \tag{4.17}
$$

There are a couple of things that should be mentioned about this equation. First, this equation is in so-called "delta" form. We will actually be solving this equation for $\Delta\hat{Q}^n$ and recovering $\hat{Q}^{n+1}$ from $\hat{Q}^{n+1} = \Delta\hat{Q}^n + \hat{Q}^n$. And second, in the coefficients of the cross derivative viscous terms the time differencing parameter θ_1 has been replaced by θ_3. For second-order time differencing (i.e., if $\theta_1 = \theta_2 + 1/2$), θ_3 should be set equal to θ_1. For first-order time differencing, however, θ_3 can be set equal to zero without losing accuracy.

5.0 SPACE DIFFERENCING

To solve equation (4.17) an evenly spaced grid is defined in the computational (ξ, η) coordinate system. Spatial derivatives are then approximated by finite difference formulas. First derivatives in the ξ direction are approximated using the following second-order central difference formula.

$$\left(\frac{\partial f}{\partial \xi} \right)_{i,j} \simeq \delta_\xi f_{i,j} = \frac{f_{i+1,j} - f_{i-1,j}}{2\Delta\xi} \tag{5.1}$$

The subscripts i and j represent grid point indices in the ξ and η directions. The computational grid spacing $\Delta\xi$ is constant, and equal to $1/(N_1 - 1)$, where N_1 is the number of grid points in the ξ direction. A similar formula is used for first derivatives in the η direction.

The non-cross derivative viscous terms in the ξ direction in equation (4.17) all have the form

$$\frac{\partial}{\partial \xi} \left[f \frac{\partial}{\partial \xi} (g\Delta Q) \right]$$

where Q represents one of the elements of $\hat{Q}$. Using central differences this is approximated by

$$\begin{aligned}
\frac{\partial}{\partial \xi} \left[f \frac{\partial}{\partial \xi} (g\Delta Q) \right]_{i,j} &\simeq \delta_\xi [f \delta_\xi (g\Delta Q)]_{i,j} \\
&= \frac{1}{\Delta\xi} \{ f_{i+1/2,j} \delta_\xi (g\Delta Q)_{i+1/2,j} - f_{i-1/2,j} \delta_\xi (g\Delta Q)_{i-1/2,j} \} \\
&= \frac{1}{(\Delta\xi)^2} \{ f_{i+1/2,j} [(g\Delta Q)_{i+1,j} - (g\Delta Q)_{i,j}] \\
&\quad - f_{i-1/2,j} [(g\Delta Q)_{i,j} - (g\Delta Q)_{i-1,j}] \} \\
&= \frac{1}{2(\Delta\xi)^2} \{ (f_{i,j} + f_{i+1,j})[(g\Delta Q)_{i+1,j} - (g\Delta Q)_{i,j}] \\
&\quad - (f_{i,j} + f_{i-1,j})[(g\Delta Q)_{i,j} - (g\Delta Q)_{i-1,j}] \} \\
&= \frac{1}{2(\Delta\xi)^2} \{ (f_{i-1,j} + f_{i,j})(g\Delta Q)_{i-1,j} \\
&\quad - (f_{i-1,j} + 2f_{i,j} + f_{i+1,j})(g\Delta Q)_{i,j} \\
&\quad + (f_{i,j} + f_{i+1,j})(g\Delta Q)_{i+1,j} \}
\end{aligned} \tag{5.2}$$

A similar formula is used for second derivatives in the η direction.

Cross derivative viscous terms are evaluated using the following central difference formula.

$$\frac{\partial}{\partial \xi}\left(f\frac{\partial g}{\partial \eta}\right)_{i,j} \simeq \delta_\xi(f\delta_\eta g)_{i,j}$$

$$= \frac{1}{2\Delta\xi}[f_{i+1,j}(\delta_\eta g)_{i+1,j} - f_{i-1,j}(\delta_\eta g)_{i-1,j}]$$

$$= \frac{1}{4\Delta\xi\Delta\eta}[f_{i+1,j}(g_{i+1,j+1} - g_{i+1,j-1})$$
$$- f_{i-1,j}(g_{i-1,j+1} - g_{i-1,j-1})] \tag{5.3}$$

Note that this formula is only needed for the source terms, since the viscous cross derivative terms are lagged one time level.

When first derivatives are needed normal to a computational boundary, such as for Neumann boundary conditions, either first- or second-order one-sided differencing is used. The first-order formula at the $\xi = 0$ boundary is

$$\left(\frac{\partial f}{\partial \xi}\right)_{1,j} \simeq \frac{1}{\Delta\xi}(f_{2,j} - f_{1,j}) \tag{5.4}$$

and at the $\xi = 1$ boundary,

$$\left(\frac{\partial f}{\partial \xi}\right)_{N_1,j} \simeq \frac{1}{\Delta\xi}(f_{N_1,j} - f_{N_1-1,j}) \tag{5.5}$$

The second-order formula at the $\xi = 0$ boundary is

$$\left(\frac{\partial f}{\partial \xi}\right)_{1,j} \simeq \frac{1}{2\Delta\xi}(-3f_{1,j} + 4f_{2,j} - f_{3,j}) \tag{5.6}$$

and at the $\xi = 1$ boundary,

$$\left(\frac{\partial f}{\partial \xi}\right)_{N_1,j} \simeq \frac{1}{2\Delta\xi}(f_{N_1-2,j} - 4f_{N_1-1,j} + 3f_{N_1,j}) \tag{5.7}$$

Similar formulas are used at the $\eta = 0$ and $\eta = 1$ boundaries.

6.0 BOUNDARY CONDITIONS

Choosing boundary conditions is perhaps the most important step in solving a flow problem with *Proteus*. Since the equations being solved at interior points are the same for every problem, the boundary conditions are what determines the final flow field for steady flows.

With the difference formulas presented in Section 5.0, N_{eq} boundary conditions are required at each computational boundary, where N_{eq} is the number of equations being solved. Note, however, that this is a numerical requirement, not a mathematical one. For example, for one-dimensional Euler flow $N_{eq} = 3$. However, characteristic theory shows that, mathematically, only two conditions may be specified at a subsonic inflow boundary, and only one at a subsonic outflow boundary (Pulliam, 1986a). Some sort of extrapolation is typically used for the additional numerical boundary conditions.

A variety of boundary conditions are built into the *Proteus* code, including: (1) specified values and/or gradients of Cartesian velocities u and v, normal and tangential velocities V_n and V_t, pressure p, temperature T, and density ρ; (2) specified values of total pressure p_T, total temperature T_T, and flow angle; (3) linear extrapolation; and (4) spatial periodicity. Another useful boundary condition is a "no change from initial condition" option for u, v, p, T, ρ, p_T, and/or T_T. Provision is also made for user-written boundary conditions. The boundary conditions may be steady, unsteady, or time-periodic. The exact combination of boundary conditions to be used will depend on the problem being run.

The boundary conditions in *Proteus* are treated implicitly. They may be viewed simply as additional equations to be solved by the ADI solution algorithm. And, in general, they involve nonlinear functions of the dependent variables. They must therefore be linearized using the procedure described in Section 4.0. The following sections describe this linearization for the general types of boundary conditions currently built into *Proteus*.

6.1 NO CHANGE FROM INITIAL CONDITIONS, $\Delta g = 0$

This boundary condition simply sets the boundary value of the function g equal to its initial condition value. It can be written as

$$\Delta g^n = g^{n+1} - g^n = 0 \tag{6.1}$$

In general, g can be a nonlinear combination of the dependent variables $\hat{Q}$. Linearizing g using the procedure described in Section 4.0, we get

$$g^{n+1} = g^n + \left(\frac{\partial g}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n + O(\Delta\tau)^2 \tag{6.2}$$

Neglecting the $O(\Delta\tau)^2$ linearization error, the linearized form of equation (6.1) can thus be written as

$$\left(\frac{\partial g}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n = 0 \tag{6.3}$$

6.2 SPECIFIED FUNCTION, $g = f$

A specified function at a boundary can be written simply as

$$g^{n+1} = f \tag{6.4}$$

where g is the function being specified and f is the value being specified. Note that f can vary along the boundary, and can be time-dependent. Using equation (6.2) and neglecting the linearization error, the linearized boundary condition becomes

$$\left(\frac{\partial g}{\partial \hat{\mathbf{Q}}} \right)^n \Delta \hat{\mathbf{Q}}^n = f - g^n \tag{6.5}$$

6.3 SPECIFIED COORDINATE DIRECTION GRADIENT, $\partial g / \partial \phi = f$

A specified gradient of a function in a coordinate direction can be written as

$$\left(\frac{\partial g}{\partial \phi} \right)^{n+1} = f \tag{6.6}$$

where g is the function whose gradient is being specified, f is the specified value, and ϕ is the coordinate direction ξ or η. Note that f can vary along the boundary, and can be time-dependent.

The linearized form of g is given by equation (6.2). The linearized form of equation (6.6) can thus be written as

$$\left(\frac{\partial g}{\partial \phi} \right)^n + \frac{\partial}{\partial \phi} \left[\left(\frac{\partial g}{\partial \hat{\mathbf{Q}}} \right)^n \Delta \hat{\mathbf{Q}}^n \right] = f + O(\Delta \tau)^2 \tag{6.7}$$

Replacing differential operators with difference operators and neglecting the linearization error, the linearized boundary condition can be written as

$$\delta_\phi \left[\left(\frac{\partial g}{\partial \hat{\mathbf{Q}}} \right)^n \Delta \hat{\mathbf{Q}}^n \right] = f - \delta_\phi g^n \tag{6.8}$$

where δ_ϕ represents the one-sided difference operator to be used at the boundary. Options are available in *Proteus* to use either first-order two-point or second-order three-point differencing.

Note that this boundary condition is a specified value of the derivative with respect to the computational coordinate, not with respect to the physical distance in the direction of the computational coordinate. Following Korn and Korn (1968), and using the properties of the generalized coordinate transformation, it can be shown that for the ξ direction the two derivatives are related by

$$\frac{\partial g}{\partial s_\xi} = \frac{J}{\sqrt{\eta_x^2 + \eta_y^2}} \frac{\partial g}{\partial \xi}$$

Similarly, for the η direction,

$$\frac{\partial g}{\partial s_\eta} = \frac{J}{\sqrt{\xi_x^2 + \xi_y^2}} \frac{\partial g}{\partial \eta}$$

If the value $f = 0$, of course, the two derivatives are equivalent.

6.4 SPECIFIED NORMAL DIRECTION GRADIENT, $\nabla g \cdot \vec{n} = f$

A specified gradient of a function normal to the boundary can be written as

$$\nabla g^{n+1} \cdot \vec{n} = f \tag{6.9}$$

where g is the function whose gradient is being specified, f is the specified value, and $\vec{n}$ represents the unit vector normal to the boundary. Note that f can vary along the boundary, and can be time-dependent.

For illustrative purposes, assume we are specifying a gradient normal to a constant ξ boundary. Then

$$\vec{n} = \frac{\nabla \xi}{|\nabla \xi|} = \frac{1}{m} \xi_x \vec{i} + \frac{1}{m} \xi_y \vec{j}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

Equation (6.9) can then be written as

$$\frac{1}{m} (g_x^{n+1} \xi_x + g_y^{n+1} \xi_y) = f \tag{6.10}$$

Using the chain rule to expand g_x^{n+1} and g_y^{n+1},

$$g_x^{n+1} = g_\xi^{n+1} \xi_x + g_\eta^{n+1} \eta_x$$
$$g_y^{n+1} = g_\xi^{n+1} \xi_y + g_\eta^{n+1} \eta_y$$

Substituting into equation (6.10) and rearranging,

$$g_\xi^{n+1} (\xi_x^2 + \xi_y^2) + g_\eta^{n+1} (\xi_x \eta_x + \xi_y \eta_y) = mf$$

Solving for g_ξ^{n+1},

$$\left(\frac{\partial g}{\partial \xi} \right)^{n+1} = \frac{f}{m} - \frac{1}{m^2} (\xi_x \eta_x + \xi_y \eta_y) \left(\frac{\partial g}{\partial \eta} \right)^{n+1} \tag{6.11}$$

Now, in order to incorporate this equation into the ADI solution procedure used in *Proteus*, the $\partial g/\partial \eta$ term in equation (6.11) is lagged one level, and evaluated at time level n instead of $n+1$. Strictly speaking, this introduces an $O(\Delta\tau)$ error into the solution. In practice, however, the actual error will depend on the degree of nonorthogonality of the coordinates near the boundary. For orthogonal coordinates no error is introduced.

Using equation (6.2), and introducing difference operators and neglecting the linearization error, we can now write the linearized boundary condition as

$$\delta_\xi \left[\left(\frac{\partial g}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n \right] = \frac{f}{m} - \frac{1}{m^2} (\xi_x \eta_x + \xi_y \eta_y) \delta_\eta g^n - \delta_\xi g^n \tag{6.12a}$$

where δ_ξ represents the one-sided difference operator to be used at the boundary. Options are available in *Proteus* to use either first-order two-point or second-order three-point differencing.

Note that the unit vector $\vec{n}$ in equation (6.9) is in the direction of increasing ξ. Therefore, a positive value for f in equation (6.12a) indicates a flux in the direction of increasing ξ. Thus, a positive f at $\xi = 0$ implies a flux into the computational domain, and a positive f at $\xi = 1$ implies a flux out of the computational domain.

Specifying a gradient normal to a constant η boundary is done in an exactly analogous manner. The resulting equation is

$$\delta_\eta \left[\left(\frac{\partial g}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n \right] = \frac{f}{m} - \frac{1}{m^2} (\eta_x \xi_x + \eta_y \xi_y) \delta_\xi g^n - \delta_\eta g^n \tag{6.12b}$$

where

$$m = \sqrt{\eta_x{}^2 + \eta_y{}^2}$$

A positive value for f in equation (6.12b) indicates a flux in the direction of increasing η. Thus, a positive f at $\eta = 0$ implies a flux into the computational domain, and a positive f at $\eta = 1$ implies a flux out of the computational domain.

6.5 LINEAR EXTRAPOLATION

Linear extrapolation from the two adjacent interior points is also available as a boundary condition. At the $\xi = 0$ boundary, where $i = 1$, this can be written as

$$g_i^{n+1} - 2g_{i+1}^{n+1} + g_{i+2}^{n+1} = 0 \tag{6.13}$$

Note that this is equivalent to setting $(\partial^2 g / \partial \xi^2)_{i+1} = 0$. Using equation (6.2), we can write the linearized boundary condition as

$$\left(\frac{\partial g}{\partial \hat{Q}} \right)_i^n \Delta \hat{Q}_i^n - 2 \left(\frac{\partial g}{\partial \hat{Q}} \right)_{i+1}^n \Delta \hat{Q}_{i+1}^n + \left(\frac{\partial g}{\partial \hat{Q}} \right)_{i+2}^n \Delta \hat{Q}_{i+2}^n = - g_i^n + 2g_{i+1}^n - g_{i+2}^n \tag{6.14}$$

Analogous extrapolation boundary conditions can easily be written for the remaining boundaries.

7.0 SOLUTION PROCEDURE

7.1 ADI ALGORITHM

The governing equations, presented in linearized matrix form as equation (4.17), are solved by an alternating direction implicit (ADI) method. The form of the ADI splitting is the same as used by Briley and McDonald (1977), and by Beam and Warming (1978). Although the split equations can be developed in more than one way, in this discussion the approximate factorization approach is used.

Letting LHS(4.17) represent the left hand side of equation (4.17), we can write

$$\text{LHS(4.17)} = \left\{ \mathbf{I} + \frac{\theta_1 \Delta \tau}{1 + \theta_2} \left[\frac{\partial}{\partial \xi} \left(\frac{\partial \hat{\mathbf{E}}}{\partial \hat{\mathbf{Q}}} - \frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right) + \frac{\partial}{\partial \eta} \left(\frac{\partial \hat{\mathbf{F}}}{\partial \hat{\mathbf{Q}}} - \frac{\partial \hat{\mathbf{F}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right) \right] \right\}^n \Delta \hat{\mathbf{Q}}^n \qquad (7.1)$$

where $\mathbf{I}$ represents the identity matrix. Note that in this equation, using the $\partial / \partial \xi$ term as an example, the notation used is meant to imply

$$\left[\frac{\partial}{\partial \xi} \left(\frac{\partial \hat{\mathbf{E}}}{\partial \hat{\mathbf{Q}}} - \frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right) \right] \Delta \hat{\mathbf{Q}} = \frac{\partial}{\partial \xi} \left(\frac{\partial \hat{\mathbf{E}}}{\partial \hat{\mathbf{Q}}} \Delta \hat{\mathbf{Q}} - \frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \Delta \hat{\mathbf{Q}} \right)$$

The term in braces in equation (7.1) can be factored to give

$$\text{LHS(4.17)} = \left[\mathbf{I} + \frac{\theta_1 \Delta \tau}{1 + \theta_2} \frac{\partial}{\partial \xi} \left(\frac{\partial \hat{\mathbf{E}}}{\partial \hat{\mathbf{Q}}} - \frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right) \right]^n \left[\mathbf{I} + \frac{\theta_1 \Delta \tau}{1 + \theta_2} \frac{\partial}{\partial \eta} \left(\frac{\partial \hat{\mathbf{F}}}{\partial \hat{\mathbf{Q}}} - \frac{\partial \hat{\mathbf{F}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right) \right]^n \Delta \hat{\mathbf{Q}}^n$$

$$- \left(\frac{\theta_1 \Delta \tau}{1 + \theta_2} \right)^2 \left[\frac{\partial}{\partial \xi} \left(\frac{\partial \hat{\mathbf{E}}}{\partial \hat{\mathbf{Q}}} - \frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right) \frac{\partial}{\partial \eta} \left(\frac{\partial \hat{\mathbf{F}}}{\partial \hat{\mathbf{Q}}} - \frac{\partial \hat{\mathbf{F}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right) \right]^n \Delta \hat{\mathbf{Q}}^n \qquad (7.2)$$

The last term represents the splitting error. Note that, since $\Delta \hat{\mathbf{Q}}^n = O(\Delta \tau)$, this term can be neglected without affecting the overall time accuracy of the algorithm, even when second-order time differencing is used.

Equation (4.17) can thus be rewritten in spatially factored form, and, neglecting the temporal truncation and splitting error terms, becomes

$$
\left[\mathbf{I} + \frac{\theta_1 \Delta\tau}{1+\theta_2} \frac{\partial}{\partial\xi} \left(\frac{\partial\hat{\mathbf{E}}}{\partial\hat{\mathbf{Q}}} - \frac{\partial\hat{\mathbf{E}}_{V_1}}{\partial\hat{\mathbf{Q}}} \right) \right]^n \left[\mathbf{I} + \frac{\theta_1 \Delta\tau}{1+\theta_2} \frac{\partial}{\partial\eta} \left(\frac{\partial\hat{\mathbf{F}}}{\partial\hat{\mathbf{Q}}} - \frac{\partial\hat{\mathbf{F}}_{V_1}}{\partial\hat{\mathbf{Q}}} \right) \right]^n \Delta\hat{\mathbf{Q}}^n =
$$

$$
- \frac{\Delta\tau}{1+\theta_2} \left(\frac{\partial\hat{\mathbf{E}}}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}}{\partial\eta} \right)^n + \frac{\Delta\tau}{1+\theta_2} \left(\frac{\partial\hat{\mathbf{E}}_{V_1}}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}_{V_1}}{\partial\eta} \right)^n + \frac{(1+\theta_3)\Delta\tau}{1+\theta_2} \left(\frac{\partial\hat{\mathbf{E}}_{V_2}}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}_{V_2}}{\partial\eta} \right)^n
$$

$$
- \frac{\theta_3\Delta\tau}{1+\theta_2} \left(\frac{\partial\hat{\mathbf{E}}_{V_2}}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}_{V_2}}{\partial\eta} \right)^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta\hat{\mathbf{Q}}^{n-1} \tag{7.3}
$$

Equation (7.3) can be split into the following two-sweep sequence.

