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THE UNIVERSITY OF ALBERTA

NUMERICAL METHODS FOR A PAIR OF NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

by

CATHERINE DESCHENEAU

A THESIS

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled "Numerical Methods for a Pair of Nonlinear Partial Differential Equations" submitted by Catherine Descheneau in partial fulfillment of the requirements for the degree of Master of Science.

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Supervisor

.....

.....

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Date: September 14, 1973

DEDICATION

To my parents, Denis Ian and Winifred Irving Gough

ABSTRACT

A study is made of methods of solution of a pair of nonlinear, coupled, third-order differential equations in two dependent and two independent variables. The equations have an incomplete initial value set. Nonlinearity is a result of the interdependence of solutions and coefficients. These equations are found to be of interest in the study of compressible boundary layer theory.

The development of methods based on a technique of representing the partial differential equations as a series of ordinary differential equations in one of the independent variables is described. Application of a quasilinearization technique coupled with integration using Chebyshev polynomials to the incompressible momentum equation is outlined, as it eliminates the need for shooting to overcome the incomplete initial value set.

An extension of the quasilinearization with Chebyshev integration technique to the compressible equations is proposed. Error control in view of the difference-differential scheme is investigated, and the difficulties to be encountered in applying the method are discussed. A comparison of the conventional and proposed approaches is made and the proposed method is shown to be potentially superior.

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TABLE OF SYMBOLS

SYMBOL	DEFINITION
p	pressure
ρ	density
μ	viscosity
Pr	Prandtl number
H	enthalpy
C	$\rho\mu/\rho_e\mu_e$
subscript e	just external to the boundary layer
subscript ∞	remote from the boundary layer
T	see [5]
$\tilde{P}$	$(x/u_e)(du_e/dx)$
R	$(x/r)(dr/dx)$
N	$(\tilde{P}+1)/2+R$
β_ν	multistep integration constants

Other symbols are defined in context.

CHAPTER ONE

INTRODUCTION TO THE PROBLEM

The equations which describe the flow of a fluid must express the characteristics of this particular kind of physical problem [10, 17, 19, 26]. The cohesive nature of the fluid is expressed in the equation of continuity; a volume element in the fluid must have a balanced transfer of mass through its walls if the molecular forces between its particles are to be obeyed. Forces acting on the fluid, whether external pressures or internal stresses, must find expression in an equation of motion developed from Newton's Second Law. Such an equation is usually given in terms of momentum as the velocity of the flow in different regions of the fluid is the quantity of prime interest. If the fluid is incompressible, kinetic forces suffice to describe the system; if it is compressible, thermodynamic forces resulting from volume and pressure changes must be taken into account. An equation based upon some convenient measure of energy must be developed from the fundamental thermodynamic relationships. This latter relationship is known as the energy equation. In addition, if other phenomena such as mass transfer through a boundary of the fluid are present, further equations must be formulated to bring them into account. The equations to be studied in this paper arise in the study of the boundary layer around an axisymmetric body immersed in a compressible fluid at

hypersonic speeds. The boundary layer is that region in which flow perpendicular to the body walls is present. Although such equations are representative of a large class of problems they are apparently incapable of formal solution. Also, because of their nonlinearity, numerical techniques with well-defined systematic error control are difficult to define for the problem. However, their practical importance makes the development of methods of approximate solution vital; both the engineering design of high speed vehicles and also the extension of knowledge in a difficult scientific field are at stake. Challenges such as these have provided the motive for the development of numerical analysis throughout the history of that subject, and have laid the groundwork for most theoretical consideration of the validity of solutions of mathematically complex problems. It is in view of the importance of the interaction between an experimental, practical situation and the stimulated theoretical investigations that this paper has been written.

An effective technique for this particular problem was outlined first by Clutter and Smith in 1963 [5] and other authors have made contributions since then [11, 12, 13, 14, 28, 29]. The problem will be described and the various approaches to its solution discussed and contrasted.

The standard description of the flow around a body immersed in a fluid consists of the equations of fluid

continuity, momentum conservation and energy conservation. Included in the equations are terms which describe the physical characteristics of the fluid; here, these include the compressibility of the fluid. Transverse curvature of the body is also included; such higher order terms are usually left out when Prandtl's boundary layer equations are used. A brief outline of the derivation of these equations is given in Appendix A. The symbols used are defined in the Table of Symbols.

A two-dimensional coordinate system is sufficient to describe the problem as it is axisymmetric [28]. Steady equilibrium flow about a body of revolution is assumed. The coordinate system to be used is shown in Figure One.

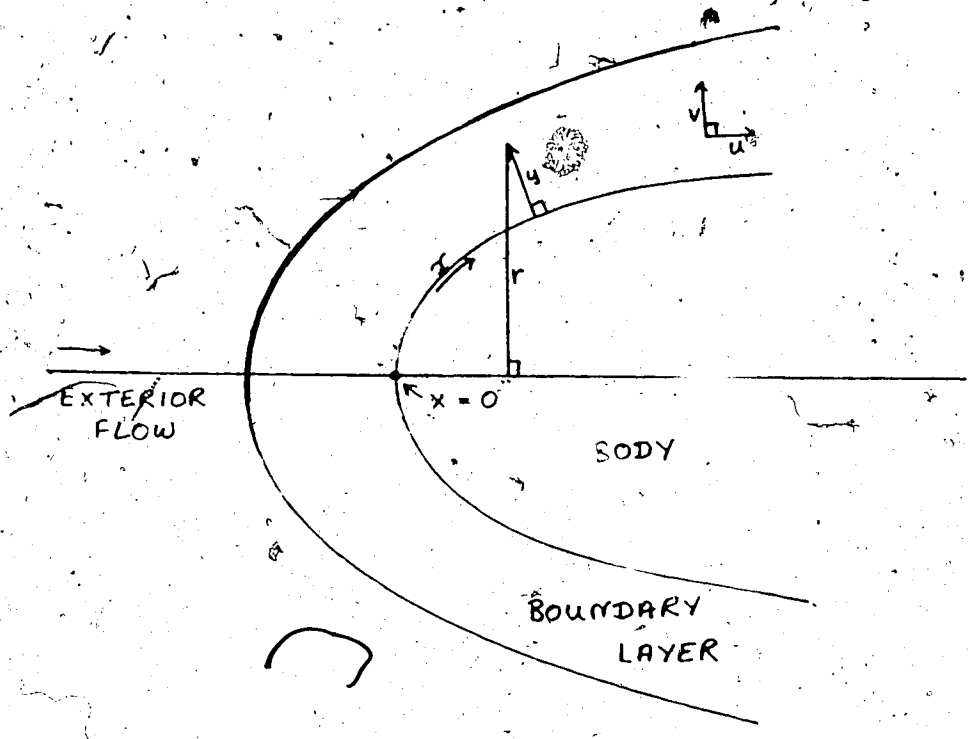

FIGURE I : x, y coordinate system

One coordinate, x, is used to represent distances from the leading edge, or stagnation point at the nose, directed along the body surface; the other, y, is used to represent distances from the body surface directed into the boundary layer perpendicular to x.

In terms of this coordinate system, and with respect to the various fluid properties and thermodynamic variables described in Appendix A and the Table of Symbols, the equations are as follows. The dependent variables u and v represent the flow speeds in the x and y directions respectively.

CONTINUITY: $$\frac{1}{r}\left[\frac{\partial}{\partial x}(r\rho u) + \frac{\partial}{\partial y}(r\rho v)\right] = 0$$

MOMENTUM: $$\rho\left[u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right] = -\frac{\partial p}{\partial x} + \frac{\mu}{r}\frac{\partial r}{\partial y}\frac{\partial u}{\partial y} + \frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right.$$

ENERGY: $$\rho\left[u\frac{\partial H}{\partial x} + v\frac{\partial H}{\partial y}\right] = \frac{1}{r}\frac{\partial r}{\partial y}\left[\frac{\mu}{pr}\frac{\partial H}{\partial y} + \mu\left(1 - \frac{1}{pr}\right)u\frac{\partial u}{\partial y}\right]$$
$$+ \frac{\partial}{\partial y}\left[\frac{\mu}{pr}\frac{\partial H}{\partial y} + \mu\left(1 - \frac{1}{pr}\right)u\frac{\partial u}{\partial y}\right]$$

The equations are awkward to integrate in this form, because the boundary layer thickness varies greatly with x, and numerical solutions will be seen to depend on values of the unknowns and fluid properties at previous positions in the x direction. Moreover as stated the equations exhibit

singularity along the curve x=0 [5]. A technique which is often used in Hydrodynamics is employed; a further transformation using potential functions combines the continuity and momentum equations while increasing the order of the problem [19]. A description of these transformations can be found in Appendix B.

The final form of the equations is:

$$\text{MOMENTUM: } \frac{\partial}{\partial\eta}(C\phi'') = -T\frac{\rho_e}{\rho}C\phi'' + C_\infty P[\phi'^2 + 2\phi' + 1 - \frac{\rho_e}{\rho}]$$

$$- C_\infty N_o(\phi+\eta)\phi'' + C_\infty x[(\phi'+1)\frac{\partial\phi'}{\partial x} - \phi''\frac{\partial\phi}{\partial x}]$$

$$\text{ENERGY: } \frac{\partial}{\partial\eta}[\frac{C}{pr}\psi' + \frac{u_e^2}{H_e}C(1-\frac{1}{P_r})(\phi'+1)\phi'']$$

$$= - C_\infty N_o(\phi+\eta)\psi' + C_\infty x[(\phi'+1)\frac{\partial\psi}{\partial x} - \psi'\frac{\partial\phi}{\partial x}]$$

$$- T\frac{\rho_e}{\rho}[\frac{C}{P_r}\psi' + \frac{u_e^2}{H_e}C(1-\frac{1}{P_r})(\phi'+1)\phi'']$$

where x, η are independent variables and ϕ, ψ are dependent. ϕ', ψ' are abbreviations for the partial derivatives of the quantities with respect to η. Other quantities are physical parameters which are supplied in tabular form or calculated with respect to position. C, Pr and ρ depend on the velocity distribution (the solution) as well as on position and must be included in the step-by-step solution of the problem.

Boundary conditions are:

$$\text{MOMENTUM EQUATION:} \begin{cases} \eta = 0: & \phi(0,x) = f(x) \\ & \phi'(0,x) = -1 \\ & (\phi'' \text{ unknown}) \\ \eta \to \infty: & \phi' \to 0 \end{cases}$$

$$\text{ENERGY EQUATION:} \begin{cases} \eta = 0: & \Psi(0,x) = g(x) - 1 \\ & \text{or } \Psi'(0,x) = g'(x) \\ \eta \to \infty: & \Psi \to 0 \text{ or } \Psi' \to 0 \end{cases}$$

Thus the problem has a free boundary with asymptotic approach to the r boundary values of the unknowns as the flow merges with the uniform external flow.

Two properties of the problem in this formulation should be noted. First, the momentum equation involves only one dependent variable, but the set of initial values is incomplete and the equation is nonlinear. Second, the energy equation involves both unknowns and is linear in ψ. It is on these two features that the method of Clutter and Smith is structured.

In setting up the discrete approximation of the equations the Hartree-Womersley technique [9] is used. That is, derivatives in x are expressed as finite differences but at each value of x the equations are treated as ordinary differential problems in η. The advantage of this treatment is that the extensive work done on the solution of ordinary differential equations can be employed, and as the equations are nonlinear, such an approach is doubly valuable.

The following is an outline of Clutter and Smith's technique:

At a given x station

(i) Assume fluid properties C, Pr, ρ/ρ_∞ from previous x station (initially given at x=0), or from latest solutions available for this value of x.

(ii) Use a shooting technique to obtain $\phi''(x,0)$ and solve the momentum equation as an O.D.E.

(a) Solve the energy equation as a linear problem in ψ using the values of ϕ, ϕ', and ϕ'' obtained from the solution of the momentum equation.

(b) Update fluid properties using latest values of all unknowns.

(c) Repeat (a)-(b) until convergence is obtained on fluid properties and ψ or iterate as desired.

(iii) Repeat (i)-(ii) until convergence is obtained on all quantities or iterate as desired.

The procedure involves certain numerical components. They are identified below together with a statement of the chosen method of attack of Clutter and Smith.

(a) Finite difference representation in x (third-order implicit differences).

(b) Integration in η (a series of Taylor's formulae of increasing step size to get started, then fourth-order Falkner-Adams predictor-corrector steps of constant step size with one use of correction).

(c) Shooting to get a complete initial value set for the momentum equation (Trial and error until three "close" trajectories are obtained).

(d) Solution of the energy equation as a linear problem (Superposition of solutions with integration as in (b)).

(e) Choice of starting values of the fluid properties for this value of x (the previous station's values are used).

A detailed description of the technique is given in Chapter Ten.

A general comment as to the nature of the Clutter and Smith method can be made. It is a direct approach which is built on the nature of the problem at hand and which makes use of the available information. Its value has been proved experimentally in a variety of situations [2,5,11,12, 13,28,29]. Theoretical consideration of the method was done after it was found to be effective.

Since this basic structure was proposed various

alternative treatments of components of the method have been suggested. In the following chapters Clutter and Smith's methods will be outlined in some detail and contrasted with these alternatives in terms of numerical characteristics.

