

SATISFACTION OF ASYMPTOTIC BOUNDARY CONDITIONS IN THE NUMERICAL SOLUTION OF BOUNDARY-LAYER EQUATIONS

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TECHNICAL PREPRINT prepared for Ninth Midwestern Mechanics Conference, Madison, Wisconsin, August 16-18, 1965

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ABSTRACT

A method for the numerical solution of differential equations of the boundary-layer type is presented. The asymptotic boundary conditions are satisfied at the edge of the boundary layer by adjusting the initial conditions so that the mean square error between the computed variables and the asymptotic values is minimized. A least squares convergence criterion is used to propose a method of solution in which the edge of the boundary layer is approached in steps. The convergence rate to a solution is rapid and appears to be insensitive to the initial guesses of the initial conditions. Use of a least-squares convergence criterion leads to the unique solution even in the case of retarded main stream flows. A description of the method is given, and two examples taken from boundary-layer theory are worked.

INTRODUCTION

The numerical integration of the ordinary differential equations of boundary-layer theory involves the satisfaction of asymptotic boundary conditions; that is, some boundary conditions are specified at the initial point or wall, and others are specified as limits that must be approached at large values of the independent variable corresponding to the

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edge of the boundary layer. In order to integrate the differential equations numerically from the wall to the edge of the boundary layer, it is necessary to specify as many additional conditions at the wall as there are conditions to be satisfied at the edge of the boundary layer. These additional initial conditions have to be varied in order to satisfy the conditions at the edge of the boundary layer. All methods that have been used to find the proper initial conditions rely on the fact that, for large values of the independent variable, the integrals of the differential equations depend on the initial conditions, called the initial-value method (ref. 1), is that of obtaining integrals of the differential equations with guessed initial conditions; that is, an attempt is made to integrate the differential equations to the edge of the boundary layer. If this can be accomplished, corrections are made for the initial guesses by the Newton-Raphson method, and the process is repeated until convergence is achieved.

In order to carry out this iteration, additional differential equations have to be integrated. There will be as many additional differential equations as there are initial conditions to be varied. The integrals of these additional equations called perturbation equations give the rate of change of the integrals of the original differential equation with respect to the initial conditions.

Another method that has been used, called quasilinearization (ref. 2), is similar in principle to the initial-value method, except that the differential equations are linearized. The resulting linear differential equations for the current approximation are inhomogeneous, since they also contain the previous approximation as members.

The perturbation equations of the initial-value method correspond to a complementary function of the linear differential equations of the quasilinearization method. In application, the two methods are different in that, in the quasilinearization method, the complementary functions are used to obtain solutions to the inhomogeneous linear differential equations, whereas in the initial-value method, the solutions to the perturbation equations are used to adjust the starting values at the initial point. A disadvantage associated with the quasilinearization method is that functions representing the previous approximation have to be stored in order to construct the current approximation. Furthermore, the solutions and a particular integral is usually not well determined except near the origin or initial point, as pointed out by Hartree (ref. 3). The solutions of the perturbation equations, however, can be used to determine the proper initial conditions closely. This is the procedure that is followed in the initial-value method.

Both methods have been used to obtain solutions of the boundary-layer equations. Neither of these methods, however, has solved the problem of when to stop the integration. Since one boundary condition is specified as a limit that must be approached at large values of the independent variable, the integration should be stopped at a value of the independent variable that is sufficiently large so that the various functions are approaching their asymptotic values. This value of the independent variable could properly be called the edge of the boundary layer. In the various methods used to solve this problem, this value of the independent variable must be guessed at beforehand. If the guessed value is too small, the integrals of the differential equation may not

be able to satisfy the imposed conditions; or, there may be more than one value of an initial condition that leads to integrals of the differential equations that satisfy the imposed boundary conditions.

If the guessed value is too large, it is possible that the integrals of the equations will diverge; or, that convergence to a solution is extremely slow.