<u>Sweep 1 (ξ direction)</u>

$$
\Delta\hat{\mathbf{Q}}^* + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{\partial}{\partial\xi} \left[\left(\frac{\partial\hat{\mathbf{E}}}{\partial\hat{\mathbf{Q}}} \right)^n \Delta\hat{\mathbf{Q}}^* \right] - \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{\partial}{\partial\xi} \left[\left(\frac{\partial\hat{\mathbf{E}}_{V_1}}{\partial\hat{\mathbf{Q}}} \right)^n \Delta\hat{\mathbf{Q}}^* \right] =
$$

$$
- \frac{\Delta\tau}{1+\theta_2} \left(\frac{\partial\hat{\mathbf{E}}}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}}{\partial\eta} \right)^n + \frac{\Delta\tau}{1+\theta_2} \left(\frac{\partial\hat{\mathbf{E}}_{V_1}}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}_{V_1}}{\partial\eta} \right)^n
$$

$$
+ \frac{(1+\theta_3)\Delta\tau}{1+\theta_2} \left(\frac{\partial\hat{\mathbf{E}}_{V_2}}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}_{V_2}}{\partial\eta} \right)^n - \frac{\theta_3\Delta\tau}{1+\theta_2} \left(\frac{\partial\hat{\mathbf{E}}_{V_2}}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}_{V_2}}{\partial\eta} \right)^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta\hat{\mathbf{Q}}^{n-1} \tag{7.4a}
$$

<u>Sweep 2 (η direction)</u>

$$
\Delta\hat{\mathbf{Q}}^n + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{\partial}{\partial\eta} \left[\left(\frac{\partial\hat{\mathbf{F}}}{\partial\hat{\mathbf{Q}}} \right)^n \Delta\hat{\mathbf{Q}}^n \right] - \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{\partial}{\partial\eta} \left[\left(\frac{\partial\hat{\mathbf{F}}_{V_1}}{\partial\hat{\mathbf{Q}}} \right)^n \Delta\hat{\mathbf{Q}}^n \right] = \Delta\hat{\mathbf{Q}}^* \tag{7.4b}
$$

In the above equations, $\hat{\mathbf{Q}}^*$ represents an intermediate solution to the governing equations.[4] It should be noted that in *Proteus*, physical (i.e, $n+1$ level) boundary conditions are used during the first ADI sweep. This introduces an $O(\Delta\tau)$ error in $\partial Q/\partial\tau$ on the boundary for unsteady flows, but no error for steady flows. This point is discussed in detail by Briley and McDonald (1980).

---

[4] The notation here is somewhat inconsistent. The quantity $\Delta\hat{\mathbf{Q}}^n = \hat{\mathbf{Q}}^{n+1} - \hat{\mathbf{Q}}^n$, but $\Delta\hat{\mathbf{Q}}^* = \hat{\mathbf{Q}}^* - \hat{\mathbf{Q}}^n$, not $\hat{\mathbf{Q}}^{n+1} - \hat{\mathbf{Q}}^*$.

Applying the spatial differencing formulas of Section 5.0 results in

Sweep 1 (ξ direction)

$$\Delta\hat{Q}_i^* + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\xi}\left[\left(\frac{\partial\hat{E}}{\partial\hat{Q}}\right)_{i+1}^n \Delta\hat{Q}_{i+1}^* - \left(\frac{\partial\hat{E}}{\partial\hat{Q}}\right)_{i-1}^n \Delta\hat{Q}_{i-1}^*\right]$$

$$-\frac{\theta_1\Delta\tau}{(1+\theta_2)2(\Delta\xi)^2}\left[(f_{i-1}+f_i)^n g_{i-1}^n \Delta\hat{Q}_{i-1}^* - (f_{i-1}+2f_i+f_{i+1})^n g_i^n \Delta\hat{Q}_i^* + (f_i+f_{i+1})^n g_{i+1}^n \Delta\hat{Q}_{i+1}^*\right] =$$

$$-\frac{\Delta\tau}{1+\theta_2}\left(\delta_\xi\hat{E} + \delta_\eta\hat{F}\right)^n + \frac{\Delta\tau}{1+\theta_2}\left(\delta_\xi\hat{E}_{V_1} + \delta_\eta\hat{F}_{V_1}\right)^n$$

$$+\frac{(1+\theta_3)\Delta\tau}{1+\theta_2}\left(\delta_\xi\hat{E}_{V_2} + \delta_\eta\hat{F}_{V_2}\right)^n - \frac{\theta_3\Delta\tau}{1+\theta_2}\left(\delta_\xi\hat{E}_{V_2} + \delta_\eta\hat{F}_{V_2}\right)^{n-1} + \frac{\theta_2}{1+\theta_2}\Delta\hat{Q}^{n-1} \qquad (7.5a)$$

Sweep 2 (η direction)

$$\Delta\hat{Q}_j^n + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\eta}\left[\left(\frac{\partial\hat{F}}{\partial\hat{Q}}\right)_{j+1}^n \Delta\hat{Q}_{j+1}^n - \left(\frac{\partial\hat{F}}{\partial\hat{Q}}\right)_{j-1}^n \Delta\hat{Q}_{j-1}^n\right]$$

$$-\frac{\theta_1\Delta\tau}{(1+\theta_2)2(\Delta\eta)^2}\left[(f_{j-1}+f_j)^n g_{j-1}^n \Delta\hat{Q}_{j-1}^n - (f_{j-1}+2f_j+f_{j+1})^n g_j^n \Delta\hat{Q}_j^n + (f_j+f_{j+1})^n g_{j+1}^n \Delta\hat{Q}_{j+1}^n\right] =$$

$$\Delta\hat{Q}^* \qquad (7.5b)$$

The subscripts i and j represent grid point indices in the ξ and η directions. For notational convenience, terms without an explicitly written i or j subscript are understood to be at i or j. In the viscous terms on the left hand side, f is the coefficient of $\partial/\partial\xi$ (or $\partial/\partial\eta$, depending on the sweep) in the $\partial\hat{E}_{V_1}/\partial\hat{Q}$ (or $\partial\hat{F}_{V_1}/\partial\hat{Q}$) Jacobian coefficient matrix. Similarly, g is the term in the parentheses following $\partial/\partial\xi$ (or $\partial/\partial\eta$) in the $\partial\hat{E}_{V_1}/\partial\hat{Q}$ (or $\partial\hat{F}_{V_1}/\partial\hat{Q}$) Jacobian coefficient matrix. Equations (7.5a) and (7.5b) represent the two-sweep alternating direction implicit (ADI) algorithm used to advance the solution from time level n to $n+1$.

7.2 MATRIX INVERSION PROCEDURE

7.2.1 Non-Periodic Boundary Conditions

The complete set of algebraic equations for the first ADI sweep with non-periodic boundary conditions can be written in the following block matrix form.[5]

---

[5] Although this discussion is written for the first ADI sweep, an exactly analogous procedure is followed for the second sweep.

$$
\begin{bmatrix}
\mathbf{B}'_1 & \mathbf{C}'_1 & \mathbf{A}'_1 & & & & & \\
\mathbf{A}_2 & \mathbf{B}_2 & \mathbf{C}_2 & & & & & \\
& \mathbf{A}_3 & \mathbf{B}_3 & \mathbf{C}_3 & & & & \\
& & & \bullet & & & & \\
& & & & \bullet & & & \\
& & & & & \bullet & & \\
& & & \mathbf{A}_{N_1-2} & \mathbf{B}_{N_1-2} & \mathbf{C}_{N_1-2} & & \\
& & & & \mathbf{A}_{N_1-1} & \mathbf{B}_{N_1-1} & \mathbf{C}_{N_1-1} \\
& & & & \mathbf{C}'_{N_1} & \mathbf{A}'_{N_1} & \mathbf{B}'_{N_1}
\end{bmatrix}
\begin{bmatrix}
\Delta\hat{\mathbf{Q}}^*_1 \\
\Delta\hat{\mathbf{Q}}^*_2 \\
\Delta\hat{\mathbf{Q}}^*_3 \\
\bullet \\
\bullet \\
\bullet \\
\Delta\hat{\mathbf{Q}}^*_{N_1-2} \\
\Delta\hat{\mathbf{Q}}^*_{N_1-1} \\
\Delta\hat{\mathbf{Q}}^*_{N_1}
\end{bmatrix}
=
\begin{bmatrix}
\mathbf{S}'_1 \\
\mathbf{S}_2 \\
\mathbf{S}_3 \\
\bullet \\
\bullet \\
\bullet \\
\mathbf{S}_{N_1-2} \\
\mathbf{S}_{N_1-1} \\
\mathbf{S}'_{N_1}
\end{bmatrix}
\qquad (7.6)
$$

These equations result from the application of equation (7.5a) for $i = 2$ to $N_1 - 1$, with boundary conditions added at $i = 1$ and $i = N_1$. The parameter $\Delta\hat{\mathbf{Q}}^*$ is the N_{eq}-element vector containing the unknown dependent variables; $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are the $N_{eq} \times N_{eq}$ coefficient submatrices at $i - 1$, i, and $i + 1$, respectively; and $\mathbf{S}$ is the N_{eq}-element subvector containing the explicit source terms. Also, $\mathbf{A}'$, $\mathbf{B}'$, and $\mathbf{C}'$ are the coefficient submatrices and $\mathbf{S}'$ the source term subvector for the boundary conditions. A variety of boundary conditions may be used. They are described briefly in Section 6.0, and in greater detail in Volumes 2 and 3.

Note that the equations at the boundaries may contain coefficients at the boundary point and the two adjacent interior points. This occurs, for example, when extrapolation or second-order gradient boundary conditions are specified. As written, therefore, the coefficient matrix in equation (7.6) is not block tridiagonal. However, $\mathbf{A}'_1$ can be eliminated by multiplying the second row of the matrix by $\mathbf{A}'_1 \mathbf{C}_2^{-1}$ and subtracting from the first row. $\mathbf{C}'_{N_1}$ can be eliminated in a similar manner. Doing this, we define

$$\mathbf{B}_1 = \mathbf{B}'_1 - \mathbf{A}'_1 \mathbf{C}_2^{-1} \mathbf{A}_2$$

$$\mathbf{C}_1 = \mathbf{C}'_1 - \mathbf{A}'_1 \mathbf{C}_2^{-1} \mathbf{B}_2 \qquad (7.7)$$

$$\mathbf{S}_1 = \mathbf{S}'_1 - \mathbf{A}'_1 \mathbf{C}_2^{-1} \mathbf{S}_2$$

and

$$\mathbf{A}_{N_1} = \mathbf{A}'_{N_1} - \mathbf{C}'_{N_1} \mathbf{A}_{N_1-1}^{-1} \mathbf{B}_{N_1-1}$$

$$\mathbf{B}_{N_1} = \mathbf{B}'_{N_1} - \mathbf{C}'_{N_1} \mathbf{A}_{N_1-1}^{-1} \mathbf{C}_{N_1-1} \qquad (7.8)$$

$$\mathbf{S}_{N_1} = \mathbf{S}'_{N_1} - \mathbf{C}'_{N_1} \mathbf{A}_{N_1-1}^{-1} \mathbf{S}_{N_1-1}$$

The set of algebraic equations solved during the first ADI sweep can now be written as

$$
\begin{bmatrix}
\mathbf{B}_1 & \mathbf{C}_1 \\
\mathbf{A}_2 & \mathbf{B}_2 & \mathbf{C}_2 \\
& \mathbf{A}_3 & \mathbf{B}_3 & \mathbf{C}_3 \\
& & & \cdot \\
& & & & \cdot \\
& & & & & \cdot \\
& & & \mathbf{A}_{N_1-2} & \mathbf{B}_{N_1-2} & \mathbf{C}_{N_1-2} \\
& & & & \mathbf{A}_{N_1-1} & \mathbf{B}_{N_1-1} & \mathbf{C}_{N_1-1} \\
& & & & & \mathbf{A}_{N_1} & \mathbf{B}_{N_1}
\end{bmatrix}
\begin{bmatrix}
\Delta\hat{\mathbf{Q}}_1^* \\
\Delta\hat{\mathbf{Q}}_2^* \\
\Delta\hat{\mathbf{Q}}_3^* \\
\cdot \\
\cdot \\
\cdot \\
\Delta\hat{\mathbf{Q}}_{N_1-2}^* \\
\Delta\hat{\mathbf{Q}}_{N_1-1}^* \\
\Delta\hat{\mathbf{Q}}_{N_1}^*
\end{bmatrix}
=
\begin{bmatrix}
\mathbf{S}_1 \\
\mathbf{S}_2 \\
\mathbf{S}_3 \\
\cdot \\
\cdot \\
\cdot \\
\mathbf{S}_{N_1-2} \\
\mathbf{S}_{N_1-1} \\
\mathbf{S}_{N_1}
\end{bmatrix}
\tag{7.9}
$$

Since the coefficient matrix is now block tridiagonal, the equations can be solved using the block matrix version of the Thomas algorithm (e.g., see Anderson, Tannehill, and Pletcher, 1984). The procedure can be summarized as follows:

1. Define $\mathbf{D}_1 = \mathbf{B}_1$.

2. Compute $\mathbf{E}_1 = \mathbf{D}_1^{-1}\mathbf{C}_1$ and $\Delta\hat{\mathbf{Q}}_1' = \mathbf{D}_1^{-1}\mathbf{S}_1$.

3. For $i = 2$ to N_1, compute

   $$\mathbf{D}_i = \mathbf{B}_i - \mathbf{A}_i\mathbf{E}_{i-1}$$

   $$\mathbf{E}_i = \mathbf{D}_i^{-1}\mathbf{C}_i$$

   $$\Delta\hat{\mathbf{Q}}_i' = \mathbf{D}_i^{-1}(\mathbf{S}_i - \mathbf{A}_i\Delta\hat{\mathbf{Q}}_{i-1}')$$

   (Actually, $\mathbf{E}_i$ is only needed for $i = 2$ to $N_1 - 1$).

4. Then, set $\Delta\hat{\mathbf{Q}}_{N_1} = \Delta\hat{\mathbf{Q}}_{N_1}'$.

5. Finally, for $i = N_1 - 1$ to 1, compute $\Delta\hat{\mathbf{Q}}_i = \Delta\hat{\mathbf{Q}}_i' - \mathbf{E}_i\Delta\hat{\mathbf{Q}}_{i+1}$.

In the *Proteus* code, in step 2 $\mathbf{E}_1$ and $\Delta\hat{\mathbf{Q}}_1'$ are actually obtained by solving $\mathbf{D}_1\mathbf{E}_1 = \mathbf{C}_1$ and $\mathbf{D}_1\Delta\hat{\mathbf{Q}}_1' = \mathbf{S}_1$ using LU decomposition of $\mathbf{D}$. A similar procedure is used to compute $\mathbf{E}_i$ and $\Delta\hat{\mathbf{Q}}_i'$ in step 3.

7.2.2 Spatially Periodic Boundary Conditions

In computational coordinates a spatially periodic boundary condition in the ξ direction may be represented as shown in Figure 7.1.[6]

---

[6] As in Section 7.2.1, this discussion is written for the first ADI sweep, but an exactly analogous procedure is followed for spatially periodic boundary conditions in the second sweep.
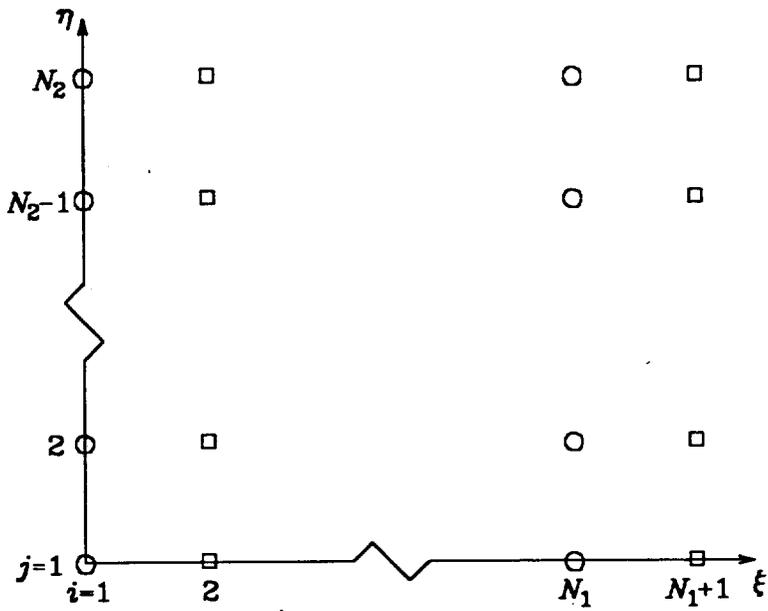
Figure 7.1 - Spatially periodic boundary condition.

The grid points along the $i = 1$ and $i = N_1$ lines are "similar" in the geometric sense, and have the same flow solution. Therefore, for a spatially periodic boundary condition in the ξ direction, $\hat{Q}_1 = \hat{Q}_{N_1}$.

To implement this boundary condition, an additional set of points is added at $i = N_1 + 1$, setting $\hat{Q}_{N_1 + 1} = \hat{Q}_2$. This allows us to use central differencing in the ξ direction at $i = N_1$, computing the coefficients in the same way as at the interior points.

The resulting set of algebraic equations will consist of $N_1 - 1$ equations (for $i = 2$ to N_1), with $N_1 + 1$ unknowns. The block coefficient matrix thus has $N_1 - 1$ rows and $N_1 + 1$ columns, as follows:

$$
\begin{bmatrix}
\mathbf{A}_2 & \mathbf{B}_2 & \mathbf{C}_2 & & & & & \\
& \mathbf{A}_3 & \mathbf{B}_3 & \mathbf{C}_3 & & & & \\
& & \mathbf{A}_4 & \mathbf{B}_4 & \mathbf{C}_4 & & & \\
& & & \cdot & & & & \\
& & & & \cdot & & & \\
& & & & & \cdot & & \\
& & & \mathbf{A}_{N_1-2} & \mathbf{B}_{N_1-2} & \mathbf{C}_{N_1-2} & & \\
& & & & \mathbf{A}_{N_1-1} & \mathbf{B}_{N_1-1} & \mathbf{C}_{N_1-1} & \\
& & & & & \mathbf{A}_{N_1} & \mathbf{B}_{N_1} & \mathbf{C}_{N_1}
\end{bmatrix}
\begin{bmatrix}
\Delta\hat{\mathbf{Q}}_1^* \\
\Delta\hat{\mathbf{Q}}_2^* \\
\Delta\hat{\mathbf{Q}}_3^* \\
\Delta\hat{\mathbf{Q}}_4^* \\
\cdot \\
\cdot \\
\cdot \\
\Delta\hat{\mathbf{Q}}_{N_1-2}^* \\
\Delta\hat{\mathbf{Q}}_{N_1-1}^* \\
\Delta\hat{\mathbf{Q}}_{N_1}^* \\
\Delta\hat{\mathbf{Q}}_{N_1+1}^*
\end{bmatrix}
=
\begin{bmatrix}
\mathbf{S}_2 \\
\mathbf{S}_3 \\
\mathbf{S}_4 \\
\cdot \\
\cdot \\
\cdot \\
\mathbf{S}_{N_1-2} \\
\mathbf{S}_{N_1-1} \\
\mathbf{S}_{N_1}
\end{bmatrix}
\tag{7.10}
$$

These equations result from the application of equation (7.5a) for $i = 2$ to N_1. As in the previous section, parameter $\Delta\hat{\mathbf{Q}}^*$ is the N_{eq}-element vector containing the unknown dependent variables; $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are the $N_{eq} \times N_{eq}$ coefficient submatrices at $i - 1$, i, and $i + 1$, respectively; and $\mathbf{S}$ is the N_{eq}-element subvector containing the explicit source terms.

