Accurate Numerical Solutions of Boundary Layer Flows by the Finite-Difference Method of Hermitian Type

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An accurate and efficient method for the numerical computation of boundary layer flows is developed. The finite-difference approximation of the differential equation uses the grid point values of the function and of the first derivative. In order to obtain the finite-difference schemes of higher order the collocation method of Falk is applied with Hermitian interpolating polynomials. This results in a system of finite-difference equations for the unknown function and first derivative. The equations are solved by means of a Gaussian elimination procedure. In order to verify the accuracy and efficiency of this finite-difference method of Hermitian type an ordinary differential equation of second order is solved as a test example. Then this technique is applied to equations of boundary layer flows, in particular to the Falkner-Skan equation and to Howarth's retarded flow. Numerical results are presented for each test example. Comparisons with results of other authors indicate a gain in accuracy for the finite-difference method of Hermitian type.

1. INTRODUCTION

Various numerical techniques have been developed for the computation of boundary layer flows. In order to generate accurate results even for complex flows, e.g., a turbulent chemical reacting flow, ordinary second order methods have to use a high number of grid points and, thus, become less efficient. Hence, higher order methods are required.

The concept of the ordinary finite-difference method aims at replacing all derivatives by the corresponding difference quotients. Keeping the mesh spacing constant the accuracy increases if finite-difference expressions of higher order are used for the replacement of all derivatives. In general, however, each of these resulting finitedifference equations involve a greater number of unknown variables. Yet without increasing the number of unknown variables in the finite-difference equations a greater accuracy is obtained by applying the Hermitian finite-difference method [1]. This method makes use of the finite-difference approximation of the differential equation given by a Taylor series expansion, at several grid points. A different approach of setting up the Hermitian finite-difference equations applies the collocation method by Falk [2]. For the general case of ordinary differential equations of second order Zurmühl [3] has derived Hermitian finite-difference expressions by the collocation method whereby the function is approximated by Lagrange's interpolation formulas.

Additionally, the truncation error of the finite-difference expression can be reduced by replacing the higher order derivatives by the grid point values of the function and of the first, the second, etc., derivatives. Such expressions follow from Hermite's generalization of Taylor's formulas. Here, the finite-difference approximation of the differential equation is obtained by the collocation method [2] which is simple to handle and requires no special previous knowledge. The approximation is based upon Hermite's interpolation formulas. In addition to the grid point values of the function as in the case of the Lagrangian interpolation formulas, the finite equations involve the grid point values of the derivatives. Therefore, the derived method is called "finite-difference method of Hermitian type," abbreviated FMH.

To illustrate what is outlined above the system of finite-difference equations for an ordinary differential equation of second order is set up by the FMH. Furthermore, a Gaussian elimination procedure is given for the direct solution of the system of these equations. A linear second order differential equation is solved as an example. With respect to the accuracy and the computation time the numerical results are compared with those obtained by known second and fourth order methods. The main purpose of the paper presented is to demonstrate the numerical virtues of accuracy and efficiency by means of applying FMH to similar and nonsimilar boundary layer flows. The advantage of the FMH is illustrated by the solution of the Falkner–Skan equation for various pressure-gradient parameters, for blowing and suction at the wall, and for flows with surface curvature. The application to more general boundary layer flows is demonstrated, in particular for Howarth's retarded flow.

2. The Finite-Difference Schemes of Hermitian Type Using the Collocation Method

Consider an ordinary linear differential equation (ODE) of second order

$$ay'' + by' + cy = r \tag{1}$$

with the boundary conditions

$$y(x_1) = y_1, \qquad (2a)$$

$$y'(x_M) = y'_M, \qquad (2b)$$

where y_1 , y'_M are given boundary values and the coefficients of the ODE *a*, *b*, *c* and *r* depend on *x*. The dash denotes differentiation of the function with respect to the independent variable *x*. The interval $[x_1, x_M]$ is divided into a uniform mesh with mesh spacing $h = (x_M - x_1)/(M - 1)$, where *M* is the number of grid points x_j (j = 1,..., M).

For the numerical solution of equation (1) with a = 1 and b = 0, finite-difference expressions of fourth order have been developed by Collatz [1] employing the three point Mehrstellen method (Hermitian finite-difference method). These Hermitian

finite-difference expressions can also be constructed with the collocation method of Falk [2]. Approximating the solution of Eq. (1) between three grid points with a fourth order polynomial, Zurmühl [3] has obtained the Hermitian finite-difference expressions using Falk's method. The Hermitian finite-difference procedure of Zurmühl has been applied by Peters [4] to boundary layer calculations. Another approach in constructing the Hermitian finite-difference approximations to equation (1) is the Mehrstellen procedure of Krause [5], which is based upon Taylor series expansions. In addition to the method of Zurmühl the Mehrstellen procedure does provide the truncation error of the Hermitian finite-difference expressions, but the derivation is more complicated. Therefore, the finite-difference method of Hermitian type described below is obtained by applying the collocation method of Falk with Hermitian interpolating polynomials. This procedure differs from those employed by Zurmühl using Lagrangian interpolating polynomials.

According to Falk [2] we consider the approximation to the differential equation of the form

$$y(x) \approx Y(x) = S(x) + P(x) Z(x).$$
(3)

The finite-difference expressions of Hermitian type for the numerical solution of equation (1) may be constructed by the collocation procedure using polynomials. Here, the Hermitian interpolating polynomial of first order between the three grid points x_{j-1} , x_j and x_{j+1} is used for the function S

$$S(x) = \sum_{l=-1}^{1} \{H_{j+l}(x) S_{j+l} + K_{j+l}(x) S'_{j+l}\} + O(h^{6}).$$
(4)

The Hermitian function H and K are polynomials of fifth order which satisfy the conditions

$$H_k(x_{j+l}) = \begin{cases} 1 & \text{for } l = k, \\ 0 & \text{for } l \neq k, \end{cases} \quad H'_k(x_{j+l}) = 0 \quad \text{for all } l, \tag{5}$$

$$K_k(x_{j+l}) = 0 \quad \text{for all } l, \qquad K'_k(x_{j+l}) = \begin{cases} 1 & \text{for } l = k, \\ 0 & \text{for } l \neq k. \end{cases}$$
(6)

