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Campylotropic Coordinates

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In boundary value problems for ordinary differential equations the finite-difference calculations for solutions having large variation over a narrow region often lose accuracy because of mesh irregularity, short steps being needed in the boundary layer and large steps elsewhere. This loss is eliminated by transformation to coordinates where a uniform mesh can be used. Several examples show that it is advantageous to take a linear combination of length and angular variation along the solution curve as the transformed coordinate for the one-dimensional case, only one-tenth as many nodes being needed in some cases as for other current methods.

1. INTRODUCTION

The truncation error of a compact finite-difference approximation to a boundary value problem for an ordinary differential equation is controlled by refining the mesh in regions where derivatives of the solution are large while retaining as smooth a mesh as possible to raise the order of the approximation. These conflicting requirements may be reconciled by employing a uniform mesh in a transformed coordinate system that expands the scale in regions where the solution has rapid variation. The particular transformation proposed here is defined intrinsically along with the solution so that the region for mesh refinement need not be known in advance. This makes the method applicable to cases with internal boundary layers.

Current mesh adjustment and node addition schemes, such as those of deBoor [1], and Pereyra and co-workers [2], or Pearson [3], require mesh widths small enough to counter the nearly singular behavior in the boundary layer so that the use of thousands of nodes in a unit interval is common [3]. No more than 129 nodes have been needed to achieve acceptable accuracy for any of the examples treated here. This small memory requirement makes the present method attractive for extension to systems of ordinary differential equations or to partial differential equations.

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2. The Transformation

Let the differential equation relate dependent variable y to independent variable x. The solution of the differential equation is represented by a curve in the (x, y) plane. It is assumed that, by some preliminary scaling, x and y have become comparable quantities with variations contributing about equally to the total length of the solution curve. The distance variable s along the curve is found from

$$x_s^2 + y_s^2 = 1. \tag{1}$$

Distance is an attractive candidate coordinate because the derivatives x_s and y_s are bounded by 1, whatever the magnitude of y_x.

A difference method based on s will be less accurate in a region where the solution curve has a large change of direction over a short distance. For this reason, a coordinate t is proposed that increases with s and with changes in θ, the inclination of the solution curve:

$$t = s + C \int |\, d\theta \,|$$

or

$$t_s = 1 + C\,|\,\theta_s\,| \tag{2}$$

where C is a nonnegative constant length to be chosen. The relation of t to x and y is found from Eqs. (1) and (2) to be

$$(x_t^2 + y_t^2)(1 + C\,|\,\theta_s\,|)^2 = 1. \tag{3}$$

Variable t is the campylotropic (curvature-seeking) coordinate being presented.

3. Differential Equations

The differential equations considered here are of second order,

$$y_{xx} = f(x, y, y_x). \tag{4}$$

Introducing t as independent variable gives

$$x_t y_{tt} - y_t x_{tt} = x_t^3 f(x, y, y_t/x_t). \tag{5}$$

Now

$$\begin{aligned} \theta_s &= y_{xx}/(1 + y_x^2)^{3/2}, \\ &= x_t^3 f/(x_t^2 + y_t^2)^{3/2}. \end{aligned} \tag{6}$$

Let σ be the sign of f and assume that s and t increase in the direction of increasing x. Then

$$|\,\theta_s\,| = x_t^3 \sigma f/(x_t^2 + y_t^2)^{3/2} \tag{7}$$

so that Eq. (3) becomes

$$(x_t^2 + y_t^2)^{3/2} + C\sigma x_t^3 f = x_t^2 + y_t^2. \tag{8}$$

Except where σ is discontinuous, one may differentiate to obtain

$$(x_t x_{tt} + y_t y_{tt})[3(x_t^2 + y_t^2)^{1/2} - 2] + C\sigma x_t^2(3x_{tt} f + x_t f_t) = 0 \tag{9}$$

where

$$f_t = f_y y_t + (f_x + f_{y_x} f)\, x_t\,. \tag{10}$$

Equations (5) and (9) are a pair of second-order differential equations for the variables x and y as functions of independent coordinate t. Considered as a quasilinear system for x_{tt} and y_{tt}, the determinant of the coefficients is

$$-\{[3(x_t^2 + y_t^2)^{1/2} - 2](x_t^2 + y_t^2) + 3C\sigma f x_t^3\}.$$

By Eq. (8) the expression equals $-(x_t^2 + t_t^2)$ which by Eq. (3) is bounded and bounded away from zero for solutions of bounded curvature. The system of differential equations (5) and (9) is, therefore, nonsingular.

