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Attn: H. Wilson, MS/ED31
Marshall Space Flight Center, AL 35812

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Technical Report

ANALYSIS OF BOUNDARY CONDITIONS FOR SSME SUBSONIC INTERNAL VISCOUS FLOW ANALYSIS

By

A. J. Baker

Prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
George C. Marshall Space Flight Center
Huntsville, AL 35812

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COMPUTATIONAL MECHANICS CORPORATION
3601a Chapman Highway
Knoxville, TN 37920

I. SUMMARY

A study has been completed of mathematically proper boundary conditions for unique numerical solution of internal, viscous, subsonic flows in the SSME. The study has concentrated on well-posed considerations, with emphasis on computational efficiency and numerically stable boundary condition statements. The method of implementing the established boundary conditions is applicable to a wide variety of finite difference and finite element codes, as demonstrated. The results of this study are reported herein.

II. TECHNICAL DISCUSSION

A. Introduction

Over the past several years a focus at NASA Marshall Space Flight Center has been adaptation and application of computational fluid dynamics (CFD) analysis techniques to flowfield prediction in components of the SSME. Several "olympiads" have been held, wherein purveyors of CFD codes have developed and compared solutions for model problem definition analyses to the turn-around duct-transfer duct SSME geometry. The SSME geometry is defined to these codes via construction of meshes that possess boundary segments roughly coincident with solid walls and containing convenient flow inlet and outlet planes. The numerical simulation of the associated flowfield is defined via appropriate specification of constraints on the (Navier-Stokes) conservation law system variables, e.g., velocity and pressure, over the entire boundary of the mesh.

This study examined boundary condition specifications for the CFD models, with emphasis on mathematical well-posedness with physical consistency. The SSME flowfield is characterized as complex turbulent three-dimensional and unsteady, at high Reynolds number and low subsonic Mach number, ie., essentially incompressible. Mathematically, the CFD algorithms/codes applied to this problem definition fall into two distinguishable categories. One family (GIM, PAGE, VAST, ...) sets up solution as the unsteady evolution of a hyperbolic conservation law system with the assumption of a compressible fluid satisfying a polytropic gas law statement. Conversely, the second family (INS3D, PHOENIX, SIMPLE, FIDAP) specifically assumes an incompressible fluid, and directly seeks the steady-state solution without specifying a (physically significant) equation of state. The PHOENIX and SIMPLE algorithms seek the steady-state through a pressure relaxation procedure that explicitly requires pressure boundary condition specifications. FIDAP uses a finite element penalty method to totally replace the appearance of pressure. Alternatively, the INS3D theory employs a pseudo-compressibility concept, yielding a hyperbolic conservation law-appearing statement for pressure that (only) requires approximation of the normal pressure gradient at boundaries. Thus, the mathematical boundary condition aspect of INS3D is more analogous to that of GIM, et.al., than PHOENIX, et.al.

The following sections examine CFD algorithm boundary condition issues from the standpoint of, a) hyperbolic conservation law systems, and, b) pressure relaxation in an incompressible flow specification.

B. Hyperbolic Conservation Law Algorithms

The conservation law system governing the kinematics, kinetics and thermodynamics of a viscous, heat-conducting fluid is generally termed the Navier-Stokes equations. The Cartesian tensor indicial form is,

$$L(\rho) = \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(u_j \rho) = 0 \tag{1}$$

$$L(\rho u_i) = \frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}(u_j \rho u_i + p\delta_{ij} - \sigma_{ij}) = 0 \tag{2}$$

$$L(\rho e) = \frac{\partial(\rho e)}{\partial t} + \frac{\partial}{\partial x_j}(u_j \rho e + u_j p - \sigma_{ij} u_i + q_j) = 0 \tag{3}$$

$$p = p(e, \rho, \gamma) \tag{4}$$

where ρ is density, ρu_i is the momentum vector, p is pressure, δ_{ij} is the Kronecker delta, e is specific total energy, and γ is the ratio of specific heats for a polytropic gas law fluid. The expression of constitutive properties of the fluid is contained in the stress tensor σ_{ij} and heat flux vector q_j. For simple fluids and laminar flow, the accepted forms are,

$$\sigma_{ij} = \frac{\mu}{Re}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right] \tag{5}$$

$$q_j = -k\frac{\partial T}{\partial x_j} \tag{6}$$

where the dynamic (molecular) viscosity $\mu(T)$, and the thermal conductibity $k(T)$, are weak functions of temperature T, and the Reynolds number is $Re=(\rho UL/\mu)$ ref.

