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Memoirs: Obtaining the Right Solution to Thermophysics Problems

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Nomenclature

C	=	constant in linear viscosity, $(\mu_r/\mu_\infty)/(T_r/T_\infty)$
c	=	speed of sound, m/s
c_f	=	skin friction, $2\tau/\rho_e u_e^2$
c_p	=	specific heat at constant pressure, J/(kg · K)
$\bar{c}_p$	=	frozen specific heat at constant pressure, J/(kg · K)
c_{P_s}	=	specific heat at constant pressure of species s, J/(kg · K)
c_s	=	mass fraction of species s, ρ_S/ρ
e	=	discretization error of numerical scheme
F	=	velocity ratio, u/u_e
H	=	stagnation enthalpy, m^2/s^2
h	=	enthalpy of gas, for perfect gas equals $c_p T$, J/kg
h_j	=	grid spacing, $y_j - y_{j-1}$, m
I, J	=	maximum values of i and j
j_s	=	mass flux relative to mass-average velocity
k	=	thermal conductivity of gas mixture, W/(m · K)
L	=	reference length, m
l	=	density–viscosity ratio, $(\rho\mu)/(\rho\mu)_r$
M	=	Mach number
M_w	=	molecular weight of gas mixture, kg/kg · mole
M_{ws}	=	molecular weight of species s, kg/kg · mole
Ne	=	electron number density, electrons/m^3
N_r	=	number of chemical reactions
p	=	static pressure of gas mixture, N/m^2
Pr	=	Prandtl number, $\mu c_p/k$
q	=	local heat flux, $k\partial T/\partial y$, W/m^2
R	=	gas constant, R_u/M_w, J/(kg · K)
Re_x	=	Reynolds number, $\rho_e u_e x/\mu_e$
R_u	=	universal gas constant, 8314.3 J/(kg · mole K)
r_b	=	radius of body, m
r_n	=	nose radius of body, m
S	=	constant in Sutherland viscosity, K
St_∞	=	Stanton number, $q_w/\rho_\infty u_\infty (H_\infty - H_w)$
s	=	distance along body surface (same as x), m
T	=	temperature, K, or total time, s
t	=	time, s
u, v	=	velocities tangential and normal to wall, m/s
V	=	transformed normal velocity
$\boldsymbol{v}_s$	=	velocity vector of species s, m/s
W	=	dependent variable matrix
$\dot{w}_s$	=	mass rate of formation of species s, kg/(m^3 · s)
x, y	=	coordinates along and normal to wall, m
γ	=	ratio of specific heats
γ_s	=	mole-mass ratio of species s, kg · mole/kg
Δx, Δy	=	grid size in x and y coordinate directions, m
$\Delta\xi$, $\Delta\eta$	=	grid size in ξ, (kg m^{j-1}/s)^2, and η coordinate directions
$\xi.\eta$	=	transformed x, (kg m^{j-1}/s)^2, and y coordinates
θ	=	temperature ratio, T/T_e
κ	=	ratio of adjacent grid spacing, h_j/h_{j+1}
μ	=	viscosity of gas mixture, kg/(m · s)
ρ	=	density of gas mixture, kg/m^3
ρ_s	=	density of species s, kg/m^3
τ	=	shear stress, $\mu\partial u/\partial y$, N

Subscripts

A	=	atoms
ad	=	adiabatic wall conditions
c, u	=	coupled and uncoupled values
e	=	local flow at edge of boundary layer
$f(0) = 0$	=	no mass transfer at wall
i	=	grid index for x or ξ coordinate
ic	=	value of variables at initial conditions
j	=	grid index for y or η coordinates
p	=	peak value in boundary layer
r	=	reference value
s	=	value for species s
w	=	wall or surface value
∞	=	freestream conditions

Introduction

A COMBINATION of experimental studies, engineering analysis, and numerical simulations are appropriate for solving thermophysics and computational fluid dynamics (CFD) problems. The experimental approach might be appropriate and the only approach available for some problems. The present paper is concerned with

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using numerical approaches, especially for boundary-layer flows, for obtaining accurate solution to thermophysics and CFD problems. Projects, research, and studies that the author has worked on will be used to illustrated how the solution methodology and solution accuracy have evolved with time.

In engineering problems, various assumptions are used to model physical phenomena, and experimental data are usually required to determine the error introduced. Because computational techniques are used to solve the governing equations, the results must be numerically accurate so that the assumptions employed can be evaluated without being contaminated by the solution procedure. Therefore, not only must the numerical results be accurate for evaluation of the modeling error, but one must also have a method to determine the precision of the numerical results. This is the verification problem. Whereas numerical solutions need not be extremely accurate in many cases, they should at least exhibit an accuracy that is compatible with the physical approximations of the model and the uses to which the results will be applied. Therefore, to get the right solution to thermophysics and CFD problems requires that the right governing equations are being used for the intended answers and that they are being solved with sufficient accuracy. Validation is concerned with the accuracy of the governing equations used to model the physics required in the simulation. If the governing equations are simplified to allow an easier solution approach, for example, Navier–Stokes equations reduced to Euler/boundary-layer equations, then a comparison of the numerical results from the two approaches can be used to evaluate or indicate the error of the reduced equations.

The emphasis of this paper is on solution of the compressible and chemically reacting boundary-layer equations. The review is initially concerned with the numerical solution of the compressible boundary-layer equations for a perfect gas and begins with the activities at Stanford University under the direction of Irmgard Flügge-Lotz. As a student at Stanford, the author worked on the development of the implicit Crank–Nicolson type finite difference scheme, which is described. When the author was at General Electric, additional physics were added to the boundary-layer equations to simulate chemically reacting flows. The governing equations were written in Levy–Lees form to allow the solution to start at stagnation points and tips of cones. This work produced a CFD code that could provide useful engineering predictions that were needed at that time. When the author returned to Sandia National Laboratories, a new chemically reacting boundary-layer code was developed with improved capabilities. Development of numerical schemes for boundary layers with variable grid spacing and issues involved with the linearization and complete coupling of the governing equation is reviewed. Also described is the approach used by the author to estimate the discretization error of the numerical solution and to verify the numerical scheme.

For a more complete review of boundary-layer theory and solution techniques, see the books by Schlichting,[1] Schetz,[2] Tannehill et al.,[3] Anderson,[4] and Cebeci and Cousteix.[5] A review of numerical techniques for solving the boundary-layer equations and a finite difference method developed by the author is given in a paper[6] published in 1970. Also, the 1975 AGARD review article by the author[7] has extensive coverage of numerical techniques for boundary layers.

Compressible Boundary-Layer Equations

The boundary-layer equations for a perfect gas are presented at this time because these equations will be referenced throughout the paper.

Physical Coordinate Form of Boundary-Layer Equations

The boundary-layer equations were initially developed by Prandtl in 1904. Development of the first-order and second-order boundary-layer equations for planar and axisymmetric flows over blunt bodies was performed by Van Dyke[8] in 1961. The dependent variables in the Navier–Stokes equations are expanded with a small perturbation parameter

$$\varepsilon = \left[(\gamma - 1)M_\infty^2\right]^{\omega/2} \Big/ \sqrt{Re}$$

where Re is the Reynolds number based on the freestream conditions and the body nose radius, M_∞ is the freestream Mach number, and the viscosity is proportional to a power ω of temperature. The procedure uses singular perturbation theory with inner and outer expansion and matching between the inner and outer flow regions. The first-order boundary-layer equations are an approximation to the Navier–Stokes equation in the inner flow region next to the wall. The coordinate system uses x as the distance along the wall and y is the normal distance from the wall. The compressible first-order boundary-layer equations for a perfect gas and two-dimensional flow are as follows, where planar $r_b = 1$ or axisymmetric r_b is body radius.

Continuity:

$$\frac{\partial}{\partial x}(r_b \rho u) + \frac{\partial}{\partial y}(r_b \rho v) = 0 \tag{1}$$

The x momentum:

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = -\frac{\mathrm{d}p}{\mathrm{d}x} + \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right) \tag{2a}$$

The y momentum:

$$\frac{\partial p}{\partial y} = 0 \tag{2b}$$

There are several forms of the energy equation depending on the dependent variable that is chosen. Because c_p is constant, the formulation with the temperature is

$$\rho u c_p \frac{\partial T}{\partial x} + \rho v c_p \frac{\partial T}{\partial y} = u \frac{\mathrm{d}p}{\mathrm{d}x} + \frac{\partial}{\partial y}\left(\frac{\mu c_p}{Pr}\frac{\partial T}{\partial y}\right) + \mu\left(\frac{\partial u}{\partial y}\right)^2 \tag{3}$$

The formulation with the enthalpy is

$$\rho u \frac{\partial h}{\partial x} + \rho v \frac{\partial h}{\partial y} = u \frac{\mathrm{d}p}{\mathrm{d}x} + \frac{\partial}{\partial y}\left(\frac{\mu}{Pr}\frac{\partial h}{\partial y}\right) + \mu\left(\frac{\partial u}{\partial y}\right)^2 \tag{4}$$

The equation of state for air is

$$p = R\rho T, \qquad R = R_u / M_w = 287.0 \tag{5}$$

The second-order boundary-layer equations are not considered in this paper but include effects due to *interaction with the outer flow* (vorticity at the outer edge and displacement thickness) and *surface effects* (transverse curvature, longitudinal curvature, surface slip, and temperature jump). The first-order boundary-layer equations become more accurate as the Reynolds number becomes very large with the second-order effects becoming smaller. The first-order boundary-layer equations are the right governing equations to use for many flow problems and are an accurate approximation of the full Navier–Stokes equations in the near-wall region. Both the first- and second-order boundary-layer equations are partial differential equations of the parabolic type that allows the numerical solution to be obtained along a wall with a marching technique.

Thermodynamic and Transport Properties

The specific heat at constant pressure for a perfect gas is obtained from $c_p = \gamma R/(\gamma - 1)$. For air, the ratio of specific heats $\gamma = 1.4$ and $c_p = 1004.5$. The Prandtl number is assumed constant, $Pr = 0.72$. The viscosity of a perfect gas is usually specified with Sutherland viscosity law, which gives the viscosity and thermal conductivity as

$$\mu = C_\mu T^{\frac{3}{2}} \Big/ (T + S), \qquad k = C_k T^{\frac{3}{2}} \Big/ (T + S), \qquad C_k = c_p C_\mu / Pr$$

For air the coefficients are $C_\mu = 1.458 \times 10^{-6}$ and the Sutherland constant $S = 110.4$ K.

Boundary and Initial Conditions

At the wall the velocity components are zero, and the wall temperature T_w or heat flux q_w is specified:

$$u(x,0)=0, \qquad v(x,0)=0$$

$$T(x,0)=T_w(x) \qquad \text{or} \qquad q_w=-\left(k\frac{\partial T}{\partial y}\right)_w$$

At the edge of the boundary layer, the velocity u_e and temperature T_e are specified. There is no boundary condition on the v_e velocity, and it is obtained as part of the numerical solution

$$u(x,y_e)=u_e(x)=-\left(\frac{1}{\rho_e}\right)\left(\frac{\mathrm{d}p}{\mathrm{d}x}\right), \qquad T(x,y_e)=T_e(x)$$

Initial conditions of the dependent variables across the boundary layer are required to start the marching solution along a wall at $x=x_{\mathrm{ic}}$:

$$u(x_{\mathrm{ic}},y)=u_{\mathrm{ic}}(y), \qquad v(x_{\mathrm{ic}},y)=v_{\mathrm{ic}}(y), \qquad T(x_{\mathrm{ic}},y)=T_{\mathrm{ic}}(y)$$

Crocco Form of the Boundary Layer Equations

In the initial development of numerical schemes for solving the boundary-layer equations, the Crocco form of the equations was used. The preceding boundary-layer equations in physical coordinates with independent variables x and y are replaced by $\xi=x$, u, and the dependent variables are the temperature T and the viscous stress $\tau=\mu(\partial u/\partial y)$. The development of these equations is given by Lagerstrom in the book edited by Moore.[9] The continuity and momentum equations are combined with ρv eliminated and are written in terms of the new dependent and independent variables. The resulting continuity-momentum equation and enthalpy form of the energy equations become

$$\rho\mu u\frac{\partial \tau}{\partial x}=f \qquad \rho\mu u\frac{\partial h}{\partial x}=g \qquad p'=\frac{\mathrm{d}p}{\mathrm{d}x}$$

$$f=\tau^2\frac{\partial^2\tau}{\partial u^2}+p'\mu\frac{\partial\tau}{\partial u}+\left[u\frac{\partial}{\partial x}(\rho\mu)-p'\frac{\partial\mu}{\partial u}\right]\tau$$

$$g=\left(\frac{1}{Pr}\frac{\partial^2 h}{\partial u^2}+1\right)\tau^2+\left(\frac{1-Pr}{Pr}\right)\tau\frac{\partial\tau}{\partial u}\frac{\partial h}{\partial u}+\mu\left(\frac{\partial h}{\partial u}+u\right)p' \qquad (6)$$

The extension of these equations for axisymmetric flow are given by Kramer and Lieberstein.[10] These equations have the properties of parabolic partial differential equation like the heat conduction equation except they are nonlinear and more complex. The independent variable u varies from zero at the wall to unity at the edge of the boundary layer, which gives a well-defined solution region. However, there are several disadvantages with this transformation because there is a singularity at the outer edge of the boundary layer. In addition, for the case with velocity overshoot, it is difficult to apply the Crocco form because quantities are double valued as a function of u.