4. Difference Equations

Difference approximations of second-order accuracy in the mesh length h are

$$\begin{aligned} x_t &\doteq (x_1 - x_{-1})/2h, \\ x_{tt} &\doteq (x_1 - 2x_0 + x_{-1})/h^2, \end{aligned} \tag{11}$$

with the similar equations for the y derivatives, where the subscripts -1, 0, 1 denote adjacent mesh nodes in order of increasing t.

The difference forms for Eqs. (5) and (9) are obtained by substitution for the derivatives of the approximations given by Eq. (11) and evaluation of functions f, f_x, f_y, f_{y_x} and σ at each point. The solution is then computed by the iterative Newton-Raphson method as described by Henrici [4] starting from an initial approximation to the solution. The total length in t of the curve is computed for the initial approximation and for each succeeding iterate. Corresponding values of h are obtained by dividing by the given number of mesh intervals.

The effect of the introduction of the curvature dependent terms may be assessed by considering the local truncation error of one of the difference approximations in Eq. (11). Thus the error in y_t due to using the first of those approximations is

$$\text{Error} = Ah^2 y_{ttt}$$

where A is a constant. If the curve has total length S and total angular variation Θ, then

$$h = (S + C\Theta)/N \tag{12}$$

where N is the number of mesh intervals. Also,

$$y_{ttt} = [(t_s y_{sss} - y_s t_{sss})\, t_s - 3(t_s y_{ss} - y_s t_{ss})\, t_{ss}]/t_s^5.$$

For curves with positive curvature, Eq. (2) becomes

$$t_s = 1 + C\theta_s$$

so that the local error may be written

$$\begin{aligned}\text{Error} = A(S/N)^2 (1 + C\Theta/S)^2 \{&[(1 + C\theta_s)\, y_{sss} - C\theta_{sss} y_s](1 + C\theta_s) \\ &- 3[(1 + C\theta_s)\, y_{ss} - C\theta_{ss} y_s]\, C\theta_{ss}\}/(1 + C\theta_s)^5. \end{aligned} \tag{13}$$

Where the solution curve is so straight that the derivatives of θ appearing in Eq. (13) are negligibly small, the error depends on C only through the factor $(1 + C\Theta/S)^2$ and therefore increases as C increases.

At the point of maximum curvature, where $|\theta_s| = K$ and $\theta_{ss} = 0$, one finds

$$\begin{aligned} |\text{Error}| &\leqslant |A|(S/N)^2 |y_{sss}| E, \\ E &= (1 + \alpha\gamma)^2 (1 + \beta\gamma)/(1 + \gamma)^4, \\ \alpha &= \Theta/SK, \beta = 1 + |y_s \theta_{sss}|/|y_{sss}| K, \gamma = CK. \end{aligned}$$

Since Θ/S is the average curvature, $0 < \alpha \leqslant 1$. Also, from their formulas, $\beta \geqslant 1$ and $\gamma \geqslant 0$. Differentiation gives

$$\frac{d \ln E}{d\gamma} = \frac{2\alpha + \beta - 4 + (3\alpha\beta - 2\alpha - 3\beta)\,\gamma - \alpha\beta\gamma^2}{(1 + \gamma)(1 + \alpha\gamma)(1 + \beta\gamma)}.$$

One sees that an increase in C can decrease the error. This decrease occurs near $C = 0$ if $(2\alpha + \beta - 4)$ is negative and also occurs in any case if C is large enough that the term $(-\alpha\beta\gamma^2)$ dominates the numerator of the fraction.

In summary, increasing the contribution of the curvature to the coordinate definition by increasing C increases the local truncation error on straight sections of the solution curve but can reduce the error on curved sections.

5. Examples

Differential equation (4) is of boundary layer type if there are short sections of the solution curve on which f is very large relative to its average value. The large value of f is produced in the present examples by a parameter p.

Other parameters governing the computations are the number N of mesh intervals and the constant C in the campylotropic coordinate specification. The relation between

N and p in the given coordinates has been explored by Dorr [5] who shows that, if N is not large enough, the numerical solution may be grossly inaccurate. In each case here, N is chosen sufficiently large so that reasonable accuracy is obtained.