The purpose of this exposition will be to illustrate the numerical complexity of a problem of this difficulty. The effectiveness of a technique developed under conditions of engineering necessity must not be denied; rather the desireability of a priori knowledge of the behavior of the numerical components of a method will be emphasised. Finding an experimental method which gives experimentally verifiable results is an art; developing techniques within a context of knowledge of the homomorphisms between the mathematical spaces of exact and approximate solutions is a science and can therefore be used with confidence in a variety of situations and under known criteria for validity. The more complex a problem, the more necessary it is to have a guarantee of the behavior of numerical methods, and yet the harder it is to obtain one. A method which offers a degree of confidence which appears to be as high as may be obtained will be discussed. The application of remarks on the numerical solution of the problem under discussion to a wider class of problems of some similarity will be emphasised.

CHAPTER TWO

FINITE DIFFERENCE APPROXIMATIONS IN X

The Hartree-Womersley technique [9] consists of the replacement of stream-wise (x) derivatives by finite difference approximations to produce ordinary differential equations in η. Derivatives are approximated at x=x(n) using quantities previously calculated upstream at x(n-1), x(n-2), etc., so the error of approximation is cumulative. There is no difficulty in starting the solution as terms involving x derivatives disappear at x=0. At x=x(2) a two-point formula must be used.

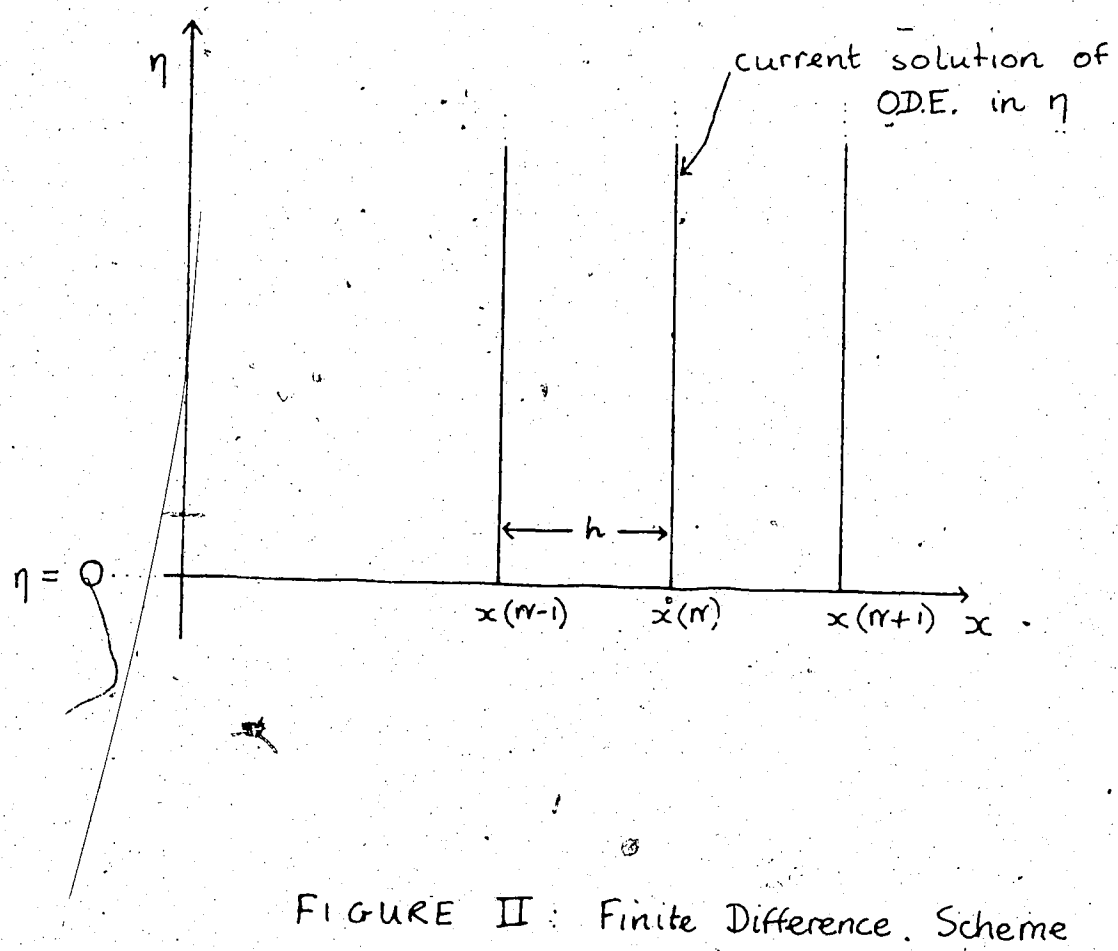

FIGURE II: Finite Difference Scheme in x

Two-point formula for function f:

$$\left(\frac{\partial f}{\partial x}\right)_N = \frac{f_N - f_{N-1}}{(x(N)-x(N-1))}$$

Error:

$$\frac{x(N) - x(N-1)}{2} \quad \frac{\partial^2 f(\xi)}{\partial x^2} \quad , \xi \in [x(N-1), x(N)]$$

At x=x(3) a three point scheme may be initiated:

Lagrangian three-point formula:

$$\left(\frac{\partial f}{\partial x}\right)_N \simeq \left[\frac{1}{x(N)-x(N-1)} + \frac{1}{x(N)-x(N-2)}\right] f_N$$

$$- \left[\frac{x(N) - x(N-2)}{(x(N)-x(N-1))(x(N-1)-x(N-2))}\right] f_{N-1}$$

$$+ \left[\frac{x(N) - x(N-1)}{(x(N)-x(N-2))(x(N-1)-x(N-2))}\right] f_{N-2}$$

Error: $\frac{(x(N)-x(N-1))(x(N)-x(N-2)}{6} \quad \frac{\partial^3 f(\xi)}{\partial x^3}$, $\xi \in [x(N-2), x(N)]$

or, for constant differences $x(n)-x(n-1)=h$, $n=1, 2, \ldots$,

$$\left(\frac{\partial f}{\partial x}\right)_N \simeq \frac{3f_N - 4f_{N-1} \quad f_{N-2}}{2h}$$

Clutter and Smith decided to use the three-point form throughcut. The three-point form is contrasted with a four-point formulae of the same type and with what is called the 'mean form' using average values of derivatives over a range of points to estimate the derivative at the next point [28]. It was found that the point form is more desireable than the mean form as the latter process tends to diverge wildly as the step size h decreases. The four-point form, secondly, was found not to give significantly more accuracy for the additional computation and storage involved.

Consider the constant differences formula (1). Under this approximation the momentum equation becomes

$$C_\infty x(N)\,[(\phi'+1)\,\frac{(3\phi'_N-4\phi'_{N-1}+\phi'_{N-2})}{2h} - \phi''_N\frac{(3\phi_N-4\phi_{N-1}+\phi_{N-2})}{2h}\,]$$

$$= \frac{\partial}{\partial\eta}\,(C_N\phi''_N) + T\,\frac{\rho_e}{\rho}\,C_N\phi''_N - C_\infty P\,[\phi'^2_N + 2\phi'_N + 1 - \frac{\rho_e}{\rho}]$$

$$+ C_N\,N(\phi_N+\eta)\phi''_N \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (2)$$

Terms in ϕ_N , ϕ_{N-1}, and ϕ_{N-2} can be seen to involve the multiplicative factor $x(n)/h$.

Clutter and Smith find experimentally [28] that if the ratio $x(n)/h$ is bounded above by 25 the accuracy of the method can be sustained. However, a different approach to the problem of truncation error growth is taken by Jaffe and Okamura [12]. They use one two-point and one three-point formula to start (their three-point formula is a linear least squares approximation). Thereafter they proceed with a four-point quadratic least-squares finite difference scheme. Under their formulation the left-hand side of the momentum equation becomes
$C_\infty x(N)\,[(\phi_N+1)p'_N(x)+\phi''_N p_N(x)]$, where

$$p'_1 = 0 \quad , \quad p'_2 = \frac{\phi'_2 - \phi'_1}{x(1)} \quad ,$$

$$p'_3 = \frac{1}{2(x(3)^2+x(2)^2-x(2)x(3))}\,[(2x(3)-x(2))\phi'_3+(2x(2)-x(3))\phi'_2$$
$$-(x(2)+x(3))\phi'_1]$$

$N = 4, 5, \ldots$

$$P_N' = D_N^{-1}(A_N + 2B_N\, x(N)) \qquad \text{where}$$

$$D_N = \begin{vmatrix} 4 & \Sigma\, x(i) & \Sigma\, x(i)^2 \\ \Sigma\, x(i) & \Sigma\, x(i)^2 & \Sigma\, x(i)^3 \\ \Sigma\, x(i)^2 & \Sigma\, x(i)^3 & \Sigma\, x(i)^4 \end{vmatrix}$$

$$A_N = \begin{vmatrix} 4 & \Sigma \phi_i' x(i) & \Sigma\, x(i)^2 \\ \Sigma\, x(i) & \Sigma \phi_i' x(i)^2 & \Sigma\, x(i)^3 \\ \Sigma\, x(i)^2 & \Sigma \phi_i' x(i)^3 & \Sigma\, x(i)^4 \end{vmatrix}$$

$$B_N = \begin{vmatrix} 4 & \Sigma\, x(i) & \Sigma \phi_i' x(i) \\ \Sigma\, x(i) & \Sigma\, x(i)^2 & \Sigma \phi_i' x(i)^2 \\ \Sigma\, x(i)^2 & \Sigma\, x(i)^3 & \Sigma \phi_i' x(i)^3 \end{vmatrix}$$

where summation is over I and i=n-3, n-2, n-1, n. Similar formulae hold for p_N (differences for ϕ_N).

It should be noted that each of the terms D_N, A_N, and B_N is of order x^6, and so $\bar{P}_N'$ is of order ϕ'. Then the left-hand side of the momentum equation involves the multiplicative factor x(n) instead of x(n)/h.

Error analysis of a theoretical nature is impractical due to the nonlinear form of the momentum equation. Experimental results [5,11,12,13,28,29] show that the method depends on local Lipschitz conditions on the unknowns, as is

to be expected for this type of difference scheme.

CHAPTER THREE

INTEGRATION IN η

In the Hartree-Womersley technique [9] integration with respect to is done along lines of constant x value. The x derivatives are approximated by finite differences. The equations are dealt with in a form in which the thickness of the boundary layer remains nearly constant with respect to the variation of x, that is, along the body. Under the transformation given in Chapter One the range of the integration variable η is $[0,\infty)$ and the method of Clutter and Smith depends on choosing a finite final value for η so that the range is approximated by $[0,\eta_\infty)$. Such choice is done by experimentation with the method and comparison of solutions generated with results obtained in wind-tunnel studies. Then the need for timing decisions to change step size and the asscciated use of interpolation on starting values of fluid properties are eliminated as the range of η is constant. Clutter and Smith [5] decide therefore to apply a multistep extrapolation-interpolation (predictor-corrector) scheme suitable for this type of problem. Allied to the use of this kind of integration is the establishment of starting values for the process.

The integration problem can be restated as follows:

MOMENTUM EQUATION:

$$\frac{\partial}{\partial \eta}(C\phi'') = -T\frac{\rho_e}{\rho_l} C\phi'' + C_\infty P[\phi'^2 + 2\phi' + 1 - \frac{\rho_e}{\rho}]$$

$$- C_\infty N(\phi+\eta)\phi'' + C_\infty x[(\phi'+1)\frac{\partial \phi'}{\partial x} - \phi''\frac{\partial \phi}{\partial x}]$$

$\eta = 0$: $\phi_N = f_w$, $\phi'_w = g_w$ (w-wall value)

$\eta \to \infty$: $\phi' \to 0$, $\phi'' \to 0$

Steps in Integration:

$$C\phi'' = \int_o^\eta \frac{\partial}{\partial \eta}(C\phi'')\, d\eta + C_w\phi''_w$$

Thus $$\phi' = \int_o^\eta \phi'' d\eta - 1$$

$$\phi = \int_o^\eta \phi' d\eta + \phi_w$$

ENERGY EQUATION: Let $\pi = \frac{C}{pr}\psi' + \frac{u_e^2}{H_e} C(1 - \frac{1}{pr})(\phi' + 1)\phi''$

Then $\pi' = -T\frac{\rho_e}{\rho}\pi - C_\infty N(\phi+\eta)\psi' + C_\infty x[(\phi'+1)\frac{\partial \psi}{\partial x} - \psi'\frac{\partial \phi}{\partial x}]$

$\eta = 0$: $\psi_w = g_w - 1$ or $\psi'_w = g'_w$

$\eta \to \infty$: $\psi \to 0$, $\psi \to 0$

Steps in Integration: $\pi = \int_o^\eta \pi' d\eta + \pi_w$

$$\psi' = \frac{P_r}{C}[\pi - \frac{u_e^2}{H_e}(1 - \frac{1}{pr})(\phi+1)\phi'']$$

$$\psi = \int_o^\eta \psi' d\eta + \psi_w$$

The procedure selected by Clutter and Smith to integrate these equations is outlined by Collatz [4]. It consists of the Falkner extrapolation formula followed by a single use of the Adams interpolation formula. For reasons

of desired accuracy and speed discussed in [5], four point forms were used. They are:

EXTRAPOLATION:

$$(C\phi'')_{r+1} = (C\phi'')_r + \frac{h}{24}\left[55(C\phi'')'_r - 59(C\phi'')'_{r-1} + 37(C\phi'')'_{r-2} - 9(C\phi'')'_{r-3}\right]$$

$$\phi'_{r+1} = \phi'_r + \frac{h}{24}\left[55\phi''_r - 59\phi''_{r-1} + 37\phi''_{r-2} - 9\phi''_{r-3}\right]$$

$$\phi_{r+1} = \phi_r + h\phi'_r + \frac{h^2}{360}\left[323\phi''_r - 264\phi''_{r-1} + 159\phi''_{r-2} - 38\phi''_{r-3}\right]$$

INTERPOLATION

$$(C\phi'')_{r+1} = (C\phi'')_r + \frac{h}{24}\left[9(C\phi'')'_{r+1} + 19(C\phi'')'_r - 5(C\phi'')'_{r-1} + (C\phi'')'_{r-2}\right]$$

$$\phi'_{r+1} = \phi'_{r+1} + \frac{h}{24}\left[9\phi''_{r+1} + 19\phi''_r - 5\phi''_{r-1} + \phi''_{r-2}\right]$$

$$\phi_{r+1} = \phi_r + h\phi'_r + \frac{h^2}{360}\left[38\phi''_{r+1} + 19\phi''_r - 5\phi''_{r-1} + \phi''_{r-2}\right]$$

$$\phi_{r+1} = \phi_r + h\phi'_r + \frac{h^2}{360}\left[38\phi''_{r+1} + 171\phi''_r - 36\phi''_{r-1} + 7\phi''_{r-2}\right]$$

The starting procedure consists of a series of Taylor's formulae of increasing step size starting with step size $h/16$ and building up to the establishment of four values spaced at h, where h is the appropriate step size in η. The intricacy of this procedure is necessary if accuracy

of the Falkner Adams scheme is to be preserved at the beginning. A detailed description of these starting formulae and the accuracy requirements can be found in [5].

