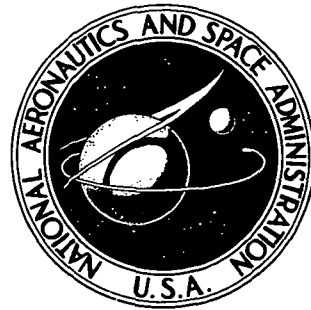


N72-33268

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**NUMERICAL METHOD FOR THE SOLUTION
OF LARGE SYSTEMS OF DIFFERENTIAL
EQUATIONS OF THE BOUNDARY-LAYER TYPE**

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION • WASHINGTON, D. C. • OCTOBER 1972

1. Report No. NASA TN D-7068	2. Government Accession No.	3. Recipient's Catalog No.	
4. Title and Subtitle NUMERICAL METHOD FOR THE SOLUTION OF LARGE SYSTEMS OF DIFFERENTIAL EQUATIONS OF THE BOUNDARY-LAYER TYPE		5. Report Date October 1972	
		6. Performing Organization Code	
7. Author(s) Michael J. Green and Philip R. Nachtsheim		8. Performing Organization Report No. A-4544	
		10. Work Unit No. 186-68-51-01	
9. Performing Organization Name and Address NASA-Ames Research Center Moffett Field, CA 94035		11. Contract or Grant No.	
		13. Type of Report and Period Covered Technical Note	
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, D. C. 20546		14. Sponsoring Agency Code	
		15. Supplementary Notes	
16. Abstract <p>A numerical method for the solution of large systems of nonlinear differential equations of the boundary-layer type is described. The method is a modification of the technique developed by Nachtsheim and Swigert for satisfying asymptotic boundary conditions. The present method employs inverse interpolation instead of the Newton method to adjust the initial conditions of the related initial-value problem. This eliminates the so-called perturbation equations required in Nachtsheim's and Swigert's application of Newton's method. The elimination of the perturbation equations not only reduces the user's preliminary work in the application of the method, but also reduces the number of time-consuming initial-value problems to be numerically solved at each iteration. Thus, although the rate of convergence of inverse interpolation is in general less than that obtained by the Newton method, the total number of required initial-value solutions may be reduced. For further ease of application, the solution of the overdetermined system for the unknown initial conditions is obtained automatically by applying Golub's linear least-squares algorithm. The relative ease of application of the proposed numerical method increases directly as the order of the differential-equation system increases. Hence, the method is especially attractive for the solution of large-order systems. After the method is described, it is applied to a fifth-order problem from boundary-layer theory.</p>			
17. Key Words (Suggested by Author(s)) Boundary-layer equations Shooting method for solution of boundary-value problems Inverse Aitken interpolation Linear least-squares solution		18. Distribution Statement Unclassified - Unlimited	
19. Security Classif. (of this report) Unclassified	20. Security Classif. (of this page) Unclassified	21. No. of Pages 9	22. Price* \$3.00

SYMBOLS

f	stream function
S	enthalpy
u	$u(x,y) \equiv f'_F(x,y) - f'(\infty)$
v	$v(x,y) \equiv S'_F(x,y) - S(\infty)$
w	$w(x,y) \equiv f''_F(x,y)$
X	x that satisfies equations (7) through (11)
x	$x \equiv f''(o)$
Y	y that satisfies equations (7) through (11)
y	$y \equiv S'(o)$
z	$z(x,y) \equiv S'_F(x,y)$
β	pressure gradient parameter
η	measure of distance from wall

Subscripts

F	evaluation at a finite value of η
i	$i = 1, 2, \text{ or } 3; i^{\text{th}}$ numerical value
u	partial differentiation with respect to u
v	partial differentiation with respect to v
w	partial differentiation with respect to w
z	partial differentiation with respect to z

Superscripts

$()'$	differentiation with respect to η
$(\bar{ })$	iterated value

**NUMERICAL METHOD FOR THE SOLUTION OF LARGE
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THE BOUNDARY-LAYER TYPE**

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SUMMARY

A numerical method for the solution of large systems of nonlinear differential equations of the boundary-layer type is described. The method is a modification of the technique developed by Nachtsheim and Swigert for satisfying asymptotic boundary conditions. The present method employs inverse interpolation instead of the Newton method to adjust the initial conditions of the related initial-value problem. This eliminates the so-called perturbation equations required in Nachtsheim's and Swigert's application of Newton's method. The elimination of the perturbation equations not only reduces the user's preliminary work in the application of the method, but also reduces the number of time-consuming initial-value problems to be numerically solved at each iteration. Thus, although the rate of convergence of inverse interpolation is in general less than that obtained by the Newton method, the total number of required initial-value solutions may be reduced. For further ease of application, the solution of the overdetermined system for the unknown initial conditions is obtained automatically by applying Golub's linear least-squares algorithm. The relative ease of application of the proposed numerical method increases directly as the order of the differential-equation system increases. Hence, the method is especially attractive for the solution of large-order systems. After the method is described, it is applied to a fifth-order problem from boundary-layer theory.