The method has been applied to four examples: The parabola provides the simplest case since f is constant; the hyperbola is typical for boundary layer problems since, as the vertex curvature increases, the curve approaches two straight lines joined by a boundary layer; the exponential is a case with very large parameter similar to problems that have been previously treated; and the practical problem formulated by Troesch and solved numerically only with great difficulty, if certain standard approaches are used, has been the subject of several analyses,

The calculations were begun in each case by a computation with parameter $C = 0$ and a small number of mesh intervals, $N = 4$ or 8. Initial values of the x_i and y_i could be taken almost arbitrarily for cases of moderate curvature with $p < 5$. Less than 10 Newton-Raphson iterations then converged to a change of less than 10^{-8} out of a total range of 1 or 2 in either variable. Number N was then doubled, linear interpolation provided initial values at the added nodes and the iterative solution process repeated. The error in the numerical solution was computed using the analytic solution. Sufficient accuracy was obtained with N no more than 128 in every case. Steps were then taken to increase C until the error passed through its minimum. For cases of large curvature, $p > 5$, the iterations fail to converge unless the initial values are chosen to be sufficiently accurate. The solution points for a not too much smaller value of p are satisfactory.

A. *Parabola Example*

The differential equation and boundary conditions are

$$y'' = p,\ y = 0 \text{ at } x = \pm(2/p)^{1/2}.$$

The exact solution is

$$y = (p/2)\, x^2 - 1,$$

and the maximum curvature is

$$K = p.$$

The error, defined as the maximum of the absolute value of the difference between the exact and computed values of y at each computed value of x, is plotted in Fig. 1 as a function of the nondimensional product CK. One sees that the difference scheme is less accurate as the curvature of the solution increases but that a proper choice of C can greatly reduce the error.

The change to campylotropic coordinates is not recommended for use with linear equations since it introduces nonlinearities. The solution to this particular example would be found exactly by a second order method in the original variable.

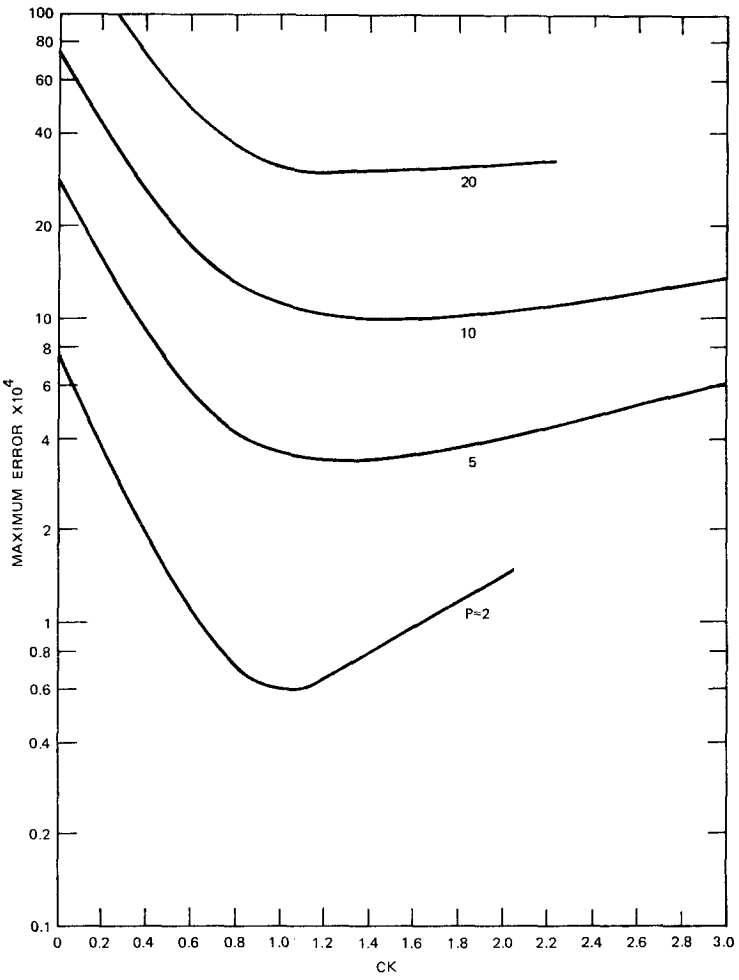

FIG. 1. Error variation with parameter C: Parabola example, $N = 32$.