In the limit of large Reynolds number, an inviscid, non-heat conducting assumption renders equations 5-6 identically zero. The resulting form of eqn 1-4 is termed the Euler equations, a homogeneous hyperbolic conservation law system. Alternatively, enforcing a statistical averaging procedure yields a Reynolds-averaged Navier-Stokes system that introduces the concept of a Reynolds stress tensor and additional governing partial differential equations, eg., the two-equation turbulent kinetic energy-isotropic dissipation function system.

In either instance the generic form of the governing equation system is,

$$\frac{\partial q}{\partial t} + \frac{\partial f_j}{\partial x_j} + s = 0 \tag{7}$$

where q contains the Navier-Stokes/Euler/Reynolds-averaged Navier-Stokes dependent variable set, f_j is the corresponding flux vector and s is a source/sink term, eg.,

$$q = \begin{Bmatrix} \rho \\ \rho u_i \\ \rho H - p/\gamma_o \\ \rho k \\ \rho\varepsilon \end{Bmatrix}, \quad f_j = \begin{Bmatrix} u_j\rho \\ u_j\rho u_i + p\delta_{ij}/\gamma_o - \sigma_{ij} \\ u_j\rho H - q_j \\ u_j\rho k + k_j \\ u_j\rho\varepsilon + \varepsilon_j \end{Bmatrix}, \quad s = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ -P + \rho\varepsilon \\ \frac{\varepsilon}{k}\left(-C_\varepsilon^1 P + C_\varepsilon^2\rho\varepsilon\right) \end{Bmatrix} \tag{8}$$

The single-point closure equations for σ_{ij}, q_j, k_j and ε_j are (cf., Baker, 1986),

$$\sigma_{ij} = \bar{\sigma}_{ij} - \overline{\rho u'_i u'_j}$$
$$q_j = \bar{q}_j + \overline{\rho H' u'_j} - \overline{u'_i \sigma_{ij}} - u_i \bar{\sigma}_{ij}$$
$$k_j = \left(C_k \, \overline{\rho u'_i u'_j} \, \frac{k}{\varepsilon} - \frac{\bar{\mu}}{Re} \delta_{ij} \right) \frac{\partial k}{\partial x_i}$$
$$\varepsilon_j = \left(C_\varepsilon \, \overline{\rho u'_i u'_j} \, \frac{k}{\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \tag{9}$$

The Euler equation form is contained in eqn 22 by deletion of k, ε, k_j, ε_j, q_j, σ_{ij} and s, and replacement of ρH by $\rho e + \gamma p$.

A familiar alternative form for eqn 7 is established following imposition of a coordinate transformation $x_i = x_i(\eta_j)$, where $_j = (\xi, \eta, \zeta)$ is any (curvilinear) coordinate system. One particularly useful form is to align the coordinate ξ with the direction of principal flow, whereupon eqn 7 can be written as

$$\frac{\partial q}{\partial t} + \frac{\partial (E - E_v)}{\partial \xi} + \frac{\partial (F - F_v)}{\partial \eta} + \frac{\partial (G - G_v)}{\partial \zeta} + s = 0 \tag{10}$$

where E, F and G are the (Euler) flux vector components, E_v, F_v and G_v are the constitutive closure model components (containing σ_{ij}, q_j, k_j and ε_j). Both are expressed in terms of scalar components in the η_j coordinate system, ie.,