Since $\hat{\mathbf{Q}}_1 = \hat{\mathbf{Q}}_{N_1}$ and $\hat{\mathbf{Q}}_2 = \hat{\mathbf{Q}}_{N_1+1}$, equation (7.10) can be rewritten with $N_1 - 1$ unknowns as:

$$
\begin{bmatrix}
\mathbf{B}_2 & \mathbf{C}_2 & & & & & & & \mathbf{A}_2 \\
\mathbf{A}_3 & \mathbf{B}_3 & \mathbf{C}_3 & & & & & & \\
& \mathbf{A}_4 & \mathbf{B}_4 & \mathbf{C}_4 & & & & & \\
& & & \cdot & & & & & \\
& & & & \cdot & & & & \\
& & & & & \cdot & & & \\
& & & & \mathbf{A}_{N_1-2} & \mathbf{B}_{N_1-2} & \mathbf{C}_{N_1-2} & & \\
& & & & & \mathbf{A}_{N_1-1} & \mathbf{B}_{N_1-1} & \mathbf{C}_{N_1-1} & \\
\mathbf{C}_{N_1} & & & & & & \mathbf{A}_{N_1} & \mathbf{B}_{N_1}
\end{bmatrix}
\begin{bmatrix}
\Delta\hat{\mathbf{Q}}_2^* \\
\Delta\hat{\mathbf{Q}}_3^* \\
\Delta\hat{\mathbf{Q}}_4^* \\
\cdot \\
\cdot \\
\cdot \\
\Delta\hat{\mathbf{Q}}_{N_1-2}^* \\
\Delta\hat{\mathbf{Q}}_{N_1-1}^* \\
\Delta\hat{\mathbf{Q}}_{N_1}^*
\end{bmatrix}
=
\begin{bmatrix}
\mathbf{S}_2 \\
\mathbf{S}_3 \\
\mathbf{S}_4 \\
\cdot \\
\cdot \\
\cdot \\
\mathbf{S}_{N_1-2} \\
\mathbf{S}_{N_1-1} \\
\mathbf{S}_{N_1}
\end{bmatrix}
\tag{7.11}
$$

An efficient algorithm to solve this system can be derived that is similar to the Thomas algorithm for block tridiagonal systems. The procedure can be summarized as follows:

1. Define $\mathbf{D}_2 = \mathbf{B}_2$ and $\mathbf{F}_2 = \mathbf{C}_{N_1}$.

2. Compute $\mathbf{E}_2 = \mathbf{D}_2^{-1}\mathbf{C}_2$, $\mathbf{G}_2 = \mathbf{D}_2^{-1}\mathbf{A}_2$, and $\Delta\hat{\mathbf{Q}}_2' = \mathbf{D}_2^{-1}\mathbf{S}_2$.

3. For $i = 3$ to $N_1 - 1$, compute

$$\mathbf{D}_i = \mathbf{B}_i - \mathbf{A}_i \mathbf{E}_{i-1}$$

$$\mathbf{E}_i = \mathbf{D}_i^{-1} \mathbf{C}_i$$

$$\mathbf{F}_i = -\mathbf{F}_{i-1} \mathbf{E}_{i-1}$$

$$\mathbf{G}_i = -\mathbf{D}_i^{-1} \mathbf{A}_i \mathbf{G}_{i-1}$$

$$\Delta \hat{\mathbf{Q}}_i' = \mathbf{D}_i^{-1} (\mathbf{S}_i - \mathbf{A}_i \Delta \hat{\mathbf{Q}}_{i-1}')$$

4. Compute

$$\mathbf{G}_{N_1-1} = \mathbf{D}_{N_1-1}^{-1} (\mathbf{C}_{N_1-1} - \mathbf{A}_{N_1-1} \mathbf{G}_{N_1-2})$$

$$\mathbf{F}_{N_1-1} = \mathbf{A}_{N_1} - \mathbf{F}_{N_1-2} \mathbf{E}_{N_1-2}$$

$$\mathbf{D}_{N_1} = \mathbf{B}_{N_1} - \sum_{i=2}^{N_1-1} \mathbf{F}_i \mathbf{G}_i$$

$$\Delta \hat{\mathbf{Q}}_{N_1}' = \mathbf{D}_{N_1}^{-1} \left(\mathbf{S}_{N_1} - \sum_{i=2}^{N_1-1} \mathbf{F}_i \Delta \hat{\mathbf{Q}}_i' \right)$$

5. Then, set $\Delta \hat{\mathbf{Q}}_{N_1} = \Delta \hat{\mathbf{Q}}_{N_1}'$.

6. Compute $\Delta \hat{\mathbf{Q}}_{N_1-1} = \Delta \hat{\mathbf{Q}}_{N_1-1}' - \mathbf{G}_{N_1-1} \Delta \hat{\mathbf{Q}}_{N_1}$.

7. Finally, for $i = N_1 - 2$ to 2, compute $\Delta \hat{\mathbf{Q}}_i = \Delta \hat{\mathbf{Q}}_i' - \mathbf{E}_i \Delta \hat{\mathbf{Q}}_{i+} - \mathbf{G}_i \Delta \hat{\mathbf{Q}}_{N_1}$.

In the *Proteus* code, in step 2 $\mathbf{E}_2$, $\mathbf{G}_2$, and $\Delta \hat{\mathbf{Q}}_2'$ are actually obtained by solving $\mathbf{D}_2 \mathbf{E}_2 = \mathbf{C}_2$, $\mathbf{D}_2 \mathbf{G}_2 = \mathbf{A}_2$, and $\mathbf{D}_2 \Delta \hat{\mathbf{Q}}_2' = \mathbf{S}_2$ using LU decomposition of $\mathbf{D}$. A similar procedure is used to compute $\mathbf{E}_i$, $\mathbf{G}_i$, and $\Delta \hat{\mathbf{Q}}_i'$ in step 3, and $\mathbf{G}_{N_1-1}$ and $\Delta \hat{\mathbf{Q}}_{N_1}'$ in step 4.

7.3 UPDATING BOUNDARY VALUES

7.3.1 Non-Periodic Boundary Conditions

With the ADI algorithm described in Section 7.1, if gradient or extrapolation boundary conditions are used for the first sweep, the boundary values from the first sweep must be updated after the second sweep. This point is easiest to illustrate by looking at the following figure.
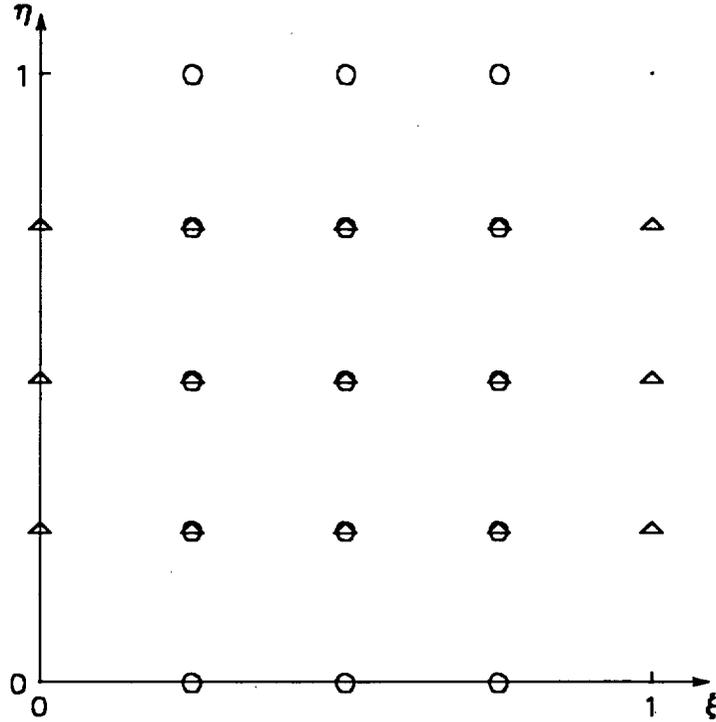
Figure 7.2 - Updating boundary values for non-periodic
boundary conditions.

In Figure 7.2, a 5 x 5 grid is shown in computational space. The triangles represent grid points at which the intermediate values $\hat{Q}^*$ are computed during the first ADI sweep. These include the boundary points at $\varsigma = 0$ and $\xi = 1$. The circles represent grid points at which the final values $\hat{Q}^{n+\cdot}$ are computed during the second ADI sweep, including the boundary points at $\eta = 0$ and $\eta = 1$. If gradient or extrapolation boundary conditions are used during the first sweep, so that the boundary values depend on the interior values, then the intermediate values at $\xi = 0$ and $\xi = 1$ must be updated after the second sweep to be consistent with the final values at the interior points.

To do this, after the second sweep the boundary condition equations are rewritten and solved at the ζ boundaries. At the $\xi = 0$ boundary,

$$\mathbf{B}_1'^n \Delta\hat{\mathbf{Q}}_1^n + \mathbf{C}_1'^n \Delta\hat{\mathbf{Q}}_2^n + \mathbf{A}_1'^n \Delta\hat{\mathbf{Q}}_3^n = \mathbf{S}_1'^n \tag{7.12}$$

The subscripts refer to the value of i, the index in the ξ direction. This equation is applied for $j = 2$ to $N_2 - 1$ in the η direction. For notational convenience, however, the subscript j has been omitted.

All the terms in equation (7.12) are known except $\Delta\hat{\mathbf{Q}}_1^n$. Solving,

$$\Delta\hat{\mathbf{Q}}_1^n = (\mathbf{B}_1'^n)^{-1}\left(\mathbf{S}_1'^n - \mathbf{C}_1'^n \Delta\hat{\mathbf{Q}}_2^n - \mathbf{A}_1'^n \Delta\hat{\mathbf{Q}}_3^n\right) \tag{7.13}$$

At the $\xi = 1$ boundary,

$$\mathbf{C}_{N_1}'^n \Delta\hat{\mathbf{Q}}_{N_1-2}^n + \mathbf{A}_{N_1}'^n \Delta\hat{\mathbf{Q}}_{N_1-1}^n + \mathbf{B}_{N_1}'^n \Delta\hat{\mathbf{Q}}_{N_1}^n = \mathbf{S}_{N_1}'^n \tag{7.14}$$

$$\Delta \hat{Q}^n_{N_1} = (\mathbf{B}'^n_{N_1})^{-1}\left(\mathbf{S}'^n_{N_1} - \mathbf{C}'^n_{N_1}\Delta \hat{Q}^n_{N_1-2} - \mathbf{A}'^n_{N_1}\Delta \hat{Q}^n_{N_1-1}\right)\tag{7.15}$$

Finally, note from Figure 7.2 that new corner point values are never computed in the solution algorithm. To make the corner values consistent with the rest of the flow field, in *Proteus* the corner values of density ρ and total energy E_T are arbitrarily defined by linearly extrapolating from the two adjacent points in both the ξ and η directions, and averaging the two results. The corner values of the velocities are updated by doing the same type of extrapolation. Instead of averaging, however, the extrapolated velocity whose absolute value is lower is used. This was done to maintain no-slip conditions at duct inlets and exits.

7.3.2 Spatially Periodic Boundary Conditions

Updating boundary values from the first sweep is complicated somewhat when spatially periodic boundary conditions are used.
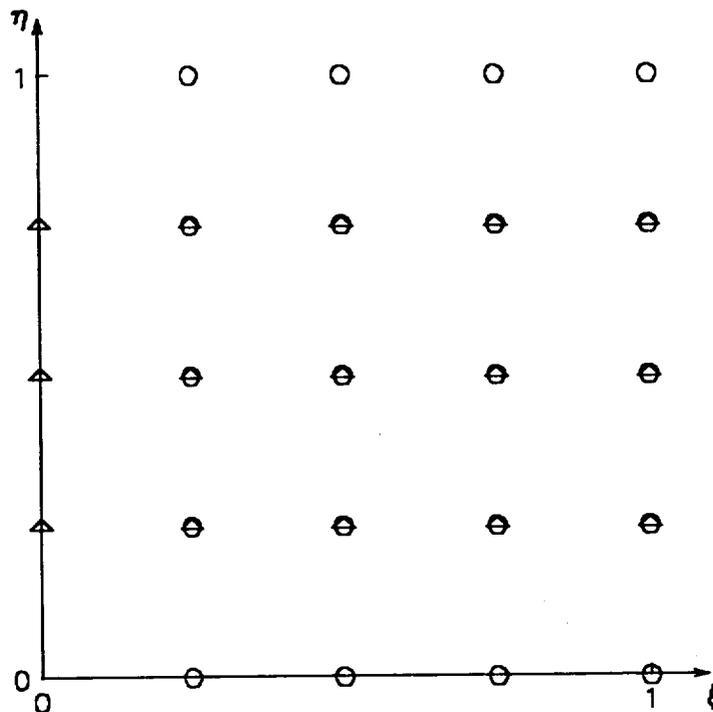
Figure 7.3 - Updating boundary values for periodic
boundary conditions in the ξ direction only.

The situation for a periodic boundary condition in the ξ direction but not in the η direction is shown in Figure 7.3. The triangles again represent grid points at which intermediate values are computed, and the circles represent grid points at which final values are computed. As can be seen from the figure, the intermediate values at $\xi = 0$ must be updated after the second sweep to be consistent with the final values at the interior points. This is easily done by setting $\hat{Q}_1 = \hat{Q}_{N_1}$ for $j = 1$ to N_2.
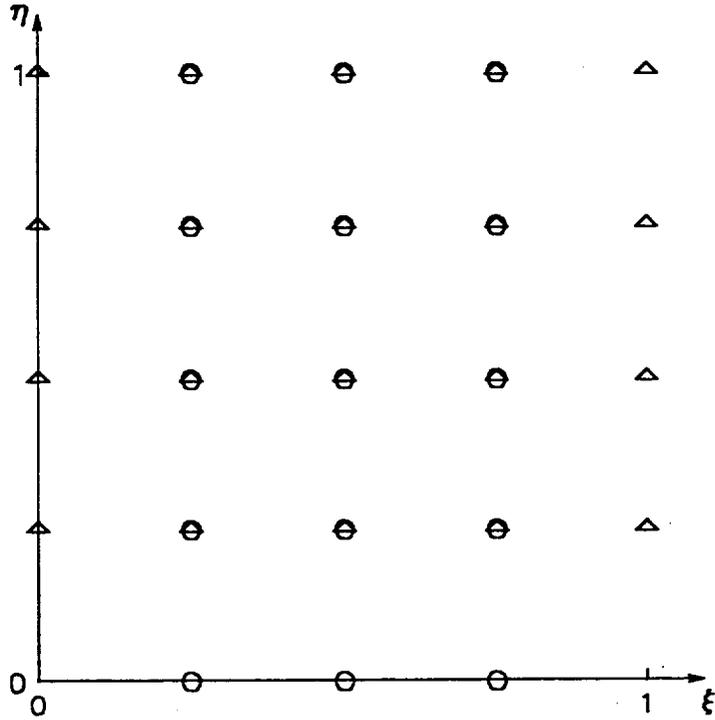
Figure 7.4 - Updating boundary values for periodic boundary conditions in the η direction only.

The situation for a periodic boundary condition in the η direction but not in the ξ direction is shown in Figure 7.4. In this case, the intermediate values at $\xi = 0$ and at $\xi = 1$ must be updated after the second sweep. To do this, the same procedure described in Section 7.3.1 for non-periodic boundary conditions is used, but for $j = 2$ to N_2 instead of $N_2 - 1$. Then, for the lower corner values, $\hat{Q}_{1,1} = \hat{Q}_{1,N_2}$ and $\hat{Q}_{N_1,1} = \hat{Q}_{N_1,N_2}$.
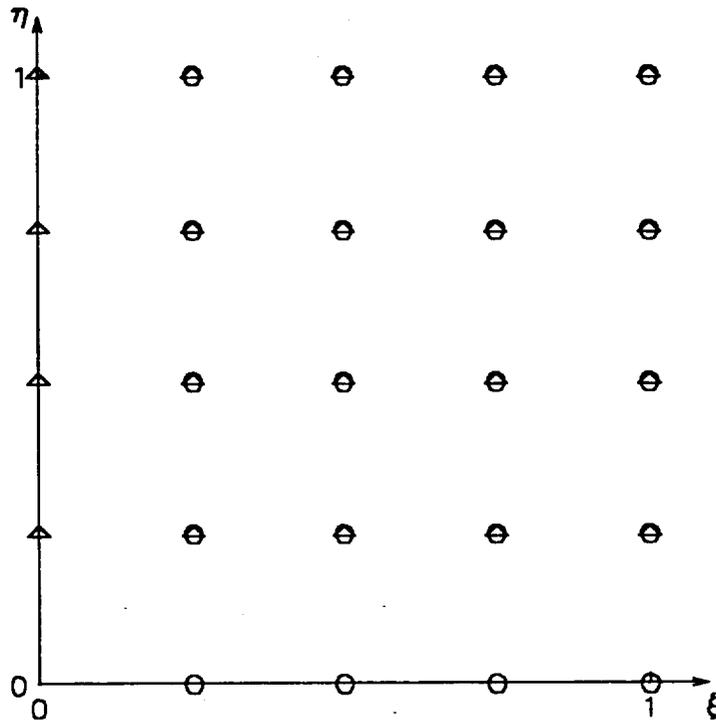
Figure 7.5 - Updating boundary values for periodic boundary conditions in both the ξ and η directions.

And finally, the situation for periodic boundary conditions in both the ξ and η directions is shown in Figure 7.5. Like the case with periodic boundary conditions only in the ξ direction, the intermediate values at $\xi = 0$ must be updated after the second sweep. This is again done by setting $\hat{Q}_1 = \hat{Q}_{N_1}$ for $j = 1$ to N_2.

8.0 ARTIFICIAL VISCOSITY

With the numerical algorithm of Section 7.0, high frequency nonlinear instabilities can appear as the solution develops. For example, in high Reynolds number flows oscillations can result from the odd-even decoupling inherent in the use of second-order central differencing for the inviscid terms. In addition, physical phenomena such as shock waves can cause instabilities when they are captured by the finite difference algorithm. Artificial viscosity, or smoothing, is normally added to the solution algorithm to suppress these high frequency instabilities. Two artificial viscosity models are currently available in the *Proteus* computer code - a constant coefficient model used by Steger (1978), and the nonlinear coefficient model of Jameson, Schmidt, and Turkel (1981). The implementation of these models in generalized nonorthogonal coordinates is described by Pulliam (1986b).

8.1 CONSTANT COEFFICIENT ARTIFICIAL VISCOSITY

The constant coefficient model uses a combination of explicit and implicit artificial viscosity. The standard explicit smoothing uses fourth-order differences, and damps the high frequency nonlinear instabilities. Second-order explicit smoothing, while not used by Steger or Pulliam, is also available in *Proteus*. It provides more smoothing than the fourth-order smoothing but introduces a larger error, and is therefore not used as often. The implicit smoothing is second order and is intended to extend the linear stability bound of the fourth-order explicit smoothing.

The explicit artificial viscosity is implemented in the numerical algorithm by adding the following terms to the right hand side of equation (7.5a) (i.e., the source term for the first ADI sweep.)

$$\frac{\varepsilon_E^{(2)}\Delta\tau}{J}(\nabla_\xi\Delta_\xi Q + \nabla_\eta\Delta_\eta Q) - \frac{\varepsilon_E^{(4)}\Delta\tau}{J}\left[(\nabla_\xi\Delta_\xi)^2 Q + (\nabla_\eta\Delta_\eta)^2 Q\right] \tag{8.1}$$

where $\varepsilon_E^{(2)}$ and $\varepsilon_E^{(4)}$ are the second- and fourth-order explicit artificial viscosity coefficients. The symbols ∇ and Δ are backward and forward first difference operators. Thus,

$$\nabla_\xi Q_i = Q_i - Q_{i-1}$$
$$\Delta_\xi Q_i = Q_{i+1} - Q_i$$
$$\nabla_\xi\Delta_\xi Q_i = Q_{i+1} - 2Q_i + Q_{i-1}$$
$$(\nabla_\xi\Delta_\xi)^2 Q_i = Q_{i+2} - 4Q_{i+1} + 6Q_i - 4Q_{i-1} + Q_{i-2}$$

Equivalent formulas are used for differences in the η direction.

A few details should be noted at this point. First, the sign in front of the artificial viscosity term being added to equation (7.5a) depends on the sign of the *"i"* term in the difference formula. For damping, that term must be negative when added to the right hand side of the equations (i.e., explicit artificial viscosity), and positive when added to the left hand side (i.e., implicit artificial viscosity.) See Anderson, Tannehill, and Pletcher (1984) for details. Second, the terms being added are differences only, and not finite difference approximations to derivatives. They are therefore not divided by $\Delta\xi$, etc. Third, the variables being differenced are Q, not $\hat{Q}$. As noted by Pulliam (1986b), scaling the artificial viscosity terms by $1/J$ makes them consistent with the form of the remaining terms in the equations. Fourth, the terms are also scaled by $\Delta\tau$. This makes the steady state solution independent of the time step size (Pulliam, 1986b). And finally, note that the fourth-order difference formula cannot be used at grid points adjacent to boundaries. At these points, therefore, the appropriate fourth-order term in expression (8.1) is replaced by a second-order term. Thus, for points adjacent to the $\xi = 0$ and $\xi = 1$ boundaries, $-\varepsilon_E^{(4)}\Delta\tau[(\nabla_\xi\Delta_\xi)^2 Q]/J$ is replaced by

$$+\frac{\varepsilon_E^{(4)}\Delta\tau}{J}\nabla_\xi\Delta_\xi Q \tag{8.2}$$

A similar expression is used at points adjacent to the $\eta = 0$ and $\eta = 1$ boundaries.