The grid for the numerical schemes in the initial boundary-layer work used a uniform grid, and the index notation is shown in Fig. 1.

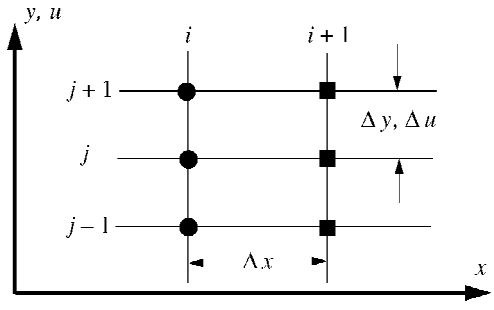

Fig. 1 Uniform grid notation.

For the Crocco variables, u is the independent variable coordinate across the boundary layer.

Early Numerical Solution Techniques and Digital Computers

A brief indication of the status of numerical techniques and digital computers when the author was a student at Stanford University (from July 1959 to January 1962) is now given.

Numerical Solution of Partial Differential Equations

The numerical solution of differential equations with finite differences was investigated by Boole (1815–1864), and a book[11] was published on this work in 1860. Boole showed that analytical solutions can be obtained to linear difference equations. The early work on the numerical solution of partial differential equations (PDEs) was mainly concerned with the stability of difference approximations. There are several classic papers such as one by Courant, Friedrichs, and Lewy[12] (CFL) (1928) where the stability of linear hyperbolic PDEs was determined, which requires that the numerical domain of influence be equal or larger than analytical domain of influence. This stability restriction is the CFL condition. Crank and Nicolson[13,14] (1947 and 1953) studied the stability of a linear parabolic PDE (unsteady heat conduction equation) and showed that implicit difference schemes are stable, whereas explicit difference schemes have restrictions on the allowable time-step size that can be used. The alternating direction implicit method for time-dependent parabolic and elliptic PDEs was initially developed by Peaceman and Rachford[15] in 1955. A paper by O'Brien et al.[16] (1951) is also noteworthy because it provided a description of the von Neumann method of stability analysis of numerical schemes that was not readily available at this time.

The later books concerned with the numerical solution of PDEs were by Hildebrand[17] (1952), Richtmyer[18] (1957), and Forsythe and Wasow[19] (1960). In addition, Hamming[20] spent the academic year 1960/1961 at Stanford writing a book and teaching a course on numerical methods and numerical solution techniques for ordinary differential equations. The theme of his book and course is given on a foreword page in the book: "The Purpose of Computing Is Insight Not Numbers."[20]

Digital Computers

A significant motivation for the numerical solution of fluid dynamic problems originated with the Manhattan Project at Los Alamos National Laboratory during World War II. This group had a significant impact on the development of digital computers that would make it feasible to use numerical solution techniques for solving flow problems. The development of computers provided a new opportunity for the utilization of the numerical techniques that had been investigated for a number of years. The governing equations of fluid dynamics are more complex than the equations that had been studied, but the initial work on numerical solution techniques provided a foundation to build upon. Evolution of computers has determined the computation capabilities that have become available.

In the late 1950s, the availability of digital computers was occurring at universities and the Stanford Computer Center had an IBM 650 computer. In this time period, more advanced computers were available at government laboratories. In the book by Tannehill et al.,[3] the IBM 650 is the first computer given in their Fig. 1.1 for the trend of relative computation cost. The relative computation cost (RCC) for a given flow and algorithm from 1953 to 1995 can be approximated as

$$\mathrm{RCC}=10^{1-5(\mathrm{year}-1953)/42}$$

In 1953 an IBM 650 computer had a RCC = 10, whereas in 1992 a Cray C90 had a RCC = 0.00023. The computer speed and memory capacity have increased significantly during this time period, whereas cost has a much slower increase. This trend has continued with the introduction of parallel computers.

Initial Numerical Solution Techniques for Boundary Layers

Numerical Work at Stanford University on Boundary Layers

In 1938 Prandtl and later in 1948 Gortler suggested that the boundary-layer equations should be solved with a numerical procedure. At the meeting "Fifty Years of Boundary Layer Research," in 1955, Flügge-Lotz[21,22] presented a paper on a difference method for the computation of the laminar compressible boundary layer. The Crocco form of the boundary-layer equations was solved with an explicit difference scheme. Equations (6) are of the form where various derivatives with respect to u and dependent variables appear on the right-hand side, and these terms are evaluated from the known solution across the boundary layer:

$$\frac{\partial \tau}{\partial x} = \frac{f(\tau_{uu}, \tau_u, \tau, \rho, \mu)}{\rho \mu u} \qquad \frac{\partial h}{\partial x} = \frac{g(h_{uu}, h_u, \tau_u, \tau, \mu)}{\rho \mu u}$$

The complete governing equations are replaced with an explicit difference equations as follows:

$$\left(\frac{\tau_{i+1} - \tau_i}{\Delta x}\right)_i = \left(\frac{f}{\rho \mu u}\right)_{i,j}, \qquad \left(\frac{h_{i+1} - h_i}{\Delta x}\right)_j = \left(\frac{g}{\rho \mu u}\right)_{i,j}$$

With initial profiles of the shear stress and enthalpy at $i = 1$, the right-hand side of these equations can be evaluated. New values of the shear stress and enthalpy across the boundary layer are determined downstream at $i + 1$ with the preceding relations. There are problems with obtaining the numerical solution near the wall where u goes to zero as the grid is refined. The numerical scheme becomes unstable if the marching step size is greater than some critical value. An important conclusion given by Flügge-Lotz[22] is "The use of finite differences for the computation of the boundary layer flow provides a good means for checking the assumptions often made to shorten boundary layer computations." These solutions were usually computed with a mechanical calculator because a digital computer was not available for some of the early solutions of the boundary-layer difference equations. One of the coarse grid solutions had 5 marching steps and 11 grid points across the layer for a total of 55 grid points.

The numerical solution techniques for the compressible boundary-layer equations was developed by a group of graduate students at Stanford University under the direction of Flügge-Lotz over a number of years. The evolution of this work is described next. The work of Flügge-Lotz was continued by Flügge-Lotz and Baxter[23,24] and Baxter and Flügge-Lotz.[25] The stability of the numerical solution was carefully investigated with the following restriction on the marching grid-size determined:

$$\left(\frac{\Delta x}{x}\right) < \frac{\left[2Pr(\Delta u/u_e)^3\right]}{c_f \sqrt{Re_x / C}}$$

This result shows that if the grid across the boundary layer is refined by a factor of two, the grid size Δx must be reduced by a factor of eight. The new solution required 16 times as many grid points as the original solution. There were 60 examples of boundary-layer problems solved, and the numerical solutions were compared to integral solutions and other approximate solutions. Some of the problems solved were 1) flat plate with a variety of wall temperature variation, 2) flat plate with various pressure gradients, and 3) solutions away from a stagnation point. The results of these studies showed that integral and approximate methods in many cases give poor results, whereas the numerical approach has the potential to provide very accurate solutions to the first-order boundary-layer equations. However, these solutions were obtained on the IBM 650 computer (with 2000 word memory) and required significant time to run and significant time to write the computer code because computer languages such as FORTRAN were not available. Most of the solutions in these works started at $x/L = 1$ and would go to $x/L = 1.04$, where L is a reference length. It was estimated that a boundary-layer solution to $x/L = 2$ would require 10–400 h of computer time. *At that time, the limitations of the digital computers and numerical schemes made the numerical solution too costly and were not the right solution for engineering problems.*

As part of the work at Stanford University, Flügge-Lotz and Howe[26] were applying the finite difference method to boundary-layer flows with suction or blowing at the wall. Further work on this problem is given in a report by Howe.[27] The solutions presented were obtained on the IBM 650 computer. One problem solved was Mach 3 flow over a flat plate in this work with transpiration cooling (mass injection at the wall) from $x/L = 0$ to 1 and no mass transfer from $x/L = 1$ to 2. The solution was started at $x/L = 1$ with a similarity solution obtained by Low.[28] The numerical solution was compared to integral solutions, and again there were significant differences in the results.

Because of the difficulties introduced by the Crocco form of the boundary-layer equations, Flügge-Lotz decided to solve the boundary-layer equations in physical coordinates. Yu was the student assigned this problem. Flügge-Lotz and Yu[29] were aware that implicit difference schemes would give a stable numerical scheme for the unsteady heat conduction problem. They did not consider the implicit approach for the nonlinear boundary-layer equation because the resulting difference equations would be nonlinear and Hartree[30] had indicated that the coefficient matrix for the system of difference equations for some problems could be ill conditioned. They believed the solution of the implicit difference equation were too difficult to solve. The idea was to use the previous explicit difference scheme experience with the Crocco equations to solve the new set of governing equations. The explicit approach can be applied to the momentum and energy equation except for the evaluation of ρv, which occurs in both equations. The value of ρv is obtained from the continuity equation, which is written in difference form. The formulation of a stable numerical scheme was a new problem and became a very difficult task. A significant effort was devoted to evaluation of the stability of the numerical scheme with various difference schemes for the continuity equation. Two approaches were chosen after a variety of methods were considered. One approach used the continuity equation in integral form and replaced ρv in the momentum and energy equations with the integral relation

$$(\rho v)_{i,j} = \int_0^y \left(\frac{\partial \rho u}{\partial x}\right)_j \mathrm{d}y$$

This is an explicit evaluation of ρv, and then a forward difference is used to evaluate the derivative in the integral. The second approach used a difference equation to approximate the PDE as

$$\frac{\partial \rho v}{\partial y} = -\frac{\partial \rho u}{\partial x}$$

$$\left[\frac{(\rho v)_j - (\rho v)_{j-1}}{\Delta y}\right]_i = -\left[\frac{(\rho u)_{i+1} - (\rho u)_i}{\Delta x}\right]_{j-1}$$

Both of these approaches determined ρv at i, j, whereas the other dependent variables are evaluated at $i + 1$. These approaches result in a lagging of ρv in the i direction. Most of the Flügge-Lotz and Yu results[29] were obtained with the first method but the second approach was much faster. The explicit schemes developed in Ref. 29 did not prove to be completely satisfactory, especially at high Mach numbers and with a heated wall. Under these conditions the step-size requirements were so severe that it was impossible to obtain stable solutions. For the four cases solved in this work on an IBM 650, the time required for a single marching step was 50–100 s. For a problem with a solution from $x/L = 1$ to 2 would require 400 steps and take 5.5–11 h of computer time. It was estimated that these solutions on an IBM 704 would require approximately 1 h.

Author's Work on Numerical Solution of Boundary Layers at Stanford University

In March of 1959, I received a letter from Dr. Flügge-Lotz on the work I would be participating in as a graduate student at Stanford

University. She wrote, "We are planning now to attack problems in which interaction of the boundary layer flow and the exterior has to be considered. A problem, which in the present development of missiles, is highly interesting and should be pushed ahead with all intensity." When I started working under Flügge-Lotz, my initial assignment was to understand the numerical scheme that Irving Yu was developing and then see whether there were any ways to improve the scheme. She realized that the explicit scheme for the boundary-layer equations in physical coordinates was not adequate. A implicit numerical scheme had been used by Rouleau and Osterle[31] to solve the incompressible boundary-layer equations in physical coordinates with a relaxation or iteration procedure. A paper had been published by Kramer and Lieberstein[10] that solved the Crocco transformed equations with an implicit finite difference scheme to eliminate stability problems. Dr. Flügge-Lotz and I met with Professor George Forsythe to seek help from a mathematician who was a leader in the field of numerical solution of PDEs. He did not provide any well-defined method for solving the boundary-layer equations but encouraged further investigation of the implicit approach. As it turned out, a large part of the authors dissertation[32,33] was concerned with developing a stable numerical scheme with reasonable computational time. A fully implicit scheme and a Crank–Nicolson-type scheme were investigated with a uniform grid spacing in both coordinate directions. Initially the implicit numerical scheme was applied to the boundary-layer equations in physical coordinates. For hypersonic laminar boundary-layer flows, a uniform grid was not appropriate due to computer limitations. For this case, the velocity varies almost linearly over a large portion of the layer except near the outer edge, where there is a rapid change in the velocity gradient. This behavior requires a small grid size across the entire boundary layer. The comment in the dissertation is "The immediate conclusion is that the grid size should vary with distance from the wall, but this is rather inconvenient." The solution to this problem was to use the Howarth–Dorodnitsyn coordinate transformation to obtain a new set of governing equations where the velocity varies more smoothly across the layer.