Another problem that sometimes besets the numerical integration of the boundary-layer equations is the apparent insensitivity of the integrals of the boundary-layer equations to the initial conditions. This difficulty appears in the integration of the Falkner-Skan differential equation (ref. 4). All the integrals of the Falkner-Skan equation for the case of nonretardèd flows in the main stream tend to diverge except the ones with the proper initial conditions; however, for the case of retarded flows, a solution with any value of the initial condition near the correct one will eventually meet the proper boundary condition at infinity. The unique solution was found by Hartree (ref. 4) for retarded flows by imposing the additional condition that the desired solution is the one that approaches the boundary condition most rapidly from below. However, this behavior of the solutions can only be learned from several trial runs.

In an effort to adapt the initial-value method to the solution of differential equations with asymptotic boundary conditions, a method was developed to eliminate the problem of when to stop the integration. This method of solution is capable of satisfying the boundary conditions at the edge of the boundary layer correctly; that is, the boundary values are approached asymptotically. This is accomplished by choosing the additional initial conditions

so that the mean square error between the computed variables and the asymptotic values is minimized. A least-squares convergence criterion is used to propose a method of solution in which the edge of the boundary layer is approached in steps. The convergence rate to a solution is rapid, and convergence appears to be insensitive to the initial guesses of the initial conditions. Use of a least-squares convergence criterion leads to the unique solution even in the case of retarded main stream flows. A description of the method is given and two examples taken from boundary-layer theory are worked.

DESCRIPTION OF METHOD

A description of the method can best be achieved by referring to a definite example of a boundary-value problem with an asymptotic boundary condition. In Falkner and Skan's treatment of the laminar boundary layer of an incompressible fluid, the following equation arises (see ref. 4)

$$f'' = - ff'' + \beta(f'^2 - 1)$$
 (1)

with the boundary conditions

 $\eta = 0; \qquad \mathbf{f} = \mathbf{f}' = 0$ $\eta \to \infty; \qquad \mathbf{f}' \to \mathbf{l}$

The primes denote differentiation with respect to η , a measure of the distance from the wall. The dependent variable f is related to the usual stream function. The potential flow is given by a power law. The flow velocity outside the boundary layer in the main stream is proportional to the distance along the wall raised to the power $\beta/(2 - \beta)$. For retarded main stream flow $\beta < 0$, and for nonretarded flow $\beta \ge 0$.

In practice, the asymptotic boundary condition is replaced by the condition that f' = 1 to a sufficient degree of accuracy at $\eta = \eta_{edge}$, where η_{edge} is the value of the independent variable at the edge of the boundary layer. The boundary-value problem is equivalent to the problem of finding a value of f''(0) for which the boundary condition at the edge of the boundary layer is satisfied; that is, it is desired to find a solution of the nonlinear equation

$$f'_{edge} \left[f''(0) \right] = 1$$

at $\eta = \eta_{edge}$, where $f'_{edge} = f'(\eta_{edge})$. The function $f'_{edge} \left[f''(0) \right]$ in this problem is not in general explicit, it will be expressed as a function of f''(0) through an integration of equation (1). With the notation $x \equiv f''(0)$, observe that a small change Δx in x changes f' by the amount

$$\frac{\partial f'}{\partial x} = \Delta x$$

so that the necessary correction to a first approximation comes from the solution of the linear equation

$$l = f' + \frac{\partial f'}{\partial x} \Delta x$$

at $\eta = \eta_{edge}$.

The solution of the equation for Δx can be performed provided the partial derivative of f' with respect to x can be evaluated at η_{edge} . The partial derivative can be evaluated by forming the perturbation equation for the function f'. This equation is obtained by differentiating the terms in equation (1) appropriately. With the notation

$$f_x = \frac{\partial f}{\partial x}, f'_x = \frac{\partial f'}{\partial x}, etc.$$

The following perturbation equation is obtained

$$\mathbf{f}_{\mathbf{X}}^{'''} = - \left(\mathbf{f}\mathbf{f}_{\mathbf{X}}^{''} + \mathbf{f}^{''}\mathbf{f}_{\mathbf{X}}\right) + 2\beta\mathbf{f}^{'}\mathbf{f}_{\mathbf{X}}^{'}$$
(2)

with the initial conditions

$$\eta = 0: f_{x} = f'_{x} = 0, f''_{x} = 1$$

Given an initial estimate of x = f''(0), the subsequent values of x are computed automatically in the iteration procedure described previously.