The stability and convergence of the application of the predictor-corrector pair must be established. A discussion of the derivation of the formulae can be found in [4]. An interpretation of the error growth is given by Collatz and the applicable theory restated here.

Error bounds can be established for a repeated series of formulae if the problem being solved satisfies a Lipschitz condition on the convex domain of solution D. The nonlinearity of the problem and the nature of solutions for some boundary values will actually prevent the problem from satisfying a Lipschitz condition in most cases; however the method of error prediction used in this type of numerical solution will be outlined in order to illustrate how and why difficulties occur.

If the n-th order equation

$$y^{(n)} = f(x,y,y',\ldots,y^{(n-1)})$$

satisfies a relation

$$|f(x,y,y',\ldots,y^{(n-1)}) - f(x,y^*,y^{*\prime},\ldots,y^{*(n-1)})| \leq \sum_{v=0}^{n-1} k_v |y^{(v)} - y^{*(v)}|$$

for all pairs

$$(x,y,y',\ldots,y^{(n-1)}),\ (x,y^*,y^{*'},\ldots,y^{*(n-1)})$$

in D (the K_ν are often regarded as

$$K_\nu = \left|\frac{\partial f}{\partial y^{(\nu)}}\right|_{\max \text{ in } D}$$

$\nu = 0, 1, 2, \ldots, n-1$) , then if D is a space containing solutions and approximations to those solutions, an idea can be obtained as to the rate of error growth.

Repeated uses of the corrector can be shown to converge under the Lipschitz condition and by suitably restricting the step size. Clutter and Smith point out that on experimental investigation one use of the corrector leads to convergence within their tolerance at a reasonable stepsize. They choose therefore to ignore the problem of convergence. It remains to investigate the stability of the process and the growth of truncation error.

Consider the error $e_{r+1}^{(m)}$ in the mth derivative of y at x_{r+1}:

$$e_{r+1}^{(m)} = y_{r+1}^{(m)} - y^m(x_{r+1})$$

this is given by

$$e_{r+1}^{(m)} = \sum_{\nu=0}^{n-m-1} \frac{h^\nu}{\nu!} e_r^{(m+\nu)} - R^*_{n-m,p+1}$$

$$+ h^{n-m} \sum_{\sigma=0}^{p} \beta^*_{n-m,\sigma,p} \left(f_{r+1-\sigma} - F(x_{r+1-\sigma})\right)$$

by the Lipschitz condition

$$|e_{r+1}^{(m)}| - h^{n-m} \sum_{v=0}^{n-1} K_v B_{n-m,o,p} |e_{r+1}^{(v)}| \leq e_m \quad . \quad . \quad . \quad . \quad (1)$$

or, as Collatz writes it,

$$|e_{r+1}^{(m)}| \leq \sum_{v=0}^{n-m-1} \frac{h^2}{v!} |e_r^{(m+v)}| + h^{n-m} \sum_{\sigma=0}^{p} \sum_{v=0}^{n-1} |\beta^*_{n-m,\sigma,p}| K_v |e_{r+1-\sigma}^{(v)}|$$

$$+ |R^*_{n-m,p+1}|$$

where

$$e_m = \sum_{v=0}^{n-m-1} \frac{h^v}{v!} |e_r^{(m+v)}| + h^{n-m} \sum_{\sigma=1}^{p} \sum_{v=0}^{n-1} K_v |\beta^*_{n-m,\sigma,p}| |e_{r+1-\sigma}^{(v)}|$$

$$+ |R^*_{n-m,p+1}|$$

Upper bounds are known for e_m provided they are known for the previous absolute errors $|e_r^{(m)}|$, $|e_{r-1}^{(m)}|$, etc. Consider the n equations for $e_{r+1}^{(m)}$ (that is, the formulae for all the different order derivatives). This system will provide a systematic error estimation process if the coefficient matrix on the left-hand side is monotonic (a matrix A is monotonic if it is such that when $(Az)_i \geq 0$ then $z_i \geq 0$ for all elements I for all real vectors $\vec{z}$), because in the case that it is monotonic, the solution can be bounded above.

That is, if A represents the coefficient matrix and if an approximation to $\vec{e}_{r+1}$ can be found such that

$$(A\bar{v})_i \geq (A\bar{e}_{r+1})_i$$

then

$$(\bar{v})_i \geq (\bar{e}_{r+1})_i$$

Collatz shows that A is monotonic if the step size h is chosen so that the diagonal elements of

$$\begin{bmatrix} d_{00} & d_{01} & \cdots & d_{0,n-1} \\ d_{10} & d_{11} & \cdots & \\ \vdots & & & \\ d_{n-1,0} & d_{n-1,1} & & d_{n-1,n-1} \end{bmatrix} \begin{bmatrix} e_{r+1}^{(0)} \\ e_{r+1}^{(1)} \\ \vdots \\ e_{r+1}^{(m)} \\ \vdots \\ e_{r+1}^{(n-1)} \end{bmatrix} \leq \begin{bmatrix} e_0 \\ e_1 \\ \vdots \\ e_m \\ \vdots \\ e_{n-1} \end{bmatrix}$$

$$d_{ij} = -h^{n-i} K_j \beta_{n-j,p} \qquad i \neq j$$

$$d_{ii} = 1 - h^{n-i} K_i \beta_{n-i,p}$$

$$d_{mm} = 1 - h^{n-m} K_m \beta_{n-m,p}$$

are such that

$$h^{n-m} < 1/(K_m \beta_{n-m,p})$$

Then we can write

$$Y_{r+1}^{(m)} - h^{n-m} \sum_{v=0}^{n-1} K_v \beta_{n-m,p} \, Y_{r+1}^{(v)} = E_m$$

where $|Y_r^{(m)}| \geq |e_r^{(m)}|$

and

$$E_m = \sum_{v=0}^{n-m-1} \frac{h^v}{v!} Y_r^{(m+v)} + h^{n-m} \sum_{\sigma=1}^{p} \sum_{v=0}^{n-1} K_v |\beta^*_{n-m,\sigma,p}| Y_{r+1-\sigma}^{(v)}$$

$$+ |R^*_{n-m,p+1}|$$

Such an expression is tedious to apply recursively. A more convenient guide to the growth of error can be obtained by applying a standard technique to solve the difference equations for the error terms. That is, a particular solution is added to a homogeneous solution of the form

$$Y_r^{(m)} = C_m z^r$$

A particular solution is

$$Y_r^{(m)} = \gamma_m = \text{constant}$$

where the C_m are determined by

$$C_m z^p - h^{n-m} \left(\sum_{v=0}^{n-1} K_v C_v \right) \left(\sum_{\sigma=0}^{p} |\beta^*_{n-m,\sigma,p}| z^{p-\sigma} \right)$$

$$- z^p - h^{n-m} \left(\sum_{v=0}^{n-m-1} \frac{h^v}{v!} C_{m+v} \right) = 0$$

The region where error growth is bounded is the region where these equations have a nontrivial solution. This region is defined where the coefficient matrix for the vanishes. If the equations under present study are concerned the system will take the form, where n=3, p=3, m=0, 1, 2

$$C_m z^p - \left(h^{3-m} \sum_{v=0}^{n-1} K_v C_v \right) \left(\sum_{\sigma=0}^{3} |\beta^*_{3-m,\sigma,3}| \; z^{3-\sigma} \right|$$

$$- z^2 \sum_{v=0}^{z-m} \frac{h^v}{v!} C_{m+v} \neq 0$$

Now as stated in terms of backward differences in their early paper [28] Clutter and Smith are using the Adams interpolator and the above theory is applicable. In their later paper [5] a method closely linked to the Adams interpolator but not identical to it is stated in terms of the Lagrangian form. After the calculation of ϕ''_{r+1} in terms of ϕ'''_{r+1}, the lower order derivatives are calculated in terms of ϕ'' instead of ϕ'''. A study of the error growth in line with that above for a second-order problem could be done instead of for a third order problem consistently, but the Lipschitz condition would then have to be applied to ϕ'', which quantity is to be calculated at each step.

The conditions for the determinant to vanish in the second-order problem are

$$0 = z^{p+1} - 2z^{p} + z^{p-1} - z(h^2 K_o \sum_{\sigma=o}^{3} |\beta^*_{3,\sigma,3}| z^{3-\sigma}$$

$$+ h K_1 \sum_{\sigma=0}^{3} |\beta^*_{2,\sigma,3}| z^{3-\sigma}) + h^2 K_o \sum_{\sigma=0}^{3} |\beta_{3,\sigma,3}| z^{3-\sigma}$$

$$+ h K_1 \sum_{\sigma=0}^{3} |\beta^*_{2,\sigma,3}| z^{3-\sigma} - h^2 K_o \sum_{\sigma=0}^{3} |\beta^*_{2,\sigma,3}| z^{3-\sigma}$$

$$\beta^*_{3,0,3} = \frac{38}{360} \quad \beta^*_{3,1,3} = \frac{171}{360} \quad \beta^*_{3,2,3} = \frac{-36}{360} \quad \beta^*_{3,3,3} = \frac{7}{360}$$

$$\beta^*_{2,0,3} = \frac{9}{24} \quad \beta^*_{2,1,3} = \frac{19}{24} \quad \beta^*_{2,2,3} = \frac{-5}{24} \quad \beta^*_{2,3,3} = \frac{1}{24}$$

and the roots z can be found as functions of the Lipschitz constants K_o, K_1 for ϕ, ϕ'. The general solution of the difference equation for $y_r^{(m)}$ will become dominated by the root largest in absolute value as r becomes large, and thus this root provides a guide to the growth of error. Such an analysis using the formulae of Clutter and Smith takes no account of the boundedness of ϕ'', however, nor can it govern the error growth in ϕ'' at the first step in the interpolation. All that can be said is that assuming the existence of K_2 throughout the process the error in ϕ and ϕ' will grow approximately as $|Z|^r$ where Z is the largest root of the above process.

It should be noted that in regions where there are singularities in the flow, that is where ϕ and ϕ' become unbounded, the error will have unbounded growth as expected.

It has been found that the solutions can be extremely sensitive to initial conditions for some values of physical parameters in the equations. This is the problem of inherent instability of the differential equations. In such cases the approach of Clutter and Smith to the problem breaks down as the shocting method needs final values of ϕ'' within some finite range to allow interpolation. The situation is aggravated if small increments in x are desired (see Chapter Two). The most effective approach to the problem of instability of the equations in such cases seems to be linearization of the equations; this approach is discussed in Chapter Six.

The question as to the presence of partial instability in the finite difference equations is not so easy to answer. Clutter and Smith find that with too large a stepsize with some flows they are not able to obtain meaningful results. They attribute this to growth of truncation error. Certainly according to their results there does not seem to be a sudden threshhold in increasing step size where there is sudden growth of round-off error.

There appear to be two investigations of alternative methods of integration of the equations. Jaffe and Okamura

[12] suggest the use of Runge- Kutta integration for third-order differential equations. Jaffe and Thomas [14] use the radically different approach of Chebyshev integration on a linearized version of the problem. The latter technique is discussed as a separate topic in Chapter Six.

Runge-Kutta integration is well-known. The procedure used by Jaffe and Okamura is taken from Collatz's book [4] and is outlined below.

x	y	$hy' = v_1$	$\frac{h^2}{2}y'' = v_2$	$\frac{h^3}{6}f(x,y,\frac{v_1}{h},\frac{2v_2}{h^2})$	
x_0	y_0	v_{10}	v_{20}	k_1	k
$x_0 + \frac{1}{2}h$	$y_0 + v_{10}/2 + v_{20}/4 + k_1/8$	$v_{10} + v_{20} + \frac{3}{4}k_1$	$v_{20} + \frac{3}{2}k_1$	k_2	k'
$x_0 + \frac{1}{2}h$	$y_0 + v_{10}/2 + v_{20}/4 + k_1/8$	$v_{10} + v_{20} + \frac{3}{4}k_1$	$v_{20} + \frac{3}{2}k_2$	k_3	k''
$x_0 + h$	$y_0 + v_{10} + v_{20} + k_3$	$v_{10} + 2v_{20} + 3k_3$	$v_{20} + 3k_3$	k_4	
$x_1 = x_0 + h$	$y_1 = y_0 + v_{10} + v_{20} + k$	$v_{11} = v_{10} + 2v_{20} + k'$	$v_{21} = v_{20} + k''$		

$$k = \frac{1}{20}(9k_1 + 6k_2 + 6k_3 - k_4), \quad k' = k_1 + k_2 + k_3$$

$$k'' = \frac{1}{2}(k_1 + 2k_2 + 2k_3 + k_4)$$

The main advantage of Runge Kutta integration is that stepsize can be changed easily without interpolation on previous steps as it is a one-step method. According to Jaffe and Okamura this property is valuable as even under the transformed version of the equation the thickness of the boundary layer begins to change significantly in flows where integration proceeds far downstream. They can also economise on calculations by making use of the fact that as

increases away from the body changes in the dependent variables become less rapid and therefore the step size can be increased. In their application of the integration formulae they include a means of testing these rates of change as integration proceeds at each x station and automatically adjusting the step size.

