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On the Numerical Solution of Elliptic Partial Differential Equations by the Method of Lines

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The technique called the method of lines is used for solving elliptic partial differential equations. To illustrate the technique solutions are obtained for one linear example and for three nonlinear examples. A stability and convergence analysis is made in the linear case.

1. INTRODUCTION

The numerical solution of elliptic partial-differential equations is usually carried out by expressing all derivatives in terms of finite differences and solving the resulting simultaneous algebraic equations by methods such as successive over-relaxation. For linear equations the methods of solution are well developed and are efficient in most cases. However, the finite-difference representation of nonlinear partial-differential equations may lead to the problem of solving a large number of simultaneous nonlinear algebraic equations. This is, in most cases, difficult and *ad hoc* methods are often used for a particular problem.

Another method of solving elliptic partial-differential equations is the finite-element technique which again is well developed for linear systems.

The method employed in this paper is called the method of lines (from here on we refer to the method as MOL) in the Soviet Union where it has been used for some thirty years. The basic feature of the method is that derivatives with respect to one of the independent variables remain continuous, while derivatives with respect to the other independent variables are replaced by finite-difference approximations. In a two-dimensional problem in a rectangle the region could be considered as divided into strips by dividing lines (hence the name) parallel to one of the axes. At each line the derivatives normal to that line would be replaced by finite differences and the other variable left continuous. Thus the system of partial differential equations is replaced by a system of ordinary differential equations. The resulting ordinary differential equations may then be solved, at least in some cases, by analytic methods. For instance Poisson's equation with linear boundary conditions has received much attention [1, 2]. In the case of more general equations, particularly those of nonlinear type, analytic solutions of the ordinary differential equations may be impossible and the problem must be treated as a two-point boundary-value problem to be solved numerically. This problem may then be solved by either a boundary-value technique such as finite differences or by the shooting method for two-point boundary-value problems. The former technique would be equivalent to solving the original problem by the grid finite-difference method and is thus avoided. The shooting method involves estimating unknown conditions at the initial point and integrating the ordinary differential equations across to the end point. The required boundary conditions at the end point can then be satisfied by iterating on the missing initial conditions. Because of the elliptic nature of the partial differential equations this initial-value integration is strictly improper. Indeed it can be shown (Section 3) that the ordinary differential equations are inherently unstable. One of the purposes of this paper is to convince the reader that in many physical problems of interest accurate solutions can readily be obtained by MOL even though the problem is incorrectly posed. It is shown that if the region of interest is divided into sufficiently few strips by the dividing lines then accurate solutions can be obtained by using high-order finite-difference approximations. As more and more strips are taken the results may at first improve but they will eventually become meaningless and the iteration technique will not not converge to a solution. In this sense the technique is analogous to an asymptotic series solution.

The work done in the Soviet Union on MOL has largely been limited to solving linear equations of elliptic (as well as parabolic and hyperbolic) type. A 1965 review paper by Liskovets [1] gives an extensive list of references to provide the mathematical background and development of MOL. These workers have developed analytic solutions of the linear ordinary differential equations for certain cases. More recently solutions of Poisson's equation with linear boundary conditions have been obtained in the United States by Leser and Harrison [2] again using analytic solutions of the ordinary differential equations.

It appears that MOL (and a similar technique called the method of integral relations) was first used in nonlinear problems for the supersonic blunt-body problem which is of interest to aerodynamicists [3]. Klunker, South and Davis [4] have discussed more recent applications of the method to the solution of equations of elliptic type such as the supersonic blunt-body problem and conical flow problems which are of great importance in aerodynamics. In general the method has received more attention for solving the correctly posed parabolic type of equation [5–7]. Thus it seems opportune to present here the experiences of the authors in applying MOL to various problems involving equations of elliptic (and mixed) type and to emphasize the advantages and disadvantages of the method which become evident in actual numerical computations.

Before discussing the advantages of MOL over grid techniques it should be pointed out that MOL can be easily applied in simple regions such as circular annuli or sectors, and rectangles. Application of the method to more complicated regions is generally limited only by the degree of ingenuity of the user, since an appropriate choice of coordinates and various transformations can be used to map most regions into one of the simple regions just mentioned. However it may be in some cases that a region cannot be suitably transformed and one would then presumably have to use the grid method.