B. *Hyperbola Example*

The hyperbola

$$y = (1/p)[1 + (p^2 - 1)\, x^2]^{1/2}$$

exhibits the general properties of boundary-layer-type solution curves most clearly. For large p, the solution follows the broken line $y = | x |$ except for a sharp bend at the corner. The differential system reads

$$y'' = [(p^2 - 1)/p][1 + (p^2 - 1)\, x^2]^{-3/2},\ y(\pm 1) = 1.$$

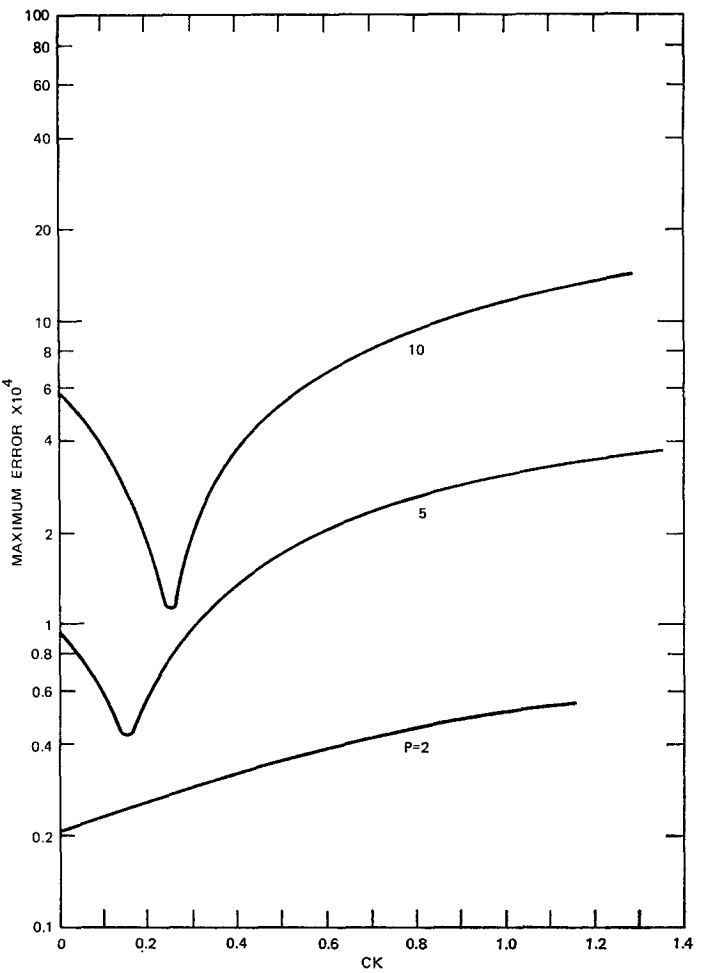

FIG. 2. Error variation with parameter C: Hyperbola example, $N = 128$.

The maximum curvature is

$$K = (p^2 - 1)/p.$$

In every case computed, the error was found to be greatest at a point near the vertex. The error is plotted in Fig. 2. One sees that the use of positive C is more effective the more curved the solution, i.e., the larger p is.

C. *Exponential Example*

A simple example that has been carried to very large values of p is the differential equation for exponentials,

$$y'' = p^2 y.$$

The solution with $y(0) = 0$ and $y(1) = 1$ is

$$y = (\sinh px)/\sinh p.$$

The corresponding curve lies close to $y = 0$ and to $x = 1$, fitting more tightly into the corner as p increases. The curvature κ is

$$\kappa = p^2 y[1 + p^2 y^2 + p^2/\sinh^2 p]^{-3/2}.$$

For $p > 5$, the third term in the bracket is negligible with respect to the first. If that