With the abbreviation $t = (x - x_j)/h$ the polynomials read

$$H_{j-1} = t^2 - \frac{5}{4}t^3 - \frac{1}{2}t^4 + \frac{3}{4}t^5, \qquad (7a)$$

$$H_j = 1 - 2t^2 + t^4, (7b)$$

$$H_{j+1} = t^2 + \frac{5}{4}t^3 - \frac{1}{2}t^4 - \frac{3}{4}t^5, \qquad (7c)$$

$$K_{j-1} = \frac{h}{4} \left(t^2 - t^3 - t^4 + t^5 \right), \tag{8a}$$

$$K_j = h(t - 2t^3 + t^5),$$
 (8b)

$$K_{j+1} = \frac{h}{4} \left(-t^2 - t^3 + t^4 + t^5 \right). \tag{8c}$$

The function P in Eq. (3) is defined as

$$P(x) = (x - x_{j-1})^2 (x - x_j)^2 (x - x_{j+1})^2$$
(9)

such that for any arbitrary function Z the grid point values of Y_j and S_j as well as of Y'_j and S'_j are the same. In the general case the function Z contains a number of freely chosen coefficients depending on the number of the finite-difference equations for the unknown grid point values of the function and of the first derivative. For the example chosen we put

$$Z(x) = \alpha. \tag{10}$$

By differentiation of Eq. (4) the following finite-difference expressions of Hermitian type are obtained at each grid point

$$S_{j-1}'' = \frac{1}{2h^2} \left(-23S_{j-1} + 16S_j + 7S_{j+1} \right) - \frac{1}{h} \left(6S_{j-1}' + 8S_j' + S_{j+1}' \right) + TE_{j-1}, \quad (11a)$$

$$S''_{j} = \frac{2}{h^{2}} \left(S_{j-1} - 2S_{j} + S_{j+1} \right) + \frac{1}{2h} \left(S'_{j-1} - S'_{j+1} \right) + TE_{j}, \qquad (11b)$$

$$S_{j+1}'' = \frac{1}{2h^2} \left(7S_{j-1} + 16S_j - 23S_{j+1}\right) + \frac{1}{h} \left(S_{j-1}' + 8S_j' + 6S_{j+1}'\right) + TE_{j+1}, \quad (11c)$$

where TE_{j-1} , TE_j and TE_{j+1} are the truncation errors (see Appendix A). The approximation (3) is required to satisfy the differential equation (1) exactly at three distinct points ("Collocation"). The points of collocation which, in general, can be chosen somewhere within the interval $[x_{j-1}, x_{j+1}]$, are taken to be the grid points x_{j-1} , x_j and x_{j+1} .

$$x = x_{j-1}:$$

$$\left(c_{j-1} - \frac{23}{2h^2} a_{j-1}\right) Y_{j-1} + \frac{16}{2h^2} a_{j-1}Y_j + \frac{7}{2h^2} a_{j-1}Y_{j+1} + \left(b_{j-1} - \frac{6}{h} a_{j-1}\right) Y'_{j-1} - \frac{8}{h} a_{j-1}Y'_j - \frac{1}{h} a_{j-1}Y'_{j+1} + (8h^4 a_{j-1}) \alpha = r_{j-1} - TE_{j-1}.$$
(12a)

$$x = x_{j}:$$

$$\frac{2}{h^{2}} a_{j}Y_{j-1} + \left(c_{j} - \frac{4}{h^{2}}a_{j}\right)Y_{j} + \frac{2}{h^{2}}a_{j}Y_{j+1} + \frac{1}{2h}a_{j}Y'_{j-1}$$

$$+ b_{j}Y'_{j} - \frac{1}{2h}a_{j}Y'_{j+1} + (2h^{4}a_{j})\alpha = r_{j} - TE_{j}.$$
(12b)

$$x = x_{j+1};$$

$$\frac{7}{2h^2} a_{j+1} Y_{j-1} + \frac{16}{2h^2} a_{j+1} Y_j + \left(c_{j+1} - \frac{23}{2h^2} a_{j+1}\right) Y_{j+1} + \frac{1}{h} a_{j+1} Y'_{j-1} + \frac{8}{h} a_{j+1} Y'_j + \left(b_{j+1} + \frac{6}{h} a_{j+1}\right) Y'_{j+1} + (8h^4 a_{j+1}) \alpha = r_{j+1} - TE_{j+1}.$$
(12c)

The free coefficient α is eliminated by multiplying the finite-difference equations at the grid points x_{j-1} and x_j by the factors a_j and $4a_{j-1}$, respectively, and subtracting one equation from the other. To simplify the representation we choose a = 1, b = c = r = 0 in Eq. (1).

$$-\frac{39}{2h^2}Y_{j-1}+\frac{24}{h^2}Y_j-\frac{9}{2h^2}Y_{j+1}-\frac{8}{h}Y'_{j-1}-\frac{8}{h}Y'_j+\frac{1}{h}Y'_{j+1}=\frac{h^5}{630}Y_j^{\text{VII}}\cdots.$$
 (13a)

In the same way the elimination of α from the finite-difference equations at the grid points x_j and x_{j+1} yields

$$-\frac{9}{2h^2}Y_{j-1} + \frac{24}{h^2}Y_j - \frac{39}{2h^2}Y_{j+1} - \frac{1}{h}Y'_{j-1} + \frac{8}{h}Y'_j + \frac{8}{h}Y'_{j+1} = \frac{-h^5}{630}Y_j^{\text{VII}}\cdots.$$
(13b)

The application of the collocation method of Falk provides a truncation error $O(h^5)$ for the finite-difference equations (13a) and (13b). This will also be shown by the numerical results in Section 4. In the general case similar equations are obtained for the finite-difference expressions of the differential equation (1). But it is much more efficient to perform the elimination numerically.

For the sake of simplicity, the finite-difference method of Hermitian type was applied to a uniform mesh spacing. The extension to nonuniform grids and to finite-difference schemes for more than three grid points is described in [6].

3. THE SYSTEM OF FINITE-DIFFERENCE EQUATIONS AND ITS SOLUTION

At each grid point x_j the value of the function Y_j and the value of the first derivative Y'_j are the unknowns of the derived finite-difference method of Hermitian type. For the differential equation (1) with two boundary conditions 2M - 2 finite-difference equations are necessary to determine the grid point values Y_j and Y'_j . In order to match the number of equations to the number of unknowns, we let $\alpha = 0$ when j = 2 in Eq. (10). Thus, collocation at the grid points x_1 , x_2 and x_3 leads to the three finite-difference equations (12a) till (12c). Correspondingly, there are three equations for j = M - 1. Further 2M - 8 equations are obtained with use of Eq. (10) for j = 3, ..., M - 2.

The system of finite-difference equations can be written in the general form

$$A_i Y_{j-1} + B_i Y'_{j-1} + C_i Y_j + D_i Y'_j + E_i Y_{j+1} + F_i Y'_{j+1} = R_i, \quad j = 2, ..., M - 1,$$
(14)

where the index *i* is

$$i = 2j + k$$
 with $\begin{cases} k = -3, -2, -1 & \text{for } j = 2, \\ k = -2, -1 & \text{for } j = 3, ..., M - 2, \\ k = 0, 1, 2 & \text{for } j = M - 1. \end{cases}$

The coefficients A_i to R_i are the coefficients that appear in Eqs. (12a) to (12c) for

j = 2 and j = M - 1, i.e., Z = 0, $\alpha = 0$, as well as in Eqs. (13a) and (13b) for j = 3, ..., M - 2. The coefficient structure of the developed system is shown in Fig. 1 where the boundary conditions Y_1 and Y'_M are incorporated. As the first derivative Y'_j explicitly appears in the system, the boundary condition Y'_M requires no finite-difference approximation.