The problem of where to stop the integration remains; that is, η_{edge} is unknown. Figure l(a) illustrates the difficulties that arise when the boundary condition f' = l is applied at a finite value of η .

The data for figure 1(a) were obtained from calculations that are described in detail subsequently. For the purpose of understanding the results presented in this figure, the reader should know that equation (1) was integrated for specified values of f''(0) with $\beta = 1$. The integration was stopped at $\eta = 5$. Tentative values of η_{edge} will hereinafter be referred to as η_{stop} .

Figure 1(a) shows f' and f" as a function of x = f"(0) at $\eta_{stop} = 5$. It can be seen that there are two values of x that satisfy the condition f' = 1 when η_{stop} is taken to be 5, namely x = 0.85 and x = 1.23. Figures 1(b) and (c) show the two solutions corresponding to the two values of x. The proper value of x can be determined by observing where f" = 0. From figure 1(a) it can be seen that the correct value of x is approximately 1.23. It can be concluded from this illustration that the satisfaction of the boundary condition f' = 1 at $\eta_{stop} = 5$ does not ensure the satisfaction of the asymptotic boundary condition on f', namely that the value of f' approaches the value 1 asymptotically. In order to satisfy the asymptotic condition at a finite value of η , the condition f' = 1 and f" = 0 should both be imposed (examination of the differential equation (1) will reveal that all higher derivatives will be zero also); that is, Δx should be chosen so that both equations

$$1 = f' + f'_{x} \Delta x \tag{3}$$

$$0 = \mathbf{f}'' + \mathbf{f}''_{\mathbf{x}} \Delta \mathbf{x} \tag{4}$$

are satisfied at $\eta = \eta_{\text{stop}}$. This is in general impossible since there are two conditions and only one adjustable parameter, Δx . However, a satisfactory solution that is consistent with the idea that the boundary condition cannot be satisfied exactly at a finite value of η is to seek the least-squares solution of the preceding equations (ref. 5); that is

$$\Delta x = \frac{f'_{x} (1 - f') - f''f'_{x}}{f'_{x}^{2} + f''_{x}^{2}}$$
(5)

In this way all the information contained in equations (3) and (4) is retained.

The least-squares solution of equations (3) and (4) attempts to minimize the sum of the squares of the errors in these equations as a function of Δx . The value of x that gives $\Delta x = 0$ corresponds to the minimum with respect to x of the quantity

$$E = (1 - f')^2 + f''^2$$
(6)

as can be seen from equation (5). In figure 2, the quantity E is shown plotted as a function of x for various values of η_{stop} . The data for figure 2 were also obtained from the calculations described subsequently.

For this example ($\beta = 1$ and $\eta_{stop} = 5$) it is seen that the least-squares solution gives a unique solution for x. It is this property, that the minimum of the sum of the squares of the appropriate boundary functions corresponds to no change in the required initial conditions, that enables satisfaction approximately of the asymptotic boundary condition at a finite value of the independent variable. The edge of the boundary layer could be defined as that value of η for which the minimum E is less than some preassigned small value as the range of integration is increased. This gives a value of η_{adma} .

The concept of convergence in the least-squares sense permits modification of the initial-value method in order to solve a wide class of boundary-layer problems. To understand why the initial value method requires modification, consider how the method can fail when it is applied to boundary-layer type problems.

Recall that in the initial-value method, corrections are obtained to the guessed initial conditions after integrating the differential equations to the edge of the boundary layer. This method can fail if the initial guess is so poor that the integration "blows up" (i.e., diverges beyond a prescribed limit) before reaching the edge of the boundary layer.

This problem can be avoided and corrections to the initial conditions can be obtained by attempting to minimize the mean square error between the computed solution and the asymptotic values before reaching the edge of the boundary layer. The modification of the initial-value method consists then of carrying out the minimizing process at any arbitrary value of η_{stop} . When

this modified procedure is used, the choice of η_{stop} , where the minimizing process is first carried out, may be dictated by other considerations than where the edge of the boundary layer is, such as keeping the variables within prescribed limits so that the solution does not diverge. After the minimum has been found and corrections to the initial conditions made at the chosen value of η_{stop} , the range of integration can be increased if necessary.