The numerical scheme for the governing equation in physical or transformed coordinates used the same numerical scheme. The nonlinear derivative terms are replaced such that linear difference equations resulted, and coefficients in the governing equations are lagged. To make the implicit method feasible, the resulting difference equations need to be of tridiagonal form, which are well suited for solution on digital computers. The problems used for the *verification* of the numerical scheme and code either had exact solutions or had been solved numerically by other procedures.

One of the issues as discussed earlier was obtaining linear difference equations. Because the viscosity is a function of the enthalpy $\mu = \mu(h)$, the second derivative term was expressed as

$$\frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right) = \mu\frac{\partial^2 u}{\partial y^2} + \mu_h\left(\frac{\partial u}{\partial y}\right)\left(\frac{\partial h}{\partial y}\right), \qquad \mu_h = \frac{\partial \mu}{\partial h}$$

The nonlinear terms with derivatives were approximated as follows for the *fully implicit* scheme:

$$(\varphi\psi)_{i+1} = \varphi_i\psi_{i+1} + \varphi_{i+1}\psi_i + \varphi_i\psi_i + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta y^2)$$

$$\varphi_i = \frac{\partial u}{\partial y} = \frac{(u_{j+1} - u_{j-1})}{\Delta y}, \qquad \psi_i = \frac{\partial h}{\partial y} = \frac{(h_{j+1} - h_{j-1})}{\Delta y}$$

Central differences were used for the derivatives in the y direction. The nonlinear terms with derivatives were approximated as follows for the *Crank–Nicolson* scheme:

$$(\varphi\psi)_{i+\frac{1}{2}} = (\varphi_i\psi_{i+1} + \varphi_{i+1}\psi_i)/2 + \mathcal{O}(\Delta y^2) + \mathcal{O}(\Delta y^2)$$

When the boundary conditions were included, the difference equations for the momentum and energy equations become a block tridiagonal equation of the form

$$\begin{aligned} B_1W_1 - C_1W_2 &= D_1 \\ -A_jW_{j-1} + B_jW_j - C_jW_{j+1} &= D_j, \qquad W_j = \begin{bmatrix} u_j \\ h_j \end{bmatrix} \\ -A_JW_{J-1} + B_JW_J &= D_J \end{aligned} \tag{7}$$

where $j = 2, 3, \ldots, J-1$. The coefficients are 2×2 matrices. The solution was obtained with the Thomas algorithm (1949), which was given in the book by Richtmyer.[18] In this solution technique, the following relation were evaluated by starting at the wall:

$$\alpha_j = B_j - A_jE_{j-1}$$

$$e_j = \alpha_j^{-1}(D_j + A_je_{j-1}), \qquad j = 2, 3, \ldots, J$$

$$E_j = \alpha_j^{-1}C_j, \qquad j = 2, 3, \ldots, J-1$$

$$\alpha_j = \begin{bmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{bmatrix}_j, \qquad E_j = \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix}_j, \qquad e_j = \begin{bmatrix} e_1 \\ e_2 \end{bmatrix}_j$$

Then the solution of the dependent variables u and h was started at the edge of the boundary layer and was marched toward the wall:

$$W_j = E_jW_{j+1} + e_j, \qquad j = J-1, J-2, \ldots, 1$$

The details of how the boundary conditions were handled have not been included in this paper. The solution was completed with the velocity v obtained from the finite difference form of the continuity equation and the density from the equation of state.

The coefficients in front of the derivatives in the governing equations should be evaluated at $i+1$ for the fully implicit scheme and at $i+\frac{1}{2}$ for the Crank–Nicolson scheme. The coefficients were lagged and evaluated at i, which results in a first-order truncation error. However, the effect of iteration at each marching step was investigated for the Crank–Nicolson scheme. One iteration was performed with predicted values at $i+1$ averaged with the values at i to obtain a better estimate of the coefficients at the midpoint. The procedure was shown to improve the solution accuracy, and the truncation error would become second-order if sufficient iterations were performed.

With the boundary-layer equations in physical or transformed coordinates, the edge of the boundary moves away from the wall as the solution proceeds along the wall. Because of computer limitations, it was desirable to match the computational domain with the boundary-layer region. In the tridiagonal solution, the elements in e_j become constant as the edge of the boundary layer is reached. The change in e_j is monitored, and when this change is less than some small number, the solution across the layer is stopped with this location used as the boundary-layer edge.

For a hypersonic boundary layer in physical coordinates, the rapid change of the velocity near the boundary-layer edge was reduced with the *Howarth–Dorodnitsyn transformation*, which introduces the new coordinates (see work by Lagerstrom in Ref. 9)

$$\xi = x, \qquad \eta = \int_0^y \left(\frac{\rho}{\rho_r}\right) \mathrm{d}y$$

The compressible boundary-layer equations in the transformed plane become

$$\frac{\partial u}{\partial \xi} + \frac{\partial V}{\partial \eta} = 0$$

$$u\frac{\partial u}{\partial \xi} + V\frac{\partial u}{\partial \eta} = -\frac{1}{\rho}\frac{dp}{d\xi} + \frac{1}{\rho_r^2}\frac{\partial}{\partial \eta}\left(l\frac{\partial u}{\partial \eta}\right), \qquad l = \rho\mu$$

$$u\frac{\partial h}{\partial \xi} + V\frac{\partial h}{\partial \eta} = \frac{u}{\rho}\frac{dp}{d\xi} + \frac{1}{\rho_r^2}\frac{\partial}{\partial \eta}\left(\frac{\mu}{Pr}\frac{\partial u}{\partial \eta}\right) + \frac{l}{\rho_r^2}\left(\frac{\partial u}{\partial \eta}\right)^2$$

A new dependent variable V was introduced as follows:

$$V = \frac{\rho}{\rho_r} v + u \frac{\partial \eta}{\partial x} = \frac{\rho}{\rho_r} \left(v - u \frac{\partial y}{\partial \xi} \right)$$

The normal velocity v or the transformed normal velocity V was obtained from the continuity equation. The difference approximation is illustrated for the transformed continuity equation. The fully implicit approach evaluates the equation at $(i+1, j-\frac{1}{2})$, which gave a first-order approximation as

$$\frac{1}{2}\left(\frac{u_{i+1}-u_i}{\Delta\xi}\right)_j + \frac{1}{2}\left(\frac{u_{i+1}-u_i}{\Delta\xi}\right)_{j-1} + \left(\frac{V_j - V_{j-1}}{\Delta\eta}\right)_{i+1} = 0$$

$$j = 2, 3, \ldots, J$$

The preceding equation was used to obtain V_j across the layer starting at the wall where V_1 is known from the wall boundary condition. The Crank–Nicolson approach evaluates the equation at $(i+\frac{1}{2}, j-\frac{1}{2})$, which gave a second-order approximation and is the box scheme approach:

$$\frac{1}{2}\left(\frac{u_{i+1}-u_i}{\Delta\xi}\right)_j + \frac{1}{2}\left(\frac{u_{i+1}-u_i}{\Delta\xi}\right)_{j-1}$$

$$+ \frac{1}{2}\left(\frac{V_j - V_{j-1}}{\Delta\eta}\right)_{i+1} + \frac{1}{2}\left(\frac{V_j - V_{j-1}}{\Delta\eta}\right)_i = 0$$

If there were any inaccuracies in the initial values of V, this approach gave wiggles that were slowly damped.

The outer edge behavior of the tangential velocity profile was illustrated in the author's dissertation,[32] and is reproduced in Fig. 2 for physical coordinates (nondimensional y coordinate) and in Fig. 3 for the transform coordinates. Figures 2 and 3 include the initial profile (solid curve), the numerical solution at downstream location (symbols), and the similar solution at the same downstream location (dashed curve). The transformed approach allows a significant reduction in the number of grid points required across the boundary layer, especially at large Mach numbers. In addition, the result in Fig. 3 shows the finite difference solution is in excellent agreement with the similarity solution of Low[34] and helps to provide verification of the code.

After a significant part of the implicit difference scheme had been developed, Stanford University acquired a Burroughs 220 computer,

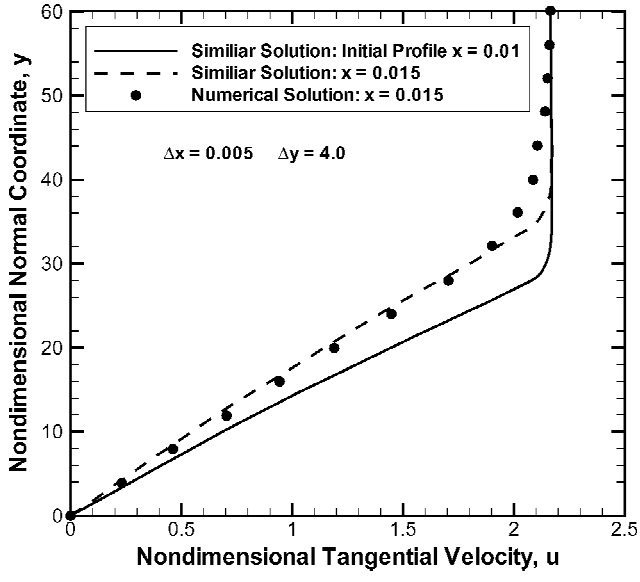

Fig. 2 Physical coordinate solution for velocity across boundary layer on a flat plate with $M_\infty = 9.6$.

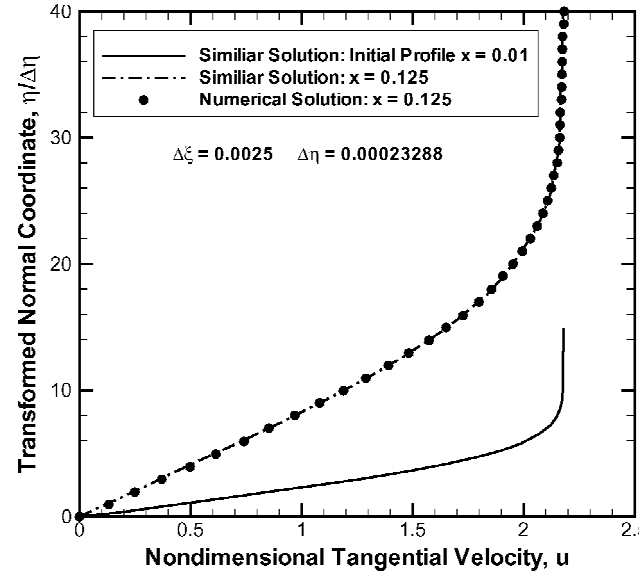

Fig. 3 Transformed coordinate solution for velocity across boundary layer on a flat plate with $M_\infty = 9.6$.