Y¦	^Y 2	۲,	Y ₃	۲ż	Y ₄	۲¦	 Ч _{М-3}	Υ, M-3	Ч _{М-2}	^ү м-2	^ү м-1	Y: M-1	Y _M	
^B 1 ^B 2 ^B 3	c ₁ c ₂ c ₃ A ₄ A ₅	D ₁ D ₂ D ₃ B ₄ B ₅	E ₁ E ₂ E ₃ C ₄ C ₅	F ₁ F ₂ F ₃ D ₄ D ₅	E ₄ E ₅	F ₄ F ₅	А _{2М-6} А _{2М-5}	^В 2М-6 ^В 2М-5	С _{2М-6} С _{2М-5} ^А 2М-4 ^А 2М-3 ^А 2М-2	D _{2M-6} D _{2M-5} B _{2M-4} B _{2M-3} B _{2M-2}	E _{2M-6} E _{2M-5} C _{2M-4} C _{2M-3} C _{2M-2}	F _{2M-6} F _{2M-5} D _{2M-4} D _{2M-3} D _{2M-2}	Е _{2М-4} Е _{2М-3} Е _{2М-2}	 $\begin{array}{c} R_{1}-A_{1}Y_{1} \\ R_{2}-A_{2}Y_{1} \\ R_{3}-A_{3}Y_{1} \\ R_{4} \\ R_{5} \\ \vdots \\ R_{2M-6} \\ R_{2M-5} \\ R_{2M-5} \\ R_{2M-5} - F_{2M-4}Y_{M} \\ R_{2M-3}-F_{2M-3}Y_{M} \\ R_{2M-2}-F_{2M-2}Y_{M} \end{array}$

FIG. 1. Coefficient structure of the system of finite-difference equations.

Because of the hepta-diagonal structure the system of finite-difference equations can be solved by means of a Gaussian elimination procedure. In order to get the recursion formulas the rewritten first finite-difference equation is set into the second and third equation. This yields the coefficients

$$Z_{i} = B_{1}C_{i+1} - B_{i+1}C_{1},$$

$$BK_{j} = (B_{1}D_{j+1} - B_{j+1}D_{1})/Z_{j},$$

$$CK_{j} = (B_{1}E_{j+1} - B_{j+1}E_{1})/Z_{j}, \qquad j = 1, 2,$$

$$DK_{j} = (B_{1}F_{j+1} - B_{j+1}F_{1})/Z_{j},$$

$$RK_{j} = (B_{1}R_{j+1} - B_{j+1}R_{1})/Z_{j}.$$

Now, with the help of the second equation Y_2 is eliminated from the third till the fifth equation. The elimination procedure continued up to the (2M - 2)th equation the coefficients

$$Z_{j} = (C_{2j+e} - A_{2j+e}CK_{2j-5}) ZB_{j-2} + (A_{2j+e}BK_{2j-5} - B_{2j+e}) ZC_{j-2},$$

$$j = 3, ..., M-2; e = -2, -1; m = e - 1.$$

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$$BK_{2j+m} = (D_{2j+e} - A_{2j+e}DK_{2j-5}) ZB_{j-2} + (A_{2j+e}BK_{2j-5} - B_{2j+e}) ZD_{j-2}/Z_j,$$

$$CK_{2j+m} = E_{2j+e}ZB_{j-2}/Z_j, \quad j = M-1; \ e = -2, -1, 0; \ m = e-1.$$

$$DK_{2j+m} = F_{2j+e}ZB_{j-2}/Z_j,$$

$$RK_{2j+m} = (R_{2j+e} - A_{2j+e}RK_{j-5}) ZB_{j-2} + (A_{2j+e}BK_{j-5} - B_{2j+e}) ZR_{j-2}/Z_j$$

are obtained, where the abbreviations are

$$ZB_{j-2} = BK_{2j-4} - BK_{2j-5},$$

$$ZC_{j-2} = CK_{2j-4} - CK_{2j-5},$$

$$ZD_{j-2} = DK_{2j-4} - DK_{2j-5},$$

$$ZR_{j-2} = RK_{2j-4} - RK_{2j-5}.$$

$$j = 3,..., M,$$

Then, the solution of the system of finite-difference equations reads

$$Y_{M} = \frac{(RK_{2M-3} - RK_{2M-5}) ZB_{M-2} + (BK_{2M-5} - BK_{2M-3}) ZB_{M-2}}{(CK_{2M-3} - CK_{2M-5}) ZB_{M-2} + (BK_{2M-5} - BK_{2M-3}) ZB_{M-2}},$$

$$Y'_{j} = (ZR_{j-1} - Y_{j+1}ZC_{j-1} - Y'_{j+1}ZD_{j-1})/ZB_{j-1},$$

$$Y_{j} = RK_{2j-3} - Y'_{j}BK_{2j-3} - Y_{j+1}CK_{2j-3} - Y'_{j+1}DK_{2j-3},$$

$$Y'_{1} = (R_{1} - Y_{2}C_{1} - Y'_{2}D_{1} - Y_{3}E_{1} - Y'_{3}F_{1})/B_{1}.$$

(15)

4. A COMPARISON OF FINITE-DIFFERENCE METHODS

In order to compare the efficiency of the finite-difference methods the differential equation

$$ay'' + y' + y = 1 (16)$$

with $a = (y'(0) - 1)/y'^{2}(0)$ is numerically solved as an example [5]. Equation (16) has the solution

$$y(x) = 1 - e^{-y'(0)x},$$
(17)

where y'(0) simulates the steep velocity gradient of turbulent boundary layers near the wall. In the present investigation the numerical calculations were performed for y'(0) = 2 and the interval [0, 1] with the boundary conditions given by Eq. (17).

The criterion for accuracy is the relative maximum of the difference from the analytical solution y_j of Eq. (17) for all grid points

$$\epsilon = \max_{1 < j < M} \frac{|Y_j - y_j|}{y_j}.$$

In order to assess the accuracy and the computation time the analytical solution (17) of Eq. (16) is compared to three numerical solutions of Eq. (16), by means of

- (I) ordinary finite-difference method (OFM), $O(h^2)$, Ref. [1],
- (II) Hermitian finite-difference method (HFM), $O(h^4)$, Ref. [3],
- (III) finite-difference method of Hermitian type (FMH), $O(h^5)$.