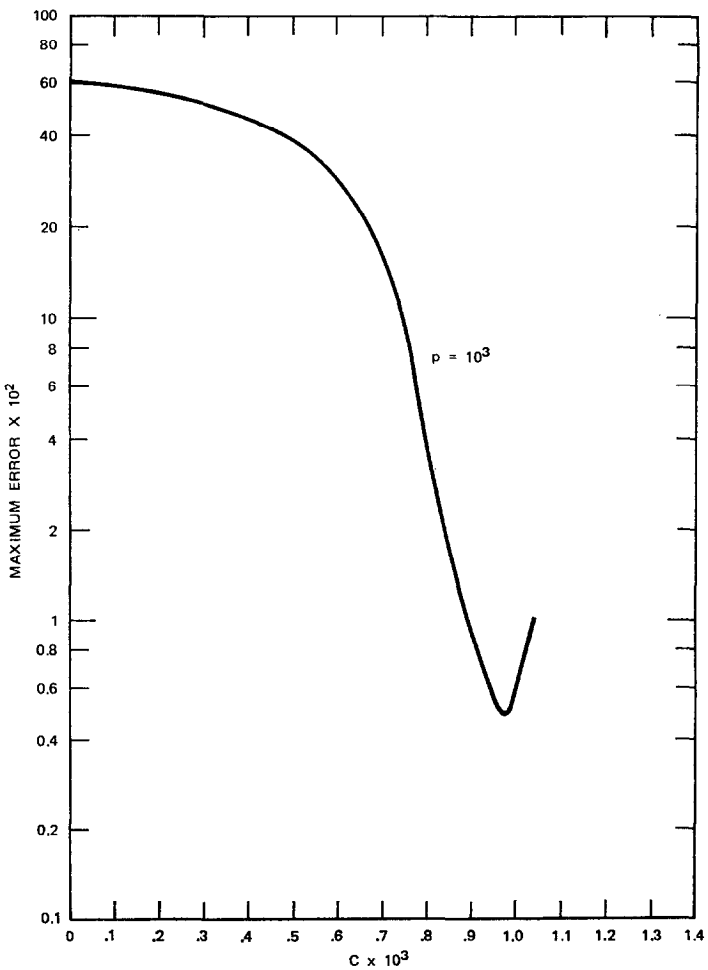

FIG. 3. Error variation with parameter C: Exponential example, $N = 128$.

third term is deleted, (κ/p) becomes a simple function of py with maximum at $py = 2^{-1/2}$. The maximum curvature K is then approximately

$$K = 2p(3)^{-3/2}.$$

The computations for a given p start with estimated values of x and y at each node. As observed by Pearson [3], the accuracy of these values is less critical for small p. The calculations were, therefore, begun with p of the order of 10. The results of the computation with one value of p were used as starting values for the next larger p. The process worked properly with p increased by a factor of $2^{1/2}$ at each step. These steps were taken to reach $p = 10^3$ using $N = 128$ mesh intervals and $C = 0$. An error of 0.60 was obtained, the error being defined as the maximum difference between exact and computed values of y at the computed node values of x. (Such a large error implies that it is an accurate representation of the solution to the difference equations rather than the differential equation that is needed for the starting values.) Convergence to a change between iterates of less than 10^{-8} was obtained generally in five or fewer iterations.

Steps in parameter C were then taken to find the least error of 0.005 at $C = 0.96 \times 10^{-3}$ as shown in Fig. 3. This error is of the same order of magnitude as that obtained by Pearson [3] using a few thousand mesh intervals in x. Mesh lengths in x for the present method may be computed as follows.

For large p the solution curve lies close to $y = 0$ and $x = 1$ so that its length S is approximately 2 and angular variation is $\pi/2$. Then h, the step size in t, is given by Eq. (12). Near $x = 0$, dy/dt and $d\theta/ds$ are nearly zero so that by Eq. (3) the step Δx in x equals h. Near $x = y = 1$, dx/dt and $d\theta/ds$ are nearly zero so that the step in y is h. The corresponding Δx found using the slope of the solution curve, is $\Delta x = h/p$. In the corner, near $x = 1$, $y = 0$, $dx/ds = dy/ds$ and $d\theta/ds = K$ so that $\Delta x = 2^{-1/2}h/(1 + CK)$.

Numerical values for Δx in the present case are

$$\Delta x = \begin{cases} 1.56 \times 10^{-2} & \text{at } (0, 0), \\ 0.81 \times 10^{-2} & \text{at } (1, 0), \\ 1.56 \times 10^{-5} & \text{at } (1, 1). \end{cases}$$

It is noteworthy that the best value of C is found to give CK near 1 in this as in the previous examples. Nondimensional quantities influencing CK include the total angular variation Θ and SK where S is the length of the curve.

D. *Troesch's Problem*

This problem arose in a study by B. A. Troesch of the confinement of a plasma column by radiation pressure and has been the subject of the several numerical investigations, among them those of Roberts and Shipman [6] and of Troesch [7]. The algorithm of Sincovec and Madsen [8] for solving two-dimensional partial differential equations by the method of lines has been used to solve Troesch's one-dimensional

space problem as the eventual steady state solution of an associated partial differential equation in space and time.