If the value of the minimum found is not small enough, it will be necessary to increase the range of integration. In this way, the edge of the boundary layer is approached in steps by successively increasing the range of integration until the correct initial conditions and the value of η_{edge} are found.

For this example, the Falkner-Skan solution with $\beta = 1$, it appears the quantity E has a definite minimum at each value of η including $\eta = 0$ as can be seen from figure 2. The numerical solution of this example will be described in the next section.

NUMERICAL SOLUTION

The method described in the previous section was programed in FORTRAN IV, double precision on the IBM 7094II-7040 direct-couple system. The boundary-layer and perturbation differential equations were rewritten as systems of first-order differential equations and integrated with a predictor-corrector (Adams-Moulton) subroutine using one correction per step and a fixed increment.

The boundary-layer equations along with the perturbation equations were integrated to the specified value of the independent variable. The

corrections were then determined, and the process was repeated until the relative change in the correction term equation (5) was less than a small preassigned value.

Extreme accuracy was not required at the smaller values of η_{stop} since the boundary conditions cannot be well satisfied there. A value of 1×10^{-8} was used at the larger values of η_{stop} to check the relative change in the correction term. This small value seemed reasonable since convergence is so rapid.

RESULTS OF NUMERICAL SOLUTION FOR EXAMPLE 1

Figure 3 shows the solution f' of equation (1) with $\beta = 1$ as a function of the independent variable η , for the first five trials needed for convergence. With an initial guess of 1.0 for f"(0), the equations were integrated to a value of $\eta_{stop} = 2$ twice and to a value of $\eta_{stop} = 5$ three times. Observe that, for the first integration, the values of f' tend to deviate radically from the correct solution at a relatively small value of η . If these calculations had been carried out to a larger value of η , the values of f' would have attained a magnitude so large that any use of these large numbers in a Newton-Raphson scheme would be meaningless.

The effect of η_{stop} on the convergence process is illustrated in figures 2 and 4. Figure 2 shows the error, equation (6), as a function of f"(0) for different values of η_{stop} . Observe that by initially using a small value for η_{stop} ($\eta_{stop} = 2$ in fig. 2) the range of meaningful initial guesses is increased, that is, initial guesses that yield a relatively small error. For extremely large values of η_{stop} the parabola-like curves in figure 2 degenerate to a vertical line, and the initial guess is limited to the correct answer.

Figure 4 shows the effect of η_{stop} on the convergence rate. The value of f"(0) after two trials is plotted against the initial guess of f"(0) for different values of η_{stop} . The distance of a point on these curves from the straight line shown in the figure is a measure of the rate of convergence. If a point remains on this line after two trials, there is no tendency toward convergence at all. It can be seen from figure 4 that the points on the curve for $\eta_{\text{stop}} = 2$ are always farther from the straight line than the points on the curve for $\eta_{\text{stop}} = 5$. This indicates that the rate of convergence is much greater for $\eta_{\text{stop}} = 2$ than for $\eta_{\text{stop}} = 5$ for all initial guesses of f"(0).

To give an idea of the rate of convergence to a solution for this example using an initial guess of f''(0) = 1, table I(a) is presented. Using quasilinearization and five corrections Radbill (ref. 2) obtains a value of f''(0)accurate to one decimal place compared with Yohner and Hansen (ref. 6), whereas the method developed herein reached an answer after two corrections that agrees with that of Yohner and Hanson to two decimal places. After two more corrections, the value of f''(0) agrees with that of Yohner and Hansen (ref. 6) to within 2 units in the seventh decimal place. The last integration was performed as a stopping criteria for the computer.

Computer time for the complete solution, using a step size of 2^{-4} was approximately 0.05 minute.

This example was also programed by single precision with good results. The difficulty in using single precision presented itself in the form of reducing

the range of initial guesses that could successfully be used to obtain the correct answer.