The programs were written in FORTRAN IV and the numerical calculations were run on the CDC 6500 Computer at the Technische Universität Berlin. Table I

Number of		Computation time t (sec)				
grid points	Step size h	OFM	HFM	FMH		
11	0.1	0.006	0.010	0.013		
26	0.04	0.014	0.023	0.034		
51	0.02	0.026	0.045	0.066		
101	0.01	0.052	0.090	0.119		
126	0.008	0.069	0.113	0.155		
201	0.005	0.117	0.178	0.233		

TABLE I

Comparison of the Computation Time for the Methods OFM, HFM, and FMH

presents the required computation time for the three finite-difference methods. These data plotted in Fig. 2 show that for all methods the computation time t rises linearly with the number of grid points M. Furthermore, for example, with M = 101 FMH needs about 1.4 times of the computation time of HFM and about 2.1 times of the computation time of OFM. This is due to the larger cost in setting up the finite-difference equation, and in solving a greater system of finite-difference equations for FMH.



FIG. 2. Computation time for the finite-difference methods.

Figure 3 presents the percentage error ϵ , plotted versus the step size h. For h = 0.01 the percentage errors are $\epsilon_{OFM} \approx 10^{-2} \%$, $\epsilon_{HFM} \approx 5.10^{-7} \%$ and $\epsilon_{FMH} \approx 10^{-9} \%$. To achieve a constant error, say $\epsilon = 2.10^{-3} \%$ for the three finite-difference methods, the step sizes are $h_{OFM} \approx 0.0045$, $h_{HFM} \approx 0.083$ and $h_{FMH} \approx 0.2$. A comparison of these results shows that the step size h_{FMH} is about twice as large as h_{HFM} and forty times as large as h_{OFM} . The number of required grid points is $M_{OFM} = 223$, $M_{HFM} = 13$ and $M_{FMH} = 6$, respectively. This leads to a high reduction in grid points for the derived FMH.

Despite a higher computation time the high accuracy of FMH provides a remarkable overall advantage. This will be demonstrated as follows. For the above mentioned example the computation time obtained by means of interpolation in Fig. 3 gives $t_{\rm OFM} \approx 0.13$ sec, $t_{\rm HFM} \approx 0.011$ sec and $t_{\rm FMH} \approx 0.006$ sec. In comparison, the computation time of FMH decreases by a factor of two for HFM and by a factor of twenty for OFM.

In spite of the fourth order approximation near the boundaries (j = 2 and j = M - 1) the overall order of the scheme is not effected. The slope of the error



FIG. 3. Errors of the numerical solution.

curves in Fig. 3 demonstrates that the truncation error of the FMH still is fifth order accurate. In order to show the effect of the new interpolation the calculations have also been performed for the FMH with $\alpha = 0$ in Eq. (10) everywhere. As predicted by Eq. (11) the order of the truncation error is 4, as for the HFM. Hence, the collocation method of Falk [2] yields a reduction of the truncation error. The FHM may be significantly improved by using more accurate 4-point approximations [6] near the boundaries (j = 2 and j = M - 2)

$$Y''_{j-1} = \frac{1}{6h^2} \left(-97Y_{j-1} + 81Y_{j+1} + 16Y_{j+2}\right) + \frac{1}{3h} \left(-22Y'_{j-1} - 54Y'_j - 27Y'_{j+1} - 2Y'_{j+2}\right) + 72h^6\alpha, \qquad (18a)$$
$$Y''_{j} = \frac{1}{54h^2} \left(56Y_{j-1} - 297Y_j + 216Y_{j+1} + 25Y_{j+2}\right) + \frac{1}{9h} \left(2Y'_{j-1} - 18Y'_j - 18Y'_{j+1} - Y'_{j+2}\right) + 8h^6\alpha, \qquad (18b)$$

$$Y''_{j+1} = \frac{1}{54h^2} \left(25Y_{j-1} + 216Y_j - 297Y_{j+1} + 56Y_{j+2} \right) + \frac{1}{9h} \left(Y'_{j-1} + 18Y'_j + 18Y'_{j+1} - 2Y'_{j+2} \right) + 8h^6 \alpha, \qquad (18c)$$

$$Y_{j+2}'' = \frac{1}{6h^2} \left(16Y_{j-1} + 81Y_j - 97Y_{j+2} \right) + \frac{1}{3h} \left(2Y_{j-1}' + 27Y_j' + 54Y_{j+1}' + 22Y_{j+2}' \right) + 72h^6 \alpha.$$
(18d)

By collocation at four points the additional unknown α is eliminated so that three finite-difference equations of Hermitian type remain. Applying Eq. (18) the overall order of the scheme is 6, as the slope of the curve shows.

5. THE FALKNER-SKAN EQUATION

Similarity solutions of boundary layers are of great interest for getting information about the behavior of boundary layer phenomena. For two-dimensional flows the incompressible laminar boundary layer equations can be reduced to

$$f''' + ff'' + \beta[1 - (f')^2] = 0$$
⁽¹⁹⁾

with the boundary conditions

$$\eta = 0$$
: $f = -K$, $f' = 0$, (20a)

$$\eta \to \infty; f' \to 1,$$
 (20b)

where primes denote the differentiation with respect to η .

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In the case K = 0 the well-known Falkner–Skan equation is obtained. In practice results were required for the pressure-gradient parameter in the range of $-0.19884 \le \beta \le 2$, where $\beta > 0$ means accelerating, $\beta = 0$ constant and $\beta < 0$ decelerating flows. In the Falkner–Skan problem with mass transfer [7] positive values of K indicate "blowing" or fluid injections, while negative values indicate "suction" or mass transfer to the wall.

The application of FMH to nonlinear ordinary differential equations of third order such as equation (19) does not pose any problems. The finite-difference expressions are obtained from the differentiated equation (5) with $x = \eta$ and $h = \Delta \eta$

$$S_{j-1}^{\prime\prime} = \frac{1}{2\Delta\eta^3} \left(99S_{j-1} - 48S_j - 51S_{j+1}\right) + \frac{1}{2\Delta\eta^2} \left(39S_{j-1}' + 96S_j' + 15S_{j+1}'\right), \quad (21a)$$

$$S_{j}''' = \frac{1}{2\Delta\eta^{3}} \left(-15S_{j-1} + 15S_{j+1} \right) - \frac{1}{2\Delta\eta^{3}} \left(3S_{j-1}' + 24S_{j}' + 3S_{j+1}' \right), \tag{21b}$$

$$S_{j+1}^{\prime\prime} = \frac{1}{2\Delta\eta^3} \left(51S_{j-1} + 48S_j - 99S_{j+1} \right) + \frac{1}{2\Delta\eta^2} \left(15S_{j-1}^{\prime} + 96S_j^{\prime} + 39S_{j+1}^{\prime} \right), \quad (21c)$$

and Eq. (9)

$$P_{j-1}^{''} = -72 \Delta \eta^3, \quad P_j^{''} = 0, \quad P_{j+1}^{''} = 72 \Delta \eta^3.$$
 (22)