The advantage of MOL over grid techniques is that an order-of-magnitude fewer unknowns are required to complete the solution. Grid techniques solve for the unknown (or unknowns) at each grid point; MOL solves for the unknown (or unknowns) at one end of each dividing line. Since there are many fewer unknowns in MOL they can be found by direct matrix inversion if the problem is linear and in the nonlinear case methods such as iteration by Newton–Raphson or minimization can be used effectively. The above methods are usually ineffective in the grid methods and iteration techniques such as successive overrelaxation (SOR) are used. Depending on the equations SOR may be efficient but there is no rigorous method for finding the optimum SOR parameter except in certain linear cases and in nonlinear cases the theories are not at all well developed.

The disadvantage of MOL compared to grid techniques is that the solution may not be obtained to such a high accuracy. The accuracy of grid techniques is theoretically limited only by round-off error so that by using double precision a result of high accuracy could be obtained. As pointed out earlier the MOL system of ordinary differential equations is inherently unstable and the instability becomes worse if the finite-difference strip size is too small, thus one has to accept results using a certain strip size at which the instability is insignificant. These results may not be sufficiently accurate for the user's purpose but it has been found by the authors that results of sufficient accuracy have been obtained in a number of problems of physical interest. Some of these results are illustrated in Sections 3 and 4.

The following section describes MOL in detail. This will be followed by a stability and convergence analysis and the results of the examples (one linear and three nonlinear) will be discussed.

2. The Method of Lines

We consider the application of MOL in a rectangular region in two dimensions. Application to either a region which lies between concentric circles or a circular sector region using polar coordinates is obvious and therefore omitted. Application to other regions is possible after transformation to one of the above regions (for example, see Fig. 1 and Example 4.C). Problems in higher dimensions can be treated by using finite differences for partial derivatives with respect to all variables except one.

A. *The Method*

Notation

(x, y)	coordinate system
ψ	a function of (x, y)
x_0, x_1	lower and upper limits on x
y_0, y_1	lower and upper limits on y
$F(y)$	a function of y at $x = x_0$
$\epsilon(y)$	a function of y at $x = x_1$
ϵ_k	value of $\epsilon(y)$ at the k-th line at $x = x_1$
F_i	value of $F(y)$ at the i-th line at $x = x_0$
ψ_i	a value of ψ on the i-th line
p_i	a value of p on the i-th line
$f(y, \psi, \partial\psi/\partial x)$	boundary condition at $x = x_1$ is that $f(y, \psi, \partial\psi/\partial x)$ is zero
ψ^{I}, ψ^{II}, etc.	first, second, etc., derivatives of ψ with respect to y.

Suppose (x, y) are independent variables and ψ is a function of (x, y) defined by partial differential equations within a region $x_0 \leqslant x \leqslant x_1$, $y_0 \leqslant y \leqslant y_1$. Boundary conditions for ψ or its normal derivatives or some combination are given on the bounds of the above region.

By estimating an unknown function (or functions) at one of the boundaries [say, for example, $\partial\psi/\partial x = F(y)$ at $x = x_0$, $y_0 \leqslant y \leqslant y_1$], and by replacing the derivatives in the y direction by differences, thus making the partial differential equations into ordinary differential equations, the equations can be integrated from x_0 to x_1. At $x = x_1$ there are given boundary conditions, of the form $f(y, \psi, \partial\psi/\partial x) = 0$ say, to be satisfied, but the preceding integration, assuming the estimate at $x = x_0$ is not correct, will give a residual of $f(y, \psi, \partial\psi/\partial x) = \epsilon(y)$, say. To solve the elliptic problem completely the estimated function at $x = x_0$ must be improved until $\epsilon(y)$ is sufficiently small.

To carry out the above integration the region is first divided (by dividing lines hence the name MOL) into strips of width δy and first or second derivatives replaced by differences

$$\left(\frac{\partial \psi}{\partial y}\right)_{x,y} = \frac{\psi(x, y + \delta y) - \psi(x, y - \delta y)}{2\delta y} + O(\delta y^2 \psi^{\mathrm{III}}), \tag{2.1a}$$

$$\left(\frac{\partial^2 \psi}{\partial y^2}\right)_{x,y} = \frac{\psi(x, y + \delta y) - 2\psi(x, y) + \psi(x, y - \delta y)}{\delta y^2} + O(\delta y^2 \psi^{\mathrm{IV}}), \tag{2.1b}$$

or alternatively by more accurate formulas such as

$$\left(\frac{\partial \psi}{\partial y}\right)_{x,y} = \frac{4}{3}\left[\frac{\psi(x, y + \delta y) - \psi(x, y - \delta y)}{2\delta y}\right] - \frac{1}{3}\left[\frac{\psi(x, y + 2\delta y) - \psi(x, y - 2\delta y)}{4\delta y}\right] + O(\delta y^4 \psi^{\mathrm{V}}) \tag{2.2a}$$

and

$$\left(\frac{\partial^2 \psi}{\partial y^2}\right)_{x,y} = \frac{4}{3}\left[\frac{\psi(x, y + \delta y) + \psi(x, y - \delta y) - 2\psi(x, y)}{\delta y^2}\right] - \frac{1}{3}\left[\frac{\psi(x, y + 2\delta y) + \psi(x, y - 2\delta y) - 2\psi(x, y)}{4\delta y^2}\right] + O(\delta y^4 \psi^{\mathrm{VI}}). \tag{2.2b}$$