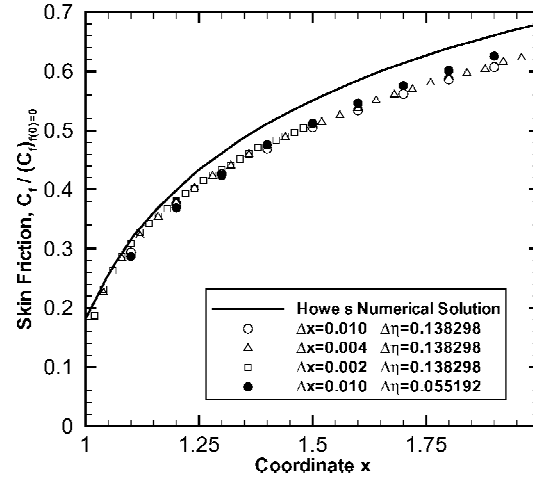

Fig. 4 Skin-friction parameter with Sutherland viscosity law for flow downstream of transpiration cooled region.

which used ALGOL programming language. This computer was about five times as fast as the IBM 650, and it was significantly easier and faster to write codes with the ALGOL language. As further verification of the implicit solution procedure and the new ALGOL code for the Burroughs 220 computer, a problem that had been carefully solved by Howe[27] with the Flügge-Lotz and Baxter[23] explicit scheme was investigated. The problem was the Mach 3 flow over a flat plate where the wall was porous from the leading edge to $x/L = 1$ with mass injection in this region. The plate was solid from $x/L = 1$ to $x/L = 2$. The initial conditions were obtained from Low[28] and were applied at $x/L = 1$. The Low similarity solutions use a linear viscosity law. When both of the numerical solutions use a linear viscosity law, the Howe explicit code[27] and the implicit code results for skin friction appear to be converging to the same result. However, when the explicit code and the implicit code used the Sutherland viscosity law, the skin friction results from the two codes do *not* appear to converge to the same answer, as shown in Fig. 4. Although the differences were less than 5%, it was disturbing that the solutions do not become the same as the grid was refined. The grid refinement studies of the implicit code indicated that these results were within 1% of the exact solution. To obtain a better estimation of the accuracy of the explicit code solutions, a further grid refinement was needed to determine if the available solution was sufficiently converged. Howe's code was written for the IBM 650

and required a significant amount of computer time. Flügge-Lotz convinced the director of the Stanford computer center to give us the IBM computer for a day. John Howe kindly agreed to help and came to the computer center early in the morning and started his code, which he had not used for a year or two. I stayed at the computer center all day in case there were any problems and checked on the progress of the solution. Late that afternoon Howe showed up, and we were convinced that the new solution was not significantly different from his original solution. The difference between the explicit code and the implicit code with Sutherland viscosity law was never resolved. The original solution by Howe used 2500 steps along the flat plate and 20 grid points across the boundary layer. This solution on the IBM 650 required 7.5 h. The implicit solution for this problem used as many as 500 steps along the flat plate and from 10 to 25 points were used across the boundary layer. The implicit solutions on the Burroughs 220 required 11–22 min. It is estimated that the explicit code would require 90 min on the Burroughs 220. The implicit code had proven to be stable and faster than the explicit solution approach.

The numerical solution of the hypersonic boundary-layer flow along a flat plate with interaction with the inviscid flow was the original objective of the author's dissertation. For this problem, the pressure along the plate must be determined as part of the solution. See Hayes and Probstein[35] for more information on this problem. With a reasonable computational technique developed, it became feasible to solve this problem. A procedure was developed to obtain the pressure as the solution was marched along the flat plate. At each marching step, an iterative method was used to obtain the pressure due to the displacement thickness of the boundary layer influencing the exterior flow and changing the pressure. The numerical predictions were compared with experimental and analytical results, and good agreement between the numerical predictions and data was obtained. Finally the original objective of my work had been completed. One of Flügge-Lotz's departing comments was, "The problem of turbulence should be avoided, as one could spend their career on the subject without producing very much."

Further Work at Stanford University on the Numerical Solution of Boundary-Layer Flows

About six months before the author finished at Stanford University, two new students started to work under Flügge-Lotz. Both Davis and Fannelop began investigating the finite-difference solution of the first- and second-order boundary-layer equations. This work received significant help from Van Dyke because he had developed the fundamental theory and was interested in obtaining solutions to these equations. The implicit solution technique was extended by Davis and Flügge-Lotz[36,37] to the second-order boundary-layer equations for hypersonic flow over axisymmetric blunt bodies. A significant observation in this work was made by Davis that one could write a set of parabolic governing equations that could be used to solve the complete shock layer. This approach was later developed by Davis into the viscous shock layer method with the numerical solution obtained with the implicit finite difference marching approach. Fannelop and Flügge-Lotz[38,39] investigated second-order boundary-layer flow over two-dimensional blunt bodies at low densities. The predictions were compared to experimental data. In both of these studies, the governing equations are solved in physical coordinates.

Two other students continued the boundary-layer studies for two problems that Flügge-Lotz had indicated that she wanted me to investigate. The first problem was given to Reyhner (see Reyhner and Flügge-Lotz[40,41]) and was concerned with solving the laminar boundary layer near the region where an impinging shock wave interacts with the boundary-layer flow. This problem requires the ability to handle separated flow with a region of reverse flow. The problem also required that displacement interaction with the inviscid flow be included with the pressure gradient obtained as part of the solution. A technique was developed for the reverse flow region where $\rho u(\partial u/\partial x)$ in the momentum equation and $\rho u(\partial u/\partial x)$ in the energy equation were neglected. This procedure allows marching of the solution through the reverse flow region and still provided reasonably accurate results. This approach was called the FLARE approximation by Williams.[42] The second problem was given to Plotkin (see Plotkin and Flügge-Lotz[43,44]) and was concerned with the prediction of the wake behind a finite length flat plate. Near the trailing edge, the Navier–Stokes equations are required to model this flow correctly. In this work, the boundary-layer equations were initially solved with the implicit finite difference scheme. Then the momentum equation was modified with a second derivative term that makes the equation elliptic. This equation was solved with an iterative procedure and provided an improved solution for this flow problem.

Other Numerical Work on Boundary Layers

There were several other people investigating numerical techniques for solving the boundary layer equations. Flügge-Lotz was in contact with A. M. O. Smith at Douglas Aircraft Company and was aware of their efforts. The first paper in 1962 from this group was by Wu[45,46] where an explicit difference scheme was being used to solve the compressible equations in physical coordinates. The Howarth–Dorodnitsyn transformed equations were also used to improve the stability requirements. A flat plate boundary-layer solution was presented that starts at the leading edge, and the solution was obtained 1 m downstream. The initial condition at the leading edge was uniform freestream flow with zero velocity at the wall. This solution approach has a transition region where the solution was not the correct Blasius solution until a sufficient number of steps have been taken along the wall. The length of this transition region was a function of the marching step size, and the solution was grid dependent. The numerical technique for the continuity equation was an implicit approach and was the same as used by Flügge-Lotz and Blottner[32] for the fully implicit scheme. This form of the difference equation for the continuity equation appears to be what was missing in the explicit scheme developed by Flügge-Lotz and Yu.[29]

Smith and Clutter[47] (also Jaffe and Smith[48]) investigated a solution technique that reduced the PDEs to ordinary differential equations across the boundary layer. This reduction was achieved by replacing the derivatives in the direction along the wall with finite difference relations. The resulting ordinary differential equations were first written as a system of first-order equations and were then solved with a shooting technique. For the incompressible case, the two velocity components are zero, and the shear stress is specified at the wall. A ordinary differential equation solver was used to march the solution across the boundary layer where the u velocity should match the inviscid u velocity. The shear stress is adjusted until the boundary edge boundary condition has been satisfied. This approach never worked very well because the solutions tend to blow up as the solution is marched across the boundary layer. The problem with this approach was nicely explained by Fay and Kaye[49] several years later. They showed that a simplified model equation for the momentum, energy or species was of the form

$$\frac{d^2w}{d\eta^2} + \alpha_1 \frac{dw}{d\eta} - \alpha_2 w = 0, \qquad \begin{matrix} w(0) = w_0 \\ w(\infty) = 0 \end{matrix}$$

From the theory of two-point boundary-value problems, a unique solution exist if $\alpha_2 > 0$. The general solution was

$$w = C_1 e^{-\tau_1 \eta} + C_2 e^{\tau_2 \eta}$$

$$\tau_1 = \left(\alpha_1 + \sqrt{\alpha_1^2 + 4\alpha_2}\right)/2 > 0$$

$$\tau_2 = \left(-\alpha_1 + \sqrt{\alpha_1^2 + 4\alpha_2}\right)/2 > 0$$

The exact solution to this problem gave the constants as $C_1 = w_0$ and $C_2 = 0$. The boundary conditions for the shooting technique were

$$w(0) = w_0, \qquad \left(\frac{dw}{d\eta}\right)_{\eta=0} = w_0'$$

The constant $C_2 = (w_0\tau_1 + w_0')/(\tau_1 + \tau_2)$, whereas the correct value of this constant is zero. This requires that $w_0' = -\tau_1 w_0$. If this condition is not satisfied exactly, the second term in the solution goes

to infinity as $\eta \to \infty$. The shooting technique was not the appropriate approach for solving two-point boundary-value problems of this type. As the boundary layer work evolved at Douglas Aircraft Company, Smith and Cebeci went to the implicit box scheme that had been developed by Keller[50] in 1970.

Additional Physics and Improved Numerical Scheme

The author worked at the General Electric Company in the Space Sciences Laboratory in King of Prussia, Pennsylvania, from 1962 to 1966. Initially I worked on three-dimensional method of characteristics for solving supersonic and hypersonic inviscid flows. However at that time, there was a critical need to predict the electron density around reentry vehicles and soon I was working on chemically reacting boundary-layer flows. *This is a problem that has not been possible to investigate experimentally in a ground facility.* The U.S. Air Force had a large effort under the direction of The Aerospace Corporation to develop numerical solution techniques for hypersonic aerodynamics. The previous boundary-layer work had indicated the need for further development of the numerical scheme and the problem of interest required that the boundary-layer equations had to be extended with new physics. Also the boundary-layer code had to handle problems where the solutions could start at the stagnation point of a blunt body or at the tip of a sharp cone. The development of the General Electric (GE) laminar, chemically reacting, boundary-layer code resulted from previous work done at Stanford and with the help of many GE colleagues. Some of the different features of the boundary-layer code are described subsequently.

Additional Physics for Chemically Reacting Boundary-Layer Flows

The major objective of the work was the prediction of the electron density in the boundary layer on slender vehicles by employing the available numerical solution scheme developed at Stanford University. For high-speed vehicles, the presence of ionized species in the boundary layer contributes to transmission interference of electromagnetic signals to and from the vehicle. The boundary-layer problem is particularly important for slender configurations because it is the principal source of high-temperature gas where chemical reactions occur. In addition, a detailed knowledge of the boundary layer at the rear of the vehicle was a necessary initial condition for the prediction of wake properties that have important impact on problems of detection and discrimination of reentry vehicles. For these problems, the gas was at sufficiently high temperatures that the gas becomes dissociated and ionized and chemical nonequilibrium effects had to be included.

To handle the additional physics, modifications to the perfect gas boundary-layer equations were required. The perfect gas boundary-layer equations for continuity and momentum stay in the same form, but the density ρ and the velocity $\boldsymbol{v}$ were obtained from the relations

$$\rho = \sum_{s=1}^{N_s} \rho_s, \qquad \rho \boldsymbol{v} = \sum_{s=1}^{N_s} \rho_s \boldsymbol{v}_s$$

where N_s is the number of chemical species and $\boldsymbol{v}_s$ is the velocity of species s relative to a fixed coordinate system. The Sutherland viscosity law must be replaced with a viscosity that is appropriate for the gas mixture. The energy equation requires two additional terms (underlined) and becomes

$$\rho u \bar{c}_p \frac{\partial T}{\partial x} + \rho v \bar{c}_p \frac{\partial T}{\partial y} = u \frac{\mathrm{d}p}{\mathrm{d}x} + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) + \mu \left(\frac{\partial u}{\partial y}\right)^2 + \underline{\frac{\partial T}{\partial y} \sum_{s=1}^{N_s} c_{p_s} j_s} - \underline{\sum_{s=1}^{N_s} h_s \dot{w}_s}$$

The first underlined term added takes into account the transport of energy due to diffusion of all of the chemical species, whereas the second underlined term accounts for energy produced or consumed due to chemical reactions. For the boundary layer, the relative mass flux j_s becomes, for multicomponent diffusion with ordinary (concentration gradients) and thermal diffusion effects included,

$$j_s = -\frac{\mu}{Pr}\left\{ \sum_{t=1}^{N_s} \bar{L}_{st} \frac{\partial c_t}{\partial y} + \frac{L_s^T}{T} \frac{\partial T}{\partial y} \right\}$$

$$\bar{L}_{st} = \begin{Bmatrix} \mathrm{Le}_s & t = s \\ \Delta L_{st} & t \neq s \end{Bmatrix}, \qquad Pr = \frac{\bar{c}_p \mu}{k}$$

where L_{st} is an effective Lewis–Semenov number for ordinary diffusion and L_s^T is a thermal Lewis–Semenov number. If Fick's law of diffusion is assumed, then $\Delta L_{st} = 0$ and Le_s must be the same for all species to have a consistent approximation with the sum of j_s over all species equal to zero. The procedure to calculate the effective Lewis–Semenov numbers $\bar{L}_{st}$ was described in a paper by the author.[6]

The governing conservation equations were completed with the addition of N_s conservation of species equations and the first-order boundary layer theory gives

$$\frac{\partial}{\partial x}(r_b \rho_s u) + \frac{\partial}{\partial y}(r_b \rho_s v) = -r_b \frac{\partial}{\partial y}(j_s) + r_b \dot{w}_s$$

$$S = 1, 2, \ldots, N_s, \qquad r_b = r_b(x)$$

where $\dot{w}_s$ is the chemical production term for species s. Because the following relations must be satisfied:

$$\sum_{s=1}^{N_s} j_s = 0, \qquad \sum_{s=1}^{N_s} \dot{w}_s = 0$$

the sum of the preceding species equations for all of the species gives the continuity equation as given in Eq. (1). The species equations were written in terms of the species mass fraction $c_s = \rho_s / \rho$ and become

$$\rho u \frac{\partial c_s}{\partial x} + \rho v \frac{\partial c_s}{\partial y} = -\frac{\partial}{\partial y}(j_s) + \dot{w}_s, \qquad s = 1, 2, \ldots, N_s$$

Only $N_s - 1$ of the species equations were required because the sum of all of the species must equal unity, and this relation can be used to find the last species (usually molecular nitrogen for air).