The implicit artificial viscosity is implemented by adding the following terms to the left hand side of the equations specified.

$$-\frac{\varepsilon_I\Delta\tau}{J}\left[\nabla_\xi\Delta_\xi(J\Delta\hat{Q}^*)\right] \quad \text{to equation (7.5a)}$$

$$\tag{8.3}$$

$$-\frac{\varepsilon_I\Delta\tau}{J}\left[\nabla_\eta\Delta_\eta(J\Delta\hat{Q}^n)\right] \quad \text{to equation (7.5b)}$$

Note that the addition of the artificial viscosity terms, in effect, changes the original governing partial differential equations. At steady state, the difference equations with the artificial viscosity terms added actually correspond to the following differential equations.[7]

$$\frac{\partial\hat{E}}{\partial\xi} + \frac{\partial\hat{F}}{\partial\eta} = \frac{\partial\hat{E}_V}{\partial\xi} + \frac{\partial\hat{F}_V}{\partial\eta} + \frac{\varepsilon_E^{(2)}}{J}\left[(\Delta\xi)^2\frac{\partial^2(J\hat{Q})}{\partial\xi^2} + (\Delta\eta)^2\frac{\partial^2(J\hat{Q})}{\partial\eta^2}\right]$$

$$-\frac{\varepsilon_E^{(4)}}{J}\left[(\Delta\xi)^4\frac{\partial^4(J\hat{Q})}{\partial\xi^4} + (\Delta\eta)^4\frac{\partial^4(J\hat{Q})}{\partial\eta^4}\right]$$

The implicit terms do not appear, since they difference $\Delta\hat{Q}$, and in the steady form of the equations $\Delta\hat{Q} = 0$. The artificial viscosity terms do not represent anything physical. The coefficients should therefore be as small as possible, but still large enough to damp any instabilities. Although optimum values will vary from problem to problem, recommended levels are $\varepsilon_E^{(4)} = O(1)$ and $\varepsilon_I = 2\varepsilon_E^{(4)}$ (Pulliam, 1986b). The recommended level for $\varepsilon_E^{(2)}$, when used, is $\varepsilon_E^{(2)} = O(1)$.

8.2 NONLINEAR COEFFICIENT ARTIFICIAL VISCOSITY

The nonlinear coefficient artificial viscosity model is strictly explicit. Using the model as described by Pulliam (1986b), but in the current notation, the following terms are added to the right hand side of equation (7.5a).

$$\nabla_\xi\left\{\left[\left(\frac{\psi}{J}\right)_{i+1} + \left(\frac{\psi}{J}\right)_i\right](\varepsilon_\xi^{(2)}\Delta_\xi Q - \varepsilon_\xi^{(4)}\Delta_\xi\nabla_\xi\Delta_\xi Q)_i\right\}$$

$$+\nabla_\eta\left\{\left[\left(\frac{\psi}{J}\right)_{j+1} + \left(\frac{\psi}{J}\right)_j\right](\varepsilon_\eta^{(2)}\Delta_\eta Q - \varepsilon_\eta^{(4)}\Delta_\eta\nabla_\eta\Delta_\eta Q)_j\right\} \tag{8.4}$$

The difference operation $\Delta_\xi\nabla_\xi\Delta_\xi Q$ is given by

$$\Delta_\xi\nabla_\xi\Delta_\xi Q_i = Q_{i+2} - 3Q_{i+1} + 3Q_i - Q_{i-1}$$

In the expression (8.4), ψ is defined as

$$\psi = \psi_x + \psi_y \tag{8.5}$$

---

[7] These equations represent the use of the constant coefficient artificial viscosity model presented in this section. The nonlinear coefficient model to be presented in Section 8.2 is more complicated, but the same principle applies.

where ψ_x and ψ_y are spectral radii defined by[8]

$$\psi_x = \frac{|U| + a\sqrt{\xi_x{}^2 + \xi_y{}^2}}{\Delta\xi}$$
$$\psi_y = \frac{|V| + a\sqrt{\eta_x{}^2 + \eta_y{}^2}}{\Delta\eta} \tag{8.6}$$

Here U and V are the contravariant velocities without metric normalization, defined by

$$U = \xi_t + \xi_x u + \xi_y v$$
$$V = \eta_t + \eta_x u + \eta_y v \tag{8.7}$$

and $a = \sqrt{\gamma RT}$, the speed of sound.

The parameters $\varepsilon^{(2)}$ and $\varepsilon^{(4)}$ are the second- and fourth-order artificial viscosity coefficients. Instead of being specified directly by the user, as they are in the constant coefficient model, in the nonlinear coefficient model they are a function of the pressure field. For the coefficients of the ξ direction differences,

$$\left(\varepsilon_\xi^{(2)}\right)_i = \kappa_2 \Delta\tau \max(\sigma_{i+1}, \ \sigma_i, \ \sigma_{i-1}) \tag{8.8a}$$

$$\left(\varepsilon_\xi^{(4)}\right)_i = \max\left[0, \ \kappa_4 \Delta\tau - \left(\varepsilon_\xi^{(2)}\right)_i\right] \tag{8.8b}$$

where

$$\sigma_i = \left| \frac{p_{i+1} - 2p_i + p_{i-1}}{p_{i+1} + 2p_i + p_{i-1}} \right| \tag{8.9}$$

Similar formulas are used for the coefficients of the η direction differences.

The parameter σ is a pressure gradient scaling parameter that increases the amount of second-order smoothing relative to fourth-order smoothing near shock waves. The logic used to compute $\varepsilon^{(4)}$ switches off the fourth-order smoothing when the second-order smoothing term is large.

The parameters κ_2 and κ_4 are user-specified constants. Like the coefficients in the constant coefficient model, the optimum values will be problem-dependent, and are best chosen through experience. Cases have been run with values of κ_2 ranging from from 0.01 for flows without shocks to 0.1 for flows with shocks, and κ_4 ranging from 0.0002 for flows computed with spatially constant second-order time differencing to 0.005 for flows computed with spatially varying first-order time differencing. Pulliam (1986b) gives $\kappa_2 = 0.25$ and $\kappa_4 = 0.01$ as typical values for an Euler analysis.

Like the constant coefficient artificial viscosity model, the nonlinear coefficient model requires special formulas near boundaries. To apply (8.4) at $i = 2$, $\varepsilon_\xi^{(2)}$ is needed at $i = 1$. It is defined as

$$\left(\varepsilon_\xi^{(2)}\right)_1 = \kappa_2 \Delta\tau \max(\sigma_2, \ \sigma_1)$$

With the above definition, applying (8.4) at $i = 2$ and $i = N_1 - 1$ requires σ at $i = 1$ and $i = N_1$. They are defined as

---

[8] It should be noted that the grid increments $\Delta\xi$ and $\Delta\eta$ in these definitions do not appear in the corresponding formulas presented by Pulliam (1986b). This is because the grids used by Pulliam are constructed such that $\Delta\xi = \Delta\eta = 1$, while in *Proteus* $\Delta\xi = 1/(N_1 - 1)$ and $\Delta\eta = 1/(N_2 - 1)$. The definitions used here for ψ_x and ψ_y result in an artificial viscosity level equivalent to that described by Pulliam.

$$\sigma_1 = \left| \frac{-p_4 + 4p_3 - 5p_2 + 2p_1}{p_4 + 4p_3 + 5p_2 + 2p_1} \right|$$

$$\sigma_{N_1} = \left| \frac{-p_{N_1-3} + 4p_{N_1-2} - 5p_{N_1-1} + 2p_{N_1}}{p_{N_1-3} + 4p_{N_1-2} + 5p_{N_1-1} + 2p_{N_1}} \right|$$

And, finally, applying (8.4) at $i = 2$ and $i = N_1 - 1$ requires $\Delta_\xi \nabla_\xi \Delta_\xi Q$ at $i = 1$ and $i = N_1 - 1$. There are numerous formulas that could be used. The ones currently in the *Proteus* code are

$$\Delta_\xi \nabla_\xi \Delta_\xi Q_1 = -Q_5 + 5Q_4 - 9Q_3 + 7Q_2 - 2Q_1$$

$$\Delta_\xi \nabla_\xi \Delta_\xi Q_{N_1-1} = Q_{N_1-4} - 5Q_{N_1-3} + 9Q_{N_1-2} - 7Q_{N_1-1} + 2Q_{N_1}$$

9.0 TURBULENCE MODELS

As noted briefly in Section 2.0, for turbulent flow the Reynolds stress and turbulent heat flux terms are modeled using the Boussinesq approach. An effective viscosity is thus defined as $\mu = \mu_l + \mu_t$, where μ_l is the laminar, or molecular, viscosity coefficient, and μ_t is the turbulent viscosity coefficient. Similarly, an effective second coefficient of viscosity is defined as $\lambda = \lambda_l + \lambda_t$, and an effective thermal conductivity coefficient is defined as $k = k_l + k_t$.

The turbulent coefficients must be computed using a turbulence model appropriate for the flow being computed. In *Proteus*, turbulence is modeled using either a generalized version of the Baldwin and Lomax (1978) algebraic eddy viscosity model, or the Chien (1982) low Reynolds number k-ε model.

9.1 BALDWIN-LOMAX MODEL

For wall-bounded flows, (i.e., boundary layers), the Baldwin-Lomax turbulence model is a two-layer model, with

$$\mu_t = \begin{cases} (\mu_t)_{inner} & \text{for } y_n \leq y_b \\ (\mu_t)_{outer} & \text{for } y_n > y_b \end{cases} \tag{9.1}$$

where y_n is the normal distance from the wall, and y_b is the smallest value of y_n at which the values of μ_t from the inner and outer region formulas are equal. For free turbulent flows (i.e., mixing layers, jets, and wakes), $\mu_t = (\mu_t)_{outer}$. In the inner region, in addition to the Baldwin-Lomax model, an alternate expression first presented by Spalding (1961), and later by Kleinstein (1967), is also available.

In a simple boundary layer analysis, with only one solid surface, the procedure for computing μ_t is relatively straightforward. In a general Navier-Stokes analysis, however, any or all of the boundaries may be solid surfaces. If both boundaries in a given coordinate direction are solid surfaces, the turbulence model is applied separately for each surface. An averaging procedure is used to combine the resulting two μ_t profiles into one. If neither boundary in a given direction is a solid surface, the formulation for free turbulent flows is used. In addition, values of μ_t are computed separately for both the ξ and η directions. This results in two complete turbulent viscosity fields. Another averaging procedure is then used to compute a single value of μ_t at each point in the flow.[9]

9.1.1 Outer Region

The outer region turbulent viscosity at a given ξ or η station is computed from

$$(\mu_t)_{outer} = K C_{cp} \rho F_{Kleb} F_{wake} Re_r \tag{9.2}$$

where K is the Clauser constant, taken as 0.0168, C_{cp} is a constant taken as 1.6, and ρ is the static density.

The parameter F_{wake} is computed from

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[9] This discussion is for the most general situation. When the flow is expected to be predominantly in one direction, input parameters in the *Proteus* code should be used to specify that direction.

$$F_{wake} = \begin{cases} y_{max} F_{max} & \text{for wall-bounded flows} \\ C_{wk} V_{diff}^2 \dfrac{y_{max}}{F_{max}} & \text{for free turbulent flows} \end{cases} \quad (9.3)$$

where C_{wk} is a constant taken as 0.25, and

$$V_{diff} = \left| \vec{V} \right|_{max} - \left| \vec{V} \right|_{min}$$

where $\vec{V}$ is the total velocity vector.

The parameter F_{max} in equation (9.3) is the maximum value of

$$F(y_n) = \begin{cases} y_n \left| \vec{\Omega} \right| \left(1 - e^{-y^+/A^+} \right) & \text{for wall-bounded flows} \\ y_n \left| \vec{\Omega} \right| & \text{for free turbulent flows} \end{cases} \quad (9.4)$$

and y_{max} is the value of y_n corresponding to F_{max}. It has been found that for wall-bounded flows the function $F(y_n)$ can have two peaks. As noted by Kirtley (1987), using the second peak as the location of F_{max} yields the best results.

For wall-bounded flows, y_n is the normal distance from the wall. For free turbulent flows, two values of F_{max} and y_{max} are computed - one using the location of $\left| \vec{V} \right|_{max}$ as an origin for y_n, and one using the location of $\left| \vec{V} \right|_{min}$. The origin giving the smaller value of y_{max} is the one finally used for computing y_n, F_{max}, and y_{max}.

In equation (9.4), $\left| \vec{\Omega} \right|$ is the magnitude of the total vorticity, defined for two-dimensional planar flow as

$$\left| \vec{\Omega} \right| = \left| \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right| \quad (9.5)$$

The parameter A^+ is the Van Driest damping constant, taken as 26.0. The coordinate y^+ is defined as

$$y^+ = \frac{\rho_w u_\tau y_n}{\mu_w} Re_r = \frac{\sqrt{\tau_w \rho_w Re_r}}{\mu_w} y_n \quad (9.6)$$

where $u_\tau = \sqrt{\tau_w / \rho_w Re_r}$ is the friction velocity, τ is the shear stress, and the subscript w indicates a wall value. In *Proteus*, τ_w is set equal to $\mu_w \left| \vec{\Omega} \right|_w$.

The function F_{Kleb} in equation (9.2) is the Klebanoff intermittency factor. For free turbulent flows, $F_{Kleb} = 1$. For wall-bounded flows,

$$F_{Kleb} = (C_{Kleb})_{min} + [1 - (C_{Kleb})_{min}] \left[1 + B \left(\frac{C_{Kleb} y_n}{y_{max}} \right)^6 \right]^{-1} \quad (9.7)$$

This factor accounts for the experimentally observed fact that, as the free stream is approached, the fraction of time the flow is turbulent decreases. In equation (9.7), B and C_{Kleb} are constants taken as 5.5 and 0.3, respectively. $(C_{Kleb})_{min}$ is a constant normally equal to 0.0. However, when using the Baldwin-Lomax model to generate initial turbulent viscosity values for the Chien k-ε model (discussed in Section 9.2), $(C_{Kleb})_{min}$ is set equal to 0.1. This yields a small positive value for μ_t in the free stream, and has been found to minimize starting problems with the k-ε model.

9.1.2 Inner Region

The inner region turbulent viscosity in the Baldwin-Lomax model is

$$(\mu_t)_{inner} = \rho l^2 \left| \vec{\Omega} \right| Re_r \tag{9.8}$$

where l is the mixing length, normally given by

$$l = \kappa y_n \left(1 - e^{-y^+/A^+} \right) \tag{9.9}$$

and κ is the Von Karman constant, taken as 0.4.

A modified form of equation (9.9), proposed by Launder and Priddin (1973), may also be used. This formula is most useful for flows with steep negative gradients of shear stress normal to the wall, such as accelerated flows or flows with suction. Their modified formula for l is

$$l = \kappa y_n \left(1 - e^{-y^+(\tau^+)^n/A^+} \right) \tag{9.10}$$

where

$$\tau^+ = \frac{\tau}{\tau_w} = \frac{\mu \left| \vec{\Omega} \right|}{\mu_w \left| \vec{\Omega} \right|_w}$$

and n is a constant taken as 1.7.

The inner region turbulent viscosity may also be computed using an alternate expression first presented by Spalding (1961), and later by Kleinstein (1967). In this model,

$$(\mu_t)_{inner} = \mu_l \kappa e^{-\kappa B} \left[e^{\kappa u^+} - 1 - \kappa u^+ - \frac{1}{2} \left(\kappa u^+ \right)^2 \right] \tag{9.11}$$

where

$$u^+ = \frac{\left| \vec{V} \right|}{u_\tau} = \frac{\left| \vec{V} \right|}{\sqrt{\tau_w/\rho_w Re_r}}$$

Again, in *Proteus*, τ_w is set equal to $\mu_w \left| \vec{\Omega} \right|_w$.

9.1.3 Averaging Procedures for Multiple Boundaries

As noted earlier, if both boundaries in a given coordinate direction are solid surfaces, the turbulence model equations are applied separately at each surface. It is assumed that the two inner regions do not overlap. The outer regions, of course, do overlap, and an averaging procedure is used to combine the two outer region μ_t profiles into one. For example, if the $\eta = 0$ and $\eta = 1$ boundaries are both solid surfaces,[10] the two values of F_{wake} at a particular ζ station are combined using the following averaging formula:

$$F_{wake} = \frac{(F_{wake})_1 f_1 + (F_{wake})_2 f_2}{f_1 + f_2} \tag{9.12}$$

Here $(F_{wake})_1$ and $(F_{wake})_2$ are the separate values computed for the $\eta = 0$ and $\eta = 1$ surfaces using equation (9.3). The parameters f_1 and f_2 are defined by

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[10] An analogous procedure is used for solid surfaces in the ζ direction.

$$f_1 = \left(\frac{2D_1}{(y_n)_1} \right)^n$$

$$f_2 = \left(\frac{2D_2}{(y_n)_2} \right)^n$$

where n is a constant taken as 2.0, $(y_n)_1$ and $(y_n)_2$ are the normal distances to the $\eta = 0$ and $\eta = 1$ surfaces, respectively, and D_1 and D_2 are the normal distances from the two η surfaces to the location of $\left| \vec{V} \right|_{max}$. In addition, the y_n/y_{max} value needed in equation (9.7) for F_{Kleb} is computed for both η surfaces, and the minimum is used. These values of F_{wake} and F_{Kleb} are then used in equation (9.2) to compute $(\mu_t)_{outer}$.

The averaging procedure described above computes a single μ_t profile from the two profiles that are computed when both boundaries in a given coordinate direction are solid surfaces. We still must average the two values that result from computing μ_t separately for both coordinate directions.[11] Following Goldberg and Chakravarthy (1987), this is done using the following formula:

$$\mu_t = \frac{(\mu_t/y_n)_1 + (\mu_t/y_n)_2}{[(1/y_n)_1^2 + (1/y_n)_2^2]^{1/2}} = \frac{(y_n)_2(\mu_t)_1 + (y_n)_1(\mu_t)_2}{[(y_n)_1^2 + (y_n)_2^2]^{1/2}} \tag{9.13}$$

Here $(\mu_t)_1$ and $(\mu_t)_2$ are the separate values computed due to the presence of boundaries at $\xi = 0$ and $\xi = 1$, and at $\eta = 0$ and $\eta = 1$, respectively. If there is only one solid surface in the ξ direction, $(y_n)_1$ is taken as the normal distance to that surface. If both ξ boundaries are solid surfaces, $(y_n)_1$ is taken as the normal distance to the closest one. If there are no solid surfaces in the ξ direction, $(y_n)_1$ is the normal distance to the location of either $\left| \vec{V} \right|_{max}$ or $\left| \vec{V} \right|_{min}$, as described in Section 9.1.1. Analogous rules are used for $(y_n)_2$.

9.1.4 Transition Model

After μ_t has been computed using the procedure described in the previous sections, a transition intermittency factor may be applied to simulate laminar-turbulent transition. The transition model is based on one given by Cebeci and Bradshaw (1984) for boundary layer analyses, and assumes that a geometric leading edge exists at either $\xi = 0$ or $\eta = 0$. They report that the model is valid for adiabatic flows at Mach numbers less than 5. In this transition model,

$$\mu_t = \begin{cases} 0 & \text{for } x \leq x_{tr} \\ \gamma_{tr}\,\mu_t & \text{for } x > x_{tr} \end{cases} \tag{9.14}$$

where x is the distance from the leading edge, the subscript tr indicates a value at the start of the transition region, and γ_{tr} is a transition intermittency factor given by

$$\gamma_{tr} = 1 - \exp\left[-G(x - x_{tr}) \int_{x_{tr}}^{x} \frac{1}{u_e} \, dx \right] \tag{9.15}$$

In equation (9.15), u_e is the velocity at the edge of the boundary layer. The factor G is given by

$$G = 8.33 \times 10^{-4} \frac{u_e^3}{\nu^2} Re_{x_{tr}}^{-1.34}$$

where $Re_{x_{tr}} = (u_e x/\nu)_{tr} Re_r$, and ν is the laminar kinematic viscosity at the edge of the boundary layer.

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[11] As noted earlier, this discussion is for the most general situation. When the flow is expected to be predominantly in one direction, input parameters in the *Proteus* code should be used to specify that direction.