$$E = \frac{1}{J} \left\{ \begin{array}{c} \rho U \\ \rho u U + \xi_x p/\gamma_0 \\ \rho v U + \xi_y p/\gamma_0 \\ \rho w U + \xi_z p/\gamma_0 \\ \rho H U \\ \rho k U \\ \rho \varepsilon U \end{array} \right\}, \quad F = \frac{1}{J} \left\{ \begin{array}{c} \rho V \\ \rho u V + \eta_x p/\gamma_0 \\ \rho v V + \eta_y p/\gamma_0 \\ \rho v V + \eta_z p/\gamma_0 \\ \rho H V \\ \rho k V \\ \rho \varepsilon V \end{array} \right\}$$

$$G = \frac{1}{J} \left\{ \begin{array}{c} \rho W \\ \rho u W + \zeta_x p/\gamma_0 \\ \rho v W + \zeta_y p/\gamma_0 \\ \rho w W + \zeta_z p/\gamma_0 \\ \rho H W \\ \rho k W \\ \rho \varepsilon W \end{array} \right\}, \quad s = \frac{1}{J} \left\{ \begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -P + \rho\varepsilon \\ \frac{\varepsilon}{k}(-C_\varepsilon^1 P + C_\varepsilon^2 \rho\varepsilon) \end{array} \right\} \tag{11}$$

where J is the Jacobian of the coordinate transformation, and the convection velocity (**U**) vector contravariant scalar components parallel to the (ξ, η, ζ) coordinate system are,

$$
\begin{aligned}
U &= \xi_x u + \xi_y v + \xi_z w \\
V &= \eta_x u + \eta_y v + \eta_z w \\
W &= \zeta_x u + \zeta_y v + \zeta_z w
\end{aligned}
\tag{12}
$$

The constitutive scalar components E_V, F_V and G_V are formed in the similar manner.

The conservation law system, eqn 7 or 10, is either hyperbolic or an initial-valued, incompletely elliptic boundary value problem, dependent upon the constitutive closure definitions (inviscid, viscous/turbulent). The solution domain $\Omega \times t$ is a bounded subregion of a portion of the SSME duct region, and the boundary conditions on $\partial\Omega$, mathematically consistent with a well-posed problem, have been examined by Dutt(1985) following a dependent variable transformation to "entropy variables." The entropy transformation of the primitive (Euler) dependent variable set $q = \{\rho, \rho u_i, \rho e\}$, eqn 1-3, has been examined, cf., Harten(1981), Osher, et.al. (1984). For a family of strictly convex entropy functions, Mallet(1985) and others show that for the (Euler) extension to viscous and heat-conducting fluids, the sole "useful" entropy function is the thermodynamic entropy ρs. Hence, the transformation is,

$$V(q) = -\rho s = -\rho \ \log \ (p/\rho^{\delta}) \tag{13}$$

and the entropy flux functions are

$$f_j = -\rho u_i (\rho s) = - m_i (\rho s) \tag{14}$$

The transformation to V(q) symmetrizes the conservation law statement, eqn 1-3, yielding a nonlinear energy estimate (for sufficiently smooth solutions to the mixed initial-boundary value problem) that corresponds to the Clausius-Duhem inequality (second law of thermodynamics).

For the (Euler equation) hyperbolic conservation law form, the appropriate number of boundary conditions on oo is (Strickwerda, 1977): supersonic inflow (5), subsonic inflow (4), supersonic outflow (none), subsonic outflow (1). For the Navier Stokes equations, 5 (4) boundary conditions are required at inflow (outflow). Dutt(1985) develops the set of "maximal dissipative" boundary conditions for eqn 1-6 for the (Navier-Stokes) boundary condition statement form,

$$\varepsilon R \frac{\partial q}{\partial \xi} + Sq = b \tag{15}$$

where R is a matrix of rank at most 4, ξ is the coordinate normal to $\partial\Omega$, and for the Euler definition ($\varepsilon = 0$), Sq=b is a proper form for the (unperturbed Euler) hyperbolic problem. The derived outflow boundary conditions are inner (dot) products of eqn 5-6 with the outward pointing unit normal vector $\hat{n}_j$, ie.,

$$\begin{aligned} \sigma_{ij}.\hat{n}_j - a_i U_1 &= b_i \ , \quad 1 \le i \le 3 \\ q_j.\hat{n}_j &= 0 \end{aligned} \tag{16}$$

where U_1 is the velocity contravariant scalar component parallel to ξ. Any SSME application involves only subsonic outflow, hence $a_1 (= a\xi\ ) \geq 0$ and b_1 is a constant and all other components of a_i and b_i vanish as does the normal heat flux. The derived inflow boundary condition couples the influx definition $\rho U_1 = b_o$ with the more general form of eqn 16.