Starting from Eq. (1) whose coefficients are chosen as $a_j = f_j$, $b_j = -\beta f'_j$, $c_j = 0$ and $r_j = -\beta$ the terms of the third derivatives (4) at the grid point x_{j-1} , x_j and x_{j+1} are added to the corresponding equations (12a) till (12c)

$$\bar{A}_{j+k}f_{j-1} + \bar{B}_{j+k}f'_{j-1} + \bar{C}_{j+k}f_j + \bar{D}_{j+k}f'_j + \bar{E}_{j+k}f_{j+1} + \bar{F}_{j+k}f'_{j+1} + \bar{G}_{j+k}\alpha = \bar{R}_{j+k},$$

$$k = -1, 0, 1, \quad (23)$$

where

$$\begin{split} \bar{A}_{j-1} &= \frac{99}{2 \Delta \eta^3} - \frac{23}{2 \Delta \eta^2} f_{j-1} , & \bar{A}_j &= -\frac{15}{2 \Delta \eta^3} + \frac{2}{\Delta \eta^2} f_j , \\ \bar{A}_{j+1} &= \frac{51}{2 \Delta \eta^3} + \frac{7}{2 \Delta \eta^2} f_{j+1} ; \\ \bar{B}_{j-1} &= \frac{39}{2 \Delta \eta^2} - \beta f'_{j-1} - \frac{6}{\Delta \eta} f_{j-1} , & \bar{B}_j &= \frac{-3}{2 \Delta \eta^2} + \frac{1}{2 \Delta \eta} f_j , \\ \bar{B}_{j+1} &= \frac{15}{2 \Delta \eta^2} + \frac{1}{\Delta \eta} f_{j+1} ; \\ \bar{C}_{j-1} &= -\frac{24}{\Delta \eta^3} + \frac{8}{\Delta \eta^2} f_{j-1} , & \bar{C}_j &= -\frac{4}{\Delta \eta^2} f_j , \\ \bar{C}_{j+1} &= \frac{24}{\Delta \eta^3} + \frac{8}{\Delta \eta^2} f_{j+1} ; \end{split}$$

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$$\begin{split} \bar{D}_{j-1} &= \frac{48}{\Delta\eta^2} - \frac{8}{\Delta\eta} f_{j-1} , & \bar{D}_j &= -\frac{12}{\Delta\eta^2} - \beta f_j , \\ & \bar{D}_{j+1} &= \frac{48}{\Delta\eta^2} + \frac{8}{\Delta\eta} f_{j+1} ; \\ \bar{E}_{j-1} &= -\frac{51}{2\Delta\eta^3} + \frac{7}{2\Delta\eta^2} f_{j-1} , & \bar{E}_j &= \frac{15}{2\Delta\eta^3} + \frac{2}{\Delta\eta^2} f_j , \\ & \bar{E}_{j+1} &= -\frac{99}{2\Delta\eta^3} - \frac{23}{\Delta2\eta^2} f_{j+1} ; \\ \bar{F}_{j-1} &= \frac{15}{2\Delta\eta^2} - \frac{1}{\Delta\eta} f_{j-1} , & \bar{F}_j &= -\frac{3}{2\Delta\eta^2} - \frac{1}{2\Delta\eta} f_j , \\ & \bar{F}_{j+1} &= \frac{39}{2\Delta\eta^2} - \beta f'_{j+1} + \frac{6}{\Delta\eta} f_{j+1} ; \\ \bar{G}_{j-1} &= 8\Delta\eta^4 f_{j-1} - 72\Delta\eta^3 , & \bar{G}_j &= 2\Delta\eta^4 f_j , \\ & \bar{R}_{j+1} &= -\beta , & \bar{R}_j &= -\beta , \\ & \bar{R}_{j+1} &= -\beta . \end{split}$$

As described in Section 2, the elimination of the parameter α at the grid points j = 2, ..., M - 2 which is performed numerically leads to higher order expressions for the Falkner-Skan equation (19). Because of the lengthiness these equations are not written out. For j = M - 1 Eqs. (23) are applied with $\alpha = 0$. As $f'_1 = 0$ is the known boundary condition the first (i = 1) of the finite-difference equations in (14) will not be used. Apart from this boundary condition, the coefficient structure of the system of finite-difference equations is the same as shown in Fig. 1. Thus, the solution procedure described in Section 3 may also be applied to differential equations of third order. In order to obtain a system of linear finite-difference equations the differential equation (19) must be linearized. Assuming an initial guess for f_i and f'_i the linearization is performed by using the Newton-Raphson procedure (see e.g. [8]). The iteration cycle is repeated until two consecutive solutions of f'_i differ by less than a chosen error ϵ . For all calculations a linear velocity profile is simply assumed for the initial values ${}^{0}f'_{j}$ from which ${}^{0}f_{j}$ is obtained by integration. The convergence criterion is $\epsilon = |v+1f'_j - vf'_j| < 10^{-6}$ at all grid points x_j , which will also be used for all calculation in this paper.

In boundary layer calculation the shear on the wall is of great interest. This most sensitive quantity is determined from $d^2f(0)/d\eta^2 = f''_w$ given by equation (11a) with the truncation error $O(\Delta \eta^4)$. Thus, only f''_w is compared with the results of other numerical methods which have been developed for the solution of the Falkner-Skan equation.

The classical Blasius equation is obtained for the pressure-gradient parameter $\beta = 0$. In Table II the calculated values of f''_w are compared with the best methods available, the Keller and Cebeci box scheme [9] with second order accuracy and the

$\Delta\eta$	Present FMH	Number of iterations	Kreiss (Ref. [10])	Box (Ref. [9])
1.0	0.454130	6	0.430834	0.506065
0.8	0.466982	6		
0.5	0.469453	6	0.465713	0.478914
0.4	0.469558	6	0.468430	
0.333	0.469584	6		0.473753
0.3	0.469591	6	0.469381	
0.2	0.469601	9	0.469582	
0.1			0.469599	0.469975
0.05				0.469694
0-extrapola	ted			0.469601

TA]	BLE	п

Comparison of Calculated Values of f''_w for Blasius Flow

Kreiss method [10] with fourth order accuracy. The Kreiss method is of the same order as the Hermitian finite-difference method [3] cited in Section 4. An accuracy to five decimal places is achieved by FMH with $\Delta \eta = 0.2$ whereas the Kreiss method obtains this result with $\Delta \eta = 0.1$ and the box method by means of an extrapolation. For all comparable mesh spacing, e.g., $\Delta \eta = 0.5$, the FMH gives more accurate (third decimal place) results than the box method and even than the fourth order Kreiss method. No difficulties arise from the nonlinearities as the Newton-Raphson procedure converges for all values of $\Delta \eta$ within few iterations.

Table III presents the results for accelerating and decelerating flows. For nearly all values of the pressure-parameter β the values of f''_w , calculated by FMH with $\Delta \eta = 0.1$, agree in six significant digits with the findings of Smith [11]. The disagreement in the results of Cebeci and Keller [12] is in the sixth decimal place and probably due to the single precision arithmetic used. Even for crude mesh spacing of $\Delta \eta = 0.4$, FMH gives a third till fourth decimal place accuracy depending on β .