If we assume that, through the transition region, $u_e \simeq (u_e)_{tr}$ and $v \simeq v_{tr}$, then equation (9.15) may be rewritten as

$$\gamma_{tr} = 1 - \exp\left[-8.33 \times 10^{-4} Re_{x_{tr}}^{0.66} \left(\frac{x}{x_{tr}} - 1 \right)^2 \right] \tag{9.16}$$

To implement equation (9.16) in *Proteus*, we replace x/x_{tr} with $Re_x/Re_{x_{tr}}$, where Re_x is defined as

$$Re_x = \frac{|\vec{V}|_{max} D}{v} Re_r$$

For flows predominantly in the ξ direction, $|\vec{V}|_{max}$ is the maximum total velocity magnitude at the current ξ station, D is the distance from the point where $|\vec{V}| = |\vec{V}|_{max}$ to the leading edge at $\xi = 0$, and v is evaluated at the point where $|\vec{V}| = |\vec{V}|_{max}$. An analogous definition of Re_x is used for flows predominantly in the η direction.

9.1.5 Turbulent Values of λ and k

The turbulent second coefficient of viscosity is simply defined as

$$\lambda_t = -\frac{2}{3} \mu_t \tag{9.17}$$

The turbulent thermal conductivity coefficient is defined using Reynolds analogy as

$$k_t = \frac{c_p \mu_t}{Pr_t} Pr_r \tag{9.18}$$

where c_p is the specific heat at constant pressure, and Pr_t is the turbulent Prandtl number. In *Proteus*, the turbulent Prandtl number may be treated as constant, or as a variable using the following formula (Wassel and Catton, 1973):

$$Pr_t = \frac{C_{Pr3}}{C_{Pr1} Pr_l} \frac{1 - \exp\left(-\dfrac{C_{Pr4}}{\mu_t/\mu_l} \right)}{1 - \exp\left(-\dfrac{C_{Pr2}}{Pr_l \mu_t/\mu_l} \right)} \tag{9.19}$$

Here C_{Pr1}, C_{Pr2}, C_{Pr3}, and C_{Pr4} are constants taken as 0.21, 5.25, 0.20, and 5.0, respectively, and $Pr_l = c_p \mu_l/k_l$ is the laminar Prandtl number.

9.2 CHIEN k-ε TURBULENCE MODEL

9.2.1 k-ε Equations

The low Reynolds number k-ε formulation of K. Y. Chien (1982) was chosen because of its reasonable approximation of the near wall region and because of its numerical stability. Here k and ε are the turbulent kinetic energy and the turbulent dissipation rate, respectively.[12] In addition, the Chien k-ε turbulence model was frequently used in past Navier-Stokes computations with good results (Nichols, 1990, 1991; Patel, Rodi, and Scheuerer, 1985; Sahu, 1984.) The set of k-ε equations are lagged in time and solved separately from the Navier-Stokes equations to allow for code modularity in turbulence modeling. In Cartesian coordinates, the two-dimensional planar equations for the Chien k-ε model can be written using vector notation as

---

[12] It should be noted that in the Chien model, ε is actually the isotropic portion of the turbulent dissipation rate. Throughout this manual, however, it is referred to as simply the turbulent dissipation rate.

$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{S} + \mathbf{T} \tag{9.20}$$

where

$$\mathbf{W} = \begin{bmatrix} \rho k \\ \rho \varepsilon \end{bmatrix} \tag{9.21a}$$

$$\mathbf{F} = \begin{bmatrix} \rho u k - \dfrac{1}{Re_r} \mu_k \dfrac{\partial k}{\partial x} \\[2ex] \rho u \varepsilon - \dfrac{1}{Re_r} \mu_\varepsilon \dfrac{\partial \varepsilon}{\partial x} \end{bmatrix} \tag{9.21b}$$

$$\mathbf{G} = \begin{bmatrix} \rho v k - \dfrac{1}{Re_r} \mu_k \dfrac{\partial k}{\partial y} \\[2ex] \rho v \varepsilon - \dfrac{1}{Re_r} \mu_\varepsilon \dfrac{\partial \varepsilon}{\partial y} \end{bmatrix} \tag{9.21c}$$

$$\mathbf{S} = \begin{bmatrix} P_k - Re_r \rho \varepsilon \\[2ex] C_1 P_k \dfrac{\varepsilon}{k} - Re_r C_2 \rho \dfrac{\varepsilon^2}{k} \end{bmatrix} \tag{9.21d}$$

$$\mathbf{T} = \begin{bmatrix} -\dfrac{2}{Re_r} \dfrac{\mu}{y_n^2} k \\[3ex] -\dfrac{2}{Re_r} \dfrac{\mu e^{-y^+/2}}{y_n^2} \varepsilon \end{bmatrix} \tag{9.21e}$$

and

$$\mu_k = \mu + \frac{\mu_t}{\sigma_k} \tag{9.22a}$$

$$\mu_\varepsilon = \mu + \frac{\mu_t}{\sigma_\varepsilon} \tag{9.22b}$$

$$C_1 = 1.35 \tag{9.22c}$$

$$C_2 = C_{2_r} \left(1 - \frac{2}{9} e^{-R_t^2/36} \right) \tag{9.22d}$$

$$\sigma_k = 1.0 \tag{9.22e}$$

$$\sigma_\varepsilon = 1.3 \tag{9.22f}$$

$$C_{2_r} = 1.8 \tag{9.22g}$$

$$R_t = \frac{\rho k^2}{\mu \varepsilon} \tag{9.22h}$$

$$P_k = \frac{\mu_t}{Re_r} P_1 - \frac{2}{3} \rho k P_2 \tag{9.23a}$$

$$P_1 = 2\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2\right] - \frac{2}{3}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 \qquad (9.23b)$$

$$P_2 = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \qquad (9.23c)$$

The turbulent viscosity is given by

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \qquad (9.24a)$$

$$C_\mu = C_{\mu_r}\left(1 - e^{-C_3 y^+}\right) \qquad (9.24b)$$

$$C_{\mu_r} = 0.09 \qquad (9.24c)$$

$$C_3 = 0.0115 \qquad (9.24d)$$

Note that the vectors **W**, **F**, **G**, and **S** are used in most standard k-ε formulations (with different constants), and the vector **T** is unique to the low Reynolds number formulation of Chien. The parameter y_n is the minimum distance to the nearest solid surface, and y^+ is computed from y_n. The production of turbulent kinetic energy P_k includes the full Boussinesq approximation for compressible flows. All of the above equations have been nondimensionalized using appropriate normalizing conditions. Nondimensionalization of mean flow properties is discussed in Section 2.1. The turbulent kinetic energy k and the turbulent dissipation rate ε have been nondimensionalized by u_r^2 and $\rho_r u_r^4 / \mu_r$, respectively.

Following the procedure of Section 2.3, the following generalized grid transformation is used to transform the k-ε equations from physical (x, y, t) coordinates to computational (ξ, η, τ) coordinates.

$$
\begin{aligned}
\xi &= \xi(x, y) \\
\eta &= \eta(x, y) \\
\tau &= t
\end{aligned}
\qquad (9.25)
$$

Applying the generalized grid transformation to equation (9.20) yields

$$\mathbf{W}_\tau + \mathbf{F}_\xi \xi_x + \mathbf{F}_\eta \eta_x + \mathbf{G}_\xi \xi_y + \mathbf{G}_\eta \eta_y = \mathbf{S} + \mathbf{T} \qquad (9.26)$$

Although the above equations can not be put into exact strong conservation law form, the procedure used to do so for the mean flow equations, described in Section 2.4, is nonetheless applied to equation (9.26). The result is

$$\frac{\partial \hat{\mathbf{W}}}{\partial \tau} + \frac{\partial \hat{\mathbf{F}}}{\partial \xi} + \frac{\partial \hat{\mathbf{G}}}{\partial \eta} = \hat{\mathbf{S}} + \hat{\mathbf{T}} \qquad (9.27)$$

where

$$\hat{\mathbf{W}} = \frac{1}{J}\begin{bmatrix} \rho k \\ \rho \varepsilon \end{bmatrix} \qquad (9.28a)$$

$$\hat{\mathbf{F}} = \hat{\mathbf{F}}_C - \hat{\mathbf{F}}_D - \hat{\mathbf{F}}_M \qquad (9.28b)$$

$$\hat{\mathbf{F}}_C = \frac{1}{J}\begin{bmatrix} \xi_x \rho u k + \xi_y \rho v k \\ \xi_x \rho u \varepsilon + \xi_y \rho v \varepsilon \end{bmatrix} \qquad (9.28c)$$

$$\hat{\mathbf{F}}_D = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} \mu_k(\xi_x^2 + \xi_y^2)k_\xi \\ \mu_\varepsilon(\xi_x^2 + \xi_y^2)\varepsilon_\xi \end{bmatrix} \qquad (9.28d)$$

$$\hat{\mathbf{F}}_M = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} \mu_k(\xi_x\eta_x + \xi_y\eta_y)k_\eta \\ \mu_\varepsilon(\xi_x\eta_x + \xi_y\eta_y)\varepsilon_\eta \end{bmatrix} \qquad (9.28e)$$

$$\hat{\mathbf{G}} = \hat{\mathbf{G}}_C - \hat{\mathbf{G}}_D - \hat{\mathbf{G}}_M \qquad (9.28f)$$

$$\hat{\mathbf{G}}_C = \frac{1}{J} \begin{bmatrix} \eta_x\rho uk + \eta_y\rho vk \\ \eta_x\rho u\varepsilon + \eta_y\rho v\varepsilon \end{bmatrix} \qquad (9.28g)$$

$$\hat{\mathbf{G}}_D = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} \mu_k(\eta_x^2 + \eta_y^2)k_\eta \\ \mu_\varepsilon(\eta_x^2 + \eta_y^2)\varepsilon_\eta \end{bmatrix} \qquad (9.28h)$$

$$\hat{\mathbf{G}}_M = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} \mu_k(\xi_x\eta_x + \xi_y\eta_y)k_\xi \\ \mu_\varepsilon(\xi_x\eta_x + \xi_y\eta_y)\varepsilon_\xi \end{bmatrix} \qquad (9.28i)$$

$$\hat{\mathbf{S}} = \frac{1}{J} \begin{bmatrix} P_k - Re_r\rho\varepsilon \\ C_1 P_k \dfrac{\varepsilon}{k} - Re_r C_2\rho \dfrac{\varepsilon^2}{k} \end{bmatrix} \qquad (9.28j)$$

$$\hat{\mathbf{T}} = \frac{1}{J} \begin{bmatrix} -\dfrac{2}{Re_r} \dfrac{\mu}{y_n^2} k \\[3mm] -\dfrac{2}{Re_r} \dfrac{\mu e^{-y^+/2}}{y_n^2} \varepsilon \end{bmatrix} \qquad (9.28k)$$

Note that in equation (9.28j), the term P_k involves derivatives with respect to the Cartesian coordinate directions (see equations (9.23a-c.) These are evaluated using the chain rule.

9.2.2 Linearization of the k-ε Equations

Solving equation (9.27) for $\partial\hat{\mathbf{W}}/\partial\tau$ and substituting the result into the time differencing scheme of Beam and Warming (1978), given by equation (3.1), for $\partial(\Delta\hat{\mathbf{W}}^n)/\partial\tau$ and $\partial\hat{\mathbf{W}}^n/\partial\tau$ yields

$$\Delta\hat{\mathbf{W}}^n = \frac{\theta_1\Delta\tau}{1+\theta_2}\left(-\frac{\partial(\Delta\hat{\mathbf{F}}_C)}{\partial\xi} + \frac{\partial(\Delta\hat{\mathbf{F}}_D)}{\partial\xi} + \frac{\partial(\Delta\hat{\mathbf{F}}_M)}{\partial\xi} - \frac{\partial(\Delta\hat{\mathbf{G}}_C)}{\partial\eta} + \frac{\partial(\Delta\hat{\mathbf{G}}_D)}{\partial\eta} + \frac{\partial(\Delta\hat{\mathbf{G}}_M)}{\partial\eta} + \Delta\hat{\mathbf{S}} + \Delta\hat{\mathbf{T}}\right)^n$$

$$+ \frac{\Delta\tau}{1+\theta_2}\left(-\frac{\partial\hat{\mathbf{F}}_C}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}_D}{\partial\xi} + \frac{\partial\hat{\mathbf{F}}_M}{\partial\xi} - \frac{\partial\hat{\mathbf{G}}_C}{\partial\eta} + \frac{\partial\hat{\mathbf{G}}_D}{\partial\eta} + \frac{\partial\hat{\mathbf{G}}_M}{\partial\eta} + \hat{\mathbf{S}} + \hat{\mathbf{T}}\right)^n$$

$$+ \frac{\theta_2}{1+\theta_2}\Delta\hat{\mathbf{W}}^{n-1} + O\left[\left(\theta_1 - \frac{1}{2} - \theta_2\right)(\Delta\tau)^2, (\Delta\tau)^3\right] \qquad (9.29)$$

Equation (9.29) is then linearized using the procedure described in Section 4.0. Let

$$A = \frac{\partial\hat{\mathbf{F}}_C}{\partial\hat{\mathbf{W}}}, \quad B = \frac{\partial\hat{\mathbf{F}}_D}{\partial\hat{\mathbf{W}}}, \quad C = \frac{\partial\hat{\mathbf{G}}_C}{\partial\hat{\mathbf{W}}}, \quad D = \frac{\partial\hat{\mathbf{G}}_D}{\partial\hat{\mathbf{W}}}, \quad M = \frac{\partial\hat{\mathbf{S}}}{\partial\hat{\mathbf{W}}}, \quad N = \frac{\partial\hat{\mathbf{T}}}{\partial\hat{\mathbf{W}}} \qquad (9.30)$$

be the Jacobian coefficient matrices, where

$$
A = \begin{bmatrix} \xi_x u + \xi_y v & 0 \\ 0 & \xi_x u + \xi_y v \end{bmatrix}
\tag{9.31}
$$

$$
B = \begin{bmatrix} \dfrac{1}{JRe_r}\, \mu_k(\xi_x^2 + \xi_y^2)\left(\dfrac{J}{\rho}\right)_\xi & 0 \\[2ex] 0 & \dfrac{1}{JRe_r}\, \mu_\varepsilon(\xi_x^2 + \xi_y^2)\left(\dfrac{J}{\rho}\right)_\xi \end{bmatrix}
\tag{9.32}
$$

$$
C = \begin{bmatrix} \eta_x u + \eta_y v & 0 \\ 0 & \eta_x u + \eta_y v \end{bmatrix}
\tag{9.33}
$$

$$
D = \begin{bmatrix} \dfrac{1}{JRe_r}\, \mu_k(\eta_x^2 + \eta_y^2)\left(\dfrac{J}{\rho}\right)_\eta & 0 \\[2ex] 0 & \dfrac{1}{JRe_r}\, \mu_\varepsilon(\eta_x^2 + \eta_y^2)\left(\dfrac{J}{\rho}\right)_\eta \end{bmatrix}
\tag{9.34}
$$

$$
M = \begin{bmatrix} 2C_\mu \dfrac{k}{\varepsilon}\dfrac{P_k}{\mu_t} & -C_\mu \dfrac{k^2}{\varepsilon^2}\dfrac{P_k}{\mu_t} - Re_r \\[2ex] C_1 C_\mu \dfrac{P_k}{\mu_t} + Re_r C_2 \dfrac{\varepsilon^2}{k^2} & -2Re_r C_2 \dfrac{\varepsilon}{k} \end{bmatrix}
\tag{9.35}
$$

$$
N = \begin{bmatrix} -\dfrac{2\mu}{\rho y_n^2 Re_r} & 0 \\[2ex] 0 & -\dfrac{2\mu}{\rho y_n^2 Re_r}\, e^{-y^+/2} \end{bmatrix}
\tag{9.36}
$$

The linearized form of equation (9.29) can now be written as

$$\Delta\hat{W}^n + \frac{\theta_1\Delta\tau}{1+\theta_2}\left[\frac{\partial(A\Delta\hat{W})}{\partial\xi} - \frac{\partial(B\Delta\hat{W})}{\partial\xi} + \frac{\partial(C\Delta\hat{W})}{\partial\eta} - \frac{\partial(D\Delta\hat{W})}{\partial\eta} - M(\Delta\hat{W}) - N(\Delta\hat{W})\right]^n =$$

$$\frac{\theta_1\Delta\tau}{1+\theta_2}\left[\frac{\partial(\Delta\hat{F}_M)}{\partial\xi} + \frac{\partial(\Delta\hat{G}_M)}{\partial\eta}\right]^{n-1}$$

$$+\frac{\Delta\tau}{1+\theta_2}\left(-\frac{\partial\hat{F}_C}{\partial\xi} + \frac{\partial\hat{F}_D}{\partial\xi} + \frac{\partial\hat{F}_M}{\partial\xi} - \frac{\partial\hat{G}_C}{\partial\eta} + \frac{\partial\hat{G}_D}{\partial\eta} + \frac{\partial\hat{G}_M}{\partial\eta} + \hat{S} + \hat{T}\right)^n + \frac{\theta_2}{1+\theta_2}\Delta\hat{W}^{n-1}$$

$$+ O\left[\left(\theta_1 - \frac{1}{2} - \theta_2\right)(\Delta\tau)^2, (\Delta\tau)^3\right] \tag{9.37}$$

9.2.3 ADI Algorithm for k-ε Equations

Letting LHS(9.37) represent the left hand side of equation (9.37), we can write

$$\text{LHS}(9.37) = \left\{I + \frac{\theta_1\Delta\tau}{1+\theta_2}\left[\frac{\partial}{\partial\xi}(A-B) + \frac{\partial}{\partial\eta}(C-D) - (M+N)\right]\right\}^n \Delta\hat{W}^n \tag{9.38}$$

where I represents the identity matrix. Factoring the term in braces, and neglecting the temporal truncation and splitting errors, equation (9.37) becomes

$$\left\{I + \frac{\theta_1\Delta\tau}{1+\theta_2}\left[\frac{\partial}{\partial\xi}(A-B) - (M+N)\right]\right\}^n \left\{I + \frac{\theta_1\Delta\tau}{1+\theta_2}\left[\frac{\partial}{\partial\eta}(C-D)\right]\right\}^n \Delta\hat{W}^n =$$

$$\frac{\theta_1\Delta\tau}{1+\theta_2}\left[\frac{\partial(\Delta\hat{F}_M)}{\partial\xi} + \frac{\partial(\Delta\hat{G}_M)}{\partial\eta}\right]^{n-1}$$

$$+\frac{\Delta\tau}{1+\theta_2}\left(-\frac{\partial\hat{F}_C}{\partial\xi} + \frac{\partial\hat{F}_D}{\partial\xi} + \frac{\partial\hat{F}_M}{\partial\xi} - \frac{\partial\hat{G}_C}{\partial\eta} + \frac{\partial\hat{G}_D}{\partial\eta} + \frac{\partial\hat{G}_M}{\partial\eta} + \hat{S} + \hat{T}\right)^n + \frac{\theta_2}{1+\theta_2}\Delta\hat{W}^{n-1} \tag{9.39}$$

Using the procedure of Douglas and Gunn (1964), as written by Briley and McDonald (1977), equation (9.39) can be split into the following two-sweep sequence.

Sweep 1 (ξ direction)

$$\left\{I + \frac{\theta_1\Delta\tau}{1+\theta_2}\left[\frac{\partial}{\partial\xi}(A-B) - (M+N)\right]\right\}^n \Delta\hat{W}^* = \frac{\theta_1\Delta\tau}{1+\theta_2}\left[\frac{\partial(\Delta\hat{F}_M)}{\partial\xi} + \frac{\partial(\Delta\hat{G}_M)}{\partial\eta}\right]^{n-1}$$

$$+\frac{\Delta\tau}{1+\theta_2}\left(-\frac{\partial\hat{F}_C}{\partial\xi} + \frac{\partial\hat{F}_D}{\partial\xi} + \frac{\partial\hat{F}_M}{\partial\xi} - \frac{\partial\hat{G}_C}{\partial\eta} + \frac{\partial\hat{G}_D}{\partial\eta} + \frac{\partial\hat{G}_M}{\partial\eta} + \hat{S} + \hat{T}\right)^n + \frac{\theta_2}{1+\theta_2}\Delta\hat{W}^{n-1} \tag{9.40a}$$

Sweep 2 (η direction)

$$\left\{I + \frac{\theta_1\Delta\tau}{1+\theta_2}\left[\frac{\partial}{\partial\eta}(C-D)\right]\right\}^n \Delta\hat{W}^n = \Delta\hat{W}^* \tag{9.40b}$$

To approximate spatial partial derivatives, the spatial differencing formulas of Section 5.0 are used in equations (9.40a) and (9.40b). Following Nichols (1991), the spatial derivatives for the convective terms are approximated using first-order upwind differencing. A first-order backward difference approximation is used for the terms with positive eigenvalues, and a first-order forward difference approximation is used for the terms with negative eigenvalues.