The problem reads

$$y'' = p \sinh py,\ y(0) = 0,\ y(1) = 1.$$

The exact solution may be written

$$x = (k/p)\, F(\arctan \sinh [py/2] | 1 - k^2)$$

where F is the elliptic integral of the first kind [9] with parameter $(1 - k^2)$, and k is obtained by imposing the condition $x = 1$ when $y = 1$.

The solution to Troesch's problem presents a curve running near $y = 0$ for $0 \leqslant x \leqslant 1$ and near $x = 1$ for $0 \leqslant y \leqslant 1$. The curve fits more tightly into the corner at

TABLE I

Maximum Error, Troesch's Problem
Entry = Max $| x_{\text{computed}} - x_{\text{exact}} | \times 10^5$

	$p = 6, K = 2.45$		$p = 10, K = 4.05$			
N	32	64	32	64	128	64
C						
0	83.3	20.8	583	149.0	37.5	31.5[a]
0.05	72.8	18.3	574	147.6	37.1	22.6
0.10	64.7	16.3	565	147.0	36.9	17.2
0.15	55.7	14.0		146.7	36.9	13.8
0.20	50.6	12.6		147.0	37.1	11.5
0.25	51.3	12.8		148.9	37.4	10.0
0.30		13.4		150.9	37.9	9.0
0.35		14.4		152.8	38.4	8.2
0.40						7.6
0.45						7.2
0.50						6.83
0.55						6.53
0.60						6.53
0.65						6.54
0.70						6.58
0.75						6.63

[a] Entries in the last column are the maximum distance from a computed point to the exact solution curve multiplied by 10^5.

$x = 1$, $y = 0$ for larger p. Computational difficulties with standard methods arise for p as small as 5.

The present scheme gives results of reasonable accuracy with a fairly coarse mesh, as shown in Table I. One sees that halving the mesh interval reduces the error by very nearly a factor of 4 so that an accuracy of order h^2 has been attained with so few mesh points. Troesch [7] reports improved results with his shooting scheme when distance is introduced as a coordinate.

The error is reduced from its value for $C = 0$ if C is given a proper positive value. However, the reduction is only about 35% for $p = 6$ and much less for $p = 10$. This insensitivity to variations in C is due to the way the error has been defined. The difference between exact and computed values of x for each computed value of y has its maximum where x is a rapidly varying function of y, on the straight nearly horizontal part of the solution curve. The distance between the computed point and the nearest point on the exact solution curve is a more informative measure of the error and is more sensitive to variations in C. The last column of Table I records results using distance for error. The point with maximum error was found near the corner in every case.

6. Applications

Problems of boundary-layer type arise frequently in many branches of science and engineering. Pearson [3] computes the location and velocity distribution through an air shock wave standing in a hyperbolic nozzle.

The suitably normalized potential ψ in a semiconductor in thermal and electrical equilibrium and with a fixed charge of given density $N(x)$ is determined [10] by

$$L^2\psi'' = 2 \sinh \psi - N(x)$$

where L is a material parameter. The given voltage drop determines boundary values for ψ. One sees that this problem is very close to that of Troesch so that the present method should be readily applicable to this and similar semiconductor field effect computations.

In many combustion problems, the chemistry may be approximated by a single overall reaction between a fuel and an oxidizer [11]. The steady-state variation of concentrations of the two reactants diffusing toward one another is governed by equations of the form

$$y_1'' = k y_1 y_2 ,$$

$$y_2'' = k y_1 y_2 .$$

It follows that $(y_1 - y_2)$ is a linear function $Ax + B$ with coefficients A and B determined by the boundary conditions. Eliminating y_2 leaves the equation

$$y_1'' = k y_1 (y_1 - Ax - B)$$

from which y_1 is to be determined. Although the form of f is different from that in Troesch's problem, the solution curve has similar properties. For large k, the curve either lies close to $y_1 = 0$ or to $y_1 = Ax + B$, i.e., to $y_2 = 0$, with a sharp bend near the intersection of these lines. The success of the present method with Troesch's problem is likely to hold for the chemical diffusion problem also.

7. Conclusions

This paper presents a possible basis for designing an algorithm together with some supporting experimental evidence. The suggested introduction of an intrinsic coordinate complicates the differential system to be solved. This disadvantage can be outweighed for problems of boundary-layer type where the need for fewer mesh points than in other schemes permits computer storage and run time reductions. Some run time may be used for interpolations if results at prescribed values of the independent variable are required. Another difficulty, that the best value for C is unknown, can be overcome at further expense in run time by incorporating a method for error estimation and a search in C to reduce that error.

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