For boundary layer flows with mass transfer the usual nomenclature as in Ref. [7] is used. The mass transfer parameter is given by

$$K = v_w [(2 - \beta) x / \nu U(x)]^{1/2}$$

with $\beta < 2$ where v_w is the rate of mass transfer at the wedge surface. Calculations have been made for various values of β and K. In Table IV some of these results are shown together with the values obtained by Tan and Di Biano [13] and Elzy and Sisson [14]. In the parametric differention method of Ref. [13] the pressure-gradient parameter β or the mass transfer parameter K are to be chosen as the parameter.

TABLE III

Comparison of Calculated Values of f''_w for Accelerating and Decelerating Flows

	Present	FMH		
β	$\Delta \eta = 0.1$	$\Delta \eta = 0.4$	Ref. [12]	Ref. [11] 0.055172 0.085700 0.319270 0.400323 0.587035 0.686708 0.854421 1.120268 1.232588 1.335772 1.521514
-0.195	0.055171	0.055158	0.055177	0.055172
-0.19	0.085701	0.085705	0.085702	0.085700
-0.10	0.319270	0.319275	0.319278	0.319270
-0.05	0.400323	0.400305	0.400330	0.400323
0.10	0.587035	0.586952	0.587037	0.587035
0.20	0.686708	0.686603	0.686711	0.686708
0.40	0.854421	0.854336	0.854423	0.854421
0.80	1.120269	1.120437	1.120269	1,120268
1.00	1.232589	1.232938	1.232561	1.232588
1.20	1.335725	1.336247	1.335724	1.335772
1.60	1.521524	1.522254	1.521516	1.521514

TABLE IV

Comparison of Calculated Values of f''_w for Blowing and Suction

		Present	FMH		
β	K	$arDelta\eta=0.1$	$\Delta \eta = 0.4$	Ref. [13]	Ref. [14]
0	-2	2.194486	2.197200	2.1945	2.1945
	-1	1.283631	1.283757	1.2836	1.2836
	0.4	0.204860	0.204918	0.2048	0.2048
	0.8	0.017474	0.017473	0.0174	0.0174
0.5	-2	2.450992	2.450812	2.4512	2.3410
	-1	1.624196	1.624488	1.6246	1.6241
	0.4	0.707727	0.707667	0.7087	0.7077
	0.8	0.531357	0.531332	0.5323	0.5313
1.0	-2	2.670041	2.665105	2.6703	2,6700
	-1	1.889318	1.888862	1,8898	1.8893
	0.4	1.017943	1.018144	1.0188	1.0179
	0.8	0.835431	0.835504	0.8362	0.8354

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The calculations in Ref. [14] were performed with the multiple-step predictorcorrector type numerical integration formulas. Compared with the values of f''_w calculated by the FMH with $\Delta \eta = 0.1$, the agreement with the results of Elzy and Sisson is very good. Again, the farily large step size of $\Delta \eta = 0.4$ gives results which agree to three significant digits, at least.

6. SIMILAR SOLUTIONS OF THE EXTENDED FALKNER-SKAN EQUATION WITH SURFACE CURVATURE

The well-known Prandtl boundary layer equations do not take into account second order effects such as the surface curvature. Various papers have been published to solve the equations for a laminar incompressible boundary layer on a curved surface.

Murphy [15] was one of the first who discussed the surface curvature effects. In his investigations the Falkner–Skan equation was extended to flows over curved surfaces yielding similar solutions. Using his nomenclature the following fourth order differential equation is obtained by

$$f^{1V} + \Omega f''' + f f''' + \Omega f f'' - \gamma [f' f'' + \Omega (f')^2] = 0$$
(24)

with the boundary conditions

$$\eta = 0$$
: $f = 0$, $f' = 0$, (25a)

$$\eta \to \infty$$
: $f' \to e^{-\Omega \eta}, f'' \to -\Omega e^{-\Omega \eta}.$ (25b)

The flow over curved surfaces depends on the curvature parameter Ω and the parameter γ which is related to the pressure-gradient parameter β by $\gamma = 2\beta - 1$.

In most cases reported the numerical solution of Eq. (24) is obtained by a so-called shooting method using the Runge-Kutta step-by-step integral formulas. One difficulty in applying this method arises from the fact that initial estimates of both, f''(0) and f'''(0) have to be made. Another difficulty is that the initial estimates must only differ little from the exact values to assure convergence of the shooting method. These difficulties can be eliminated entirely by the application of the FMH to fourth order differential equations as it is illustrated below.

The finite-difference expressions for the fourth derivatives are obtained from the differentiated equation (5)

$$S_{j-1}^{IV} = \frac{1}{\Delta \eta^4} \left(-102S_{j-1} + 24S_j + 78S_{j+1} \right) - \frac{1}{\Delta \eta^3} \left(36S_{j-1}' + 120S_j' + 24S_{j+1}' \right),$$
(26a)

$$S_{j}^{IV} = \frac{1}{\varDelta \eta^{4}} \left(-12S_{j-1} + 24S_{j} - 12S_{j+1} \right) + \frac{1}{\varDelta \eta^{3}} \left(-6S_{j-1}' + 6S_{j+1}' \right), \tag{26b}$$

$$S_{j+1}^{IV} = \frac{1}{\Delta \eta^4} \left(78S_{j-1} + 24S_j - 102S_{j+1} \right) + \frac{1}{\Delta \eta^3} \left(24S_{j-1}' + 120S_j' + 36S_{j+1}' \right), \quad (26c)$$

and Eq. (9)

$$P_{j-1}^{IV} = 312 \Delta \eta^2, \quad P_j^{IV} = -48 \Delta \eta^2, \quad P_{j+1}^{IV} = 312 \Delta \eta^2.$$
 (27)

The finite-difference expressions of Eq. (24) are derived in the same way as those in Section 5 for a third order differential equation. However, the elimination of the parameter α in these expressions is accomplished at all inner grid points j = 2,...,M - 1. The missing finite-difference equation of higher order, that is the (2M - 3)rd equation, is given by the boundary condition $f''(\eta \rightarrow \infty) = -\Omega e^{-\Omega \eta}$ using Eq. (11c) for j = M - 1.

The system of finite-difference equations has the same coefficient structure as that for the Falkner-Skan equation in Section 5. Thus the recursion procedure for solving the equations can be applied. The numerical calculations indicate that no difficulties arise from the solution of Eq. (24) by the FMH and that, for this nonlinear problem, convergence is always obtained.