For a multicomponent gas mixture with N_s distinct chemical species and N_r simultaneous chemical reactions, the stoichiometric relations were written as

$$\sum_{s=1}^{N_s} \alpha_{rs} X_s \Leftrightarrow \sum_{s=1}^{N_s} \beta_{rs} X_s, \qquad r = 1, 2, \ldots, N_r \tag{8}$$

The quantities X_s represent the chemical species where α_{rs} and β_{rs} are the stoichiometric coefficients. The net rate of production of species s per unit volume is the sum of the production from all of the reactions and is

$$\dot{w}_s = M_{ws} \sum_{r=1}^{N_r} (\beta_{rs} - \alpha_{rs})(R_{fr} - R_{br}) \tag{9}$$

The forward and backward [reactions are going to right and left in Eq. (8), respectively] reaction rates for the r reactions were obtained from

$$R_{fr} = k_{fr} \prod_{s=1}^{N_s} \left(\frac{\rho c_s}{M_{ws}}\right)^{\alpha_{rs}}$$

$$R_{br} = k_{br} \prod_{s=1}^{N_s} \left(\frac{\rho c_s}{M_{ws}}\right)^{\beta_{rs}}$$

where k_{fr} and k_{br} are the forward and backward reaction rate coefficients, respectively. The reaction rates are a function of the gas

temperature when the gas is in thermal equilibrium. The rate coefficients were approximated with the curve fit relations

$$k_{fr} = T^{C_{2r}} \exp(C_{0r} + C_{1r}/T), \qquad k_{br} = T^{D_{2r}} \exp(D_{0r} + D_{1r}/T)$$

where the coefficients must be provided for each chemical reaction.

The equation of state (5) also needs a new relation for the molecular weight of the mixture and was obtained from

$$M_w = 1 \Big/ \sum_{s=1}^{N_s} \left(\frac{c_s}{M_{ws}} \right)$$

where M_{ws} is the molecular weight of species s. In addition, the thermodynamic and transport properties of the gas mixture must be determined from the species properties. The frozen specific heat at constant pressure was obtained from

$$\bar{c}_p = \sum_{s=1}^{N_s} c_s c_{ps}$$

The specific heat c_{ps} and enthalpy h_s of species s are required as a function of temperature. The individual species transport properties are required for viscosity μ_s and binary diffusion coefficients D_{ts}. The mixture viscosity μ and thermal conductivity k were determined from Wilke's mixture rules (see Refs. 51–53). The thermal conductivity is related to the species viscosity and specific heat. The species viscosity and binary diffusion coefficients were approximated with curve fits of the form

$$\mu_s = e^{C_{\mu s} T^{A_{\mu s}} \ln T + B_{\mu s}}, \qquad D_{ts} = p e^{C_{ts} T^{A_{ts}} \ln T + B_{ts}} \tag{10}$$

The least-square curve fit coefficients $A_{\mu s}$, $B_{\mu s}$, and $C_{\mu s}$ were obtained with a quadratic approximation $x = A_\mu y^2 + B_\mu y + C_\mu$, where $x = \ln \mu_s$ and $y = \ln T$. A similar approach was used for the binary diffusion coefficients.

Further Development of Boundary-Layer Solution Scheme

One of the problems with the previous boundary-layer work was obtaining initial conditions for starting the solutions. Similarity solutions were used, but the assumptions used in these solutions were not always consistent with the nonsimilar boundary-layer solution being obtained downstream. The Levy–Lees transformed boundary-layer equations provide a system of governing equations that reduce to the similar equations at the stagnation point and the tip of a cone or leading edge of a flat plate. This transformation allows larger marching step sizes in the marching direction along the wall without an increase in numerical error. In addition, the Levy–Lees transformation includes the Howarth–Doronitsyn transformation, which provides smoother hypersonic boundary-layer profiles.

Similarity coordinates were obtained with the Levy–Lees transformation

$$\xi(x) = \int_0^x (\rho\mu)_r u_e r_b^{2j} \, \mathrm{d}x, \qquad \eta(x, y) = u_e r_b^j \sqrt{\frac{K}{2\xi}} \int_0^y \rho \, \mathrm{d}y$$

A new dependent variable formulation was used with the variables F, V, and θ defined as

$$F = \frac{u}{u_e}, \qquad V = 2\xi \left[F \frac{\partial \eta}{\partial x} + \frac{\rho v r_b}{\sqrt{2\xi}} \right] \Big/ \left[(\rho\mu)_r u_e r_b^2 \right], \qquad \theta = \frac{T}{T_e}$$

In these definitions, the variable V was introduced rather than the usual stream function variable f, which gave a simpler form of the governing equations. The evaluation of the normal velocity v was not required for the boundary-layer solution and is difficult to obtain from the variable V because $\partial\eta/\partial x$ is not readily available. However, in 1993 a procedure to calculate the normal velocity was given by Pruett.[54] The governing boundary-layer equations were transformed to the $F - V - \theta$ similar form, which gave

$$2\xi \frac{\partial F}{\partial \xi} + \frac{\partial V}{\partial \eta} + F = 0$$

$$2\xi F \frac{\partial F}{\partial \xi} + V \frac{\partial F}{\partial \eta} + \beta(F^2 - \theta) - \frac{\partial}{\partial \eta}\left[l \frac{\partial F}{\partial \eta} \right] = 0$$

$$2\xi F \frac{\partial \theta}{\partial \xi} + V \frac{\partial \theta}{\partial \eta} - \frac{1}{Pr} \frac{\partial}{\partial \eta}\left[l \frac{\partial \theta}{\partial \eta} \right] - \alpha l \left[\frac{\partial F}{\partial \eta} \right]^2 = 0 \tag{11}$$

where the following notation was introduced:

$$l = \frac{(\rho\mu)}{(\rho\mu)_r}, \qquad \alpha = \frac{u_e^2}{c_p T_e} \qquad \beta = \left(\frac{2\xi}{u_e} \right) \left(\frac{\mathrm{d}u_e}{\mathrm{d}\xi} \right)$$

For flat plate flow, $\alpha = u_e^2/c_p T_e$ and $\beta = 0$, whereas at a stagnation point $\alpha = 0$ and $\beta = 1$ for two-dimensional flow and $\alpha = 0$ and $\beta = \frac{1}{2}$ for axisymmetric flow. The *similar equations* for compressible flow become Eq. (11) with the first term in each equation set to zero, since $\xi = 0$.

To improve the robustness of the numerical scheme, the variable V was evaluated at $ih = (i + \frac{1}{2})$ and the difference form of the continuity equation was written as

$$\xi_{ih} \left[\left(\frac{F_{i+1} - F_i}{\Delta\xi} \right)_j + \left(\frac{F_{i+1} - F_i}{\Delta\xi} \right)_{j-1} \right] + \left(\frac{V_j - V_{j-1}}{\Delta\eta} \right)_{ih} + \left(\frac{F_j + F_{j-1}}{4} \right)_{i+1} + \left(\frac{F_j + F_{j-1}}{4} \right)_i = 0$$

This difference equation is second order in both coordinate directions. The continuity equation was uncoupled from the other coupled equations that were solved with the tridiagonal solver.

The derivatives were linearized as done in earlier work, and the coefficients in the governing equations were lagged and evaluated at i rather than at ih. The species equations have a chemical production source term $W = \dot{w}_s/\rho$ that is a function of density, temperature, and mass fraction of chemical species. The density was replaced with the equation of state. The production term was linearized and written in implicit form as

$$W_{1+\frac{1}{2}} = W_i + \frac{1}{2} \left(\frac{\partial W}{\partial \theta} \right)_i (\theta_{i+1} - \theta_i) + \frac{1}{2} \sum_{s=1}^{N_s} \left(\frac{\partial W}{\partial c_s} \right)_i [(c_s)_{i+1} - (c_s)_i]$$

The chemical production terms produce stiff differential equations, and it is very important to use an implicit numerical scheme for these equations, as discussed by Curtiss and Hirschfelder.[55] The evaluation of the derivatives is given in a GE report,[56] and the development is somewhat lengthy. The GE boundary-layer code coupled all of the species equations, with the momentum and energy equations, but the continuity equation was uncoupled. This procedure tends to be more robust than uncoupling the equations. However, the full storage capacity of the computers were required for relatively small chemical models. Later work started to investigate the uncoupling of the species equations and how the production term should be formulated.

Another boundary-layer code based on the work already described was developed by Levine,[57] who was in the engineering group in the Missile and Space Division of GE. Later, Levine moved to the Air Force Research Laboratory in Edwards, California, and he further developed the Stanford/GE boundary-layer numerical solution methodology for analysis of rocket nozzle flows. His boundary-layer code is still being used today.

Chemically Reacting Boundary-Layer Results

The initial problem investigated was a binary gas mixture (atomic and molecular oxygen) with simplified thermodynamic and transport properties. The flow over a flat plate with insulated and noncatalytic wall with freestream conditions of Mach 15 and altitude of 100,000 ft was calculated. This problem provided a check of the formulation, numerical solution, and computer code and were compared with results from two approximate solutions developed by Chung–Anderson[58] and Rae.[59] The comparison of the finite difference solution with the approximate solutions are given in Fig. 5 which shows the three predictions are in reasonable agreement. The initial work at GE was first presented at a meeting[60] in August 1963. The material in this presentation was published as a GE report[56] and later as an article.[61]

Further development of the gas model was accomplished for ionized air with 6 chemical species, O, O_2, N, N_2, NO, and NO^+, and 11 chemical reactions. The specific heat and enthalpy of the species were obtained from analytical equations that included translation, rotation, and vibration energies. The viscosities of the species were obtained from collision integrals for dissociated air as given by Yun and Mason.[62] The viscosities were approximated with curve fits as described earlier. The boundary-layer flow on a sharp cone with 10-deg half-angle was computed with the finite difference scheme for ionized air. The freestream velocity was 22,000 fps, and the altitude was 100,000–150,000 ft. The boundary-layer edge properties were constant. At the wall, the gas was in chemical equilibrium. The solutions were obtained from the cone tip to 15 ft downstream. The maximum electron density along the body is given in Fig. 6, which

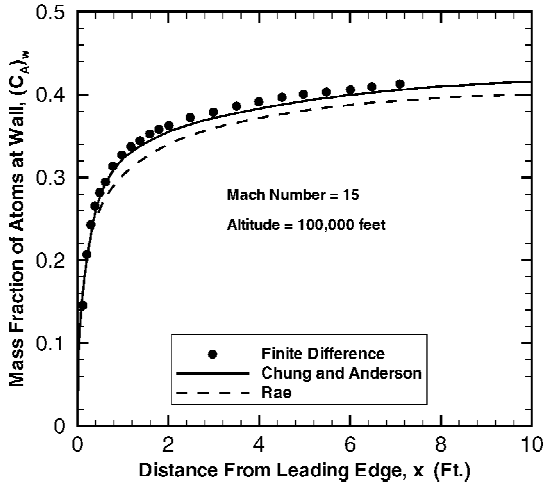

Fig. 5 Mass fraction of atomic oxygen at the wall for an insulated and noncatalytic flat plate boundary-layer flow.