9.2.4 Matrix Inversion Procedure for k-ε Equations

Non-Periodic Boundary Conditions

Explicit boundary conditions are used for ease of implementation and modification. The complete set of algebraic equations for the first ADI sweep with non-periodic boundary conditions can be written in the following block matrix form.

$$
\begin{bmatrix}
\mathbf{B}_2 & \mathbf{C}_2 & & & & & \\
\mathbf{A}_3 & \mathbf{B}_3 & \mathbf{C}_3 & & & & \\
 & \mathbf{A}_4 & \mathbf{B}_4 & \mathbf{C}_4 & & & \\
 & & & \bullet & & & \\
 & & & & \bullet & & \\
 & & & & & \bullet & \\
 & & \mathbf{A}_{N_1-3} & \mathbf{B}_{N_1-3} & \mathbf{C}_{N_1-3} & & \\
 & & & \mathbf{A}_{N_1-2} & \mathbf{B}_{N_1-2} & \mathbf{C}_{N_1-2} \\
 & & & & \mathbf{A}_{N_1-1} & \mathbf{B}_{N_1-1}
\end{bmatrix}
\begin{bmatrix}
\Delta\hat{\mathbf{W}}_2^* \\
\Delta\hat{\mathbf{W}}_3^* \\
\Delta\hat{\mathbf{W}}_4^* \\
\bullet \\
\bullet \\
\bullet \\
\Delta\hat{\mathbf{W}}_{N_1-3}^* \\
\Delta\hat{\mathbf{W}}_{N_1-2}^* \\
\Delta\hat{\mathbf{W}}_{N_1-1}^*
\end{bmatrix}
=
\begin{bmatrix}
RHS_2 - A_2\Delta\hat{\mathbf{W}}_1^* \\
RHS_3 \\
RHS_4 \\
\bullet \\
\bullet \\
\bullet \\
RHS_{N_1-3} \\
RHS_{N_1-2} \\
RHS_{N_1-1} - C_{N_1-1}\Delta\hat{\mathbf{W}}_{N_1}^*
\end{bmatrix}
\tag{9.41}
$$

In the above matrix, $\mathbf{A}_i$, $\mathbf{B}_i$, and $\mathbf{C}_i$ are the 2×2 coefficient matrices in front of $\Delta\hat{\mathbf{W}}_{i-1}^*$, $\Delta\hat{\mathbf{W}}_i^*$, and $\Delta\hat{\mathbf{W}}_{i+1}^*$, respectively, and they should not be confused with the Jacobian coefficient matrices A, B, and C defined in equations (9.30). The above block tridiagonal coefficient matrix is solved using the Thomas algorithm discussed in Section 7.2.1. An analogous procedure is used for the second ADI sweep.

Spatially Periodic Boundary Conditions

A spatially periodic boundary condition in the ζ direction may be represented as shown in Figure 7.1. Following Section 7.2.2, an additional set of grid points is added at $i = N_1 + 1$, setting $\hat{\mathbf{W}}_{N_1+1} = \hat{\mathbf{W}}_2$. This allows us to use central differencing in the ζ direction at $i = N_1$.

Since $\hat{\mathbf{W}}_1 = \hat{\mathbf{W}}_{N_1}$ and $\hat{\mathbf{W}}_2 = \hat{\mathbf{W}}_{N_1+1}$, equation (9.41) can be rewritten as:

$$
\begin{bmatrix}
\mathbf{B}_2 & \mathbf{C}_2 & & & & & & \mathbf{A}_2 \\
\mathbf{A}_3 & \mathbf{B}_3 & \mathbf{C}_3 & & & & & \\
 & \mathbf{A}_4 & \mathbf{B}_4 & \mathbf{C}_4 & & & & \\
 & & & \bullet & & & & \\
 & & & & \bullet & & & \\
 & & & & & \bullet & & \\
 & & & \mathbf{A}_{N_1-2} & \mathbf{B}_{N_1-2} & \mathbf{C}_{N_1-2} & & \\
 & & & & \mathbf{A}_{N_1-1} & \mathbf{B}_{N_1-1} & \mathbf{C}_{N_1-1} \\
\mathbf{C}_{N_1} & & & & & & \mathbf{A}_{N_1} & \mathbf{B}_{N_1}
\end{bmatrix}
\begin{bmatrix}
\Delta\hat{\mathbf{W}}_2^* \\
\Delta\hat{\mathbf{W}}_3^* \\
\Delta\hat{\mathbf{W}}_4^* \\
\bullet \\
\bullet \\
\bullet \\
\Delta\hat{\mathbf{W}}_{N_1-2}^* \\
\Delta\hat{\mathbf{W}}_{N_1-1}^* \\
\Delta\hat{\mathbf{W}}_{N_1}^*
\end{bmatrix}
=
\begin{bmatrix}
RHS_2 \\
RHS_3 \\
RHS_4 \\
\bullet \\
\bullet \\
\bullet \\
RHS_{N_1-2} \\
RHS_{N_1-3} \\
RHS_{N_1}
\end{bmatrix}
\tag{9.42}
$$

To solve the above system, the algorithm described in Section 7.2.2 is used. An analogous procedure is used for the second ADI sweep.

9.2.5 Updating Boundary Values for k-ε Equations

For easy modification and easy accommodation of complicated boundary conditions for k and ε, non-periodic boundary conditions are treated explicitly in the solver. After the k and ε values at the interior points are advanced in time, the values at the boundaries are simply computed from the new interior values using the specified boundary conditions.

Spatially periodic boundary conditions in either sweep direction are treated implicitly, as described in the previous section. For a periodic boundary condition in the ξ direction, the k and ε values at $i = 1$ are easily updated by setting $\hat{W}_1 = \hat{W}_{N_1}$. An analogous procedure is used for periodic boundary conditions in the η direction.

9.2.6 Turbulent Values of λ and k

The turbulent second coefficient of viscosity λ_t and the turbulent thermal conductivity coefficient k_t are defined as described previously in Section 9.1.5.

APPENDIX A - EXPANSION OF VISCOUS TERMS

In Section 4.2, the viscous terms in the governing equations are linearized. To do this, the elements of $\hat{E}_V$ and $\hat{F}_V$, given in equations (2.17d) and (2.17e) must first be rewritten in terms of the dependent variables, and with derivatives in the Cartesian directions transformed to derivatives in the computational directions using the chain rule. The non-cross derivative terms, involving $\hat{E}_{V_1}$ and $\hat{F}_{V_1}$, are then linearized using Taylor series expansion. The cross derivative terms, involving $\hat{E}_{V_2}$ and $\hat{F}_{V_2}$, are simply lagged one time level. This Appendix presents the fully expanded viscous terms required in the linearization procedure.

The viscous term $\hat{E}_V$ is given by equation (2.17d), which is repeated here.

$$\hat{E}_V = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} 0 \\ \tau_{xx}\xi_x + \tau_{xy}\xi_y \\ \tau_{xy}\xi_x + \tau_{yy}\xi_y \\ \beta_x\xi_x + \beta_y\xi_y \end{bmatrix} \tag{A.1}$$

where

$$\tau_{xx} = 2\mu u_x + \lambda(u_x + v_y)$$

$$\tau_{yy} = 2\mu v_y + \lambda(u_x + v_y)$$

$$\tau_{xy} = \mu(u_y + v_x)$$

$$\beta_x = u\tau_{xx} + v\tau_{xy} - \frac{1}{Pr_r} q_x$$

$$\beta_y = u\tau_{xy} + v\tau_{yy} - \frac{1}{Pr_r} q_y$$

$$q_x = -kT_x$$

$$q_y = -kT_y$$

The chain rule is used to transform derivatives in the Cartesian directions into derivatives in the computational directions, resulting in

$$\tau_{xx} = (2\mu + \lambda)(\xi_x u_\xi + \eta_x u_\eta) + \lambda(\xi_y v_\xi + \eta_y v_\eta)$$

$$\tau_{yy} = (2\mu + \lambda)(\xi_y v_\xi + \eta_y v_\eta) + \lambda(\xi_x u_\xi + \eta_x u_\eta)$$

$$\tau_{xy} = \mu(\xi_y u_\xi + \eta_y u_\eta + \xi_x v_\xi + \eta_x v_\eta)$$

$$\beta_x = (2\mu + \lambda)(\xi_x uu_\xi + \eta_x uu_\eta) + \lambda(\xi_y uv_\xi + \eta_y uv_\eta)$$
$$+ \mu(\xi_y vu_\xi + \eta_y vu_\eta + \xi_x vv_\xi + \eta_x vv_\eta) + \frac{k}{Pr_r}(\xi_x T_\xi + \eta_x T_\eta)$$

$$\beta_y = (2\mu + \lambda)(\xi_y vv_\xi + \eta_y vv_\eta) + \lambda(\xi_x vu_\xi + \eta_x vu_\eta)$$
$$+ \mu(\xi_y uu_\xi + \eta_y uu_\eta + \xi_x uv_\xi + \eta_x uv_\eta) + \frac{k}{Pr_r}(\xi_y T_\xi + \eta_y T_\eta)$$

The above expressions for the τ's and β's are next substituted into equation (A.1). The ξ derivative terms become elements of $\hat{E}_{V_1}$, and the η derivative terms become elements of $\hat{E}_{V_2}$. The resulting four elements of $\hat{E}_{V_1}$ (excluding the $1/JRe_r$ coefficient) are

$$(\hat{E}_{V_1})_1 = 0 \tag{A.2a}$$

$$(\hat{E}_{V_1})_2 = 2\mu\xi_x^2 u_\xi + \lambda\xi_x(\xi_x u_\xi + \xi_y v_\xi) + \mu\xi_y(\xi_y u_\xi + \xi_x v_\xi) \tag{A.2b}$$

$$(\hat{E}_{V_1})_3 = 2\mu\xi_y^2 v_\xi + \lambda\xi_y(\xi_x u_\xi + \xi_y v_\xi) + \mu\xi_x(\xi_y u_\xi + \xi_x v_\xi) \tag{A.2c}$$

$$(\hat{E}_{V_1})_4 = 2\mu(\xi_x^2 uu_\xi + \xi_y^2 vv_\xi) + \lambda\xi_x(\xi_x uu_\xi + \xi_y uv_\xi) + \lambda\xi_y(\xi_x vu_\xi + \xi_y vv_\xi)$$
$$+ \mu\xi_x(\xi_y vu_\xi + \xi_x vv_\xi) + \mu\xi_y(\xi_y uu_\xi + \xi_x uv_\xi) + \frac{k}{Pr_r}(\xi_x^2 + \xi_y^2)T_\xi \tag{A.2d}$$

For linearization it is convenient to rewrite the last element as

$$(\hat{E}_{V_1})_4 = \frac{(2\mu + \lambda)}{2}\left[\xi_x^2(u^2)_\xi + \xi_y^2(v^2)_\xi\right] + (\mu + \lambda)\xi_x\xi_y(uv)_\xi$$
$$+ \frac{\mu}{2}\left[\xi_x^2(v^2)_\xi + \xi_y^2(u^2)_\xi\right] + \frac{k}{Pr_r}(\xi_x^2 + \xi_y^2)T_\xi \tag{A.2e}$$

The elements of $\hat{F}_{V_1}$ have exactly the same form as those of $\hat{E}_{V_1}$, but with ξ replaced by η.

The four elements of $\hat{E}_{V_2}$ (again excluding the $1/JRe_r$ coefficient) are

$$(\hat{E}_{V_2})_1 = 0 \tag{A.3a}$$

$$(\hat{E}_{V_2})_2 = 2\mu\xi_x\eta_x u_\eta + \lambda\xi_x(\eta_x u_\eta + \eta_y v_\eta) + \mu\xi_y(\eta_y u_\eta + \eta_x v_\eta) \tag{A.3b}$$

$$(\hat{E}_{V_2})_3 = 2\mu\xi_y\eta_y v_\eta + \lambda\xi_y(\eta_x u_\eta + \eta_y v_\eta) + \mu\xi_x(\eta_y u_\eta + \eta_x v_\eta) \tag{A.3c}$$

$$(\hat{E}_{V_2})_4 = 2\mu(\xi_x\eta_x uu_\eta + \xi_y\eta_y vv_\eta) + \lambda\xi_x(\eta_x uu_\eta + \eta_y uv_\eta) + \lambda\xi_y(\eta_x vu_\eta + \eta_y vv_\eta)$$
$$+ \mu\xi_x(\eta_y vu_\eta + \eta_x vv_\eta) + \mu\xi_y(\eta_y uu_\eta + \eta_x uv_\eta) + \frac{k}{Pr_r}(\xi_x\eta_x + \xi_y\eta_y)T_\eta \tag{A.3d}$$

The elements of $\hat{F}_{V_2}$ have exactly the same form as those of $\hat{E}_{V_2}$, but with ξ replaced by η and η replaced by ξ.

The analysis used in *Proteus* for axisymmetric flow is essentially the same as for two-dimensional planar flow, described in the main body of this report. However, there are some additional terms in the axisymmetric equations that complicate things somewhat. For that reason, the axisymmetric analysis is described separately in this appendix.

B.1 GOVERNING EQUATIONS

In cylindrical coordinates, the governing equations for axisymmetric flow, with swirl, can be written using vector notation as

$$\frac{\partial(r\,\mathbf{Q})}{\partial t} + \frac{\partial(r\,\mathbf{E})}{\partial x} + \frac{\partial(r\,\mathbf{F})}{\partial r} + \mathbf{H} = \frac{\partial(r\,\mathbf{E}_V)}{\partial x} + \frac{\partial(r\,\mathbf{F}_V)}{\partial r} + \mathbf{H}_V \tag{B.1}$$

where

$$\mathbf{Q} = [\rho \quad \rho u \quad \rho v \quad \rho w \quad E_T]^T \tag{B.2a}$$

$$\mathbf{E} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (E_T + p)u \end{bmatrix} \tag{B.2b}$$

$$\mathbf{F} = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ (E_T + p)v \end{bmatrix} \tag{B.2c}$$

$$\mathbf{H} = \begin{bmatrix} 0 \\ 0 \\ -p - \rho w^2 \\ \rho vw \\ 0 \end{bmatrix} \tag{B.2d}$$

$$\mathbf{E}_V = \frac{1}{Re_r} \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xr} \\ \tau_{x\theta} \\ u\tau_{xx} + v\tau_{xr} + w\tau_{x\theta} - \frac{1}{Pr_r}q_x \end{bmatrix} \tag{B.2e}$$

$$\mathbf{F}_V = \frac{1}{Re_r} \begin{bmatrix} 0 \\ \tau_{xr} \\ \tau_{rr} \\ \tau_{r\theta} \\ u\tau_{xr} + v\tau_{rr} + w\tau_{r\theta} - \frac{1}{Pr_r} q_r \end{bmatrix}$$

(B.2f)

$$\mathbf{H}_V = \frac{1}{Re_r} \begin{bmatrix} 0 \\ 0 \\ -\tau_{\theta\theta} \\ \tau_{r\theta} \\ 0 \end{bmatrix}$$

(B.2g)

Equation (B.1) thus represents, in order, the continuity, x-momentum, r-momentum, θ-momentum (swirl), and energy equations, with dependent variables ρ, ρu, ρv, ρw, and E_T. Note that the additional terms in these axisymmetric equations destroy the strong conservation law form of the two-dimensional planar equations presented in Section 2.1. Unfortunately, the axisymmetric form of the equations cannot be put into strong conservation law form (Vinokur, 1974.)

The shear stresses and heat fluxes are given by

$$\tau_{xx} = 2\mu \frac{\partial u}{\partial x} + \lambda \left[\frac{\partial u}{\partial x} + \frac{1}{r} \left(\frac{\partial(rv)}{\partial r} \right) \right]$$

$$\tau_{rr} = 2\mu \frac{\partial v}{\partial r} + \lambda \left[\frac{\partial u}{\partial x} + \frac{1}{r} \left(\frac{\partial(rv)}{\partial r} \right) \right]$$

$$\tau_{\theta\theta} = 2\mu \frac{v}{r} + \lambda \left[\frac{\partial u}{\partial x} + \frac{1}{r} \left(\frac{\partial(rv)}{\partial r} \right) \right]$$

$$\tau_{xr} = \mu \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right)$$

(B.3)

$$\tau_{x\theta} = \mu \frac{\partial w}{\partial x}$$

$$\tau_{r\theta} = \mu \left(\frac{\partial w}{\partial r} - \frac{w}{r} \right)$$

$$q_x = -k \frac{\partial T}{\partial x}$$

$$q_r = -k \frac{\partial T}{\partial r}$$

In these equations, x, r, and θ represent the axial, radial, and circumferential directions, respectively; and u, v, and w represent the velocities in those directions. The remaining symbols are the same as those in the two-dimensional equations described in Section 2.1.

For turbulent flow, μ, λ, and k represent effective coefficients. The turbulence model is described in Section 9.0. The only modification to the model for axisymmetric flow is the definition of $\left| \bar{\Omega} \right|$, the magnitude of the total vorticity. For axisymmetric flow,

$$|\vec{\Omega}| = \left[\left(\frac{\partial w}{\partial r} + \frac{w}{r}\right)^2 + \left(\frac{\partial w}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r}\right)^2\right]^{1/2}$$

When the generalized grid transformation of Section 2.3 (with y replaced by r), is applied to equation (B.1) the result is

$$(r\,Q)_\tau + (r\,Q)_\xi \xi_t + (r\,Q)_\eta \eta_t + (r\,E)_\xi \xi_x + (r\,E)_\eta \eta_x + (r\,F)_\xi \xi_r + (r\,F)_\eta \eta_r + H$$
$$- (r\,E_V)_\xi \xi_x - (r\,E_V)_\eta \eta_x - (r\,F_V)_\xi \xi_r - (r\,F_V)_\eta \eta_r - H_V = 0 \tag{B.4}$$

Although this axisymmetric equation cannot be put into exact strong conservation law form, the procedure used to do so for the two-dimensional equation, described in Section 2.4, is nonetheless applied to equation (B.4). The result is

$$\frac{\partial(r\,\hat{Q})}{\partial\tau} + \frac{\partial(r\,\hat{E})}{\partial\xi} + \frac{\partial(r\,\hat{F})}{\partial\eta} + \hat{H} = \frac{\partial(r\,\hat{E}_V)}{\partial\xi} + \frac{\partial(r\,\hat{F}_V)}{\partial\eta} + \hat{H}_V \tag{B.5}$$

where

$$\hat{Q} = \frac{Q}{J}$$

$$\hat{E} = \frac{1}{J}(E\xi_x + F\xi_r + Q\xi_t)$$

$$\hat{F} = \frac{1}{J}(E\eta_x + F\eta_r + Q\eta_t)$$

$$\hat{H} = \frac{H}{J}$$

$$\hat{E}_V = \frac{1}{J}(E_V\,\xi_x + F_V\,\xi_r)$$

$$\hat{F}_V = \frac{1}{J}(E_V\,\eta_x + F_V\,\eta_r)$$

$$\hat{H}_V = \frac{H_V}{J}$$

Using equations (B.2a) through (B.2g) these can be expanded as

$$\hat{Q} = \frac{1}{J}[\rho \quad \rho u \quad \rho v \quad \rho w \quad E_T]^T \tag{B.6a}$$

$$\hat{E} = \frac{1}{J}\begin{bmatrix} \rho u \xi_x + \rho v \xi_r + \rho \xi_t \\ (\rho u^2 + p)\xi_x + \rho uv\xi_r + \rho u\xi_t \\ \rho uv\xi_x + (\rho v^2 + p)\xi_r + \rho v\xi_t \\ \rho uw\xi_x + \rho vw\xi_r + \rho w\xi_t \\ (E_T + p)u\xi_x + (E_T + p)v\xi_r + E_T\,\xi_t \end{bmatrix} \tag{B.6b}$$

$$\hat{F} = \frac{1}{J} \begin{bmatrix} \rho u \eta_x + \rho v \eta_r + \rho \eta_t \\ (\rho u^2 + p)\eta_x + \rho u v \eta_r + \rho u \eta_t \\ \rho u v \eta_x + (\rho v^2 + p)\eta_r + \rho v \eta_t \\ \rho u w \eta_x + \rho v w \eta_r + \rho w \eta_t \\ (E_T + p)u\eta_x + (E_T + p)v\eta_r + E_T \eta_t \end{bmatrix} \tag{B.6c}$$

$$\hat{H} = \frac{1}{J} \begin{bmatrix} 0 \\ 0 \\ -p - \rho w^2 \\ \rho v w \\ 0 \end{bmatrix} \tag{B.6d}$$

$$\hat{E}_V = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} 0 \\ \tau_{xx}\xi_x + \tau_{xr}\xi_r \\ \tau_{xr}\xi_x + \tau_{rr}\xi_r \\ \tau_{x\theta}\xi_x + \tau_{r\theta}\xi_r \\ \beta_x\xi_x + \beta_r\xi_r \end{bmatrix} \tag{B.6e}$$

$$\hat{F}_V = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} 0 \\ \tau_{xx}\eta_x + \tau_{xr}\eta_r \\ \tau_{xr}\eta_x + \tau_{rr}\eta_r \\ \tau_{x\theta}\eta_x + \tau_{r\theta}\eta_r \\ \beta_x\eta_x + \beta_r\eta_r \end{bmatrix} \tag{B.6f}$$

$$\hat{H}_V = \frac{1}{J} \frac{1}{Re_r} \begin{bmatrix} 0 \\ 0 \\ -\tau_{\theta\theta} \\ \tau_{r\theta} \\ 0 \end{bmatrix} \tag{B.6g}$$

where

$$\beta_x = u\tau_{xx} + v\tau_{xr} + w\tau_{x\theta} - \frac{1}{Pr_r} q_x$$

$$\beta_r = u\tau_{xr} + v\tau_{rr} + w\tau_{r\theta} - \frac{1}{Pr_r} q_r \tag{B.7}$$

