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Technical Notes

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Primitive Variable Implicit Approach for Compressible Chemical Vapor Deposition

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Introduction

THIS Note provides a description of a primitive variable formulation of a line-relaxation implicit scheme that has proved very useful in solving difficult compressible internal flow problems. The implementation of this solution method was motivated by efforts to model arc-heated plasma jet reactors for chemical vapor deposition of material thin films.[1,2] The low-pressure reactor flow is supersonic with strong shocks, strong viscous effects, and contains large regions of low Mach number flow. Our implementation of some standard implicit solution schemes showed poor convergence performance for the compressible multicomponent Navier–Stokes equations being solved. A line-relaxation scheme performed well for both the compressible flow aspects and the viscous flow aspects.

Traditionally, compressible schemes solve for the conservation variables (densities, momentums, and total energy). Thomas and Walters[3] present a line-relaxation scheme where they use the flux split scheme to construct a diagonally dominant implicit system. MacCormack and Candler[4] presents a line-relaxation scheme based on Steger–Warming splitting. In our opinion, the primitive variables (pressure, velocities, temperature, and mass fraction) are of more interest. The primitive variable formulation simplifies the linearization of certain terms for the implicit scheme and the evaluation of multicomponent thermophysical properties. Furthermore, the primitive variable implementation was constructed to prepare for future investigation of time preconditioning[5] to relieve the acoustic stiffness in the large low Mach number regions of the flowfield.

Most line-relaxation schemes for the compressible governing equations are diagonally enhanced to improve steady-state convergence characteristics. Implicit matrix terms are modified using some sort of upwind scheme to approximate the linearized convective terms. The diagonal enhancement is an artificial dissipation and acts to stabilize the implicit scheme. We prefer to use a simple approximation to form the upwinded implicit convective terms. A popular simplification is to use central differences with second-order artificial dissipation as presented by Shuen and Yoon[6] for a Gauss–Seidel implicit scheme. Typically, the linearization is performed in terms of conservative variables, and the convective flux Jacobian has the nice property that the diagonal terms all have the units of velocity. This makes the addition of the artificial dissipation term simple and consists of adding a velocity scale to the diagonal. The simple diagonal enhancement used by Shuen and Yoon[6] cannot be applied directly with primitive variables because the convective flux Jacobians do not scale directly with velocity. A matrix scaling is required, and it shown herein how this diagonal enhancement can be simply integrated into the flux Jacobian term.

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Time Integration and Linearization

The two-dimensional, laminar Navier–Stokes equations are written with the time derivative of the conservative variables Q and a vector function F representing the spatial conservation laws,

$$\iiint \frac{\partial Q}{\partial t}\,\mathrm{d}V + F(Q) = 0 \tag{1}$$

The equations are discretized in time using the backward Euler method and discretized in space using a finite volume method on a structured, multiple block grid. The backward Euler method is first-order accurate in time and is sufficient for time marching to steady state. The discrete system is written as a single vector function R

$$R(Q^{n+1}) = \frac{Q^{n+1} - Q^n}{\Delta t}\Delta V + F(Q^{n+1}) \tag{2}$$

The time step is denoted by the superscript n. The solution is advanced in time by driving $R(Q)$ toward zero. The nonlinear equations are linearized about time level n in terms of primitive variables and approximately inverted. It is too difficult to generate the exact linearization matrix corresponding to the flux functions in $F(Q)$ so an approximate matrix is used. In forming the approximate matrix, the following philosophy is pursued: The implicit (left-hand side) matrix is a function of the numerical method, whereas the (right-hand side) spatial conservation law reflects the actual physics. In this way, the left-hand side can approximate the discretization used for the right-hand side. The approximation should always be simpler, enhance diagonal dominance, and reduce the work and storage involved with the linear algebra. Therefore, the approximate matrix is constructed from a different discretization of the spatial conservation law $\bar{R}$, in terms of the primitive variables W. The function R, which will be driven toward zero, is expanded in a Taylor series, but the derivative of R is replaced by the derivative of $\bar{R}$. The resulting matrix problem is

$$\left.\frac{\partial \bar{R}}{\partial W}\right|^n (W^{n+1} - W^n) = -F(W^n) \tag{3}$$

The flux functions in F are constructed with the advection upwind split method (AUSM)[7] and minmod interpolation[8] for the convective terms and central differencing for the diffusive transport terms. The approximate matrix is constructed from central differencing with artificial dissipation. Once the implicit equations are linearized, the problem is reduced to an exercise in linear algebra—the line-relaxation part.