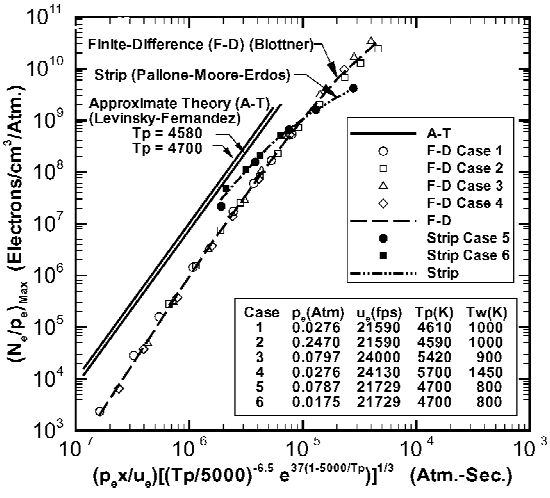

Fig. 6 Maximum electron density in the boundary layer on a sharp cone.

correlates the predictions for different cases in terms of boundary-layer edge properties and the peak temperature Tp in the boundary layer at the tip of the cone. Results from four finite difference solutions are presented. Multistrip predictions of Pallone et al.[63] and the approximate theory of Levinsky and Fernandez[64] are also shown in Fig. 6. The correlation is satisfactory, and the finite difference results are in reasonable agreement with the other predictions. The real test of the code is comparison of predictions to flight data that did not exist at that time. The work on ionized gases was published as a GE report,[65] with more details given in the report than in the *AIAA Journal*.[66]

Further Development of Codes and Numerical Techniques

Sandia Chemically Reacting Boundary-Layer Code

In 1966 the author returned to Sandia National Laboratories and continued to work on boundary layer flows with chemical reactions. The GE/U.S. Air Force boundary-layercode remained at GE due to proprietary restrictions on the code. A new code was started with the objective of developing a capability to handle arbitrary multicomponent gas mixtures. Also the interest was in solving boundary-layer flows with ablation products where there can be a large number of chemical species. The previous work had shown that a gas model with 11 species and 20 reactions required nearly the full capacity of a IBM 7094 computer with 32,000-word memory. It was decided to solve the governing equations in an uncoupled manner, where the computer memory requirements would be less demanding. The coupled method lagged the evaluation of the coefficient in the governing equation, and the truncation error was of order the step size Δx. The uncoupled method also has a truncation error of the order of step size Δx. The solution accuracy of the two approaches should be similar. The main concern with the uncoupled method was the impact on the stability of the numerical solution scheme. It was discovered that the order of solution of the governing equations was important. First the momentum equation was solved to obtain the tangential velocity. Next, the continuity equation was solved to obtain the transformed normal velocity V. Then the species equations were solved before the energy equation. The truncation error of the numerical scheme could be improved with iteration at each marching step, but calculations showed that iteration was not necessary. To improve solution accuracy, it was better to reduce the marching grid size rather than iterating at each marching step.

The Sandia code has additional capabilities and is easier to use than the previous code developed at GE. The major improvements were as follows: 1) Numerical scheme is improved. 2) Solution for the initial profiles is included. 3) Thin viscous shock layer can be solved at the stagnation point. 4) Variable grid sizes across layer and variable boundary layer thickness are available. 5) Complete multicomponent diffusion is included. 6) Additional boundary layer properties are determined. 7) Updated transport properties are employed. 8) Arbitrary body shape is available.

The linearization of the production term in the species equation has a very significant impact on the stability of the numerical scheme. The production term for species s was written as

$$\dot{w}_s/\rho = W_s^0 - W_s^1 c_s$$

In this equation, the mass fraction c_s was evaluated implicitly at $(i+1)$, whereas the coefficients were lagged and evaluated at (i). For a binary gas mixture of oxygen with the chemical reaction $O_2 + M_1 \Leftrightarrow 2O + M_1$, Eq. (9) gives for atomic oxygen, $s = O$,

$$W_s^0 = M_{ws} A\left(2\gamma_{O_2}\right), \qquad W_s^1 = 2k_b \rho^2 \gamma_s \gamma_{M_1}$$

$$\gamma_s = c_s / M_{ws}, \qquad A = k_f \rho \gamma_{M_1}$$

Because the element oxygen is constant or nearly constant in an air mixture, the relation $\gamma^O = 2\gamma_{O_2} + \gamma_s$ was used to rewrite the preceding relations as

$$W_s^0 = M_{ws} A(\gamma^O), \qquad W_s^1 = 2k_b \rho^2 \gamma_s \gamma_{M_1} + A$$

Because γ^O is a constant, the coefficient W_s^0 is independent of the mass fraction of the oxygen species. Further details of the linearization of the production terms for air mixture are given in the Sandia report.[67]

The actual time required per step for the uncoupled method as given in the review paper[6] and the earlier GE coupled method is given in Fig. 7. The uncoupled code on an IBM 7094 could handle more than twice as many species without any increase in computation time. At the time this work was being done, the coupled approach did not seem appropriate due to the rapid increase in computational time and storage requirements. Because present-day computers are significantly faster and have very large memories, a multicomponent, reacting boundary-layer code written today should consider coupling all of the equations together and include other numerical improvements that will be discussed subsequently. The coupled approach provides a more stable numerical scheme and a more robust code. *The most appropriate solution procedure should be reevaluated as the computer capabilities change.*

Initial results from the Sandia boundary-layer code were presented[68] in September 1967 at an AGARD Seminar at the National Physics Laboratory in England. As part of this meeting, Clark H. Lewis[69] had requested four investigators to use their boundary-layer codes to predict the flow on a hyperboloid. The freestream flow conditions were an altitude of 100,000 ft. and a velocity of 20,000 ft/s, with a wall temperature of 1000 K. The boundary-layer edge conditions were provided by Lewis and are given in the paper by Blottner.[6] The heat transfer (Stanton number) results along the body surface from the stagnation point to the end of the body are presented in Fig. 8. The four codes used different gas

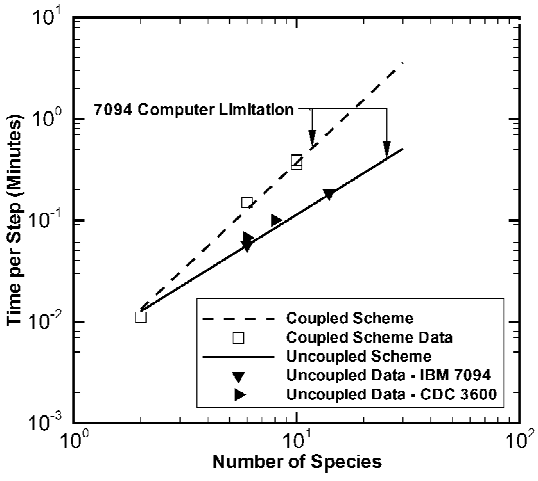

Fig. 7 Computational time on IBM 7094 for various numbers of chemical species with binary diffusion approximation.

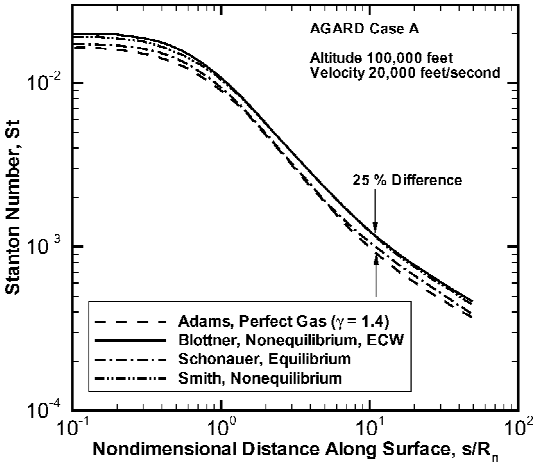

Fig. 8 Stanton number for laminar flow along a hyperboloid for AGARD test case.

models: perfect gas, equilibrium air, and nonequilibrium air with equilibrium conditions at the wall. Therefore, one would not expect perfect agreement between the results. With this type of comparison of codes, it is difficult to evaluate the accuracy of the numerical solutions from the various codes.

At this meeting the author became aware of Richardson's h^2–extrapolation method in a paper presented by Cooke and Mangler[70] on the numerical solution of boundary-layer equations for an ideal gas. The purpose of using Richardson extrapolation was to obtain more accurate results without using a large number of grid points across the boundary. Two or three coarse grid solutions could be used to obtain a solution of the desired accuracy rather than having to use a very fine grid. The fine grid solution would be impossible to obtain because the available computer capabilities were not sufficient. Another interesting paper on boundary-layer flows of a gas mixture in chemical equilibrium was presented by Kendall and Bartlett,[71] and this work developed into the well known BLIMP code.[72] Also, the author renewed his friendship with Davis, which resulted in Davis spending the summer of 1968 at Sandia, where he worked on adding the governing equations for a reacting gas mixture into his viscous shock-layer code. This provided the capability to do chemically reacting blunt-body flows.

The Sandia boundary-layer code was further developed and documented in a Sandia report,[67] with a complete discussion of the numerical scheme, physics included in the code, listing of the code, and three example problems. (Requests for this report are still being received.) The transport properties in this code are based on work performed by Yos[73] for Sandia. The collision cross sections for the atomic and molecular interactions in these results are obtained from calculations of Yun and Mason[62] and Yun et al.[74] Curve fits of the viscosity and binary diffusion coefficients of the species are of the form given in Eq. (10). The thermodynamic properties of the species are based on the calculations of Browne (see Ref. 6), where a table look-up method is used. The code includes thermodynamic properties for 20 species: O_2, N_2, O, N, NO, NO^+, CO, CO_2, CN, C_1, C_2, C_3, N^+, N_2^+, H, H_2, OH, H_2O, AR, and Ar^+. The code was written such that other gas models can be used if additional species properties are added to the code. The reactions included in the gas model are arbitrary and can be changed with input to the code. With these improvements to the physics of the code, more accurate predictions were possible. The solution of the thin viscous shock layer at the stagnation point is also an option in the code. Predictions of the flow at the stagnation point of a body at altitudes from 100,000 to 250,000 ft for air in chemical nonequilibrium using this code are presented in Ref. 75.

Variable Grid Scheme

The need for variable grid spacing across the boundary layer has already been shown to be important for hypersonic flows, with the governing equations in physical coordinates. Also the need for variable spacing is necessary for turbulent boundary-layer flows, as shown in Fig. 9. For 1% accuracy of the wall shear stress, the number of grid points goes from approximately 700 with a uniform grid to around 25 with a variable grid spacing. This result is for an algebraic turbulence model and the grid spacing is $h_{j+1} = \kappa h_j$, where $h_j = y_j - y_{j-1}$. Keller and Cebeci[76] were very successful in solving turbulent boundary layers with the box scheme that had been developed by Keller.[50] The finite difference scheme developed by the present author was extended to variable grid spacing in Ref. 77. The first derivative can be written as

$$\left(\frac{\partial W}{\partial y}\right)_j = \bar{\alpha}\left(\frac{W_{j+1} - W_j}{y_{j+1} - y_j}\right) + (1 - \bar{\alpha})\left(\frac{W_j - W_{j-1}}{y_j - y_{j-1}}\right)$$

$$- \frac{1}{2}[\bar{\alpha}(1 + \kappa) - 1]W_{yy}h_j + \cdots$$

If $\bar{\alpha} = 1/(1 + \kappa)$, then the approximation is second order. If the usual assumption is used that $\bar{\alpha} = \kappa/(1 + \kappa)$, the approximation is

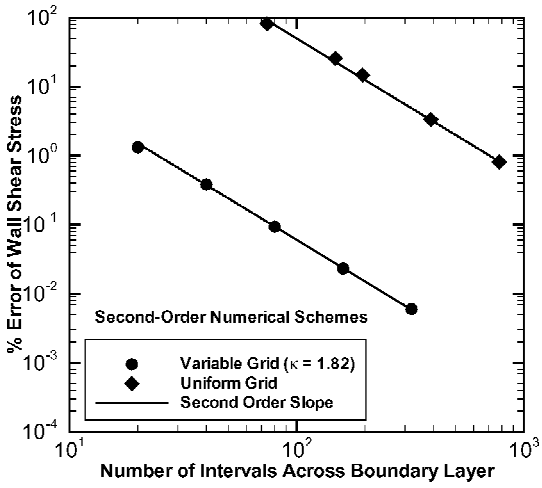

Fig. 9 Influence of grid spacing on accuracy of wall shear stress for flat plate turbulent boundary layer.

first order for a nonuniform grid and the derivative becomes

$$\left(\frac{\partial W}{\partial y}\right)_j = \frac{W_{j+1} - W_{j-1}}{y_{j+1} - y_{j-1}} - W_{yy}\frac{(\kappa - 1)h_j}{2} + \mathcal{O}\left(h_j^2\right) \quad (12)$$

Another approach is to introduce a coordinate transformation $y_j = y_j(\eta)$, where a uniform grid spacing $\Delta\eta$ is used in the new variable. The first derivative becomes, in the new coordinate system,

$$\left(\frac{\partial W}{\partial y}\right)_j = \left(\frac{\partial W}{\partial \eta} \Big/ y_\eta\right)_j$$

$$\left(\frac{\partial W}{\partial \eta}\right)_j = \frac{W_{j+1} - W_{j-1}}{2\Delta\eta} + \mathcal{O}(\Delta\eta^2)$$

The coordinate derivative is approximated as

$$(y_\eta)_j = \left(\frac{\partial y}{\partial \eta}\right)_j = \frac{y_{j+1} - y_{j-1}}{2\Delta\eta} + \mathcal{O}(\Delta\eta^2)$$

The first derivative becomes second order in terms of the η coordinate system:

$$\left(\frac{\partial W}{\partial y}\right)_j = \frac{(W_{j+1} - W_{j-1})}{(y_{j+1} - y_{j-1})} + \mathcal{O}(\Delta\eta^2)$$

This equation uses the same difference approximation for the first derivative as Eq. (12), but now the order has changed from first to second with this interpretation. Following the same procedure, the second derivative can be written as a second-order approximation in the η coordinate system. The variable grid scheme uses a nonuniform grid where one starts with the finest grid and then removes every other grid point to obtain a coarser grid. This process is repeated to obtain a series of grids. With this approach, the construction proceeds from *fine to coarse grid*. If the grid has a constant value of the grid ratio between adjacent intervals ($\kappa = \text{const}$), then the value of κ is reduced as the grid is refined. The interval ratio on the finer grid equals the square root of the interval ratio on the fine grid, $\kappa_{\text{finer}} = \sqrt{\kappa_{\text{fine}}}$. Therefore as the grid is refined, the interval ratio approaches one, and the grid approaches a uniform grid.