B.2 LINEARIZATION

Solving equation (B.5) for $\partial \hat{Q}/\partial\tau$ (assuming r is not a function of time) and substituting the result into the time differencing scheme of Beam and Warming, given by equation (3.1), for $\partial(\Delta \hat{Q}^n)/\partial\tau$ and $\partial \hat{Q}^n/\partial\tau$ yields

$$\Delta\hat{Q}^n = -\frac{\theta_1\Delta\tau}{1+\theta_2}\frac{1}{r}\left(\frac{\partial(r\Delta\hat{E}^n)}{\partial\xi} + \frac{\partial(r\Delta\hat{F}^n)}{\partial\eta} + \Delta\hat{H}^n\right) - \frac{\Delta\tau}{1+\theta_2}\frac{1}{r}\left(\frac{\partial(r\hat{E}^n)}{\partial\xi} + \frac{\partial(r\hat{F}^n)}{\partial\eta} + \hat{H}^n\right)$$

$$+ \frac{\theta_1\Delta\tau}{1+\theta_2}\frac{1}{r}\left(\frac{\partial(r\Delta\hat{E}_V{}^n)}{\partial\xi} + \frac{\partial(r\Delta\hat{F}_V{}^n)}{\partial\eta} + \Delta\hat{H}_V{}^n\right) + \frac{\Delta\tau}{1+\theta_2}\frac{1}{r}\left(\frac{\partial(r\hat{E}_V{}^n)}{\partial\xi} + \frac{\partial(r\hat{F}_V{}^n)}{\partial\eta} + \hat{H}_V{}^n\right)$$

$$+ \frac{\theta_2}{1+\theta_2}\Delta\hat{Q}^{n-1} + O\left[\left(\theta_1 - \frac{1}{2} - \theta_2\right)(\Delta\tau)^2, (\Delta\tau)^3\right] \qquad (B.8)$$

This equation must be linearized using the procedure described in Section 4.0.

B.2.1 Inviscid Terms

For the inviscid terms the Jacobian coefficient matrix $\partial\hat{E}/\partial\hat{Q}$ is

$$\frac{\partial\hat{E}}{\partial\hat{Q}} = \begin{bmatrix} \xi_t & \xi_x & \xi_r & 0 & 0 \\ \frac{\partial p}{\partial\rho}\xi_x - uf_1 & \xi_t + f_1 + u\xi_x + \frac{\partial p}{\partial(\rho u)}\xi_x & u\xi_r + \frac{\partial p}{\partial(\rho v)}\xi_x & \frac{\partial p}{\partial(\rho w)}\xi_x & \frac{\partial p}{\partial E_T}\xi_x \\ \frac{\partial p}{\partial\rho}\xi_r - vf_1 & v\xi_x + \frac{\partial p}{\partial(\rho u)}\xi_r & \xi_t + f_1 + v\xi_r + \frac{\partial p}{\partial(\rho v)}\xi_r & \frac{\partial p}{\partial(\rho w)}\xi_r & \frac{\partial p}{\partial E_T}\xi_r \\ -wf_1 & w\xi_x & w\xi_r & \xi_t + f_1 & 0 \\ -f_1\left(f_2 - \frac{\partial p}{\partial\rho}\right) & f_2\xi_x + f_1\frac{\partial p}{\partial(\rho u)} & f_2\xi_r + f_1\frac{\partial p}{\partial(\rho v)} & f_1\frac{\partial p}{\partial(\rho w)} & \xi_t + f_1\left(1 + \frac{\partial p}{\partial E_T}\right) \end{bmatrix} \qquad (B.9)$$

where $f_1 = u\xi_x + v\xi_r$ and $f_2 = (E_T + p)/\rho$. The Jacobian matrix $\partial\hat{F}/\partial\hat{Q}$ has the same form as $\partial\hat{E}/\partial\hat{Q}$, but with ξ replaced by η.

For the additional term $\hat{H}$, the linearization procedure gives

$$\frac{\partial\hat{H}}{\partial\hat{Q}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\partial p}{\partial\rho} + w^2 & -\frac{\partial p}{\partial(\rho u)} & -\frac{\partial p}{\partial(\rho v)} & -\frac{\partial p}{\partial(\rho w)} - 2w & -\frac{\partial p}{\partial E_T} \\ -vw & 0 & w & v & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad (B.10)$$

B.2.2 Viscous Terms

To linearize the viscous terms, $\hat{E}_{V_1}$, $\hat{E}_{V_2}$, etc., must first be rewritten in terms of the dependent variables, and with derivatives in the cylindrical coordinate directions transformed to derivatives in the computational directions using the chain rule. The shear stress and heat flux terms, given by equations (B.3) and (B.7), become

$$\tau_{xx} = (2\mu + \lambda)(\xi_x u_\xi + \eta_x u_\eta) + \frac{\lambda}{r}\left[\xi_r(rv)_\xi + \eta_r(rv)_\eta\right]$$

$$\tau_{rr} = 2\mu(\xi_r v_\xi + \eta_r v_\eta) + \lambda(\xi_x u_\xi + \eta_x u_\eta) + \frac{\lambda}{r}\left[\xi_r(rv)_\xi + \eta_r(rv)_\eta\right]$$

$$\tau_{\theta\theta} = 2\mu\frac{v}{r} + \lambda(\xi_x u_\xi + \eta_x u_\eta) + \frac{\lambda}{r}\left[\xi_r(rv)_\xi + \eta_r(rv)_\eta\right]$$

$$\tau_{xr} = \mu(\xi_r u_\xi + \eta_r u_\eta + \xi_x v_\xi + \eta_x v_\eta)$$

$$\tau_{x\theta} = \mu(\xi_x w_\xi + \eta_x w_\eta)$$

$$\tau_{r\theta} = \mu(\xi_r w_\xi + \eta_r w_\eta) - \mu\frac{w}{r}$$

$$\beta_x = (2\mu + \lambda)(\xi_x u u_\xi + \eta_x u u_\eta) + \frac{\lambda}{r}\left[\xi_r u(rv)_\xi + \eta_r u(rv)_\eta\right]$$
$$+ \mu(\xi_r v u_\xi + \eta_r v u_\eta + \xi_x v v_\xi + \eta_x v v_\eta) + \mu(\xi_x w w_\xi + \eta_x w w_\eta)$$
$$+ \frac{k}{Pr_r}(\xi_x T_\xi + \eta_x T_\eta)$$

$$\beta_r = 2\mu(\xi_r v v_\xi + \eta_r v v_\eta) + \frac{\lambda}{r}\left[\xi_r v(rv)_\xi + \eta_r v(rv)_\eta\right]$$
$$+ \mu(\xi_r u u_\xi + \eta_r u u_\eta + \xi_x u v_\xi + \eta_x u v_\eta) + \mu(\xi_r w w_\xi + \eta_r w w_\eta)$$
$$+ \lambda(\xi_x v u_\xi + \eta_x v u_\eta) - \mu\frac{w^2}{r} + \frac{k}{Pr_r}(\xi_r T_\xi + \eta_r T_\eta)$$

The above expressions for the shear stress and heat flux terms are substituted into equations (B.6e) through (B.6g). As in the two-dimensional planar case, the cross derivative terms are separated from the non-cross derivative terms. In addition, for the axisymmetric case the non-derivative terms are included with the cross derivatives.

The resulting five elements of $\hat{E}_{V_1}$ (excluding the $1/JRe_r$ coefficient) are

$$(\hat{E}_{V_1})_1 = 0 \tag{B.11a}$$

$$(\hat{E}_{V_1})_2 = 2\mu\xi_x^2 u_\xi + \lambda\xi_x\left[\xi_x u_\xi + \frac{1}{r}\xi_r(rv)_\xi\right] + \mu\xi_r(\xi_r u_\xi + \xi_x v_\xi) \tag{B.11b}$$

$$(\hat{E}_{V_1})_3 = 2\mu\xi_r^2 v_\xi + \lambda\xi_r\left[\xi_x u_\xi + \frac{1}{r}\xi_r(rv)_\xi\right] + \mu\xi_x(\xi_r u_\xi + \xi_x v_\xi) \tag{B.11c}$$

$$(\hat{E}_{V_1})_4 = \mu\xi_x^2 w_\xi + \mu\xi_r^2 w_\eta \tag{B.11d}$$

$$(\hat{E}_{V_1})_5 = 2\mu(\xi_x^2 u u_\xi + \xi_r^2 v v_\xi) + \lambda\xi_x\left[\xi_x u u_\xi + \frac{1}{r}\xi_r u(rv)_\xi\right] + \lambda\xi_r\left[\xi_x v u_\xi + \frac{1}{r}\xi_r v(rv)_\xi\right]$$
$$+ \mu\xi_x(\xi_r v u_\xi + \xi_x v v_\xi + \xi_x w w_\xi) + \mu\xi_r(\xi_r u u_\xi + \xi_x u v_\xi + \xi_r w w_\xi) + \frac{k}{Pr_r}(\xi_x^2 + \xi_r^2)T_\xi \tag{B.11e}$$

For linearization it is convenient to rewrite the last element as

$$(\hat{E}_{V_1})_5 = \frac{(2\mu + \lambda)}{2}\left[\xi_x^2(u^2)_\xi + \xi_r^2(v^2)_\xi\right] + (\mu + \lambda)\xi_x\xi_r(uv)_\xi + \lambda\xi_r\frac{r_\xi}{r}(\xi_r v^2 + \xi_x uv)$$
$$+ \frac{\mu}{2}\left[\xi_x^2(v^2 + w^2)_\xi + \xi_r^2(u^2 + w^2)_\xi\right] + \frac{k}{Pr_r}(\xi_x^2 + \xi_r^2)T_\xi \tag{B.11f}$$

The elements of $\hat{\mathbf{F}}_{V_1}$ have exactly the same form as those of $\hat{\mathbf{E}}_{V_1}$, but with ξ replaced by η.

The five elements of $\hat{\mathbf{E}}_{V_2}$ (again excluding the $1/JRe_r$ coefficient) are

$$(\hat{\mathbf{E}}_{V_2})_1 = 0 \tag{B.12a}$$

$$(\hat{\mathbf{E}}_{V_2})_2 = 2\mu\xi_x\eta_x u_\eta + \lambda\xi_x\left[\eta_x u_\eta + \frac{1}{r}\eta_r(rv)_\eta\right] + \mu\xi_r(\eta_r u_\eta + \eta_x v_\eta) \tag{B.12b}$$

$$(\hat{\mathbf{E}}_{V_2})_3 = 2\mu\xi_r\eta_r v_\eta + \lambda\xi_r\left[\eta_x u_\eta + \frac{1}{r}\eta_r(rv)_\eta\right] + \mu\xi_x(\eta_r u_\eta + \eta_x v_\eta) \tag{B.12c}$$

$$(\hat{\mathbf{E}}_{V_2})_4 = \mu\xi_x\eta_x w_\eta + \mu\xi_r\eta_r w_\eta - \mu\xi_r\frac{w}{r} \tag{B.12d}$$

$$\begin{aligned}(\hat{\mathbf{E}}_{V_2})_5 = {}&2\mu(\xi_x\eta_x uu_\eta + \xi_r\eta_r vv_\eta) + \lambda\xi_x\left[\eta_x uu_\eta + \frac{1}{r}\eta_r u(rv)_\eta\right] + \lambda\xi_r\left[\eta_x vu_\eta + \frac{1}{r}\eta_r v(rv)_\eta\right]\\&+ \mu\xi_x(\eta_r vu_\eta + \eta_x vv_\eta + \eta_x ww_\eta) + \mu\xi_r(\eta_r uu_\eta + \eta_x uv_\eta + \eta_r ww_\eta)\\&- \mu\xi_r\frac{w^2}{r} + \frac{k}{Pr_r}(\xi_x\eta_x + \xi_r\eta_r)T_\eta\end{aligned} \tag{B.12e}$$

The last element can be rewritten as

$$\begin{aligned}(\hat{\mathbf{E}}_{V_2})_5 = {}&2\mu(\xi_x\eta_x uu_\eta + \xi_r\eta_r vv_\eta) + \lambda\xi_x(\eta_x uu_\eta + \eta_r uv_\eta) + \lambda\xi_r(\eta_x vu_\eta + \eta_r vv_\eta) + \lambda\eta_r\frac{v}{r}(\xi_x u + \xi_r v)r_\eta\\&+ \mu\xi_x(\eta_r vu_\eta + \eta_x vv_\eta + \eta_x ww_\eta) + \mu\xi_r(\eta_r uu_\eta + \eta_x uv_\eta + \eta_r ww_\eta)\\&- \mu\xi_r\frac{w^2}{r} + \frac{k}{Pr_r}(\xi_x\eta_x + \xi_r\eta_r)T_\eta\end{aligned} \tag{B.12f}$$

The elements of $\hat{\mathbf{F}}_{V_2}$ have exactly the same form as those of $\hat{\mathbf{E}}_{V_2}$, but with ξ replaced by η and η replaced by ξ.

The five elements of $\hat{\mathbf{H}}_V$ are

$$(\hat{\mathbf{H}}_V)_1 = 0 \tag{B.13a}$$

$$(\hat{\mathbf{H}}_V)_2 = 0 \tag{B.13b}$$

$$(\hat{\mathbf{H}}_V)_3 = -2\mu\frac{v}{r} - \lambda(\xi_x u_\xi + \eta_x u_\eta) + \frac{\lambda}{r}\left[\xi_r(rv)_\xi + \eta_r(rv)_\eta\right] \tag{B.13c}$$

$$(\hat{\mathbf{H}}_V)_4 = \mu(\xi_r w_\xi + \eta_r w_\eta) - \mu\frac{w}{r} \tag{B.13d}$$

$$(\hat{\mathbf{H}}_V)_5 = 0 \tag{B.13e}$$

Performing the linearization, the Jacobian coefficient matrix $\partial \hat{E}_{V_1} / \partial \hat{Q}$ is

$$
\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} = \frac{1}{Re_r}
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\[2ex]
\left(\dfrac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{21} & \alpha_{xx} \dfrac{\partial}{\partial \xi}\left(\dfrac{1}{\rho} \right) & \alpha_{xr} \dfrac{\partial}{\partial \xi}\left(\dfrac{1}{\rho} \right) + \alpha'_{xr} \dfrac{1}{\rho} r_\xi & 0 & 0 \\[3ex]
\left(\dfrac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{31} & \alpha_{xr} \dfrac{\partial}{\partial \xi}\left(\dfrac{1}{\rho} \right) & \alpha_{rr} \dfrac{\partial}{\partial \xi}\left(\dfrac{1}{\rho} \right) + \alpha'_{rr} \dfrac{1}{\rho} r_\xi & 0 & 0 \\[3ex]
\left(\dfrac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{41} & 0 & 0 & \alpha_{zz} \dfrac{\partial}{\partial \xi}\left(\dfrac{1}{\rho} \right) & 0 \\[3ex]
\left(\dfrac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{51} & \left(\dfrac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{52} & \left(\dfrac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{53} & \left(\dfrac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{54} & \alpha_0 \dfrac{\partial}{\partial \xi}\left(\dfrac{\partial T}{\partial E_T} \right)
\end{bmatrix}
\qquad \text{(B.14)}
$$

where

$$
\alpha_{xx} = (2\mu + \lambda)\xi_x^2 + \mu \xi_r^2
$$

$$
\alpha_{rr} = \mu \xi_x^2 + (2\mu + \lambda)\xi_r^2
$$

$$
\alpha_{zz} = \mu \xi_x^2 + \mu \xi_r^2
$$

$$
\alpha_{xr} = (\mu + \lambda)\xi_x \xi_r
$$

$$
\alpha'_{xr} = \frac{\lambda}{r} \xi_x \xi_r
$$

$$
\alpha'_{rr} = \frac{\lambda}{r} \xi_r^2
$$

$$
\alpha_0 = \frac{k}{Pr_r} (\xi_x^2 + \xi_r^2)
$$

$$
\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{21} = - \alpha_{xx} \frac{\partial}{\partial \xi}\left(\frac{u}{\rho} \right) - \alpha_{xr} \frac{\partial}{\partial \xi}\left(\frac{v}{\rho} \right) - \alpha'_{xr} \frac{v}{\rho} r_\xi
$$

$$
\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{31} = - \alpha_{xr} \frac{\partial}{\partial \xi}\left(\frac{u}{\rho} \right) - \alpha_{rr} \frac{\partial}{\partial \xi}\left(\frac{v}{\rho} \right) - \alpha'_{rr} \frac{v}{\rho} r_\xi
$$

$$
\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{41} = - \alpha_{zz} \frac{\partial}{\partial \xi}\left(\frac{w}{\rho} \right)
$$

$$
\left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)_{51} = - \alpha_{xx} \frac{\partial}{\partial \xi}\left(\frac{u^2}{\rho} \right) - \alpha_{rr} \frac{\partial}{\partial \xi}\left(\frac{v^2}{\rho} \right) - \alpha_{zz} \frac{\partial}{\partial \xi}\left(\frac{w^2}{\rho} \right)
$$

$$
- 2\alpha_{xr} \frac{\partial}{\partial \xi}\left(\frac{uv}{\rho} \right) - 2\alpha'_{rr} \frac{v^2}{\rho} r_\xi - 2\alpha'_{xr} \frac{uv}{\rho} r_\xi + \alpha_0 \frac{\partial}{\partial \xi}\left(\frac{\partial T}{\partial \rho} \right)
$$

$$\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}}\right)_{52} = -\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}}\right)_{21} + \alpha_0 \frac{\partial}{\partial \xi}\left(\frac{\partial T}{\partial(\rho u)}\right)$$

$$\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}}\right)_{53} = -\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}}\right)_{31} + \alpha'_{rr}\frac{v}{\rho}r_\xi + \alpha_0 \frac{\partial}{\partial \xi}\left(\frac{\partial T}{\partial(\rho v)}\right)$$

$$\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}}\right)_{54} = -\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}}\right)_{41} + \alpha_0 \frac{\partial}{\partial \xi}\left(\frac{\partial T}{\partial(\rho w)}\right)$$

The Jacobian coefficient matrix for the remaining non-cross derivative viscous terms, $\partial \hat{\mathbf{F}}_{V_1}/\partial \hat{\mathbf{Q}}$, has the same form as $\partial \hat{\mathbf{E}}_{V_1}/\partial \hat{\mathbf{Q}}$, but with ξ replaced by η.