INTRODUCTION

Many problems in boundary-layer theory are posed mathematically as nonlinear, two-point boundary-value problems on an infinite interval. The so-called initial-value or "shooting" method, which does not require linearization of the equations, has been successfully applied to this class of problems. Basically, the shooting method adjusts the initial conditions so that the solution of the related initial-value problem satisfies the required boundary conditions at the outer boundary point.

Of fundamental importance in the application of the shooting technique is the manner in which the adjustment of the initial conditions is made. Many adjustment schemes have been proposed (see ref. 1). In particular, Nachtsheim and Swigert (ref. 2) have developed an iterative adjustment scheme for boundary-layer problems with asymptotic boundary conditions. In that scheme, the differential equations are numerically integrated to some finite outer boundary point. The initial conditions are adjusted so that the errors between the computed values and the corresponding asymptotic values of both the functions with asymptotic boundary conditions and

their derivatives are minimized in the least-squares sense. The iterative adjustments are continued until the solution converges within some prescribed accuracy. The precision of the solution is continually improved by progressively extending the range of integration. In this scheme, Newton's method is applied to the nonlinear equations. However, Newton's method requires the rate of change of the original differential equations with respect to each of the unknown initial conditions. Therefore, for each unknown initial condition, a concomitant differential-equation system (the so-called perturbation equations and their associated boundary conditions) must be formally constructed and numerically integrated simultaneously with the original differential-equation system.

This paper describes a numerical method that modifies the Nachtsheim-Swigert adjustment scheme so that the perturbational differential-equation systems are eliminated. The numerical method is similar to the one proposed by Warner (ref. 3) for the finite interval. The elimination of the perturbation equations relieves the user of the burdensome task of formally generating and coding these equations for each problem, while simultaneously reducing the total number of numerical integrations to be performed. For additional convenience and accuracy, the linear least-squares solution for the unknown initial conditions is achieved using Golub's method (ref. 4) of orthogonal transformations on the original system. So the task of finding the so-called normal equations, and then solving these linear algebraic equations for the least-squares solution, is also eliminated. The method is described and is applied to a specific problem in boundary-layer theory.

NUMERICAL METHOD

The method is best described by applying it to a specific problem. Consider Stewartson's boundary-layer equations (for which Cohen and Reshotko, ref. 5, found similar solutions) with unit Prandtl number, and with pressure gradient parameter $\beta = 1/2$:

$$f''' + ff'' + 1/2(S + 1 - f'^2) = 0 \quad (1)$$

$$S'' + fS' = 0 \quad (2)$$

$$f(o) = 0, \quad f'(o) = 0, \quad S(o) = S_w \quad (3)$$

$$f'(\infty) = 1, \quad S(\infty) = 0 \quad (4)$$

where S_w characterizes a particular solution. The generalization of the method to any order differential system follows naturally from the application to this fifth-order problem.

For notational convenience, define the unknown initial conditions by

$$x = f''(o) \quad (5)$$

$$y = S'(o) \quad (6)$$

To apply the shooting method, initial guesses are made for x and y . These estimates, along with equations (1), (2), and (3), form an initial-value problem, which can be integrated by a numerical integration algorithm (e.g., Adams-Moulton) to some specified finite value of the independent variable η . Denote this outer boundary point of the finite integration range as η_F . Further, let a function subscripted with F denote the numerical value the function takes on when evaluated at η_F .

Define

$$u(x,y) = f'_F(x,y) - f'(\infty)$$

$$v(x,y) = S_F(x,y) - S(\infty)$$

$$w(x,y) = f''_F(x,y)$$

$$z(x,y) = S'_F(x,y)$$

The boundary-value problem of equations (1) through (4) could be solved by determining the unknown initial conditions x and y such that

$$u(x,y) = 0 \tag{7}$$

$$v(x,y) = 0 \tag{8}$$

$$w(x,y) = 0 \tag{9}$$

$$z(x,y) = 0 \tag{10}$$

Note that equations (7) and (8) require that the dependent variables f' and S approach their boundary values in a finite domain, whereas equations (9) and (10) give the Nachtsheim-Swigert criteria, namely, the slopes of those variables also simultaneously approach zero. The solutions are not unique when only $f' = 1$ and $S = 0$ are specified at a finite η_F ; see reference 2.