In the work of Keller with the box scheme,[50] Richardson extrapolation was used to improve the accuracy of the numerical solutions. The objective was not to obtain highly accurate results, but to obtain reasonably accurate results from solutions on relative coarse grids. This is the same idea as discussed earlier that was used by Cooke and Mangler.[70] In the variable grid scheme work, the Richardson extrapolation procedure was used to provide an estimate of the exact solution and a way to check the order of the scheme. To determine whether the variable grid scheme was second order, a flat plate turbulent boundary-layer problem investigated by Keller and Cebeci was used. The problem was solved with five grids across the boundary layer with $\kappa = 1.82$ and $\Delta\eta = 10, 20, 40, 80$, and 160 and a fixed grid along the flat plate. For the case of halving the grid spacing as the grid is refined, the Richardson extrapolation relation is

$$W_{\text{exact}} \approx W_{\text{RE}} = w(\Delta\eta) + [w(\Delta\eta) - w(2\Delta\eta)]/3$$

where $w(\Delta\eta)$ is the numerical solution on the finest grid. The discretization error e at any grid point (x_i, η_j) is equal to the difference between the exact solution of the difference equation w and the exact solution of the differential equation W. This gives $e = w - W$. Richardson extrapolation assumes that the discretization error behavior depends on the numerical scheme, and for central differences the form for two-dimensional problems is

$$e = \left(\alpha_2\Delta x^2 + \alpha_4\Delta x^4 + \cdots\right) + \left(\beta_2\Delta\eta^2 + \beta_4\Delta\eta^4 + \cdots\right)$$

If numerical solutions on a coarse grid with intervals $(\Delta x, 2\Delta\eta)$ and a refined grid with intervals $(\Delta x, \Delta\eta)$ are obtained, combining these two results gives the exact solution as

$$W = W_{RE} - \alpha_2\Delta x^2 - \beta_4\Delta\eta^4 - \cdots$$

where the Richardson extrapolation result is equivalent to a fourth-order numerical scheme in the η coordinate direction.

The grid refinement procedure for the box scheme uses a coarse nonuniform basic grid with an arbitrary distribution of basic grid points. A refined grid is obtained by introducing uniform grids between the basic grid points. This is referred to as a piecewise-uniform grid, and construction proceeds from *coarse to fine grid*. One of the results of the variable grid scheme work is given in Fig. 10, where the skin-friction percent error at the end of the flat plate ($Re_x = 1.88 \times 10^6$) is given as the number of intervals $\Delta\eta$ is increased. The solution accuracy for the box scheme and the variable grid scheme are nearly the same, and both show second-order behavior for this problem.

The variable grid scheme has been recently used by Wilcox[78] for solving a large variety of turbulent flow problems governed by the boundary-layer equations. The boundary-layer code provided in his book is based on this numerical scheme.

Further Studies on Linearization and Coupling of Equations

The earlier work before the variable grid scheme development did not adequately investigate the accuracy of the implicit numerical scheme or try to improve the truncation error, especially in the marching direction. As indicated earlier, the emphasis was on obtaining numerical solutions to engineering problems that required answers. The implicit numerical scheme was stable, second order

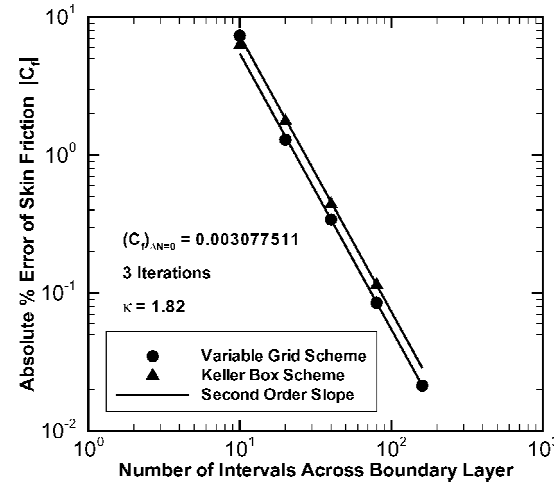

Fig. 10 Accuracy of skin friction for turbulent boundary layer with box scheme and variable grid scheme.

across the layer, the solutions were converging as the grid was refined, and the solutions appeared to be reasonably accurate. The numerical scheme lagged the evaluation of the coefficients in the differential equations that results in first-order behavior in the marching direction. With the Levy–Lees coordinates, most of the variables have a slow variation in the marching direction, and the first-order scheme in the marching direction provided the needed solutions without too much computer time. When a more accurate scheme was desired, a Picard type of iteration was performed at each marching step to increase the scheme to second order. Another error that had been neglected was due to the incomplete coupling of the governing equations with the continuity equation. With iteration at each marching step, the coupling error can be removed. However the earlier numerical scheme required a large number of iterations to improve the solution, and it seemed better to reduce the marching step size and not iterate. An investigation of the linearization and coupling issues was made by the author,[79] and a further extension of the work was documented in a Sandia report,[80] which were notes used in a course at North Carolina State University.

For the linearization investigation, the incompressible boundary-layer equations were used and transformed with the Levy–Lees variables. The governing equations become the continuity and momentum equations, which are given in Eq. (11) with $\theta = 1$ and $l = 1$. All of the dependent variables appear linearly in the continuity equation, but there are three nonlinear terms in the momentum equation. These terms are represented as a function $f(\varphi, \psi)$, where the variables φ and ψ represent the dependent variables or derivatives of the dependent variables at $(i+1)$ or $ih = i + 1/2$. If $f = \varphi\psi$, then the linearized expansion in delta form is

$$\varphi\psi = \bar{\varphi}\bar{\psi} + \bar{\psi}\delta\varphi + \bar{\varphi}\delta\psi + \cdots \tag{13}$$

where the delta-dependent variables are $\delta\varphi = \varphi - \bar{\varphi}$ and $\delta\psi = \psi - \bar{\psi}$. The variables $\bar{\varphi}$ and $\bar{\psi}$ are an initial guess of the values of the variables φ and ψ. The linearization of the three terms in the momentum equation are obtained from Eq. (13) and become in delta form

$$F^2 = \bar{F}^2 + (2\bar{F})\delta F, \qquad \delta F = F - \bar{F}$$

and variables are at $(i+1)$

$$\left[F\frac{\partial F}{\partial \xi}\right]_{ih} = \frac{\left(\bar{F}_{i+1}^2 - \bar{F}_i^2\right)}{(2\Delta\xi)} + \left(\frac{\bar{F}_{i+1}}{\Delta\xi}\right)\delta F_{i+1}$$

$$\left[V\frac{\partial F}{\partial \eta}\right]_{ih,j} = (\bar{V} + \delta V)_{ih,j}\left(\frac{\partial F}{\partial \eta}\right)_{ih} + \frac{V_{ih,j}}{2}\left(\frac{\delta F_{j+1} - \delta F_{j-1}}{2\Delta\eta}\right)_{i+1}$$

where

$$\left(\frac{\partial F}{\partial \eta}\right)_{ih} = \frac{1}{2}\left[\left(\frac{\partial \bar{F}}{\partial \eta}\right)_{i+1} + \left(\frac{\partial F}{\partial \eta}\right)_{i}\right]_j$$

$$\left(\frac{\partial F}{\partial \eta}\right)_{i,j} = \left(\frac{F_{j+1} - F_{j-1}}{2\Delta\eta}\right)_i$$

Complete linearization of the boundary-layer equations can become difficult as more physics is included. To obtain quadratic convergence with Newton's iterative solution method, complete linearization is needed. In 1989, a paper on the linearization of the incompressible turbulent boundary layer equation was published by Jang et al.[81]

For the *coupled approach*, the linearized form of the momentum and continuity equations with delta dependent variables are

$$-A_{11}\delta F_{j-1} + B_{11}\delta F_j - C_{11}\delta F_{j+1} + B_{12}\delta V_j = D_1$$

$$-A_{21}\delta F_{j-1} + B_{21}\delta F_j - A_{22}\delta V_{j-1} + B_{22}\delta V_j = D_2 \tag{14}$$

where delta variables δF are at $i+1$ and the δV variables are at ih. When these equations are completed with the boundary conditions, the equations are of block tridiagonal form given in Eq. (7), where $W_j = [\delta F_j \;\; \delta V_j]^T$. These equations are solved with the Thomas algorithm for tridiagonal equations, which can be used for scalar or block tridiagonal equations. The computer time and memory requirements for solving block tridiagonal equation is significantly larger than scalar tridiagonal equations. For the *uncoupled approach* the preceding equations become

$$-A_{11}\delta F_{j-1} + B_{11}\delta F_j - C_{11}\delta F_{j+1} = D_1$$

$$B_{22}\delta V_j = D_2 + A_{22}\delta V_{j-1} + A_{21}\delta F_{j-1} - B_{21}\delta F_j$$

These equations require one scalar tridiagonal solution and one algebraic solution for each iteration.

The importance of coupling the governing equations was investigated for the Howard problem (see Schlichting,[1] page 163) where the boundary-layer edge velocity decreases linearly as follows:

$$u_e/u_\infty = 1 - x/L = \sqrt{1 - (2\xi/L)}, \qquad \beta = (2\xi/L)[(2\xi/L) - 1] \tag{15}$$

The incompressible flow case was solved with reference length $L = 8$, $0 \le \eta \le 6$, $\Delta\eta = 0.2$, and $\Delta\xi = 0.2, 0.1, 0.05, 0.025, 0.0125$, and 0.00625. This problem was solved with both the coupled and uncoupled approach. With the uncoupled Crank–Nicolson (UCN) approach, the momentum equation was solved first, and then the continuity was solved. At each marching step, the solution was iterated various number of times (1, 5, 9, 19), and the impact on the skin friction at the wall is shown in Fig. 11. With the coupled approach, the momentum and continuity equations were solved simultaneously with one iteration at each marching step. Davis in 1972 (see Ref. 79) suggested a modified tridiagonal solution approach for coupling the momentum and continuity equations. The *Davis coupled* scheme is the same as the coupled approach, but a special form of the block tridiagonal solution method is used. The Davis coupled scheme result is also given in Fig. 11. These results show that the uncoupled approach requires approximately 20 iterations to obtain a second-order method in the marching direction.

This problem was further investigated[80] several years later with the coupled approach using no iterations and one iteration at each marching step. The solutions with one iteration were obtained with the total number of marching steps $I = 5, 9, 17, 33$, and 65. The solutions with no iterations were obtained with $I = 9, 17, 33, 65, 257$, and 513. The results of these solutions are given in Fig. 12, where the error of the wall skin-friction parameter $C_F\sqrt{Re_x}$ is shown as the number of marching steps I is changed. The solution with no iterations has first-order behavior, whereas the solution with one iteration has second-order behavior in the marching direction. From this study, the number of marching steps and computer time required for a desired accuracy of the skin friction at $\xi = 0.8$ was determined and are given in Table 1. When accurate solutions are

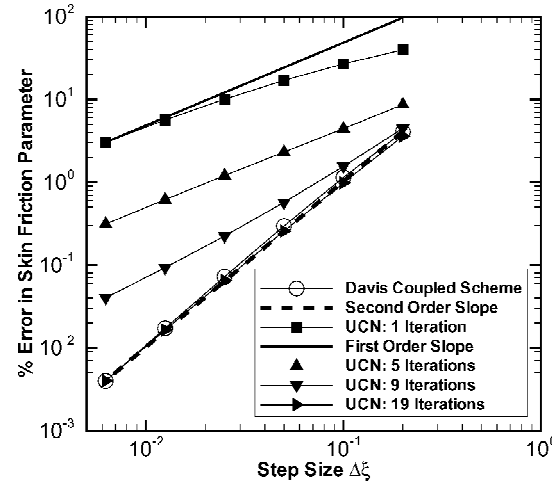

Fig. 11 Accuracy of UCN scheme and Davis coupled scheme.