The line-relaxation scheme sweeps through the grid, solving block-tridiagonal matrices for each grid line. Sweeping is continuous across grid block boundaries by keeping the grid block coupling terms in the matrix. Boundary conditions are treated as equations and coupled implicitly to the interior conservation laws. Alternating sweeping is used to help propagate boundary information quickly and is crucial for internal flow problems with low Mach number regions. To remove biasing due to preferred flow directions, the scheme sweeps through i lines and then j lines. The scheme also performs backward sweeps. Alternating sweeping continues at a particular time level until the linear problem is converged to a desired level.

Primitive Variable Linearization

The matrix operator for one finite volume in the system, linearized with respect to the primitive variables, is

$$\left[\Gamma_{i,j}\frac{\Delta V}{\Delta t} - A^{+}_{i-1,j} - A^{-}_{i,j} + A^{+}_{i,j} + A^{-}_{i+1,j} - B^{+}_{i-1,j} - B^{-}_{i,j} + B^{+}_{i,j} + B^{-}_{i+1,j} - C_{i,j} - \mathrm{VIS}_{i,j}\right]\Delta W = -\boldsymbol{R}(W^n)_{i,j} \tag{4}$$

where the inviscid flux Jacobians are defined as

$$A = \frac{\partial(F\cdot S_x)}{\partial W} \qquad B = \frac{\partial(G\cdot S_y)}{\partial W}$$
$$C = \frac{\partial(H\cdot S_\theta)}{\partial W} \qquad \Gamma = \frac{\partial Q}{\partial W} \tag{5}$$

The x-direction inviscid fluxes are F, the y-direction inviscid fluxes are G, and H represents any terms that arise when cylindrical coordinates are used. The fluxes are multiplied by the finite volume cell-face area components S_x, S_y, and S_θ. The linearization of diffusion terms, such as viscosity, heat conduction, and mass diffusion, are lumped together in the VIS term to simplify the discussion. The fluxes for the implicit left-hand side are constructed from central differences with artificial dissipation. The residual $\boldsymbol{R}$ represents the physical right-hand side, and those inviscid fluxes are constructed with the AUSM scheme.

The flux Jacobians are diagonally enhanced with an artificial dissipation term, proportional to the spectral radius of the Euler equations. The Jacobians also contain the cell-face area scaling S. Unlike the flux Jacobians with respect to conservative variables, the primitive variable Jacobians are not proportional to the spectral radius and so the scaling matrix Γ must be used:

$$A^{\pm} = \frac{1}{2}\left(\frac{\partial F}{\partial Q} \pm \cdot S|\lambda_A|\right)\Gamma = \frac{1}{2}(A \pm \Gamma\cdot S|\lambda_A|) \tag{6}$$

The scaling term Γ is the time term Jacobian and arises naturally in transforming the system from conservative variables to primitive variables.

The addition of the artificial dissipation term is simple because it mostly involves adjusting the contravariant velocity U. The contravariant velocity with area scaling is $U = k_x u + k_y v$. The k_x and k_y describe cell-face area projections in the i or j directions. The artificial dissipation comes in through the eigenvalue terms, which also have a cell-face area scaling S,

$$\bar{U} = \tfrac{1}{2}(U \pm |\bar{\lambda}_A|) \tag{7}$$

$$|\bar{\lambda}_A| = |U| + cS \tag{8}$$

The cell-face area scaling S, introduced in k_x and k_y, is also applied to the sound speed term in the eigenvalue. The implicit artificial dissipation terms are absorbed in modifications to terms for the existing central differenced flux Jacobian.