There are two main disavantages of the Runge-Kutta type of process. In the first place, there are frequent function evaluations (in a fourth-order method, four to each step). Secondly, there is a lack of systematic truncation error estimation.

Some indication of the size of the truncation error can be obtained by performing two integrations of different step size in parallel and using the fact that the method is of fourth order. Over a large number of steps it may be assumed the rate of change of the error growth is dominated by that of the highest order derivative. Then if integration is performed with step sizes h and 2h the following estimation may be made.

At each step, an error of order h^5 is made (agreement with a Taylor's series up to the fourth order term is assured, where the expansion is around the previous point). At the point $\eta = \eta_0 + 2nh$ reached in 2n steps of size h the error of truncation is $A(2n)h^5$ where A is some constant. Then at the same point $\eta_0 + 2nh$ reached in n steps with step size

$2h$ the error of truncation is $A(\eta)(2h)^5$. Then, if the process is being reasonably accurate,

$$\phi''(\eta) \simeq \tilde{\phi}''_{h,2n} - A.2nh^5 \simeq \tilde{\phi}''_{2h,n} - A.n.2^5h^5$$

where $\phi''_{h,2n}$, $\phi''_{2h,n}$ are the approximations obtained by the two integrations. Now

$$(A)(2n)(h^5) = A(2nh)h^4 = A(\eta-\eta_o)h^4$$

$$(A)(2^5n)(h^5) = A(2nh)2^4h^4 = A(\eta-\eta_o)2^4h^4$$

so

$$A(\eta-\eta_0)h^4 \simeq \frac{\tilde{\phi}''_{h,2n} - \phi''_{2h,n}}{2^4 - 1}$$

and

$$\phi''(\eta) \simeq \tilde{\phi}''_{h,2n} - \frac{\phi''_{2h,n} - \tilde{\phi}''_{h,2n}}{2^4 - 1}$$

Thus the error at each value of η should be approximately one-fifteenth of the difference between integrations performed with step size h and step size 2h. A check on the reliability of the process can be maintained throughcut by maintaining two concurrent integrations.

The use of Merson's variant of the Runge-Kutta process may be considered. The trouble is that when nonlinearities are present, the process of performing one extra calculation

in each step and using a comparison between it and the estimate of the point of interest to estimate the error has been shown to consistently over-estimate the error. This drawback makes the method unsuitable for the problem at hand where changes in step size should not be necessary frequently and reaction to changing conditions should not be over-sensitive.

The remarks that have been made about integration procedures in this chapter have centred on the treatment of the momentum equation. The same methods of integration have been used in most cases for the energy equation. In any case, since the energy equation is linear, the success of the process will be governed by the success with the nonlinear momentum equation [28, 5].

CHAPTER FOUR

THE MOMENTUM EQUATION

The solution of the nonlinear momentum equation is complicated by the fact that the initial value set is not complete. $\phi''(x,0)$ is not specified. The technique Clutter and Smith [5] introduce to deal with this situation consists of a process of shooting to obtain bracketting values of one of the final conditions within a certain range and then using interpolation to converge on the correct trajectory.

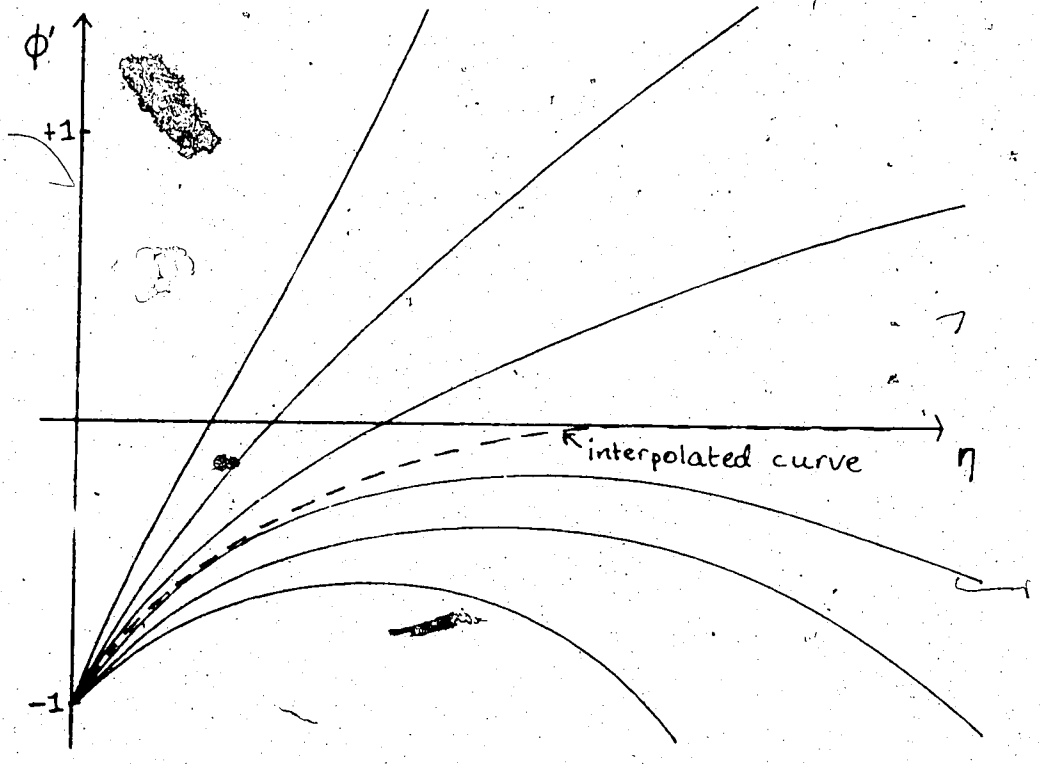

FIGURE III: Trial Values of $\phi''(x(N),0)$

Problems arise in the application of this method. In some cases, small changes in the starting values for trial trajectories lead to large changes in the resultant curves [12,29], as can be seen in Figure III. Sometimes these changes are unmanageably large due to instability of the differential equations with certain values of the physical parameters. Even when the equations are not so unstable the difference between bracketting solutions may be too large for the Lagrange interpolation used to be meaningful. Clutter and Smith [29] try to deal with this latter situation by stopping integration before the trajectories diverge too much, and repeating the process in the hope that the trajectory will gradually extend outwards to the full range of η as the correct solution is approached. In a later modification the use of 'mid-course corrections' is proposed as trajectories start to diverge. The problem is then treated as a new initial value one and interpolation done on the final trajectory segments of the resultant bracketting solutions.

Jaffe and Okamura [12] attempt to improve the situation by introducing a form of quadratic convergence to the final trajectory. They introduce the function

$$\Omega_{w,\eta}(\phi_n) = W_1(\phi_n')^2 + W_2(\phi_n'')^2 + W_3(\phi_n''')^2$$

at integration step n, where W_1, W_2 and W_3 are weights. Now at the edge of the boundary layer ϕ' is explicitly zero and the other quantities implicitly tend to zero, so W_1 is made large in comparison to W_2 and W_3. Then the minimum of the

function Ω is equal to zero, and the location of this minimum will yield the desired values of ϕ', ϕ'', and ϕ'''. Then $\phi''(x,0)$ can be improved to yield these values by a process of quadratic interpolation. The authors find that this process is rapidly convergent for problems where ϕ' is such that it is monotonically increasing to zero.

Any interpolation method is dependent on finding bracketting values of the desired solution within a reasonable range; the variations proposed can accelerate this search but they cannot eliminate the cases where inherent instability is present. It is to this end that Jaffe and Thomas [14] developed the idea of linearizing the equation. The solution of the problem in terms of the difference between succeeding trajectories in a quasi-linearization iteration means that smaller variations in the numbers concerned may be encountered in situations where instability is not extreme. However, once the problem can be treated as a linear one the need for shooting can be eliminated entirely by treating both endpoints as fixed and solving the trajectory as a system of linear algebraic equations. The one condition that has to be met is that the initial trajectory be 'sufficiently close' to the final one to ensure convergence of the quasilinearization process. Jaffe and Thomas appear to find this condition easier to meet than it is to overcome the problems involved with the more conventional approach of shooting. The

quasilinearization approach is dealt with in Chapter Six.

CHAPTER FIVE

THE ENERGY EQUATION: SUPERPOSITION OF SOLUTIONS

The energy equation can be treated as linear problem in ψ alone once ϕ, ϕ' and ϕ'' are considered supplied by the current solution of the momentum equation [28]. The integration formulae are discussed in Chapter Three. The boundary conditions are

$$\eta = 0: \quad \text{either } \psi(0,x) = g(x) \text{ or } \psi'(0,x) = g'(x)$$

$$\eta \to \infty: \quad \psi \to 0 \quad \text{or} \quad \psi' \to 0$$

Linear problems of this nature can be solved by constructing a linear combination of the solutions of two other problems. Clutter and Smith [28] and later authors [11,12,13] use this technique.

Suppose ψ_0 is given. Integrate with arbitrary $\psi_0' = \psi_{w1}'$ to obtain ψ_1', ψ_1. If ψ'' is greater than zero at the edge of the boundary layer, subtract a quantity from the arbitrary starting condition to obtain ψ_{w2}' and integrate to obtain ψ_2. Then calculate A,B such that

$$A\psi_1' + B\psi_2' = A\psi_1 + B\psi_2 = 0$$

at the edge of the boundary layer, and

$$A + B = 1, \quad B = 1 - A$$

Then since

$$\psi_{w,1} = \psi_{w,2} = \psi_w \equiv \psi(x,0)$$

then $$\psi = A\,\psi_1 + B\,\psi_2$$

and $$\psi' = A\psi_1' + B\psi_2'$$

will satisfy all boundary conditons.

A parallel procedure is followed if $\psi'(x,0)$ is given.

Once both ψ and ϕ are known, fluid properties along the constant x line can be updated. Iteration on the energy equation can be performed improving these fluid properties until desired convergence criteria are fulfilled. Then the newest fluid property values can be fed to the momentum equation and the entire double loop perfcrmed again until a final set of ccnvergence criteria is met for the x station.

Various authors [11, 3] have inserted other linear equations describing phenomena in special flows (for example, gas injection into the boundary layer), either in place of or coupled with the energy equation. The treatment of such equations is identical to that of the energy equation.

Any technique for solving "linear" ordinary differential equations could have been used in the solution of the energy equation. These techniques do not affect the fundamental nature of the Clutter and Smith [28,5] method

for solving the coupled equations, nor can a different choice of integration method for the energy equation avoid the problems that arise due to the nature of the momentum equation and its boundary values. A method of solution for both equations using a series expansion will be discussed in Chapter Seven, and this technique will be found to take full advantage of a linearized form of both equations.

CHAPTER SIX

QUASILINEARIZATION AND THE HARTREE-WOMERSLEY TECHNIQUE

The use of quasilinearization in the approximate solution of differential systems originated in the theory of dynamic programming [1, 16, 25]. The formulations most familiar to the numerical analyst are those of the Newton-Raphson and Kantorovich approximation techniques. The aim of the quasilinearization method is to set up an iterative process on a linear problem which approximates to the original nonlinear problem in the sense that the solution of the linear problem is a satisfactory approximation to the solution of the original problem. Then at each step in the iteration procedures suitable for linear problems may be used. The question of the validity of the resultant convergent solution must be investigated.

Any high-order differential equation can be considered as a system of first-order differential equations. Consider therefore the system

$$\dot{\vec{U}} = \vec{F}(\vec{U}, t)$$

where $\vec{U}$ is the 'state vector' or set of dependent variables and in this case t is the only independent variable. Let the boundary conditions be

$$\vec{G}_1(\vec{U})_{t=0} = 0 \ , \quad \vec{G}_2(\vec{U})_{t=T} = 0$$

Let $\vec{U}(1)$ be an initial guess to the solution of the system. Then $F(\vec{U}, T)$ can be expanded around $\vec{U}(1)$ in a Taylor series truncated after the linear term:

$$\bar{F}(\bar{u},t) = \bar{F}(\bar{u}_1,t) + J_1(\bar{F})\ (\bar{U} - \bar{U}_1) \ . \ . \ . \qquad (1)$$

where

$$J_1(\bar{F}) = \left(\frac{\partial F_j}{\partial U_i}\right)_{\bar{U}=\bar{U}_1}$$

where the indices I and j mean the ith and jth elements of the vectors F and U respectively.