Table 1 Number of steps and computer time for coupled scheme

% Error of $C_f\sqrt{Re_x}$	Marching steps I		Time, s	
	No iteration	One iteration	No iteration	One iteration
10	9	3	2.7	2.5
1	110	9	6.6	3.0
0.1	1200	28	49.1	4.5

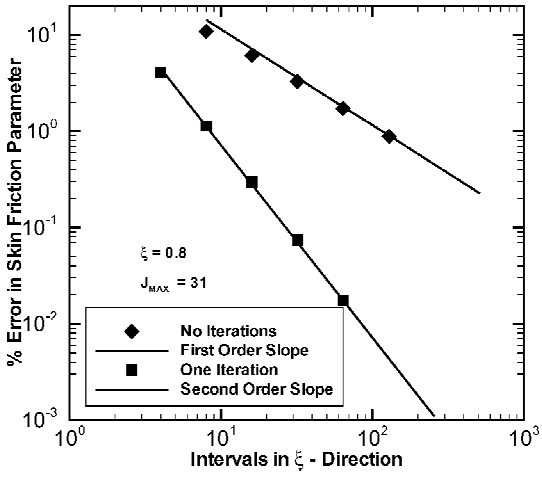

Fig. 12 Accuracy of skin friction for Howarth problem.

desired for this problem, the second-order solution with one iteration requires significantly less computer time than the first-order solution without iteration.

A comprehensive review on the numerical difficulties with solving chemically reacting flows has been made by McDonald.[82] The issue of whether to solve the equations coupled or uncoupled has been carefully addressed. McDonald states, "As a rough guide, if N partial differential equations are being solved coupled, this requires about $N^2/2$ times the labor of solving N uncoupled equations." This is written as $t_c = N^2 t_u/2$, where t_c is the time for one solution of the coupled equations and t_u is the time for solving all of the uncoupled equations once. The total time to solve the coupled equations at each marching step is $T_c = 2t_c$ due to the one iteration required. The total time to solve the uncoupled equations at each marching step is $T_u = I_u t_u$ due to I_u iterations required to obtain a second-order scheme. Combining the relations gives the ratio of total coupled time to the total uncoupled time,

$$T_c/T_u = N^2/I_u$$

The boundary-layer work has shown that $I_u \approx 20$ for two coupled equations, but when N is large, the value of I_u could increase significantly. From this time estimate, for a large number of chemical species, the uncoupled sequential solution technique could be faster than the fully coupled solution technique. This assumes that the uncoupled technique will be second order in the marching direction with $I_u < 10N$ iterations at each step. Also the uncoupled approach could become unstable and not work. The results presented in Fig. 7 can be misleading because the numerical scheme is first order in the marching direction, and all of the improvements in the numerical scheme as discussed were not included in this earlier work. A reevaluation of the linearization and coupling issues for chemically reacting flows is needed, but perhaps the importance is less significant because computer capabilities have improved considerably.

Verification of Numerical Solutions

Getting the Right Solution to a Boundary-Layer Problem

One problem that was solved by the author[79] was motivated by results presented in an earlier paper by Fitzhugh.[83] One of the results, Fig. 2 in Fitzhugh's paper, was for the Howarth problem with

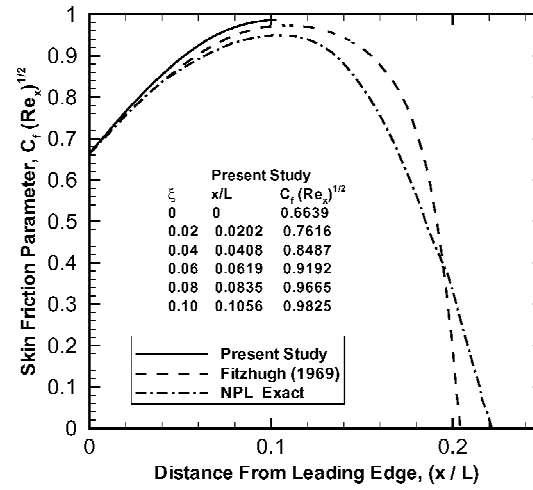

Fig. 13 Results for the numerical solution of the linearly retarded flow at Mach 4 and wall temperature equals freestream value.

Mach 4 flow where the variation of the skin-friction parameter along the wall was presented. His numerical solution was compared to a National Physics Laboratory (NPL) "exact" numerical solution and three approximate solutions. His result did not agree with any of the other results, and one had no idea what the correct solution should be. The author[79] solved the compressible boundary-layer equations with $\Delta\xi$ fixed and four values of $\Delta\eta$ and then solved with $\Delta\eta$ fixed and four values of $\Delta\xi$. The fine grid results for skin friction were estimated to have an error of approximately 0.1%. These results were further improved with Richardson extrapolation. These predictions are compared to the prediction of NPL and Fitzhugh in Fig. 13. The results of Ref. 79 are sufficiently accurate that further grid refinement will not change the curve location. Results for larger values of ξ are not given because the boundary layer grows rapidly in the region near separation and a large value of η_e is required to obtain an accurate solution. The linearly retarded freestream velocity problem has also been investigated by Werle and Senechal.[84] The boundary-layer solution technique was used to obtain a solution to a Howarth problem investigated by Werle and Senechal for the case of Mach 6 flow with the wall temperature equal to the total temperature. Three solutions with $\eta_e = 8.8$ were obtained by the present author on a series of refined grids. With Richardson extrapolation, the exact solution of the skin friction along the wall was estimated and the percent error of the skin friction determined. The author's results are in excellent agreement with the predictions of Werle and Senechal except near separation point where there is a slight difference. For small values of x/L, the skin-friction values have errors of less than 0.1%, whereas near separation the error grows to 1.7%. Because at separation the skin friction is zero, the percent error is not the appropriate quantity to measure the solution accuracy against near the separation point. The discretization error of the numerical solution might be a more appropriate measure of the solution accuracy. These problems illustrate that one can develop confidence in the accuracy of the computational solutions. *For a specified model and governing equations, one can determine an accurate numerical solution and the discretization error if sufficient computer capability is available.*

Picking the Right Benchmark Problem

As part of code verification, benchmark problems have been chosen and accurate solutions have been obtained with well-established codes. These benchmark solutions are very valuable because authors of new codes can use these solutions to help verify their codes. However, it is common practice to use the incompressible flat plate boundary-layer solution (Blasius solution) as a benchmark problem to help verify Navier–Stokes codes. It should be the other way around, where Navier–Stokes solutions are used to *validate* the accuracy of the boundary-layer equations for the flat plate problem. The incompressible Navier–Stokes equations were initially solved

Table 2 Skin friction on flat plate

$\sqrt{Re_x}$	$c_f\sqrt{Re_x}$
0	0.7549
2.0591	0.7631
12.817	0.6877
135.34	0.6645
∞	0.6641

by Davis and van de Vooren–Dijkstra for the flow over a semi-infinite flat plate. The leading-edge singularity was removed by transforming the Navier–Stokes equations into parabolic coordinates. Davis[85] and Botta et al.[86] extended the flat plate solutions to flow over a parabolic cylinder where the semi-infinite flat plate has the nose radius equal to zero. The semi-infinite flat plate results of Davis and van de Vooren are in reasonable agreement but not of benchmark quality. The variation of the skin-friction parameter $c_f\sqrt{Re_x}$ away from the leading edge in terms of the Reynolds number Re_x is given at several locations in Table 2 The data of van de Vooren are presented in Table 2. The skin friction approaches the Blasius value far downstream from the leading edge. The use of the Blasius solution to verify Navier–Stokes solutions must be used with care.

Observations on Obtaining the Right Solutions

The recent approach to obtaining accurate results to thermophysics and CFD problems has utilized numerical solutions to avoid approximate solutions techniques of the governing equations and has employed more fundamental governing equations. For example, Navier–Stokes equations are used rather than Euler/boundary-layer equations for attached flow over a body or large eddy simulation (LES) approach is used rather than the Reynolds averaged Navier–Stokes (RANS) equations for turbulent flow. As CFD moves toward more fundamental governing equations with less modeling and approximations required, numerical solution techniques are being developed for the new governing equations with a continued quest for faster and more accurate approaches. Clearly, accurate numerical solutions of the more fundamental governing equations provide a database of benchmark solutions that is very valuable and has the same importance as an experimental database. However, for the predictions needed in engineering analysis and design, the solution requirements are different. These predictions must provide reasonably accurate results in a short turn-around time. As computer memory and speed increase, the feasibility of using more fundamental governing equations will become possible.

In a recent paper by Bardos,[87] he indicated that in fluid mechanics one can introduce a "chain" of equations with the hope that the next level of equations will become relevant when the physics of the phenomena becomes too complicated to be computed by the previous equations. He also indicates the present concerns are *how to describe the phenomena with the convenient equations*, how to compute these phenomena, and how to use and visualize the results in spite of the complexity. It is the first item that is relevant to the present discussion. Bardos does not define convenient equations, but an appropriate definition is a set of governing equations that include sufficient physics that the prediction can provide a solution with the desired accuracy. The convenient equations for design might be a reduced form of the laminar Navier–Stokes (LNS) equations or a reduced form of the RANS equations. The convenient equations for research investigations might be the LNS equations for laminar flows and LES approach for turbulent flows.

At this time, the Navier–Stokes equations appear to be the convenient equations for high-fidelity thermophysics and CFD solutions, but this approach is not sufficiently fast for many design applications. The problem has been clearly illustrated in the review paper by Gnoffo et al.,[88] where design issues for hypersonic vehicles are considered. The authors have shown that a leveraging approach can be used to supplement the costly and time-consuming Navier–Stokes solutions used in recent design studies. The authors state, "*The leveraging approach* refers to the use of engineering approximations, often based on boundary-layer methods, to extend (leverage) a limited matrix of CFD solutions for better coverage of the parameter space." The two-dimensional boundary layer code LATCH was used to provide the approximate three-dimensional solutions. Boundary-layer codes are limited to attached flows, and the main difficulty is providing edge boundary conditions.

The work at NASA Langley Research Center has been successful in determining the steamlines near the wall and matching the boundary-layer to the inviscid flow. The boundary-layer approach is a efficient method to study flows with known edge conditions and various surface phenomena (see the work of Flügge-Lotz and Baxter[24]), especially if the boundary-layer edge properties are not in too much error due to the surface changes. There has been significant progress in matching the boundary layer with the inviscid flow with the work of Wuthrich and Sawley,[89] DeJarnette and Radciffe,[90] and the work of other investigators referenced in these papers. The work of Wuthrich and Sawley show that the computation time for the inviscid/boundary-layer approach is significantly less than a Navier–Stokes solution.

Another approach of coupling the boundary-layer solution to a Navier–Stokes solution was suggested by Van Dalsem and Steger,[91] and it was referred to as the fortified Navier–Stokes approach. This technique has been investigated by other authors (M. D. Bergeron and D. W. Zingg, T. H. Olsen, M. M. Hafez, and Van Dalsem), and K. Fujii refers to the approach as the fortified solution algorithm. In the fortified method, the boundary-layer equations are computed with a time-relaxation method, which allows three-dimensional and separated flows be solved.

Closing Comments

There has been the compelling desire to replace wind-tunnel experiments with CFD; this has not happened to date and will not happen in the foreseeable future. Also, for a long time, there has been an issue with the credibility of numerical solutions, and this issue is now receiving significant attention. A new issue that has not been addressed adequately is, *What convenient form of the governing equations should be used to solve engineering problems*? At this time, maybe the right governing equations for thermophysics and CFD problems should be a mixture of 1) LNS or RANS, which can provide high fidelity solutions, and 2) *reduced* forms of LNS or RANS for approximate solutions. There is a need to further investigate and improve reduced forms of the Navier–Stokes equations and to determine the error introduced by the simplified equations. When this is accomplished, there will be better engineering analysis and design capabilities for providing insight, not numbers, in a reasonable amount of time.

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