The diagonally enhanced convective flux Jacobian with respect to the primitive variables $A^{\pm}$ is given in partitioned form by

$$A^{\pm} = \begin{bmatrix} A^{\pm}_{11} & A^{\pm}_{12} \\ A^{\pm}_{21} & A^{\pm}_{22} \end{bmatrix} \tag{9}$$

$$A^{\pm}_{11} = \begin{bmatrix} \dfrac{\rho\bar{U}}{P} & \rho k_x & \rho k_y & -\dfrac{\rho\bar{U}}{T} \\ \dfrac{\rho u\bar{U}}{P} & \rho\bar{U} + \rho u k_x & \rho u k_y & -\dfrac{\rho u\bar{U}}{T} \\ \dfrac{\rho v\bar{U}}{P} & \rho v k_x & \rho\bar{U} + \rho v k_y & -\dfrac{\rho v\bar{U}}{T} \\ \dfrac{\rho H\bar{U}}{P} \mp |\lambda_A| & \rho u\bar{U} + \rho H k_x & \rho v\bar{U} + \rho H k_y & -\dfrac{\rho H\bar{U}}{T} + \rho C_p\bar{U} \end{bmatrix} \tag{10}$$

$$A^{\pm}_{12} = \begin{bmatrix} -\rho\bar{U}\dfrac{MW}{MW_1} & \cdots & -\rho\bar{U}\dfrac{MW}{MW_{n-1}} \\ -\rho u\bar{U}\dfrac{MW}{MW_1} & \cdots & -\rho u\bar{U}\dfrac{MW}{MW_{n-1}} \\ -\rho v\bar{U}\dfrac{MW}{MW_1} & \cdots & -\rho v\bar{U}\dfrac{MW}{MW_{n-1}} \\ -\rho H\bar{U}\dfrac{MW}{MW_1} + \rho\bar{U}h_1 & \cdots & -\rho H\bar{U}\dfrac{MW}{MW_{n-1}} + \rho\bar{U}h_{n-1} \end{bmatrix} \tag{11}$$

$$A^{\pm}_{21} = \begin{bmatrix} \dfrac{\rho\bar{U}y_1}{P} & \rho k_x y_1 & \rho k_y y_1 & -\dfrac{\rho\bar{U}y_1}{T} \\ \vdots & \vdots & \vdots & \vdots \\ \dfrac{\rho\bar{U}y_{n-1}}{P} & \rho k_x y_{n-1} & \rho k_y y_{n-1} & -\dfrac{\rho\bar{U}y_{n-1}}{T} \end{bmatrix} \tag{12}$$

$$A^{\pm}_{22} = \begin{bmatrix} -\rho\bar{U}y_1\dfrac{MW}{MW_1} + \rho\bar{U} & \cdots & -\rho\bar{U}y_1\dfrac{MW}{MW_{n-1}} \\ \vdots & \ddots & \vdots \\ -\rho\bar{U}y_{n-1}\dfrac{MW}{MW_1} & \cdots & -\rho\bar{U}y_{n-1}\dfrac{MW}{MW_{n-1}} + \rho\bar{U} \end{bmatrix} \tag{13}$$

Example Problem

An example solution is included to indicate the type of flowfield being investigated along with the performance of the flow solver. Temperature contours in an arc jet reactor configuration are shown in Fig. 1. Supersonic flow exits a nozzle and impinges upon a substrate where the material coating is grown, in this case diamond. The nozzle operates with a dissociated mixture of hydrogen from a plasma generator, seeded with a hydrocarbon material growth species. The nozzle is run in an overexpanded mode, but the terminating normal shock causes the boundary layer to separate inside the nozzle and set up a recirculation zone. The pressure vessel, settling tank, and outlet are not shown.

The convergence characteristics for this type of problem are shown in Fig. 2. The solution is started from a uniform flow jetting into quiescent flow. The grid system consists of five blocks with about 10,000 grid points. For the first few thousand iterations, the conservation law discretization is first-order accurate. This helps propagate shock waves faster. After the L_2 norm of the conservation laws drops below 10^{-5}, the shock waves and flow separation have set up. At this point, the minmod interpolation functions are turned on for higher order accuracy. As is typical, the shock limiters cause the residual norm to hang up.