Now it is desired to obtain a second approximate solution, $\vec{U}(2)$, which is closer to the real solution $\vec{U}$ than was $\vec{U}(1)$. This can be achieved by setting $\vec{U}$ equal to $\vec{U}(2)$ in (1) and forcing

$$\bar{F}(\bar{U}_2,t) = \dot{\bar{U}}_2$$

then

$$\dot{\bar{U}}_2 \simeq \bar{F}(\bar{U}_1,t) + J_1(\bar{F})\,(\bar{U}_2-\bar{U}_1)$$

an iterative process can then be set up of the form

$$\dot{\bar{U}}_N = \bar{F}(\bar{U}_{N-1},t) + J_{N-1}(\bar{F})\,(\bar{U}_N-\bar{U}_{N-1})$$

Since at each stage in the iteration the solution depends on a two-point boundary problem, it must be shown that this sequence exists; if it does exist, it is necessary

to examine its convergence and determine whether its limit is indeed the solution of the original problem.

The linear iterative scheme may be written

$$\dot{\bar{U}}_N - J_{N-1}\bar{U}_N = \bar{F}(\bar{U}_{N-1},t) - J_{N-1}\,\bar{U}_{N-1}$$

This is a linear first-order ordinary differential equation in the unknown $U(n)$ which has the general formal solution

$$\bar{U}_N = \exp\left(\int_0^T J_{N-1}dt\right)\left[\int_0^T(\bar{F}(\bar{U}_{N-1},t) - J_{N-1}\,\bar{U}_{N-1})\right.$$
$$\left.\exp\left(\int_0^T - J_{N-1}\,dt_1\right)dt + C_N\right]$$

where $c(n)$ is chosen so that the boundary conditions are satisfied.

Set $$\max_{||\bar{U}||\le 1} \max(||\bar{F}||,\ ||J||) = m$$

and $$\min_{||\bar{U}||\le 1} ||J|| = m_1$$

then

$$||\bar{U}_N|| \le \exp(mT)\left[\int_0^T(m + m||\bar{U}_{N-1}||)\exp(-m_1T)\,dt + C_N\right]$$

A sufficient condition for a convergent sequence to be obtained from this relation is

$$||\bar{U}_{N-1}|| \le 1$$

for all n. Then

$$||\vec{U}_N|| \leq \exp(mT)\,(2m.\int_0^T \max_{0\leq t_1\leq T} (\exp(-m_1 t_1))\,dt + C_N)$$

$$= \exp(mT)\,(2mT + C_N)$$

then if

$$m_2 = \max_{0\leq t\leq T} ||\vec{U}_N||$$

$$m_2 \leq e^{mT}(2mT + C_N)$$

for

$$m_2 \leq 1, \quad e^{-mT} \leq 2mT + C_N$$

thus, sufficient conditions for a convergent sequence to exist are

1) $\vec{a}$ to exist and be bounded

2) $\vec{U}(1)$ to be chosen so that

$$||\vec{U}_1|| \leq 1$$

3) T to obey

$$e^{-mT} \leq 2mT + C_N$$

The sequence can be shown to be monotonic as well as convergent.

The problem can usefully be rephrased in terms of the difference between succeeding approximations in the quasilinearization algorithm:

$$\vec{e}_N = \vec{U}_N - \vec{U}_{N-1}$$

with boundary conditions

$$\vec{e}_N = \vec{0} \qquad (t = 0, \quad t = T)$$

and the above discussion may be followed for the unknown $\vec{e}_N$. The latter treatment is valuable in investigating the rate of convergence of the sequence and in determining the limit point. Thus

$$\dot{\vec{U}}_{N+1} - \dot{\vec{U}}_N = \vec{F}_N - \vec{F}_{N-1} + J_N(\vec{U}_{N+1} - \vec{U}_N) - J_{N-1}(\vec{U}_N - \vec{U}_{N-1})$$

or

$$\dot{\vec{e}}_{N+1} = \vec{F}_N - \vec{F}_{N-1} + J_N \vec{e}_{N+1} - J_{N-1} \vec{e}_N$$

then

$$\vec{e}_{N+1} = \exp\left(\int_0^T J_N dt\right) \left[\int_0^T (\vec{F}_N - \vec{F}_{N-1} - J_{N-1} \vec{e}_N) \left(\exp \int_0^T - J_N dt_1\right) dt\right]$$

where $c(n)=0$ as the boundary conditions are of the form

$$\vec{e}_{N+1} = 0 \qquad \text{at} \qquad t = 0, \quad t = T$$

The mean-value theorem applied in vector form yields

$$\vec{F}_N - \vec{F}_{N-1} - J_{N-1}\vec{e}_N = \frac{1}{2} (\vec{e}_N)^T H_N(\bar{\theta}) \vec{e}_N$$

where $H(n)$ represents the Hessian tensor of second derivatives applied at a point in the interval $[\vec{U}(n-1), \vec{U}(n)]$ (element-by-element). Now

$$\max_{||\vec{U}|| \le 1} ||\tfrac{1}{2}(\vec{e}_N)^T H_N(\bar{\theta}) \vec{e}_N|| \le \frac{1}{2} (\max||\vec{e}_N^T||).K.(\max||\vec{e}_N||)$$

$$= \frac{1}{2} K \, ||\vec{e}_N||^2_{max}$$

where $K = \max_{||\vec{U}|| \le 1} ||H_N(\bar{\theta})||$

so

$$||\vec{e}_{N+1}|| \leq T \exp(mT) \int_0^T \frac{K}{2} (\max||\vec{e}_N||)^2 \, dt$$

$$= \frac{KT^2}{2} \exp(mT) (\max||\vec{e}_N||)^2$$

Thus the rate of convergence of the sequence of approximations is quadratic.

By a process of inductive reasoning it can be seen that

$$||\vec{e}_{N+1}|| \leq [\frac{KT^2}{2} \exp(mT)]^{2^N-1} (\max||\vec{e}_2||)^{2N} \ldots$$

where

$$\vec{e}_2 = \vec{U}_2 - \vec{U}_1$$

Convergence therefore depends on the quantity

$$\frac{KT^2}{2} \exp(mT) \max_{0\leq t\leq T} ||\vec{e}_2||$$

This quantity can be made less than 1 if either T is small enough or $\max_{0\leq t\leq T} ||\vec{e}_2||$ is small enough. Thus a proper choice of the initial approximation can be sufficient to ensure a quadratic rate of convergence.

If the convergence condition above is met, then the sequence of approximations $\vec{U}(n)$ has limit point C. It follows that $\vec{U}(n)$ approaches $\vec{U}(n-1)$ and

$$\dot{\vec{U}}_N = \vec{F}(\vec{U}_{N-1},t) + J_{N-1}(\vec{U}_N - \vec{U}_{N-1})$$

becomes

$$\dot{\vec{U}}_N = \vec{F}(\vec{U}_N,t) - \vec{F}(\vec{U}_{N-1},t)$$

or

$$\vec{U}_N = \vec{U}$$

The quasilinearization process is particularly appropriate when used in conjunction with the Hartree-Womersley technique [9], because at each x-value except the first an initial approximation is available from the preceeding station. Not only that, but the initial solution is known to be within a certain tolerance of the actual solution dependent on the x derivatives. For example,

$$(\emptyset)_{x=x(m)} = (\emptyset)_{x=x(m-1)} + \left(\frac{\partial \emptyset}{\partial x}\right)_{m-1} (x_m - x_{m-1}) + O(\Delta x)^2 \quad (3)$$

similarly for the other unknowns.

What this means in practice is that a bound can be put on the quantity

$$||\vec{U} - \vec{U}_1|| \geq ||\vec{U}_2 - \vec{U}_1|| = ||\vec{e}_2|| \qquad \text{by monotonicity}$$

It would be possible, indeed, to ensure convergence by keeping running estimates of the relevant quantities in equation (2) and calculating as many terms as required in equation (3). Coincident with a decision to keep such a running check on convergence would be a decision as to the appropriate kind of norm to use. A situation which would make such a process valuable would be, for example, the approach to a point of separation in the boundary layer equations. The x-array could be manipulated as well as all the other quantities involved in the convergence criteria in order to guarantee convergence and the validity of results. Problems with the use of smaller increments of x as

discussed in Chapter 2 are avoided when Chebyshev integration is used, showing again the power of the combined techniques.

The running calculations involved are as follows:

(a) suppose H and J are known on line m. Estimate them on line m+1 by element-wise Taylor expansion. (since the elements of these matrices will consist of multiples and combinations of the coefficients and unknowns $\vec{U}$ this is possible).

(b)

Ensure

$$\max_{0\le t\le T} \; ||\vec{e}_2|| \le ||\vec{U} - \vec{U}_1|| \le \frac{2}{KT^2} \exp(-mT)$$

by choice of $\vec{U}(1)$ through equation (3) and/or choice of $x(m)-x(m-1)$.

Once a quasilinearized form of the equations has been obtained the choice of a method of integration has to be reconsidered. The incomplete initial value set remains, and unless both boundaries are treated simultaneously a form of shooting must still be used. The use of the difference between trajectories as the dependent variable will reduce this problem as variation between different solutions for different initial values will be less, but the effect of this reduction is hard to predict.

A method of solution of a linearized form of the incompressible momentum equation has been described by

Cebeci and Smith[2]; it uses a finite difference scheme designed to take advantage of the nature of the incompressible problem and therefore has no application to the general problem. Other experimenters such as Radbill and McCue [25] describe the construction of solutions to this type of problem using any integration method for ordinary differential equations and superimposing homogeneous and particular solutions. The latter approach loses accuracy when the superimposed solutions are greatly different for small changes in the initial conditions; it has been demonstrated that this is precisely the difficulty with the present problem. It is imperative, therefore, that a form of solution which treats both boundaries simultaneously be selected. Such a requirement suggests a means of transforming the differential problem into a system of linear algebraic equations by means of a series solution.

The application of quasilinearization to the boundary layer equations combined with Chebyshev integration will be discussed in the following chapters. It should be added that in general nonlinear boundary conditons can be treated in exactly the same way as the nonlinear differential problem. Convergence to the actual boundary conditions follows in a similar manner.

CHAPTER SEVEN

THE USE OF CHEBYSHEV POLYNOMIALS IN INTEGRATION

At each step in the iteration of a quasilinearization process integration of a linear ordinary differential equation must be done. Although an analytic solution was presented in the previous chapter in order that convergence analysis might be done, this solution is not useful computationally.

In the problem under discussion one of the major difficulties has been the incomplete initial value set. Shooting is less risky using a quasilinearized form as differences between neighbouring trajectories are not so large when $\vec{e}$ is used instead of $\vec{U}$. It is more sensible, however, to take advantage of the linear form of the problem to the extent of using an integration technique which treats both boundaries at once. Superposition of solutions as discussed in Chapter Five might be used, but once again the accuracy of the multipliers would be called into question if a degree of inherent instability were present. Jaffe and Thomas [14] have suggested a method for the incompressible momentum equation which converts the problem into a system of linear algebraic equations, thus treating all boundary conditions simultaneously. Other interesting features of the method will be discussed. Their choice of integration technique involves expressing the dependent variables in terms of Chebyshev polynomials. In order to discuss this

choice of procedure a brief outline of approximation theory will be given.

Numerical analysis is a discipline which attempts to describe mathematical functions, which are defined either explicitly or implicitly, as a simple computational problem for various values of their independent variables. Such a description may consist of tables of values or, more economically, of an approximation function which is easily evaluated for given arguments and which has known deviation over the range of interest.

A differential equation is an implicit means of defining a function or functions. Conventional step-by-step integration builds up a table of values which describes the function at discrete values of the independent variable(s). Error in the table is cumulative, and the value of a function at an arbitrary point not in the table must be obtained by interpolation, wherein further error is introduced. These conditions are acceptable if enough is known about the error. A different approach is to assume an appropriate approximate form for the solution in terms of an easily computed function of known deviational behavior and transform the differential problem into one of determining the parameters which will ensure a reasonable approximation.

The easiest approximational form in terms of computation is the polynomial. The most compact in a given

space is the orthogonal set of polynomials spanning that space. Then, if a theory of measure for the difference between functions in the space and members of the basis or linear combinations of members of the basis is defined, any function in the space may be represented non-redundantly in terms of the basis with known deviation. Given measure definition, the linear combination of basis members representing a function may be manipulated in order to minimize the difference in some sense. That is, if f is represented by

$$f(x) \approx a_1\phi_1(x) + a_2\phi_2(x) + \ldots + a_{n+1}\phi_{n+1}$$

the coefficients a(i) will depend on the definition of f and on some error criterion. The choice of norm will result in a certain set of orthogonal functions being used.

The Chebyshev polynomials are useful in numerical analysis because of their computational form, the error criteria they may be made to obey, and their applicability to a wide class of functions. Lanczos [18] is the father of modern interest in them. Since his re-discovery of their importance many researchers have investigated their application to approximation theory. A comprehensive book on their use is by Fox and Parker [8]. In this book the means of extending known results to differential problems is discussed. The relevant theory and properties of Chebyshev polynomials is outlined briefly below.

Suppose that the Chebyshev polynomials are defined by

$$T_n(x) = \cos((n-1)\theta), \quad \cos\theta = x, \quad -1 \le x \le 1$$

or equivalently

$$T_1 = 1 \quad , \quad T_2 = x$$

and the recursion relation

$$T_{r+1}(x) = 2x\,T_r(x) - T_{r-1}(x)$$

These polynomials obey the minimax criterion, that an approximation $p_n(x)$ of $f(x)$, where $e_n(x)=f(x)-p_n(x)$, should be such that $\max_{-1\le x\le 1} |e_n(x)|$ is a minimum for all possible representations in terms of combinations of polynomials. The Chebyshev polynomials may also be made to obey a least-squares criterion

$$\sum_{i=1}^{n+1} w(x_i)\, e_n^2(x_i) = \min, \quad \text{(discrete f)}$$

or

$$\int_{-1}^{1} w(x)\, e_n^2(x)\,dx = \min, \quad \text{(continuous f)}$$

where the weighting functions are

$$w(x) = (1 - x^2)^{-\frac{1}{2}}$$

Another property of the Chebyshev polynomial approximation is that, of all polynomial expansions expressed in terms of ultraspherical polynomials, it has the fastest and most universal convergence rate.