And finally, linearizing $\hat{\mathbf{H}}_V$, the Jacobian coefficient matrix $\partial \hat{\mathbf{H}}_V/\partial \hat{\mathbf{Q}}$ is

$$\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}} = \frac{1}{Re_r}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{31} & \left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{32} & \left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{33} & 0 & 0 \\ \left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{41} & 0 & 0 & \left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad (B.15)$$

where

$$\left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{31} = \lambda \xi_x \frac{\partial}{\partial \xi}\left(\frac{u}{\rho}\right) + \lambda \xi_r \frac{\partial}{\partial \xi}\left(\frac{v}{\rho}\right) + \lambda \eta_x \frac{\partial}{\partial \eta}\left(\frac{u}{\rho}\right)$$
$$+ [2\mu + \lambda(\xi_r r_\xi + \eta_r r_\eta)]\frac{1}{r}\frac{v}{\rho} + \lambda \eta_r \frac{\partial}{\partial \eta}\left(\frac{v}{\rho}\right)$$

$$\left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{32} = -\lambda \xi_x \frac{\partial}{\partial \xi}\left(\frac{1}{\rho}\right) - \lambda \eta_x \frac{\partial}{\partial \eta}\left(\frac{1}{\rho}\right)$$

$$\left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{33} = -\lambda \xi_r \frac{\partial}{\partial \xi}\left(\frac{1}{\rho}\right) - [2\mu + \lambda(\xi_r r_\xi + \eta_r r_\eta)]\frac{1}{r}\frac{1}{\rho} - \lambda \eta_r \frac{\partial}{\partial \eta}\left(\frac{1}{\rho}\right)$$

$$\left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{41} = -\mu \xi_r \frac{\partial}{\partial \xi}\left(\frac{w}{\rho}\right) + \frac{\mu}{r}\frac{w}{\rho} - \mu \eta_r \frac{\partial}{\partial \eta}\left(\frac{w}{\rho}\right)$$

$$\left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}}\right)_{44} = \mu \xi_r \frac{\partial}{\partial \xi}\left(\frac{1}{\rho}\right) - \frac{\mu}{r}\frac{1}{\rho} + \mu \eta_r \frac{\partial}{\partial \eta}\left(\frac{1}{\rho}\right)$$

B.2.3 Equation Of State

The equation of state given in Section 4.3 must be modified slightly to add the swirl velocity w. Thus,

$$p = (\gamma - 1)\left[E_T - \frac{1}{2}\rho(u^2 + v^2 + w^2)\right] \tag{B.16}$$

or, in terms of temperature,

$$T = \frac{1}{c_v}\left[\frac{E_T}{\rho} - \frac{1}{2}(u^2 + v^2 + w^2)\right]. \tag{B.17}$$

The derivatives arising from the linearization are the same as those presented in Section 4.3, except for

$$\frac{\partial p}{\partial \rho} = \frac{\gamma - 1}{2}(u^2 + v^2 + w^2) \tag{B.18a}$$

$$\frac{\partial p}{\partial(\rho w)} = -(\gamma - 1)w \tag{B.18b}$$

$$\frac{\partial T}{\partial \rho} = -\frac{1}{c_v}\left[\frac{E_T}{\rho^2} - \frac{1}{\rho}(u^2 + v^2 + w^2)\right] \tag{B.18c}$$

$$\frac{\partial T}{\partial(\rho w)} = -\frac{w}{c_v \rho} \tag{B.18d}$$

If constant stagnation enthalpy can be assumed, the appropriate equation of state is

$$p = \frac{\gamma - 1}{\gamma}\rho\left[h_T - \frac{1}{2}(u^2 + v^2 + w^2)\right] \tag{B.19}$$

and the temperature becomes

$$T = \frac{1}{c_p}\left[h_T - \frac{1}{2}(u^2 + v^2 + w^2)\right] \tag{B.20}$$

Again, the derivatives arising from the linearization are the same as in Section 4.3, except for

$$\frac{\partial p}{\partial \rho} = \frac{\gamma - 1}{\gamma}\left[h_T + \frac{1}{2}(u^2 + v^2 + w^2)\right] \tag{B.21a}$$

$$\frac{\partial p}{\partial(\rho w)} = -\frac{\gamma - 1}{\gamma}w \tag{B.21b}$$

$$\frac{\partial T}{\partial \rho} = \frac{1}{c_p \rho} (u^2 + v^2 + w^2) \tag{B.21c}$$

$$\frac{\partial T}{\partial (\rho w)} = -\frac{w}{c_p \rho} \tag{B.21d}$$

B.2.4 Linearized Governing Equation

The linearized form of equation (B.8) can now be written as

$$\Delta \hat{Q}^n + \frac{\theta_1 \Delta \tau}{1 + \theta_2} \frac{1}{r} \left\{ \frac{\partial}{\partial \xi} \left[r \left(\frac{\partial \hat{E}}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n \right] + \frac{\partial}{\partial \eta} \left[r \left(\frac{\partial \hat{F}}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n \right] + \left(\frac{\partial \hat{H}}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n \right\}$$

$$- \frac{\theta_1 \Delta \tau}{1 + \theta_2} \frac{1}{r} \left\{ \frac{\partial}{\partial \xi} \left[r \left(\frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n \right] + \frac{\partial}{\partial \eta} \left[r \left(\frac{\partial \hat{F}_{V_1}}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n \right] + \left(\frac{\partial \hat{H}_V}{\partial \hat{Q}} \right)^n \Delta \hat{Q}^n \right\} =$$

$$- \frac{\Delta \tau}{1 + \theta_2} \frac{1}{r} \left(\frac{\partial (r \hat{E})}{\partial \xi} + \frac{\partial (r \hat{F})}{\partial \eta} + \hat{H} \right)^n + \frac{\Delta \tau}{1 + \theta_2} \frac{1}{r} \left(\frac{\partial (r \hat{E}_{V_1})}{\partial \xi} + \frac{\partial (r \hat{F}_{V_1})}{\partial \eta} + \hat{H}_V \right)^n$$

$$+ \frac{(1 + \theta_3) \Delta \tau}{1 + \theta_2} \frac{1}{r} \left(\frac{\partial (r \hat{E}_{V_2})}{\partial \xi} + \frac{\partial (r \hat{F}_{V_2})}{\partial \eta} \right)^n - \frac{\theta_3 \Delta \tau}{1 + \theta_2} \frac{1}{r} \left(\frac{\partial (r \hat{E}_{V_2})}{\partial \xi} + \frac{\partial (r \hat{F}_{V_2})}{\partial \eta} \right)^{n-1}$$

$$+ \frac{\theta_2}{1 + \theta_2} \Delta \hat{Q}^{n-1} + O\left[\left(\theta_1 - \frac{1}{2} - \theta_2 \right)(\Delta \tau)^2, (\theta_3 - \theta_1)(\Delta \tau)^2, (\Delta \tau)^3 \right] \tag{B.22}$$

B.3 SOLUTION PROCEDURE

Letting LHS(B.22) represent the left hand side of equation (B.22), we can write

$$\text{LHS(B.22)} = \left\{ K + \frac{\theta_1 \Delta \tau}{1 + \theta_2} \frac{1}{r} \left[\frac{\partial}{\partial \xi} \left(r \frac{\partial \hat{E}}{\partial \hat{Q}} - r \frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right) + \frac{\partial}{\partial \eta} \left(r \frac{\partial \hat{F}}{\partial \hat{Q}} - r \frac{\partial \hat{F}_{V_1}}{\partial \hat{Q}} \right) \right] \right\}^n \Delta \hat{Q}^n \tag{B.23a}$$

where

$$K = I + \frac{\theta_1 \Delta \tau}{1 + \theta_2} \frac{1}{r} \left(\frac{\partial \hat{H}}{\partial \hat{Q}} - \frac{\partial \hat{H}_V}{\partial \hat{Q}} \right) \tag{B.23b}$$

and I represents the identity matrix. The term in braces in equation (B.23a) can be factored to give

$$\text{LHS(B.22)} = \left[K + \frac{\theta_1 \Delta \tau}{1 + \theta_2} \frac{1}{r} \frac{\partial}{\partial \xi} \left(r \frac{\partial \hat{E}}{\partial \hat{Q}} - r \frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right) \right]^n \left[I + K^{-1} \frac{\theta_1 \Delta \tau}{1 + \theta_2} \frac{1}{r} \frac{\partial}{\partial \eta} \left(r \frac{\partial \hat{F}}{\partial \hat{Q}} - r \frac{\partial \hat{F}_{V_1}}{\partial \hat{Q}} \right) \right]^n \Delta \hat{Q}^n$$

$$- \left(\frac{\theta_1 \Delta \tau}{1 + \theta_2} \right)^2 \frac{1}{r^2} K^{-1} \left[\frac{\partial}{\partial \xi} \left(r \frac{\partial \hat{E}}{\partial \hat{Q}} - r \frac{\partial \hat{E}_{V_1}}{\partial \hat{Q}} \right) \frac{\partial}{\partial \eta} \left(r \frac{\partial \hat{F}}{\partial \hat{Q}} - r \frac{\partial \hat{F}_{V_1}}{\partial \hat{Q}} \right) \right]^n \Delta \hat{Q}^n \tag{B.24}$$

The last term represents the splitting error.

Equation (B.22) can thus be rewritten in spatially factored form, and, neglecting the temporal truncation and splitting error terms, becomes

$$
\left[K + \frac{\theta_1 \Delta\tau}{1+\theta_2} \frac{1}{r} \frac{\partial}{\partial\xi} \left(r\frac{\partial\hat{E}}{\partial\hat{Q}} - r\frac{\partial\hat{E}_{V_1}}{\partial\hat{Q}} \right) \right]^n (K^{-1})^n \left[K + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{1}{r} \frac{\partial}{\partial\eta} \left(r\frac{\partial\hat{F}}{\partial\hat{Q}} - r\frac{\partial\hat{F}_{V_1}}{\partial\hat{Q}} \right) \right]^n \Delta\hat{Q}^n =
$$

$$
-\frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E})}{\partial\xi} + \frac{\partial(r\hat{F})}{\partial\eta} + \hat{H} \right)^n + \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E}_{V_1})}{\partial\xi} + \frac{\partial(r\hat{F}_{V_1})}{\partial\eta} + \hat{H}_V \right)^n
$$

$$
+\frac{(1+\theta_3)\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E}_{V_2})}{\partial\xi} + \frac{\partial(r\hat{F}_{V_2})}{\partial\eta} \right)^n - \frac{\theta_3\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E}_{V_2})}{\partial\xi} + \frac{\partial(r\hat{F}_{V_2})}{\partial\eta} \right)^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta\hat{Q}^{n-1} \qquad (B.25)
$$

Using the procedure of Douglas and Gunn (1964), as written by Briley and McDonald (1977), equation (B.25) can be split into the following two-sweep sequence.

Sweep 1 (ξ direction)

$$
\left[K + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{1}{r} \frac{\partial}{\partial\xi} \left(r\frac{\partial\hat{E}}{\partial\hat{Q}} - r\frac{\partial\hat{E}_{V_1}}{\partial\hat{Q}} \right) \right]^n \Delta\hat{Q}^* =
$$

$$
-\frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E})}{\partial\xi} + \frac{\partial(r\hat{F})}{\partial\eta} + \hat{H} \right)^n + \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E}_{V_1})}{\partial\xi} + \frac{\partial(r\hat{F}_{V_1})}{\partial\eta} + \hat{H}_V \right)^n
$$

$$
+\frac{(1+\theta_3)\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E}_{V_2})}{\partial\xi} + \frac{\partial(r\hat{F}_{V_2})}{\partial\eta} \right)^n - \frac{\theta_3\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E}_{V_2})}{\partial\xi} + \frac{\partial(r\hat{F}_{V_2})}{\partial\eta} \right)^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta\hat{Q}^{n-1} \qquad (B.26a)
$$

Sweep 2 (η direction)

$$
\left[K + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{1}{r} \frac{\partial}{\partial\eta} \left(r\frac{\partial\hat{F}}{\partial\hat{Q}} - r\frac{\partial\hat{F}_{V_1}}{\partial\hat{Q}} \right) \right]^n \Delta\hat{Q}^n = K^n\Delta\hat{Q}^* \qquad (B.26b)
$$

Or, expanding K and rearranging,

Sweep 1 (ξ direction)

$$
\Delta\hat{Q}^* + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{1}{r} \frac{\partial}{\partial\xi} \left[r\left(\frac{\partial\hat{E}}{\partial\hat{Q}} \right)^n \Delta\hat{Q}^* \right] - \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{1}{r} \frac{\partial}{\partial\xi} \left[r\left(\frac{\partial\hat{E}_{V_1}}{\partial\hat{Q}} \right)^n \Delta\hat{Q}^* \right] + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial\hat{H}}{\partial\hat{Q}} - \frac{\partial\hat{H}_V}{\partial\hat{Q}} \right)^n \Delta\hat{Q}^* =
$$

$$
-\frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E})}{\partial\xi} + \frac{\partial(r\hat{F})}{\partial\eta} + \hat{H} \right)^n + \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E}_{V_1})}{\partial\xi} + \frac{\partial(r\hat{F}_{V_1})}{\partial\eta} + \hat{H}_V \right)^n
$$

$$
+\frac{(1+\theta_3)\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E}_{V_2})}{\partial\xi} + \frac{\partial(r\hat{F}_{V_2})}{\partial\eta} \right)^n - \frac{\theta_3\Delta\tau}{1+\theta_2} \frac{1}{r} \left(\frac{\partial(r\hat{E}_{V_2})}{\partial\xi} + \frac{\partial(r\hat{F}_{V_2})}{\partial\eta} \right)^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta\hat{Q}^{n-1} \qquad (B.27a)
$$

Sweep 2 (η direction)

$$\Delta\hat{Q}^n + \frac{\theta_1\Delta\tau}{1+\theta_2}\frac{1}{r}\frac{\partial}{\partial\eta}\left[r\left(\frac{\partial\hat{F}}{\partial\hat{Q}}\right)^n\Delta\hat{Q}^n\right] - \frac{\theta_1\Delta\tau}{1+\theta_2}\frac{1}{r}\frac{\partial}{\partial\eta}\left[r\left(\frac{\partial\hat{F}_{V_1}}{\partial\hat{Q}}\right)^n\Delta\hat{Q}^n\right] + \frac{\theta_1\Delta\tau}{1+\theta_2}\frac{1}{r}\left(\frac{\partial\hat{H}}{\partial\hat{Q}} - \frac{\partial\hat{H}_V}{\partial\hat{Q}}\right)^n\Delta\hat{Q}^n =$$

$$\Delta\hat{Q}^* + \frac{\theta_1\Delta\tau}{1+\theta_2}\frac{1}{r}\left(\frac{\partial\hat{H}}{\partial\hat{Q}} - \frac{\partial\hat{H}_V}{\partial\hat{Q}}\right)^n\Delta\hat{Q}^* \qquad\text{(B.27b)}$$

Applying the spatial differencing formulas of Section 5.0 results in

Sweep 1 (ξ direction)

$$\Delta\hat{Q}_i^* + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\xi}\frac{1}{r}\left[\left(r\frac{\partial\hat{E}}{\partial\hat{Q}}\right)_{i+1}^n\Delta\hat{Q}_{i+1}^* - \left(r\frac{\partial\hat{E}}{\partial\hat{Q}}\right)_{i-1}^n\Delta\hat{Q}_{i-1}^*\right]$$

$$- \frac{\theta_1\Delta\tau}{(1+\theta_2)2(\Delta\xi)^2}\frac{1}{r}\left[(r_{i-1}f_{i-1}+r_if_i)^ng_{i-1}^n\Delta\hat{Q}_{i-1}^* - (r_{i-1}f_{i-1}+2r_if_i+r_{i+1}f_{i+1})^ng_i^n\Delta\hat{Q}_i^* + (r_if_i+r_{i+1}f_{i+1})^ng_{i+1}^n\Delta\hat{Q}_{i+1}^*\right]$$

$$+ \frac{\theta_1\Delta\tau}{1+\theta_2}\frac{1}{r}\left(\frac{\partial\hat{H}}{\partial\hat{Q}} - \frac{\partial\hat{H}_V}{\partial\hat{Q}}\right)_i^n\Delta\hat{Q}_i^* = -\frac{\Delta\tau}{1+\theta_2}\frac{1}{r}\left[\delta_\xi(r\,\hat{E}) + \delta_\eta(r\,\hat{F}) + \hat{H}\right]^n + \frac{\Delta\tau}{1+\theta_2}\frac{1}{r}\left[\delta_\xi(r\,\hat{E}_{V_1}) + \delta_\eta(r\,\hat{F}_{V_1}) + \hat{H}_V\right]^n$$

$$+ \frac{(1+\theta_3)\Delta\tau}{1+\theta_2}\frac{1}{r}\left[\delta_\xi(r\,\hat{E}_{V_2}) + \delta_\eta(r\,\hat{F}_{V_2})\right]^n - \frac{\theta_3\Delta\tau}{1+\theta_2}\frac{1}{r}\left[\delta_\xi(r\,\hat{E}_{V_2}) + \delta_\eta(r\,\hat{F}_{V_2})\right]^{n-1} + \frac{\theta_2}{1+\theta_2}\Delta\hat{Q}^{n-1} \qquad\text{(B.28a)}$$

Sweep 2 (η direction)

$$\Delta\hat{Q}_j^n + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\eta}\frac{1}{r}\left[\left(r\frac{\partial\hat{F}}{\partial\hat{Q}}\right)_{j+1}^n\Delta\hat{Q}_{j+1}^n - \left(r\frac{\partial\hat{F}}{\partial\hat{Q}}\right)_{j-1}^n\Delta\hat{Q}_{j-1}^n\right]$$

$$- \frac{\theta_1\Delta\tau}{(1+\theta_2)2(\Delta\eta)^2}\frac{1}{r}\left[(r_{j-1}f_{j-1}+r_jf_j)^ng_{j-1}^n\Delta\hat{Q}_{j-1}^n - (r_{j-1}f_{j-1}+2r_jf_j+r_{j+1}f_{j+1})^ng_j^n\Delta\hat{Q}_j^n + (r_jf_j+r_{j+1}f_{j+1})^ng_{j+1}^n\Delta\hat{Q}_{j+1}^n\right]$$

$$+ \frac{\theta_1\Delta\tau}{1+\theta_2}\frac{1}{r}\left(\frac{\partial\hat{H}}{\partial\hat{Q}} - \frac{\partial\hat{H}_V}{\partial\hat{Q}}\right)_j^n\Delta\hat{Q}_j^n = \Delta\hat{Q}^* + \frac{\theta_1\Delta\tau}{1+\theta_2}\frac{1}{r}\left(\frac{\partial\hat{H}}{\partial\hat{Q}} - \frac{\partial\hat{H}_V}{\partial\hat{Q}}\right)^n\Delta\hat{Q}^* \qquad\text{(B.28b)}$$

These equations are solved using the same matrix inversion procedure described in Section 7.2.

B.4 CHIEN k-ε TURBULENCE MODEL

The axisymmetric k-ε equations for the Chien model can be written using vector notation as

$$\frac{\partial(r\mathbf{W})}{\partial t} + \frac{\partial(r\mathbf{F})}{\partial x} + \frac{\partial(r\mathbf{G})}{\partial r} = r(\mathbf{S} + \mathbf{T}) \qquad\text{(B.29)}$$

where $\mathbf{W}$, $\mathbf{F}$, $\mathbf{G}$, $\mathbf{S}$, and $\mathbf{T}$ are the same as the corresponding terms in the two-dimensional planar equations with the coordinate y replaced by r, and

$$P_1 = 2\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial r}\right)^2 + \left(\frac{v}{r}\right)^2\right] - \frac{2}{3}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial r} + \frac{v}{r}\right)^2$$

$$+ \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x}\right)^2 + \left(\frac{\partial w}{\partial x}\right)^2 + \left[r\frac{\partial}{\partial r}\left(\frac{w}{r}\right)\right]^2 \qquad\text{(B.30a)}$$

$$P_2 = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial r} + \frac{v}{r} \qquad (\text{B.30b})$$

The analysis for the axisymmetric k-ε equations is the same as for the two-dimensional planar k-ε equations, described in the main body of this report.

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13. ABSTRACT (Maximum 200 words)

A computer code called *Proteus 2D* has been developed to solve the two-dimensional planar or axisymmetric, Reynolds-averaged, unsteady compressible Navier-Stokes equations in strong conservation law form. The objective in this effort has been to develop a code for aerospace propulsion applications that is easy to use and easy to modify. Code readability, modularity, and documentation have been emphasized. The governing equations are solved in generalized nonorthogonal body-fitted coordinates, by marching in time using a fully-coupled ADI solution procedure. The boundary conditions are treated implicitly. All terms, including the diffusion terms, are linearized using second-order Taylor series expansions. Turbulence is modeled using either an algebraic or two-equation eddy viscosity model. The thin-layer or Euler equations may also be solved. The energy equation may be eliminated by the assumption of constant total enthalpy. Explicit and implicit artificial viscosity may be used. Several time step options are available for convergence acceleration. The documentation is divided into three volumes. This is the Analysis Description, and presents the equations and solution procedure. It describes in detail the governing equations, the turbulence model, the linearization of the equations and boundary conditions, the time and space differencing formulas, the ADI solution procedure, and the artificial viscosity models.

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