Table V presents the FMH-calculated values of f''_w and a comparison of values for the nondimensional displacement thickness

$$arDelta^+ = \int_0^\infty \left(1 - rac{f'}{e^{-\Omega\eta}}
ight) d\eta$$

TABLE V

Calculated Values of f''_w for Flows with Surface Curvature and Comparison of Integral Characteristic

β						
		$f_u^{\prime\prime}$, , ,	4	[+	4
	Ω	$\Delta \eta = 0.1$	$\Delta \eta = 0.4$	$\Delta \eta = 0.1$	$\Delta \eta = 0.4$	Δ+ (Ref. [15])
1	0.1	1.06760	1.06800	0.73853	0.73849	0.7386
1	0	1.23259	1.23311	0.64790	0.64781	0.6479
1	-0.1	1.39076	1.39135	0.58034	0.58039	0.5799
0.5	0.1	0.777417	0.777359	0.93423	0.93431	0.9342
0.5	0	0.927679	0.927599	0.80455	0.80461	0.8045
0.5	-0.1	1.07229	1.07195	0.71100	0.71169	0.7104
0.2	0.1	0.556090	0.556002	1.16040	1.16045	1.1604
0.2	0	0.686710	0.686571	0.98416	0.98422	0.9842
0.2	0.1	0.813270	0.808968	0.86066	0.87143	0.8606
0	0.1	0.367084	0.367074	1.45246	1.45245	1.4524
0	0	0.467603	0.469585	1.21678	1.21676	1.2168
0	-0.1	0.569485	0.573245	1.05353	1.04758	1.0537
-0.1	0.1	0.245411	0.245445	1.73090	1.73081	1.7282
-0.1	0	0.319269	0.319343	1.44270	1.44258	1.4427
-0.1	-0.1	0.390187	0.396656	1.25168	1.23700	1.2516

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calculated by a fourth order integration formula. For flows without pressure-gradient $(\beta = 0)$ and without surface curvature $(\Omega = 0)$, the fourth order differential equation (24) reduces to the Falkner-Skan equation (19). In this case the solution procedure by the FMH generates the same accuracy in five significant digits compared

 $\Delta \eta = 0.4$ the agreement of f''_w is very good, which is due to the high accuracy of the FMH even for differential equations of fourth order. For $\Delta \eta = 0.1$ the values of Δ^+ differ only in the fourth significant digit from those of Murphy [15] obtained by the shooting method. Except for concave surfaces ($\Omega < 0$) the same accuracy is also achieved for a larger $\Delta \eta$ -spacing ($\Delta \eta = 0.4$).

7. THE BOUNDARY LAYER EQUATIONS

In the previous sections the application of the FMH was illustrated for boundary value problems of ordinary differential equations up to the fourth order. The general boundary layer equations, however, are an excellent example for numerical checks on parabolic partial differential equations. Using the notation of Cebeci and Smith [16] by introducing the Levy-Lees transformation

$$d\xi = \mu \rho u_e \, dx, \qquad d\eta = \rho u_e / (2\xi)^{1/2} \, dy$$

and the dimensionless stream function $f(\xi, \eta) = \Psi(x, y)/(2\xi)^{1/2}$ the boundary layer equations can be written as

$$f''' + ff'' + \beta(\xi)[1 - (f')^2] = 2\xi \left[f' \frac{\partial f'}{\partial \xi} - f'' \frac{\partial f}{\partial \xi} \right].$$
(28)

Here $\partial f/\partial \eta$ is represented by f', etc., $\beta(\xi) = (2\xi/u_e) du_e/d\xi$ is the pressure-gradient parameter and u_e is the external velocity. The boundary conditions for flow without mass transfer at the wall become

$$\eta = 0$$
: $f(\xi, 0) = 0, \quad f'(\xi, 0) = 0,$ (29a)

$$\eta \to \infty$$
: $f'(\xi, \eta_{\infty}) = 1.$ (29b)

The numerical solution of the parabolic equation (28) with the FMH is obtained in the usual way of replacing the ξ derivatives by finite-differences [17]. The grid point locations used are η_j where $\eta_1 = 0$ and j = 1, 2, ..., M and ξ_i where $\xi_1 = 0$ and i = 1, 2, ..., N. At the station ξ_i the derivatives $(\partial f'/\partial \xi)_i$ and $(\partial f/\partial \xi)_i$ are approximated by the finite-difference Lagrangian formula

$$\left(\frac{\partial F}{\partial \xi}\right)_{i} = L_{i}F_{i} + L_{i-1}F_{i-1} + L_{i-2}F_{i-2}$$
(30)

2 -9 - The derivatives are of first order for two points with

$$L_i = \frac{1}{\xi_i - \xi_{i-1}}, \quad L_{i-1} = \frac{-1}{\xi_i - \xi_{i-1}}, \quad L_{i-2} = 0$$
 (30a)

and of second order for three points with

$$L_{i} = \frac{1}{\xi_{i} - \xi_{i-1}} + \frac{1}{\xi_{i} - \xi_{i-2}}, \qquad L_{i-1} = \frac{-(\xi_{i} - \xi_{i-2})}{(\xi_{i} - \xi_{i-1})(\xi_{i-1} - \xi_{i-2})},$$

$$L_{i-2} = \frac{\xi_{i} - \xi_{i-1}}{(\xi_{i} - \xi_{i-2})(\xi_{i-1} - \xi_{i-2})}$$
(30b)

As the values of f_{i-1} , f_{i-2} , f'_{i-1} , and f'_{i-2} have been determined at previous stations, all other quantities of Eq. (28) are evaluated at ξ_i . The result of this fully implicit method is an ordinary differential equation with the independent variable f at station ξ_i . Thus, Eq. (28) reads:

$$f''' + [f + 2\xi(L_if + L_{i-1}f_{i-1} + L_{i-2}f_{i-2})]f'' - [\beta + 2\xi L_i](f')^2$$

= $-\beta + 2\xi f'(L_{i-1}f'_{i-1} + L_{i-2}f'_{i-2}).$ (31)

Here the coefficients L_i , L_{i-1} and L_{i-2} are given by Eq. (30b) except at ξ_2 where the coefficients (30a) are used. At $\xi_1 = 0$, Eq. (31) reduces to the Falkner-Skan equation (19), the solution of which is described in Section 5.

The method described here was already successfully applied to calculate the most complex flow field of turbulent diffusion flames [18], where chemical reactions take place. These investigations have shown that the FMH generates numerical results of good accuracy even for a relatively crude $\Delta\eta$ -spacing. Thus, quite satisfactory calculations were accomplished, as will be demonstrated below.

One of the boundary layer flows which has been treated extensively [9, 10, 16, 19–21] is the Howarth's retarded flow [22] with $u_e(x) = 1 - x/8$. This problem will be employed as a convenient check of numerical solutions. As Keller and Cebeci [9] have published several tables of their results, the same grid point spacing is used in the present investigation, but with larger values of η_{∞} .

	1	2	3	4	5	6	7	8	9
$\xi_i \ \eta_j$	0 0	0.4 1.0	0.7 2.0	0.8 3.0	0.86 4.0	0.894 5.0	6.0	7.0	8.0

The nets $N_{r,s}$ for which each ξ -interval or η -interval is subdivided into (r + 1) or (s + 1) equal subintervals, respectively, contains (5r + 6)(8s + 9) points.