Evaluation of the coefficients for a function f involves expressions like

$$a_r = \frac{2}{n+1} \sum_{k=o}^{n} f(x_k)\, T_r(x_k), \quad \text{(discrete f)}$$

$$a_r = \frac{2}{\pi} \int_{-1}^{1} f(x)\, (1 - x^2)^{-\frac{1}{2}}\, T_r(x)\,dx, \quad \text{(continuous f)}$$

which, as given here, satisfy the least-squares error criterion. Where f is implicitly defined these expressions cannot be used. The coefficients must be calculated using other information. The differential system and knowledge of the differentiated form of a Chebyshev expansion may be used to set up a system of linear algebraic equations which may be solved for the coefficients.

In order that the differential equation may be represented as a system of algebraic equations all quantities that appear in it must be represented as Chebyshev series, and means of combining the expansions in products or quotients or in various other ways developed. This may not be a trivial task. The following chapter will illustrate the process as developed by Jaffe and Thomas [14], and the extension of the method to the more complex compressible equations will be discussed following that. A useful formula is that for the product of Chebyshev series:

$$f = \frac{a_1}{2} T_1 + \sum_{i=2}^{n} a_i T_i \qquad g = \frac{b_1}{2} T_1 + \sum_{i=2}^{n} b_i T_i$$

$$T_i \cdot T_j = \cos(i-1)\theta \cos(j-1)\theta = \frac{1}{2}[\cos(i+j-2)\theta + \cos(i-j)\theta]$$

$$= \frac{1}{2}[T_{i+j-1} + T_{|i-j|+1}]$$

$$f \cdot g = \left(\frac{a_1 b_1}{4} + \sum_{k=2}^{n} \frac{1}{2} a_k b_k\right) T_1 + \sum_{i=2}^{n} \left[\frac{a_i b_i}{2} + \sum_{k=2}^{n} \frac{a_k}{2} (b_{|k-i+1|}\right.$$

Various techniques for solving linear systems may be used tc obtain the Chebyshev coefficients. It should be borne in mind that at least part of the system, that dealing with the differentiation of a Chebyshev expansion, is upper triangular:

$$a'_{r-1} - a'_{r+1} = 2(r-1)\, a_r \qquad (2 \leq r \leq n)$$

$$a'_n = a'_{n+1} = 0$$

The solution of a finite set of equations for a truncated Chebyshev expansion involves a perturbed system and does not yield the leading terms of the infinite Chebyshev expansion. A method of estimating and partially eliminating the perturbation developed by Lanczos [18] and discussed by Fox and Parker [8] may be used but it means more calculation and in an iterative scheme such as quasilinearization may not be valuable. The alternative is to calculate succeedingly larger sets of equations and examine the sequence of coefficients for evidence of convergence of the expansion. The latter approach was used by Jaffe and Thomas .

A brief summary of the advantages of a coupling of the quasilinearization process with Chebyshev integration for the boundary layer equations will be given.

A) Quasilinearization allows the problem to be treated as a linear one.

B) Quasilinearization used in conjunction with the Hartree-Womersley technique [9] can ensure convergence to a solution where conditions on the various derivatives are satisfied.

C) The Chebyshev approach allows treatment of all boundary conditions at once, thus eliminating shooting.

D) The representation of solutions as Chebyshev expansions is compact compared to tabular values and rapidly convergent compared to other polynomial expansions.

E) Derivatives or integrals of given expansions are easily calculable.

F) Any evaluation of a solution for a given value of the independent variable is possible without interpolation.

G) Error bounds on solutions are calculable.

CHAPTER EIGHT

THE JAFFE-THOMAS TECHNIQUE FOR THE INCOMPRESSIBLE EQUATION

In 1970 Jaffe and Thomas [14] published a paper which solved the incompressible momentum equation using quasilinearization and Chebyshev integration. Their work serves as a practical illustration of the various procedures involved. If the equation is written as

$$f''' + P(1-f'^2) + Nff'' = x\left(f'\frac{\partial f'}{\partial x} - f''\frac{\partial}{\partial x}\right)$$

$$P = \left(\frac{x}{u_e}\right)\frac{du_e}{dx}$$

$$N = \frac{P+1}{2} + \frac{x}{r^k}\frac{dr^k}{dx}, \quad \begin{cases} k=0, & \text{2-dimensional} \\ k=1, & \text{axisymmetric} \end{cases}$$

with boundary conditions

$$f(x,0) = f'(x,0) = 0$$

$$f'(x,\eta_\infty) = 1$$

where the x derivatives are treated in the Hartree - Womersley manner as

$$\left(\frac{\partial f}{\partial x}\right)_N = af_N + bf_{N-1} + cf_{N-2} \qquad \left(\frac{\partial f'}{\partial x}\right)_N = af'_N + bf'_{N-1} + cf'_{N-2}$$

$$a = (x_N - x_{N-1})^{-1} + (x_N - x_{N-2})^{-1}$$

$$b = (x_{N-2} - x_N)/((x_N - x_{N-1})(x_N - x_{N-2}))$$

$$c = (x_N - x_{N-1})/((x_N - x_{N-2})(x_{N-1} - x_{N-2}))$$

then the quasilinearized form is

$$F_i = 0 = f_{i-1} + J_{i-1}\ (\bar{U}_i - \bar{U}_{i-1})$$

where

$$F(f''',f'',f',f) = 0 \quad , \quad \bar{U} = (f''',f'',f',f)^T$$

$$J = \left(\frac{\partial F}{\partial f'''} \quad \frac{\partial F}{\partial f''} \quad \frac{\partial F}{\partial f'} \quad \frac{\partial F}{\partial f}\right)$$

$$= (\ 1 \quad \alpha f+h \quad 2wf'-h' \quad \alpha f'')$$

$$\equiv (\ 1 \quad B \quad C \quad D)$$

$$\alpha = \frac{P+1}{2} + R + \Delta_1 \qquad h' = \Delta_2 f'_{N-1} + \Delta_3 f'_{N-2}$$

$$w = -(P+\Delta_1) \qquad \Delta_1 = ax \quad \Delta_2 = bx \quad \Delta_3 = cx$$

$$h = \Delta_2 f_{N-1} + \Delta_3 f_{N-2}$$

or, written in terms of

$$e_i^{(n)} = f_i^{(n)} - f_{i-1}^{(n)}$$

$$e_i''' + Be_i'' + Ce_i' + De_i + F_{i-1} = 0$$

Convergence on the iterative scheme may be expected

subject to conditions outlined in Chapter Six.

Now suppose that the solutions are of the form

$$e = \frac{a_1}{2} + \sum_{j=2}^{m} a_j T_j$$

$$e' = \frac{a'_1}{2} + \sum_{j=2}^{m-1} a'_j T_j$$

$$e'' = \frac{a''_1}{2} + \sum_{j=2}^{m-2} a''_j T_j$$

$$e''' = \frac{a'''_1}{2} + \sum_{j=2}^{m-3} a'''_j T_j$$

introducing (4m-6) unknowns.

Now $a'_{j-1} - a'_{j+1} + 2_j a_j = 0,\ j = 2,3,\ldots m \quad (a'_m = a'_{m+1} = 0)$

$a''_{j-1} - a''_{j+1} + 2_j a'_j = 0,\ j = 2,3,\ldots,m-1 \quad (a''_{m-1} = a''_m = 0)$

$a'''_{j-1} - a'''_{j+1} + 2_j a''_j = 0,\ j = 2,3,\ldots,m-2 \quad (a'''_{m-2} = a'''_{m-1} = 0)$

yielding 3m-6 equations.

Matching the coefficients for the polynomial $T(j)$, the resultant system of linear algebraic equations corresponding to the differential system is

$$\frac{a_1'''}{2} + \frac{a_1'' b_1}{4} + \sum_{j=2}^{m-3} \frac{a_j'' b_j}{2} + \frac{a_1' c_1}{4} + \sum_{j=2}^{m-3} \frac{a_j' c_j}{2}$$

$$+ \frac{a_1 d_1}{4} + \sum_{j=2}^{m-3} \frac{a_j d_j}{2} + \text{cheb}_1 (F_{i-1}) = 0$$

$$a_k''' + a_1'' \frac{b_k}{2} + \sum_{j=2}^{m-3} \frac{a_j''}{2} [b_{|j-k|+1} + b_{j+k-1}]$$

$$+ a_1' \frac{c_k}{2} + \sum_{j=2}^{m-3} \frac{a_j'}{2} [c_{|j-k|+1} + c_{j+k-1}]$$

$$+ a_1 \frac{d_k}{2} + \sum_{j=2}^{m-3} \frac{a_j}{2} [d_{|j-k|+1} + d_{j+k-1}]$$

$$+ \text{cheb}_k (F_{i-1}) = 0$$

$$k = 2,3,\ldots,m-3$$

yielding m-3 equations.

where $\text{cheb}_k (F_{i-1}) = \text{cheb}_k (F(\bar{U}_{i-1}))$

$$= \text{cheb}_k (F(\bar{U}_{i-2} + \bar{e}_{i-1}))$$

The number of equations is $3m-6+m-3=4m-9$. The boundary conditions give the remaining three equations needed for a completely determined solution and they take the form

$$e(-1) = \frac{a_1}{2} - a_2 + a_3 - \ldots (-1)^m a_m = 0$$

$$e'(1) = \frac{a_2'}{2} + a_2' + a_3' + \ldots + a_{m-1}' = 0$$

$$e'(-1) = \frac{a_1'}{2} - a_2' + a_3' + \ldots + (-1)^{m-1} a_{m-1}' = 0$$

Solution of the system can proceed for each cycle of the quasilinearization procedure given an initial solution. The following initial solution was found to work:

$$f(\eta) = \eta - \left(\frac{\eta_\infty}{5}\right)\left[1 - \left(1 - \frac{\eta}{\eta_\infty}\right)^5\right]$$

The results of Jaffe and Thomas have been duplicated both in order to correct their mistakes and as a basis for extension of the method to the compressible equation as the structure of solution is the same. It should be noted that Jaffe and Thomas obtain results which are comparable in accuracy and efficiency to both finite difference results and results obtained using Clutter and Smith's [5] methods. The advantages of storing solutions in polynomial form have already been discussed. The following chapter will be devoted to a discussion of the problems involved in extending the technique to the compressible equations.

CHAPTER NINE

EXTENSION TO THE COMPRESSIBLE EQUATIONS

The system consisting of the compressible equations, momentum and energy, may be quasilinearized in the same manner as the incompressible momentum equation. Indeed this has been done, as can be seen in references [1,25]. The equations may be written as

$$\Lambda(\phi''',\phi'',\phi',\phi,\pi',\pi,\psi) =$$

$$(C\phi'')' + T\frac{\rho_e}{\rho}C\phi'' - C_\infty P\left[\phi'^2+2\phi'+1-\frac{\rho_e}{\rho}\right] + C_\infty N(\phi+\eta)\phi''$$

$$- C_\infty x\left[(\phi'+1)\frac{\partial\phi'}{\partial x} - \phi''\frac{\partial\phi}{\partial x}\right] = 0$$

$$\Omega(\phi''',\phi'',\phi',\phi,\pi',\pi,\psi) =$$

$$\pi' + T\frac{\rho_e}{\rho} - C_\infty N(\phi+\eta)\psi' + C_\infty x\left[(\phi'+1)\frac{\partial\psi}{\partial x} - \psi'\frac{\partial\phi}{\partial x}\right] = 0$$

$$\pi = \frac{C}{P_r}\psi' + \frac{u_e^2}{H_e}C\left(1-\frac{1}{P_r}\right)(\phi'+1)\phi''$$

and then with the state vector

$$\vec{U} = (\phi''',\phi'',\phi',\phi,\pi',\pi,\psi)^T$$

the quasilinearized form is

$$\vec{F}(\vec{U}_N,\eta) = \vec{F}(\vec{U}_{N-1},\eta) + J_{N-1}(\vec{F})\,(\vec{U}_N - \vec{U}_{N-1})$$

$$\vec{F}(\vec{U},\eta) = \begin{bmatrix} \Lambda \\ \phi''' - (\phi'')' \\ \phi'' - (\phi')' \\ \phi' - (\phi)' \\ \Omega \\ \pi' - (\pi)' \\ \psi' - (\psi)' \end{bmatrix} = \vec{0}$$

where J takes the form

$$(J_{ij})_{N-1} = \frac{\partial F_i}{\partial U_j} \quad , \quad i = 1,2,\ldots 7 \ , \ j = 1,2,\ldots,7$$

Now since the terms $C, Pr, \rho e/\rho, T$ are not constants or functions of position but depend on the solutions or state vector, the Jacobian matrix must take this dependence into account. For instance,

$$\left(\frac{\partial \Lambda}{\partial \phi}\right)_{tot} = \left(\frac{\partial \Lambda}{\partial \phi}\right)_{explicit} + \frac{\partial \Lambda}{\partial C}\,\frac{\partial C}{\partial \phi} + \frac{\partial \Lambda}{\partial\left(\frac{\rho e}{\rho}\right)}\,\frac{\partial\left(\frac{\rho e}{\rho}\right)}{\partial \phi} + \ldots$$

Thus either the exact form of the dependence of these quantities must be known or some other means of updating the Jacobian at each step must be found. An alternative

approach is to treat these quantities as being constant at each step and updating them after a new solution is found without including the chain differentiation in the Jacob matrix. The effect of such a measure would be to slow do convergence of the quasilinearization algorithm an unpredictable amount.