$$\begin{aligned} \rho U_1 &= b_o \\ \sigma ij\ .\hat{n}_j - a_i U_{\underline{i}} &= b_i \quad , 1 \le i \le 3 \\ - q_j.\hat{n}_j - a_4 T &= b_4 \end{aligned} \tag{17}$$

In eqn 17, the subscript bar on the contravariant velocity vector U_i denotes the index is <u>not</u> summed, and a_i and b_i $(0 \le i \le 4)$ are constants subject to constraints. For the SSME definition of subsonic inflow ($M_\xi < 1$), $a_1 = 0 = b_1$ while a_2, $a_3 > b_o/2$ and $a_4 > 1/2\ (\gamma^2 - \gamma + 2\ )\ b_o + \varepsilon$, where ε corresponds to the inverse Reynolds number, see eqn 5. Of some interest, the last expression in eqn 17 is directly amenable to physical interpretation; in expanded form, using eqn 6,

$$-q_j \cdot \hat{n}_j = k\frac{\partial T}{\partial x} \cdot \hat{n}_j = K\nabla T \cdot \hat{n} = b_4 + a_4 T \quad = h\ (T - T_r) \tag{18}$$

Thus, a_4 is interpreted as the boundary heat convection coefficient h, and T_r is the heat exchange reference temperature.

Equations 15-18, in concert with Strickwerda's constraints, encompass the range of boundary conditions, that are mathematically well-posed and numerically stable, for SSME flow CFD simulations formulated as approximate procedures for solving the hyperbolic conservation law Euler extension to Navier-Stokes. Since SSME flowfields are uniformly subsonic, then only one exit Dirichlet boundary condition is allowed, taken as the static pressure. Up to four inlet Dirichlet boundary conditions are mathematically permitted; however, eqn 17 suggests that all but the mass influx be replaced by Neumann constraints. Further, if the mass influx is specified, then the inlet pressure may not be specified (unless a region of supersonic flow exists between inlet and outlet). Conversely, a Dirichlet specification of inlet total pressure could be made, whereupon the mass flux will become determined by the flowpath total pressure drop. The reported SSME simulations using PAGE and VAST have generally employed the former, while the INS3D simulations have generally used the latter.

C. Incompressible Navier-Stokes Algorithms

As noted at the end of Section A, the alternative SSME simulation CFD construction class utilizes incompressibility directly to recast the Navier-Stokes system into a non-hyperbolic conservation law form. In these procedures, eg., PHOENIX, SIMPLE and FIDAP, the pressure distribution is derived indirectly from the velocity constraint of divergence-freeness, hence no equation of state is (need be) assumed to exist. Thus, no (Dirichlet) pressure boundary conditions are needed or appropriate in defining the CFD simulation, although it is well published that PHOENIX and SIMPLE employ a "pressure correction equation" to achieve convergence to a numerical approximation of divergence-freeness. This is not strictly exact, as will be developed.

The mentioned class of incompressible Navier-Stokes algorithms can be viewed in a unified manner as decisions made in evaluating a Taylor series on the time evolution of the velocity field $\underline{u}_t$, where boldface defines a vector field. Assuming knowledge of the solution at time t_n, where $t_{n+1} = t_n + \Delta t$, we have,

$$\underline{u}^{n+1} = \underline{u}^n + \Delta t \underline{u}_t^n + \ldots \tag{19}$$

The incompressible form of eqn 2, plus eqn 5, provides the expression for the time-derivative $\underline{u}_t$ in eqn 19, hence,

$$\underline{u}^{n+1} = \underline{u}^n - \Delta t \, [\underline{u}^n \cdot \nabla \underline{u}^n + \nabla p - Re^{-1} \nabla^2 \underline{u}^n] + \ldots \tag{20}$$

The basic CFD algorithm theoretical choice lies in selection of ∇p in eqn 20. A finite element penalty algorithm replaces the variable p with the approximation to continuity,

$$p = - \lambda \nabla \cdot \tilde{\underline{u}} \tag{21}$$

where λ is a large $O(10^6)$ constant. The superscript tilde denotes that $\tilde{\mathbf{u}}$ is an <u>approximation</u> to a divergence-free velocity field. Finally, eqn 21 is evaluated at the new time t^{n+1}, hence eqn 20-21 is an implicit expression.