Howarth's problem was calculated by the author for various grid sizes, but only for $\Delta \eta = 0.2$ the results of f''_w are tabulated in Table VI. As is shown in Table II a smaller step size $\Delta \eta$ does not substantially improve the accuracy. The results of

		Present FMH		N (0, 0, 10)
ξn	N _{4,4}	N _{9,4}	N _{19,4}	N (9; 9, 19) (Ref. [9]) 0.469601 0.345941 0.207143 0.13924
0	0.469599	0.469599	0.469599	0.469601
0.4	0.345649	0.345893	0.345957	0.345941
0.7	0.206059	0.206881	0.207115	0.207143
0.8	0.137691	0.138876	0.139218	0.13924
0.86	0.083838	0.082268	0.082805	0.08286
0.894	0.021114	0.028728	0.030239	0.030531
Points	1066	2091	4141	9282

TABLE VI

Comparison of Calculated Values of f''_{w} for Howarth's Retarded Flow

Table VI clearly demonstrate, how the accuracy is influenced by a variation of the step size $\Delta \xi$. Comparison is made with excellent values computed by Keller and Cebeci [9] using the Richardson extrapolation. For the crude $\Delta \xi$ net $N_{4,4}$ the values of f''_w differ from the results in the column N (9; 9,19) for increasing ξ . The agreement becomes better for the more refined net $N_{9,4}$. Reducing the step size further, as for the net $N_{19,4}$, generates at least a four-decimal-place accuracy, but only half of the grid points are needed compared with Ref. [9].

One of the most significant quantities of boundary layer flows is the point of separation. The calculations performed using the FMH encountered no difficulty, even extremely close to the point of separation ξ_{sep} . Table VII shows the $f''_w = 0$ -extrapolated values of ξ_{sep} for three different nets checked against known results of other authors. The agreement is very good except for the net $N_{4,4}$ with a crude step size $\Delta \xi$.

Calculated Position of the Separation Point in Howarth's Retarded Flow

Autho	r	Ęsep	
Present FMH			
N4.4		0.956998	
$N_{9.4}$		0.958738	
N _{19.4}		0.958865	
Rosenhead	[21]	0.958504	
Hirsh	[10]	0.958544	
Keller and Ceb	eci [9]	0.958800	
Hartree	[20]	0.9589	
Smith and Clu	tter [19]	0.9600	

8. CONCLUSIONS

Using the collocation method of Falk with Hermitian interpolating polynomials the finite-difference method of Hermitian type was derived. The resulting system of finite-difference equations can be solved by a Gaussian elimination procedure. As the first derivative appears explicitly in the finite-difference scheme boundary conditions of first and second order might be used without a loss of accuracy. The application to boundary layer flows indicates an improvement of the accuracy and efficiency compared with known second and even fourth order methods. Thus, the finitedifference method of Hermitian type is of advantage for problems where other methods achieve accurate results only by means of a high number of grid points and, hence, requiring "high" storage and computing time.

APPENDIX A: TRUNCATION ERROR OF THE FINITE-DIFFERENCE EXPRESSIONS FOR THE SECOND DERIVATIVE

A Taylor series expansion of S(x) yields

$$S_{j\pm 1} = S_{j} \pm hS'_{j} + \frac{h^{2}}{2!}S''_{j} \pm \frac{h^{3}}{3!}S''_{j} + \frac{h^{3}}{4!}S_{j}^{\prime\prime\prime} + \frac{h^{4}}{4!}S_{j}^{IV} \pm \frac{h^{5}}{5!}S_{j}^{V} + \frac{h^{6}}{6!}S_{j}^{VI} \pm \frac{h^{7}}{7!}S_{j}^{VII} + \frac{h^{8}}{8!}S_{j}^{VIII} \cdots .$$
(A1)

From this equation follows

$$S_{j-1} - 2S_j + S_{j+1} = h^2 S_j'' + \frac{2}{4!} h^4 S_j^{IV} + \frac{2}{6!} h^6 S_j^{VI} + \frac{2}{8!} h^8 S_j^{VIII} \cdots,$$
(A2)

$$S_{j+1} - S_{j-1} = 2hS'_j + \frac{2}{3!}h^3S''_j + \frac{2}{5!}h^5S'_j + \frac{2}{7!}h^7S'^{\rm VII}_j \cdots .$$
 (A3)

By means of the differentiated equation (A3)

$$(S'_{j+1} - S'_{j-1}) h = 2h^2 S''_j + \frac{2}{3!} h^4 S^{IV}_j + \frac{2}{5!} h^6 S^{VI}_j + \frac{2}{7!} h^8 S^{VIII}_j \cdots$$
(A4)

we obtain from Eq. (A2) for the second derivative at the central grid point x_i

$$S_{j}'' = \frac{2}{h^{2}} \left(S_{j-1} - 2S_{j} + S_{j+1} \right) + \frac{1}{2h} \left(S_{j-1}' - S_{j+1}' \right) + TE_{j}, \qquad (A5)$$

where the truncation error is given by

$$TE_{j} = \frac{1}{360} h^{4}S_{j}^{VI} + \frac{1}{10080} h^{6}S_{j}^{VIII} \cdots .$$
 (A6)

The following Hermitian finite-difference formulas are derived by Collatz (cf. [1, p. 539]):

$$S_{j-1}'' - 8S_{j}'' + S_{j+1}'' + \frac{9}{h}(S_{j-1}' - S_{j+1}') + \frac{24}{h^2}(S_{j-1} - 2S_j + S_{j+1}) = \frac{1}{2520}h^6S_{j}^{VIII}\cdots,$$
(A7)
$$S_{j-1}'' - S_{j+1}'' + \frac{1}{h}(7S_{j-1}' + 16S_{j}' + 7S_{j+1}') + \frac{15}{h^2}(S_{j-1} - S_{j+1}) = -\frac{1}{315}h^5S_{j}^{VII}\cdots.$$
(A8)

Using Eq. (A5) the finite-difference expressions of Hermitian type at the grid points x_{j-1} and x_{j+1} may be performed from Eqs. (A7) and (A8) by adding and subtracting, respectively.

$$S_{j-1}'' = \frac{1}{2h^2} \left(-23S_{j-1} + 16S_j + 7S_{j+1} \right) - \frac{1}{h} \left(6S_{j-1}' + 8S_j' + S_{j+1}' \right) + TE_{j-1}, \quad (A9)$$

$$S''_{j+1} = \frac{1}{2h^2} \left(7S_{j-1} + 16S_j - 23S_{j+1} \right) + \frac{1}{h} \left(S'_{j-1} + 8S'_j + 6S'_{j+1} \right) + TE_{j+1} \,. \tag{A10}$$

The truncation errors are of fourth order

$$TE_{j\pm 1} = \frac{1}{90} h^4 S_j^{V1} \pm \frac{1}{630} h^5 S_j^{V11} + \frac{1}{1680} h^6 S_j^{V111} \cdots .$$
(A11)

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