Instead of using a direct Newton iteration scheme to determine the roots x and y of the nonlinear system, equations (7) through (10) apply the inverse Aitken interpolation technique as generalized in reference 3. The functions $u = u(x,y)$, $v = v(x,y)$, $w = w(x,y)$ and $z = z(x,y)$ may be inverted to give $x = x(u,v)$, $y = y(u,v)$ and also $x = x(w,z)$, $y = y(w,z)$, provided the Jacobians of the transformations do not vanish at any points in question. Denote the values of x and y when u , v , w , and z are zero as X and Y , and the values of derivatives $\partial x/\partial u$, \dots , $\partial y/\partial z$ when $x = X$ and $y = Y$ as X_u , \dots , Y_z . Expand $x(u,v)$, $y(u,v)$ and $x(w,z)$, $y(w,z)$ into their corresponding Taylor series for two variables and then truncate after linear terms to obtain:

$$x = X + uX_u + vX_v \tag{11}$$

$$y = Y + uY_u + vY_v \tag{12}$$

and

$$x = X + wX_w + zX_z \tag{13}$$

$$y = Y + wY_w + zY_z \tag{14}$$

Because each of equations (11) through (14) contains three unknowns (e.g., X , X_u , and X_v in equation (11)), it will be sufficient to specify three sets of initial trial values, (x_1, y_1) , (x_2, y_2) and (x_3, y_3) . Equations (1) and (2) with conditions (3), (5), and (6) can be integrated to obtain (u_1, v_1) and (w_1, z_1) , (u_2, v_2) and (w_2, z_2) , and (u_3, v_3) and (w_3, z_3) . Substituting these values into equations (11) through (14) and rearranging leads to the matrix equation

$$\begin{bmatrix} u_1 & v_1 & 0 & 0 & 1 \\ 0 & 0 & w_1 & z_1 & 1 \\ u_2 & v_2 & 0 & 0 & 1 \\ 0 & 0 & w_2 & z_2 & 1 \\ u_3 & v_3 & 0 & 0 & 1 \\ 0 & 0 & w_3 & v_3 & 1 \end{bmatrix} \begin{bmatrix} X_u & Y_u \\ X_v & Y_v \\ X_w & Y_w \\ X_z & Y_z \\ X & Y \end{bmatrix} = \begin{bmatrix} x_1 & y_1 \\ x_1 & y_1 \\ x_2 & y_2 \\ x_2 & y_2 \\ x_3 & y_3 \\ x_3 & y_3 \end{bmatrix} \quad (15)$$

As in reference 2, the least-squares solution is the accepted solution of this overdetermined system of 12 equations with 10 unknowns. The usual method is not used—that is, determining the system of so-called normal equations and then solving the resulting linear algebraic system to obtain the least-squares solution of the overdetermined system, as in equation (15).

As a replacement, the method developed by Golub (reference 4) is used to solve the linear least-squares problem. Golub's algorithm is based on applying orthogonal Householder transformations to the original overdetermined system. (See ref. 4 for a description of the method, as well as an error analysis.) This approach for obtaining the linear least-squares solution is numerically more stable than the solution via the normal equations.

Once the values X and Y are determined from the least-squares solution of equation (15), they can be used in equations (5) and (6) along with equation (3) to again numerically integrate equations (1) and (2) to obtain new values (\bar{u}_1, \bar{v}_1) and (\bar{w}_1, \bar{z}_1) . These values then replace the least accurate equations in equation (15). The resulting least-squares system is then solved again to determine the improved initial conditions, X and Y . This iterative procedure is continued until the errors between the computed boundary values and the specified asymptotic boundary conditions are within a prescribed tolerance, that is, until u , v , w , and z are all less than a very small prescribed number.

NUMERICAL RESULTS

A computer program was written using the proposed technique. The program was coded in FORTRAN IV for the time-sharing system (TSS/360) on the IBM 360/67 computer at Ames Research Center. As a specific example, the computer solved the problem given by equations (1) through (4) with the parameter S_w equal to -0.2 .

The estimates for the unknown initial conditions (x, y) required to start the solution were $(0.8, 0.1)$, $(0.8, 0.1001)$, and $(0.8001, 0.1)$. The solution converged in 11 iterations so that the absolute error between the computed boundary conditions and the asymptotic boundary conditions was less than 1×10^{-9} . The initial conditions for the converged solution were $f'' = 0.86228190$ and $S' = 0.1062283$, which agree with the values (five decimal places) given in reference 5. The total central processing unit (CPU) time was 6.85 seconds.

For comparison, the same problem was solved using the Nachtsheim-Swigert method. The only modifications to the computer program were those involving adjustment of the initial conditions. With the original guess of (0.8, 0.1) for the missing initial conditions, the computed values were within 1×10^{-9} of their corresponding asymptotic values in seven iterations. However, the CPU time was 9.03 seconds. The increase in computer time was caused by the integration of three fifth-order systems at each iteration (namely, the original system and the perturbational system for each of the two unknown initial conditions) whereas, in the proposed method, only the original fifth-order system was integrated at each iteration.

CONCLUSIONS

For boundary-layer problems modeled by a large system of nonlinear differential equations with asymptotic boundary conditions (e.g., multicomponent diffusion flame problems), application of the shooting method with an adjustment scheme requiring perturbation equations is laborious if not prohibitive. The use of an inverse interpolatory adjustment procedure, which eliminates the perturbation equations, appears as an attractive alternative. The technique is easily programmed since only the original differential-equation system is used. And, although ease of application is the major advantage of this method, there may also be a savings in computer time, as was illustrated in the example considered. The suitability of the method appears to increase as the order of the system increases.

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Moffett Field, Calif. 94035, June 7, 1972

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