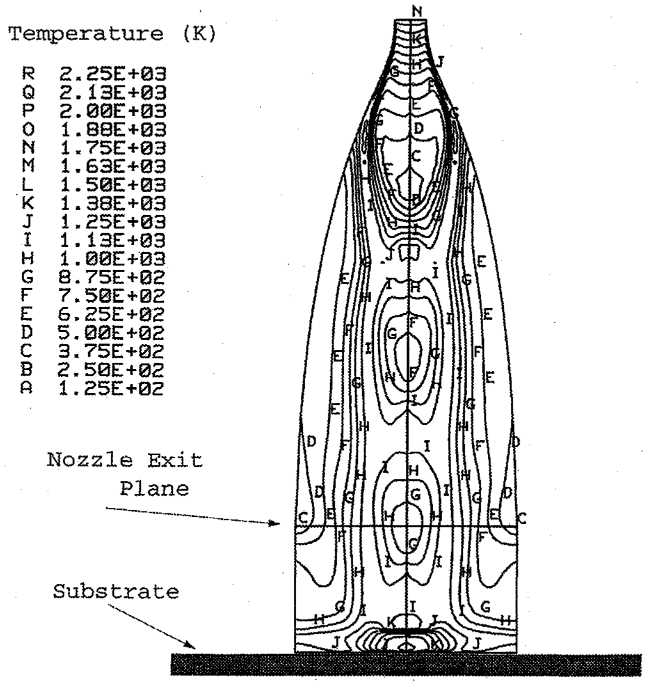

Fig. 1 Temperature contours in nozzle section.

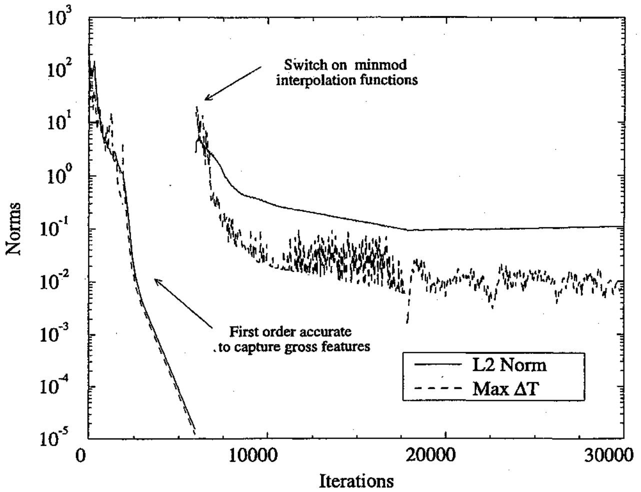

Fig. 2 Convergence characteristics for line relaxation applied to the arc jet flowfield.

Summary

A solution strategy for solving the compressible Navier–Stokes equations applied to supersonic internal flows has been presented. The implicit time-integration scheme consists of line relaxation written in terms of primitive variables. The linearized terms are a simple approximation of the flux splitting used to discretize the spatial conservation laws. The linearized implicit terms are constructed from central differencing with artificial dissipation. A matrix scaling term is introduced for the implementation of the artificial dissipation in the convective terms. The implicit scheme is effective in propagating shocks and handling interactions with the internal viscous flow features found in an arc-heated plasma jet reactor. Future efforts are directed toward investigating time preconditioning to enhance convergence in the large regions of low Mach number flow.

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Rotating Dissipation for Accurate Shock Capture

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I. Introduction

AN open problem in the simulation of supersonic flows is the capture of shocks that are, in general, oblique with respect to grid lines. Especially for upwind-biased algorithms, the use of a collection of one-dimensional operators in two or three dimensions produces poor results because of the wrong choice in the direction of propagation of the characteristic variables. The fault in the domain of dependence is easy to understand by examining a shock oblique to the mesh. With the grid-dependent schemes, the velocity component in one of the grid directions may be subsonic upstream of the shock, and the numerical information can propagate nonphysically in the upstream region, reducing the shock resolution. The spreading of the discontinuity would be reduced if a new mesh, orthogonal to the shock, was employed. This forms the basis of the so-called rotated upwind formulation, which attempts to reproduce an orthogonal shock situation without actually changing the mesh. The development of this grid-independent approach has led to a family of very promising schemes.[1] The concept of rotating the numerical scheme to follow the physical properties of the flow was introduced by Jameson[2] to solve the full potential equation. Roe[1] addressed the problem of solving a multidimensional hyperbolic system, and encouraging applications to the Euler equations have been obtained by Van Leer et al.[3] and Dadone and Grossman.[4]

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