The partial differential equations thus become a set of coupled ordinary differential equations in one independent variable x with differential equations for each of the dividing lines in the region $y_0 \leqslant y \leqslant y_1$. The terms in each equation depend on variables to both sides of that line. These resulting ordinary differential equations can then be integrated by standard techniques, for example, by the Hamming predictor-modifier-corrector method [8] with the Runge–Kutta starting procedure.

Once an integration has been made from one boundary to the other (x_0 to x_1 in the case above) the residual function $\epsilon(y)$ is known at each line for the given estimate $F(y)$. To improve the estimate $F(y)$ so that $|\epsilon(y)|$ is made smaller, the following method is used.

Suppose that n strips are used. Then the function $F(y)$ can be defined by its values $F(y_0 + j\,\delta y)$ ($j = 0, 1,..., n$; $y_0 + n\,\delta y = y_1$), and similarly $\epsilon(y)$ is represented by its values $\epsilon(y_0 + j\,\delta y)$. The minimization of $|\epsilon(y)|$ is carried out by minimizing $\sum_{k=0}^{n} \epsilon^2(y_0 + k\,\delta y)$ with respect to $F(y_0 + j\,\delta y)$, $j = 0, 1,..., n$. Many methods exist for minimization; one of the best for minimizing a sum of squares is presented by Powell [9]. This method is similar to the generalized least-squares technique given by the iterative process

$$\sum_{j=0}^{m} \left\{ \sum_{k=0}^{n} \frac{\partial \epsilon_k}{\partial F_i} \frac{\partial \epsilon_k}{\partial F_j} \right\} \delta F_j = -\sum_{k=0}^{n} \epsilon_k \frac{\partial \epsilon_k}{\partial F_i} \qquad (i = 0, 1, \ldots, m), \tag{2.3}$$

where in the above case (i.e., F estimated at each line) the number of unknowns $(m + 1)$ is equal to $n + 1$. In some cases it may be more convenient to represent $F(y)$ by a Fourier (or other) series, say $\sum_{i=0}^{m} F_i \cos iy$ with $m < n$ thus reducing the amount of work needed to obtain a solution (for instance, see Example 4.C). In the above Equation (2.3) $\epsilon_k \equiv \epsilon(y_0 + k\,\delta y)$ and $F_i \equiv F(y_0 + i\,\delta y)$ and δF_j is the improvement to be made to F_j so that $\sum_{k=0}^{n} \epsilon_k^2$ is minimized.

In the generalized least-squares technique "steps" defined by (2.3) are made until either $\sum \epsilon_k^2$ or $\delta F_j / F_j$ is sufficiently small. Each step requires calculating $\partial \epsilon_k / \partial F_i$ by differences

$$\frac{\partial \epsilon_k}{\partial F_i} \simeq \frac{\epsilon_k(F_0, \ldots, F_i + \Delta F_i, \ldots, F_m) - \epsilon_k(F_0, \ldots, F_i, \ldots, F_m)}{\Delta F_i} \tag{2.4}$$

for $i = 0, 1, 2, \ldots, m$, where ϵ_k is considered as a function of $F_0, F_1, \ldots, F_m$ since, for given values of $F_0, F_1, \ldots, F_m$, the corresponding values of ϵ_k $(k = 0, 1, \ldots, n)$ can be found by integration as described previously. ΔF_i is a small increment in F_i, say $10^{-6} F_i$ if $F_i \neq 0$. Now in Powell's method only the first step requires the use of (2.4). After the first step partial derivatives are calculated approximately from values of ϵ_k $(k = 0, 1, \ldots, n)$ already obtained on the previous step. Powell's method is more efficient than the generalized least-squares technique and it is also claimed to ensure convergence.