Equation (1) was also integrated for the case of a retarded main stream flow with $\beta = -0.1$. However, no additional conditions had to be imposed such as those used by Hartree (ref. 4) in order to obtain the unique solution. The value of f"(0), which was obtained by minimizing the mean square error, agreed with the value obtained by Smith (ref. 7) for this case to six decimal places.

EXTENSION TO SYSTEMS OF EQUATIONS

The least squares modification of the initial-value method described previously for a differential equation with a single dependent variable can easily be generalized to systems of equations. As an example of a problem with two dependent variables, consider the boundary value problem for the free-convection flow about a vertical plate. This example is taken from reference 8. It consists of solving the differential equations

$$f''' = 3ff'' + 2f'^2 - h$$
 (7)

$$h'' = -3Prfh'$$
(8)

with the boundary conditions

 $\eta = 0: \qquad f = f' = 0, h = 1$ $\eta \Rightarrow \infty: \qquad f' \Rightarrow 0, h \Rightarrow 0$

Again the primes denote differentiation with respect to η (a measure of the distance from the wall), and the dependent variable f is related to the usual stream function. The dependent variable h is proportional to the temperature excess of the fluid over the ambient temperature, and Pr denotes the Prandl number. Since there are two asymptotic boundary conditions to satisfy, two additional initial conditions at the wall will have to be adjusted; that is, values of $x \equiv f''(0)$ and $y \equiv h'(0)$ are sought that will satisfy simultaneously the nonlinear equations

$$f'_{edge} \left[f''(0), h'(0) \right] = 0$$

$$h_{edge} \left[f''(0), h'(0) \right] = 0$$
at $\eta = \eta_{edge}$, where $f'_{edge} = f'(\eta_{edge})$ and $h_{edge} = h(\eta_{edge})$. The

necessary first corrections to a first approximation x and y come from a solution of the linear equations

$$0 = \mathbf{f'} + \mathbf{f'_x} \Delta \mathbf{x} + \mathbf{f'_y} \Delta \mathbf{y}$$
$$0 = \mathbf{h} + \mathbf{h_x} \Delta \mathbf{x} + \mathbf{h_y} \Delta \mathbf{y}$$

at $\eta = \eta_{edge}$. Where $f'_x = \frac{\partial f'}{\partial x}$, $f'_y = \frac{\partial f'}{\partial y}$, etc. However, in order to satisfy the asymptotic boundary conditions, the preceding equation must be supplemented by

 $0 = f'' + f''_X \Delta x + f''_y \Delta y$ $0 = h' + h'_X \Delta x + h'_y \Delta y$

and Δx and Δy must be found such that the sum of squares of the errors in the preceding four equations be a minimum. The least-squares solution for those quantities is given by the solution of the following matrix equation:

$$\begin{bmatrix} f'_{x}^{2} + h_{x}^{2} + f_{x}^{"2} + h_{x}^{'2}, & f'_{x}f'_{y} + h_{x}h_{y} + f''_{x}f''_{y} + h'h'_{x}h'_{y} \\ f'_{x}f'_{y} + h_{x}h_{y} + f''_{x}f''_{y} + h'xh'_{y}, & f'_{y}^{'2} + h'_{y}^{2} + f''_{y}^{'2} + h'^{'2}_{y} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix}$$

$$= -\begin{bmatrix} f'f'_{x} + hh_{x} + f''f''_{x} + h'h'_{x} \\ f'f'_{y} + hh_{y} + f''f''_{y} + h'h'_{y} \end{bmatrix}$$
(9)

The values of x and y that give $\Delta x = \Delta y = 0$ correspond to the minimum with respect to x and y of the quantity

$$E = f'^{2} + h^{2} + f''^{2} + h'^{2}$$
(10)

The partial derivatives with respect to x and y that appear in the equation (9) are obtained by integrating the appropriate perturbation differential equations. The perturbation differential equations for the x derivatives are

$$f_{x}^{"'} = -3(f_{x}f^{"} + ff_{x}^{"}) + 4f'f_{x}' - h_{x}$$
(11)

and

$$h''_{X} = -3 Pr(f_{X}h' + fh'_{X})$$
 (12)

with the initial conditions

 $\eta = 0$: $f_X = f'_X = h_X = h'_X = 0$; $f''_X = 1$

The perturbation differential equations for the y derivatives are

$$f_{y}''' = -3(f_{y}f'' + ff_{y}'') + 4f'f_{y}' - h_{y}$$
(13)
$$h_{v}'' = -3Pr(f_{y}h' + fh_{y}')$$
(14)

with the initial conditions

$$\eta = 0$$
: $f_y = f'_y = f''_y = h_y = 0$; $h'_y = 1$

Note that the equations for the y derivatives are the same as the equations for the x derivatives. The integrals of these equations will differ since the initial conditions are different.