A far greater difficulty in extending the Jaffe and Thomas [14] method to the compressible equations is that of expressing the fluid properties as Chebyshev series. As far as is known to the author this has not been attempted, although the desireability of doing so is great, in order to eliminate shooting. Problems arise, for example, in

$$C = \frac{(\frac{h_e}{h_{ref}})^{0.3329} - 0.020856}{(\frac{h}{h_{ref}})^{0.3329} - 0.020856}$$

Now

$$\frac{h}{h_{ref}} = (\psi+1)\frac{H_e}{h_{ref}} - (\phi'+1)^2 \frac{u_e^2}{u_\infty^2}\frac{u_\infty^2}{2h_{ref}}$$

can be expressed in terms of the Chebyshev expansions for ψ and ϕ', but an expression for the fractional powers of a Chebyshev series is not known. The above form of dependence of the fluid properties on the solutions was deduced from tables of experimental figures by Clutter and Smith [5].

One approach to the treatment of C, μ/ρ, P_r, etc. would help in the calculation of approximations of the chain derivatives (for example, $\frac{\partial C}{\partial \phi}$,). It provides a Chebyshev

expansion for all desired quantities in the most straightforward manner at the cost of spoiling the elegance and suitability of the method and adding extra computation. However the ability to eliminate shooting is the paramount consideration.

Suppose a new value of x is to be dealt with. Initial approximations to the state vector and fluid properties are available from the preceeding x station and they are assumed to be in Chebyshev form. Then one iteration of the quasilinearization scheme with the Jacobian matrix assuming constant fluid properties will yield a new state vector in Chebyshev form. Now new fluid properties in Chebyshev form must be obtained. The only possible way to do this seems to be to calculate the actual values of the relevant solutions at various values of η, use Cohen's formulae to get the fluid properties at those points, and then fit a Chebyshev interpolation polynomial to them.

The most accurate Chebyshev interpolating polynomial of degree n joining the points x(0), x(1), ..., x(n) is that calculated for x at the zeroes of the (n+1)th-degree Chebyshev polynomial T(n+2): The collocation points are

$$x_i = \cos\left(\frac{2i+1}{n+1}\,\frac{\pi}{2}\right) \qquad i = 0,1,\ldots,n$$

then

$$f(x) = \sum_{k=1}^{n+1} a_k T_k + e_{n+2}$$

where

$$a_1 = \frac{1}{n+1} \sum_{i=0}^{n} f(x_i)$$

and

$$a_k = \frac{2}{n+1} \sum_{i=0}^{n} f(x_i)\, T_k(x_i) \qquad k = 2,3,\ldots,n+1$$

The error is then of order $T(n+2)$.

One fact serves to compensate partly for the labour of additional computation at each quasilinearization step. Once the fluid properties have been updated according to the new state vector, two succeeding expansions of the fluid proerties are known. Then an approximation of the form

$$\left(\frac{\partial C}{\partial \phi'}\right)_N \simeq \left(\frac{\Delta C}{\Delta \phi'}\right)_N \qquad \Delta C = C_N - C_{N-1} \qquad \Delta \phi'_N = \phi'_N - \phi'_{N-1}$$

can serve to correct the Jacobian matrix and the proper accelerated form of the quasilinearization scheme can be used. The above approximation can be formed, as can expansions for quantities like T,

$$T = T_w / \left(1 + T_w \int_0^{\eta} \frac{\rho_e}{\rho}\, d\eta\right)$$

by use of a quotient formula for two Chebyshev series.

The quotient problem is equivalent to the inversion problem, for

$$g/_f = \frac{1}{f} \cdot g$$

therefore if

$$f(x) = \frac{a_1}{2} + \sum_{i=2}^{n} a_i\, T_i$$

a Chebyshev expansion for $1/f$ in terms of the a(i) is desired.

Now

$$\frac{1}{f} \cdot f = 1$$

so if

$$\frac{1}{f} = \frac{c_1}{2} + \sum_{i=2}^{n} c_i T_i$$

the product formula for Chetyshev series yields

$$\frac{1}{f} \cdot f = \left[\frac{c_1 a_1}{4} + \sum_{k=2}^{n} \frac{1}{2} a_k c_k\right] T_1$$

$$+ \left[\frac{c_1 a_k}{2} + \sum_{i=2}^{n} \frac{c_i}{2} (a_{|i-k|+1} + a_{i+k-1})\right] T_k = 1$$

$$\therefore \frac{a_1 c_1}{4} + \frac{1}{2}\left[\sum_{k=2}^{n} a_k c_k\right] = 1$$

$$\frac{a_k c_1}{2} + \sum_{i=2}^{n} \frac{c_i}{2} (a_{|i-k|+1} + a_{i+k-1}) = 0 \qquad k = 2,3,\ldots,n$$

These are equations of the form

$$\begin{bmatrix} \frac{a_1}{4} & \frac{a_2}{2} & \frac{a_3}{2} & \cdots & \frac{a_n}{2} \\ \frac{a_2}{2} & \frac{a_1+a_3}{2} & \frac{a_2+a_4}{2} & \cdots & \frac{a_{n-1}}{2} \\ \vdots & \frac{a_2+a_4}{2} & \frac{a_1+a_5}{2} & \cdots & \frac{a_{n-2}}{2} \\ \vdots & \vdots & & & \\ \frac{a_n}{2} & \frac{a_{n-1}}{2} & \cdots & & \frac{a_1}{2} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \\ \\ \\ c_n \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

which can be solved by whatever routine is set up to solve the main system of linear equations for the

quasilinearization steps.

Under the suggested treatment of the fluid properties Jaffe and Thomas's [14] means of solving the incompressible equation can be extended to the compressible equations. The integration problem, with its associated error considerations, becomes a problem of solving a system of linear algebraic equations with associated questions about the well-conditionedness of the coefficient matrices. The form of the matrix is given below, and as the elements vary at each value of x and each quasilinearization step the condition of the matrix has not been investigated a priori. If it becomes ill-conditioned the method will fail.

The next chapter will compare the proposed extension of the Jaffe-Thomas technique [14], quasilinearization with Chebyshev integration, to the Clutter-Smith method [5] of solution. The design of implementations of the methods will be outlined.

CHAPTER TEN

COMPARISON OF TECHNIQUES

Flow diagrams for the two techniques are given below. A list of the routines involved and their functions follows. The basic Clutter and Smith method [5] and Jaffe and Thomas routine [14] were implemented in order to compare programming complexity. These implementations were done using Fortran IV. Extension of the proposed method to the compressible equations is represented in the form of flow diagrams and descriptions of additional routines required. The three methods will be referred to by CS, JT and EJT respectively in the following comparison. Conclusions are to be drawn with reference to a class of equations bearing the characteristics of non-linearity and an incomplete initial value set.

CS Routine Structure

MAIN: Sets up arrays

Sets N=0, M=0, E=0

Sets initial conditions as necessary

(a) Branch to treat x(i)

increment I

test for end of program, i=N ?

if not, go to (a)

Treatment Of X(i):

MOM: Set initial ϕ'' for given trial integration

Generate trial trajectory (IMOM)

Use shocting logic with several trajectories (INT) incrementing M

EN: Implement superposition logic

Generate necessary trajectories (IEN)

SETP: Generate new fluid properties using given solutions and incrementing E.

IMOM: Integration logic for ϕ

INT: Interpolation for shooting logic

IEN: Integration logic for ψ

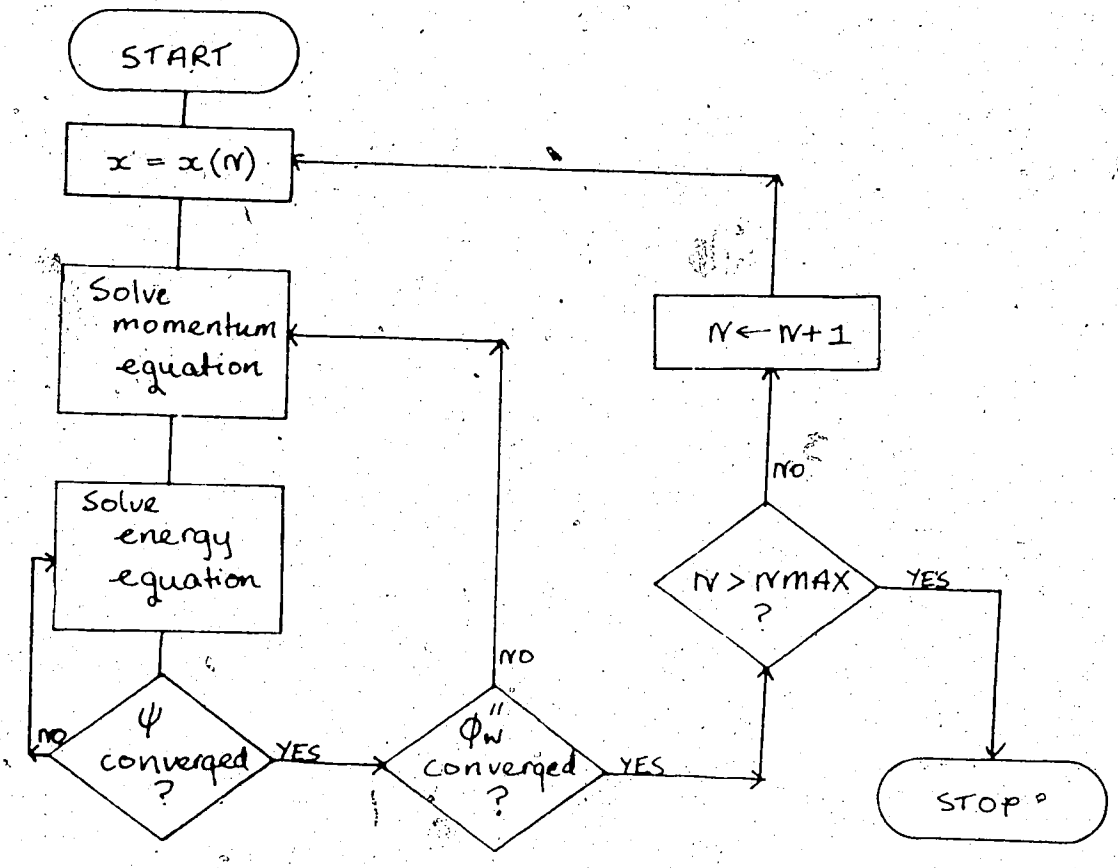

FIGURE IV The Clutter-Smith Technique

JT Routine Structure

MAIN:	Sets up arrays
	Sets up initial approximations
	Sets parameters for the particular problem (e.g. Falkner-Skan)
	Calls COVAL to set up Jacobian matrix for initial approximation
	Calls QLIN to implement method for each x value
COVAL:	Evaluates Jacobian elements for latest approximate solution
QLIN:	Sets up convergence test for line x(n)
	Replaces old solution by new solution
	Calls CHEB
CHEB:	Calls ESOL
	Calls FN
ESOL:	Uses Gaussian Elimination (for example) to solve system outlined in COEFF
FN:	Obtains expansions for solutions from those for the error terms
COEFF:	Sets up the system of linear algebraic equations for the quasilinearized version of the problem.

Additional Routines For EJT

FLUID:	Obtain Chebyshev expansions for fluid properties using evaluation

and interpolation

INT: Interpolate with Chebyshev series

Changes:

MAIN: Different initial solutions

COVAL: Different Jacobian elements

QLIN: Extended convergence tests

COEFF: Different equations to represent quasilinear form of the compressible equations

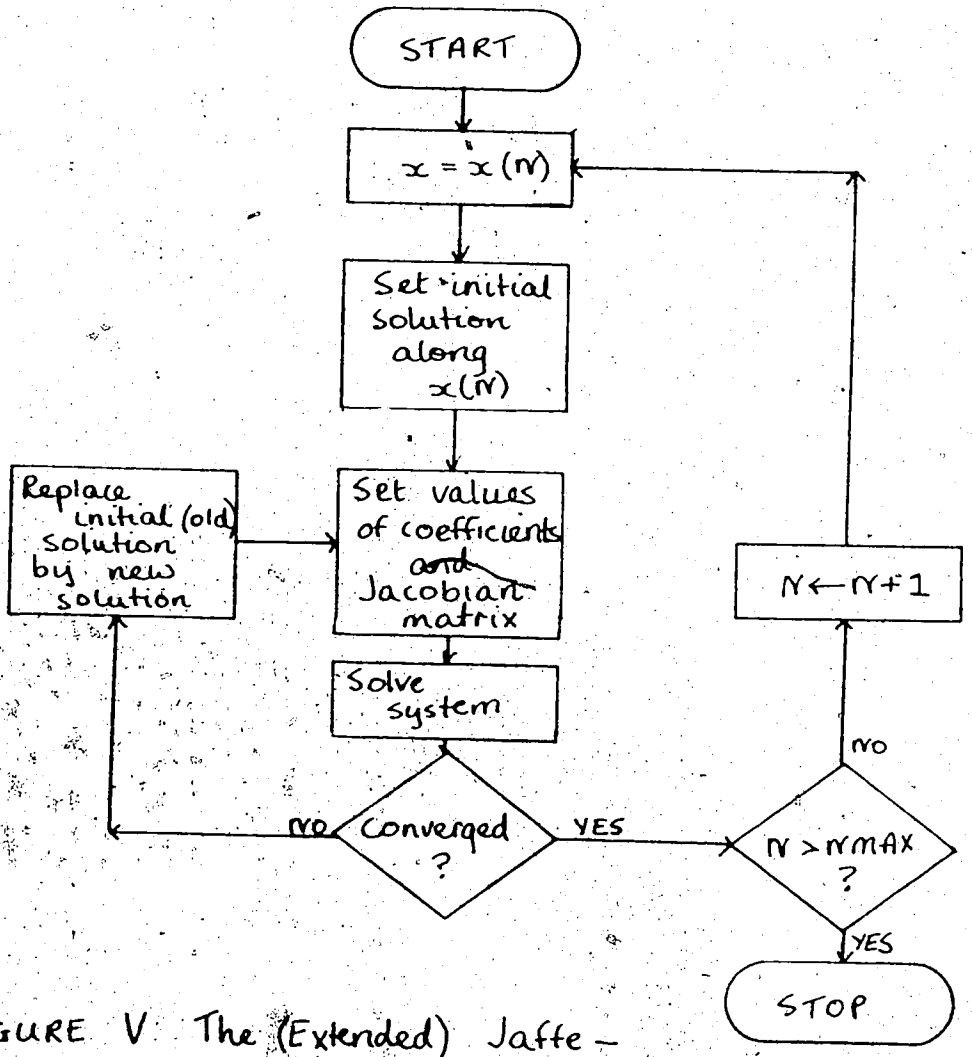

FIGURE V The (Extended) Jaffe-Thomas Technique

Comparison of the methods is to be made on the grounds of thecretical considerations, programming considerations, computing time involved, and storage involved.