The basic theory for the SIMPLE-class of incompressible Navier-Stokes CFD algorithms is similarly developed directly from eqn 20. If ∇p^n is employed, then the solution $\tilde{\underline{u}}^{n+1}$ does not satisfy the continuity equation. Hence, define a new pressure $\hat{p}^{n+1}$ that produces (assumption) a divergence-free velocity field $\underline{u}^{n+1}$. Writing eqn 20 for both pressures, taking the sum and subtracting yields,

$$\nabla \times (\underline{u}^{n+1} - \tilde{\underline{u}}^{n+1}) = \mathbf{0} \tag{22}$$

Thus, the distinction between the predicted and the continuity-satisfying velocity fields at t^{n+1} can at most be the gradient of a scalar field Φ, ie.,

$$\underline{u}^{n+1} - \tilde{\underline{u}}^{n+1} = .\Phi \tag{23}$$

Subtracting eqn 22 into the incompressible form of eqn 1 yields

$$\nabla^2 \Phi = - \nabla \cdot \tilde{\underline{u}}^{n+1} \tag{24}$$

The boundary condition for eqn 23, for the harmonic function Φ, is obtained from eqn 22 as

$$\nabla \Phi . \hat{\mathbf{n}} = (\underline{u}^{n+1} - \tilde{\underline{u}}^{n+1}) \, .\hat{\mathbf{n}} \tag{25}$$

where $\hat{n}$ is the unit outwarding pointing vector normal to the solution domain o. Once Φ^h is determined, using an appropriate (CFD) algorithm for eqn 23-24, then the "corrected pressure" field is

$$\hat{p}^{n+1} = p^n - \frac{\Phi}{\Delta t} \tag{26}$$

At steady-state convergence, eqn 23 becomes homogeneous, hence $|\Phi^h| \simeq 0$ for a (single) Dirichlet boundary specification in concert with eqn 24. Thus in the limit, $\hat{p}$ is the pressure field that coexists with a computed approximation to the divergence-free velocity field $\underline{u}^h$.

Viewing eqn 20, 22-25, there is no admissible pressure boundary condition specification for the SIMPLE-class, CFD incompressible Navier-Stokes algorithms. Equations 16-17 remain appropriate for the remaining variables, and the mass flowrate (eqn 17a) must be specified to create a SSME problem statement. The auxiliary variable Φ carries the remaining boundary condition specification, and eqn 24 is homogeneous Neumann everywhere that the distinction between $\underline{u}^h$ and $\tilde{\underline{u}}^h$ must vanish, eg., inlet, solid (no-slip) walls, symmetry planes, etc. The sole Dirichlet constraint for Φ^h therefore can only be applied at a location on the mass efflux boundary segment of oo. Assuming the CFD iteration sequence is convergent, eqn 25 yields the corresponding static pressure distribution to within an arbitrary constant, which can be specified (for example) to match $\hat{p}$ to an inlet or an outlet pressure level.

D. Concluding Discussion

The literature contains numerous results documenting the robustness of the CFD algorithm boundary conditions developed in the preceeding sections. The compressible hyperbolic conservation law formulation is exhaustively examined in Dutt(1985); Chang and Kwak(1984) document the total pressure specification option for the INS3D algorithm. To our knowleddge, the interpretation of SIMPLE-type algorithms developed in Section C is not common knowledge. The ϕ^h construction for incompressible parabolic Navier-Stokes algorithms is well established; Baker(1983, Ch. 6-7) fully documents the range of application of the solution statement given as eqn 23-24.

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