Note also that there are as many additional systems of perturbation equations to integrate as there are asymptotic boundary conditions to meet.

NUMERICAL SOLUTION OF EXAMPLE 2 AND RESULTS

The same general procedure used in the previous example was employed to solve this example. One notable difference is that five trials were needed at the larger value of η_{stop} , rather than the three trials of the first example. This is probably because of the need of adjusting two initial conditions rather than one, and because an error in one initial condition leads to an error in computing the correction term of the other.

The solutions of equations (7) and (8) are shown in figure 5 for Pr = 0.733. Note (as in the previous example) that the functions f' and h of figure 5 diverge radically from the true solutions, for the initial guesses of trial 1.

Table 1(b) shows the rapid rate of convergence for this more difficult example. With initial guesses of 1.0 and - 1.0 for f"(0) and h'(0), respectively, convergence is realized after two trials with $\eta_{stop} = 2$ and five trials with $\eta_{stop} = 8$. The results are in close agreement with the published values of Ostrach (ref. 8).

The effect of η_{stop} on the convergence process for this example is illustrated in figures 6(a) and (b). Level curves for the error, equation (10), are plotted in the f"(0) plane for $\eta_{\text{stop}} = 2$ in figure 6(a) and for $\eta_{\text{stop}} = 5$ in figure 6(b). As in the previous example, by using a small value for η_{stop} , the range of initial guesses that yields a relatively small error is again increased; that is, the area where E is less than 1 is much greater in figure 6(a) than in figure 6(b). For extremely large values of η_{stop} , the area enclosed by the level curve where E is less than 1 shrinks to a point, and the initial guess is limited to the correct answer.

Computer time for the second example was about 0.15 minutes with a step size of 2^{-4} . In both examples, the convergence was made insensitive to the initial guesses by choosing a small value of η_{stop} for the first two trials. The answer thus obtained for the initial conditions was good

enough to step η_{stop} up considerably. The error term may be made as small as desirable by continuous stepping of η_{stop} . This error term may also be used as a stopping criteria for computer calculations and findings η_{edge} automatically.

CONCLUSIONS

The two main problems of integrating the boundary-layer equations, approximating the missing initial conditions, and finding η_{edge} , have been reduced to an automatic initial-value technique that is easily programed on high-speed computers. The method appears to be insensitive to initial guesses and converges quickly to the solution.

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TABLE I. - CONVERGENCE HISTORY OF

INITIAL VALUES

Trial	Correction	^ŋ stop	f"(0)				
1 2 3 4 5	1 2 3 4 5	2.0 2.0 5.0 5.0 5.0	1.0 1.2463981 1.2266764 1.2326729 1.2325878 1.2325878				

(a) Example 1

Published values

Source	nstop	f"(0)
Radbill (ref. 2)	5.0	1.2397
(ref. 6)	4.0	1.2325876

(b) Example 2

Trial	Correction	η_{stop}	f"(0)		h'(0)					
1 2 3 4 5 6 7	l 2 3 4 5 6 7	2.0 2.0 8.0 8.0 8.0 8.0 8.0	1.0 .61735605 .63211384 .66795925 .67387305 .67412049 .67412438 .67412438		-1.0 59008297 57655550 52593128 50916398 50790411 50789273 50789273					
Published values										
	Source	η_{stop}	f"(0)	h'(0)						
	Ostrach (ref. 8)		0.6741	-0.5	080					



Figure 2. - Error as function of f"(0) for different values of η_{stop} .

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Figure 6, - Level curves of error as function of f"(0) and h'(0).

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