1) Theoretical Considerations.

(a) Both methods use the Hartree-Womersley technique to transform the problem into a series of ordinary differential equations. In the CS method, integration using predictor-corrector formulae is then used. First approximations to fluid properties are taken from the preceeding x value. In the EJT, a quasilinearization process with Chebyshev integration is then used, with first approximations to all quantities given by the previous value of x.

(b) Integration. CS uses multiple individual integrations with different initial values and fluid properties. Each integration uses complex starting formulae and involves truncation error which cannot readily be estimated . Different multistep formulae are needed for each dependent variable $\phi'', \phi', \phi, \pi, \psi$. A double iterative loop is needed to produce solutions for a given value of x. EJT uses a single iterative loop in its quasilinearization scheme , each loop involving solution of a system of linear algebraic equations, evaluation of the Jacobian elements, and peripheral treatment of fluid properties.

(c) Shooting . CS uses a shooting method to complete the initial value set. This process introduces many additional complete integrations along $x(N)$ and in some cases does not work due to the inherent nature of the problem. Suggested variants may improve the solution in borderline cases but do not eliminate the problem. EJT eliminates shooting entirely by transforming the problem into a linear one and using a method of integration which can treat both ends of the integration range at the same time.

(d) Solution of the energy equation. CS uses a second and separate iterative loop to solve the energy equation. In the EJT , the two equations are solved simultaneously in one iterative loop.

(e) Fluid properties: the fluid properties can be treated more easily in their actual form in CS , but give rise to more iterations. The interdependence of the solutions and the fluid properties is represented more accurately in the quasilinearization method, however, thus accelerating solution.

Perhaps the most significant ground of comparison of the two methods other than the shooting problem lies in the manner in which each takes advantage of the Hartree-Womersley technique. CS merely uses information from the immediately preceeding x value to obtain initial approximations to the fluid properties: The EJT can use as

many previous x values as necessary to ensure convergence of the scheme under certain conditions on the Hessian matrix of the system. The EJT makes use of all available information to give a certain credibility to the numerical results obtained, and a priori information as to the degree of truncation error involved. For CS the validity of solutions obtained has had to be established by experimental testing.

2) Programming Considerations.

The CS is very hard to program and debug due to the number of complex formulae and the subroutine structures. The EJT is simple to program, the only complex formulae being involved in the routine setting up the linear equations. All other program segments are standard ones, for example, one to solve systems of equations. The complex routine is made simpler by the use of supporting subroutines setting up product and quotient formulae and evaluating members of the Jacobian matrix. The penalty of the easier programming is prior manipulation of the problem to put it in quasilinearized form but this process is standard and a small price to pay.

3) Computing Time Involved.

An accurate comparison of the computing time involved in either method cannot be made without actual implementation of the EJT . A prediction that the EJT would be considerably more efficient can be made, however, based on the fact that it is a singly iterative method.

4) storage considerations.

The CS results are presented in tabular form at iteration arguments. Large storage arrays are required for this, and the shooting technique involves storage of more than one trajectory at each x value until the final version is obtained. Supplementary arrays are also needed to test for convergence in the iteration loops. The EJT stores a set of Chebyshev coefficients at each x value and must maintain a Jacobian matrix at all times. The set of coefficients is smaller than the corresponding table of values. Interpolation between values in a table for arbitrary values of η is avoided. Furthermore, integrals or derivatives of stored quantities are readily calculable.

CHAPTER ELEVEN

CONCLUSIONS AND RECOMMENDATIONS

The primary features of the Clutter-Smith (CS) and extended Jaffe-Thomas techniques (EJT) techniques will be summarized and conclusions drawn.

The CS method uses the Hartree-Womersley technique to transform the equations into ordinary differential equations in the independent variable η. In that form the equations have nonlinear coefficients (the fluid properties) and an incomplete initial value set. If the momentum equation is to be solved, shooting on the parameter $\phi''(x,0)$ must be performed; if this process is successful, the energy equation can then be solved as a linear problem in ψ. The solution at each value of x is refined by re-calculating the coefficients and solving the equations again until a convergence criterion is satisfied. A predictor-corrector integration technique using four points is used once suitable starting formulae have ensured accuracy at the wall $\eta = 0$. The integration formulae can be chosen so that error control depends on Lipschitz constants of the solution variables, but a priori error control is difficult to ensure as these constants are hard to calculate given the nonlinearity of the coefficients and the iterative way they are treated. Practical values of the fluid parameters in the equations make shooting a less than satisfactory technique as large variations in trajectory result from

small changes in initial values of ϕ''. Various improvements on the shooting technique have been proposed but the problem cannot be eliminated using the CS approach.

The EJT method transforms the nonlinear equations into a quasilinearized form which can be integrated using techniques for linear equations. The Hartree-Womersley technique fits well with the method, as a first approximation which ensures convergence of the quasilinearization algorithm is provided, as long as measures on the solution tendencies, which can be estimated using the quasilinearization parameters, are within a reasonable range. Thus points of irregularity in the flow can be approached more nearly using the EJT than the CS method. Advantage can be taken of the linearized form of the equation to eliminate the necessity for shooting by transforming the differential equations into a set of linear algebraic equations by means of a series form of solution. Chebyshev polynomials are suitable, and the solution representation is attractive in terms of easy maniptulation and compact storage. Difficulties encountered in representing the dependence of the fluid properties on the solution can be overcome using interpolation. The method solves both the momentum and the energy equations in a single iterative loop for each value of x and the refinement of the fluid properties is an automatic consequence of the quasilinearization process. The method is easy to im[illegible]

at the cost of prior manipulation to put the problem in quasilinear form.

It must be concluded that the EJT is potentially a much more powerful technique for solving this kind of complex problem than the CS, which is representative of a large class of empirically developed methods. It is recommended therefore that the EJT be implemented fully using a problem of practical significance. The a priori error control, avoidance of shooting, and relative ease of implementation are incentive enough, while the other advantages of the method which have been outlined during the thesis are added benefits of the method.

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APPENDIX A

DERIVATION OF THE BOUNDARY LAYER EQUATIONS

The derivation of the equations can be followed in detail in [10, 17, 21, 26]. A brief discussion of the origin of these equations is given below.

The continuity equation.

Consider a volume element in a fluid. The mass of fluid enclosed in that fluid at time t is

$$\int_V \rho dV$$

The total mass change outward due to fluid flow operates through the surface of the volume element and is given by

$$\int_S \rho \vec{U}.\vec{n} ds$$

where $\vec{n}$ is the outward normal. The law of conservation of mass in a fluid states that the outflow of mass must balance the net change of mass inside the element, or

$$\frac{\partial}{\partial t} \int_V \rho dV = - \int_S \rho \bar{U}.\bar{n} ds$$

Using Green's theorem this becomes

$$\int_V \left(\frac{\partial \rho}{\partial t} + \bar{\nabla}.(\rho \bar{U}) \right) dV = 0$$

and since the volume element is arbitrary the integrand must be 0 or

$$\frac{\partial \rho}{\partial t} + \bar{\nabla}.(\rho \bar{U}) = 0$$

If the Cartesian coordinates in two-dimensional flow are u and v, transformation to the coordinate system in r described in Chapter One yields

$$\bar{\nabla}.(\rho\bar{U}) = \frac{1}{r}\left(\frac{\partial}{\partial x}(r\rho u) + \frac{\partial}{\partial y}(r\rho v)\right)$$

and making the assumption that the flow is steady

$$\frac{\partial \rho}{\partial t} = 0$$

the continuity equation becomes

$$\frac{1}{r}\left(\frac{\partial}{\partial x}(r\rho u) + \frac{\partial}{\partial y}(r\rho v)\right) = 0$$

The momentum equation.

The Navier-Stokes equation of motion for fluids is derived from the expression

$$\rho \frac{Du_i}{Dt} = \rho F_i + \frac{\partial \sigma_{ij}}{\partial x_j}$$

where

$$\frac{D\bar{U}}{Dt} = \frac{\partial \bar{U}}{\partial t} + \bar{U}.\nabla\bar{U}$$

Here the second law of Newton is used as follows. The integral

$$\int_\tau \frac{D\bar{U}}{Dt}\rho d\tau$$

is the sum of the products of mass and acceleration over the volume element τ. (The material derivative $\frac{D}{Dt}$ is descriptive of the history of a particular collection of particles in the fluid and not of a point in the stationary Cartesian space.) The 'body force per unit mass' or 'external' force is called F and the integral

$$\int_\tau \rho \bar{F} d\tau$$

sums these forces over the volume element. It contains all external influences acting on the element. Added to the effect of these forces is the force of surface tension. A stress tensor σ_{ij} may be introduced and the sum of the effects of these forces may be written

$$\int_{\partial\tau} \sigma_{ij} n_j dS = \int_{\tau} \frac{\partial \sigma_{ij}}{\partial x_j} d\tau$$

where the double subscript summation convention is used. Newton's law may then be written

$$\int_{\tau} \frac{Du_i}{Dt} \rho d\tau = \int_{\tau} F_i \rho d\tau + \int \frac{\partial \sigma_{ij}}{\partial x_j} d\tau$$

or, since τ is arbitrary,

$$\rho \frac{Du_i}{Dt} = \rho F_i + \frac{\partial \sigma_{ij}}{\partial x_j}$$

Substitutions for the material derivative and the desired form of the stress tensor yield the momentum equation as found in Chapter One.

<u>The energy equation.</u>

The energy equation is an expression of the balance of thermodynamic energy change in a compressible fluid. It may be develcped from the relation

$$\rho \frac{Dh}{Dt} = \phi + \frac{Dp}{Dt} + \frac{\partial}{\partial x_j} (k \frac{dT}{\partial x_j})$$

where $\rho \frac{Dh}{Dt}$ expresses the energy stored in a volume element τ. Now h is enthalpy, defined by

$$h = E + p\tau$$

where E is the total internal energy of the particles in the element. And $p\tau$ is a term expressing possible variation in energy through relative changes in pressure or volume. ϕ is the dissipation function or rate of work done by viscous forces. $\frac{Dp}{Dt}$ is the material derivative of pressure with respect to time. Also k is the thermal conductivity and T the absclute temperature.

The above equation may be regarded as a statement of

the second law of thermodynamics

$$dE = TdS - pdV$$

in terms of conveniently measureable thermodynamic quantities.

The derivation of the specific expression found in Chapter One from the above form may be followed in Reference [28].

APPENDIX B

TRANSFORMATION OF THE EQUATIONS

A standard transformation used in boundary layer theory is that of Dorodnitsyn [19]

$$\eta = \int_0^y \rho dy \quad , \quad \xi = x$$

which has the effect of stretching the boundary layer coordinate normal to the body coordinate proportionally to the density, thus making the layer thickness approximately uniform along the body. Clutter and Smith [28,5] use a transformation closely related to this one:

$$\eta = \frac{u_e}{\rho_\infty \mu_\infty x} \int_0^y \rho dY \quad , \quad x = x$$

This transformation is reminiscent also of the Falkner Skan transformation [6]:

$$\eta = \left(\frac{u}{\rho \mu x}\right)^{1/2} y$$

and allows convenient parallels to be drawn with the incompressible equation of momentum.

Further treatment of the equations consists of representing the dependent variables as potential functions and thus increasing the order of the equations by one. Such treatment is standard in flow studies as it allows automatic satisfaction of the continuity equation by the stream function :

$$\rho r u = \frac{\partial(\Phi r)}{\partial y} \quad , \quad \rho r v = \frac{-\partial(\Phi r)}{\partial x}$$

Clutter and Smith use a dimensionless version of the stream function:

$$f = (\rho_\infty \mu_\infty x\, u_e)^{-1/2}\, \Phi$$

Final transformation of the momentum equation is to the quantity

$$\phi = f - \eta$$

which helps to reduce the accumulation of round-off error in the numerical calculations to be performed. Details of the conversion of the momentum equation to its final form may be found in [5].

The energy equation undergoes transformation first to the (η, x) plane as described above and then to the unknown (enthalpy) H. H is transformed by

$$g = H/H_e$$

to a dimensionless quantity and then by

$$\psi = g - 1$$

to cut down round-off error. It is then in its final form.