Powell's method has been used extensively by one of the authors (Jones) when applying MOL. South and Klunker, on the other hand, have used the Newton–Raphson technique given by

$$\sum_{j=0}^{n} \frac{\partial \epsilon_i}{\partial F_j} \delta F_j = -\epsilon_i \qquad (i = 0, 1, \ldots, n)$$

and have also had considerable success with the simplified Newton–Raphson scheme [10] in which partial derivatives $\partial \epsilon_i / \partial F_j$ are recomputed only when necessary and usually not on each iteration. The simplified scheme works well when one is sufficiently near to the solution [4].

As noted earlier it is not necessary to define the function $F(y)$ by its values at $y_0 + j\,\delta y$ $(j = 0, 1, \ldots, n)$ if Powell's method is used. In fact it is more economical to define $F(y)$ by as few unknowns as possible in order to reduce the computation required for the first step given by (2.4). For instance, the first few terms of a Fourier-series expansion can be used if it is known that $F(y)$ can be adequately represented in this way.

B. *Finite Differences and Boundary Conditions*

In this section we compare the difference schemes given by Eqs. (2.1) and (2.2) and see how to apply formulas of the same accuracy near the boundaries.

The first question of interest is to know what gains in efficiency can be made using (2.2) instead of (2.1). For this purpose the first derivatives given in (2.1) and (2.2) are compared.

Suppose E represents the exact derivative of a function ψ with respect to y and let A_1 and A_2 represent the approximations given by Eqs. (2.1) and (2.2), respectively. Then it can be shown that the error

$$\epsilon_1 = \left| 1 - \frac{A_1}{E} \right| \simeq \frac{\delta {y_1}^2}{6} \left| \frac{\psi^{\mathrm{III}}}{\psi^{\mathrm{I}}} \right|$$

and that

$$\epsilon_2 = \left| 1 - \frac{A_2}{E} \right| \simeq \frac{\delta {y_2}^4}{24} \left| \frac{\psi^{\mathrm{V}}}{\psi^{\mathrm{I}}} \right|,$$

where δy_1 and δy_2 are the finite-difference increments. Now we want to find the ratio $\delta y_2 : \delta y_1$ to give the same accuracy in both formulas, i.e., $\epsilon_1 = \epsilon_2 = \epsilon$. For this condition we have

$$\frac{\delta y_2}{\delta y_1} \simeq 0.90 \left| \frac{{\psi^{\mathrm{III}}}^2}{\psi^{\mathrm{V}} \psi^{\mathrm{I}}} \right|^{1/4} \epsilon^{-1/4}. \tag{2.5}$$

The value of $\epsilon^{1/4}\, \delta y_2/\delta y_1$ can be calculated from this formula for well-known functions. Its value is approximately 0.90 for $\sin ny$, $\cos ny$ and $\exp(ny)$, while for $\log y$ its value is 0.57. Hence provided the approximate formula (2.5) holds, it can be seen that if ϵ is, say 10^{-4} (0.01 % accuracy), then $\delta y_2/\delta y_1$ lies between 6 for the log function and 9 for the sin, cos and exp functions.

The above analysis shows that 6–9 times as many dividing lines must be used with (2.1a) to get equivalent accuracy to (2.2a) for the first derivatives. Equation (2.1a) requires about half as many computer multiplications, divisions, etc., compared to (2.2a) but this affects only one statement of the computer program and so is insignificant in terms of computer time (for instance, see Example 3.C). A similar saving in lines may be made by using the 5-point scheme (2.2b) instead of (2.1b) for second derivatives. The superiority of (2.2) over (2.1) is illustrated in Example 3.C.

To apply (2.2) on a line adjacent to a boundary line is not possible unless the boundary line is a line of symmetry when image lines are used. If the boundary line is not a line of symmetry then the following formulas are recommended.

(i) Dirichlet Boundary Condition

Use

$$\pm\delta y\,\frac{\partial\psi_1}{\partial y} = \frac{1}{4}(\psi_1-\psi_0) - \frac{3}{2}(\psi_1-\psi_2) + \frac{1}{2}(\psi_1-\psi_3) - \frac{1}{12}(\psi_1-\psi_4) + O(\delta y^5\psi^{\mathrm{V}}) \tag{2.6}$$

for a first derivative, where lines 0, 1, 2, 3, 4 are adjacent and line 0 forms the boundary. The symbols ψ_0, ψ_1, etc., refer to the values of ψ on line 0, line 1, etc., and ψ^{V} refers to the fifth derivative of ψ with respect to y in the range considered. The upper sign is used if the lines 0, 1, 2, 3, 4 are at increasing y values, otherwise the lower sign is used. For a second derivative

$$\frac{\delta y^2}{2}\frac{\partial^2\psi_1}{\partial y^2} = -\frac{1}{6}(\psi_2-\psi_1) + \frac{1.75}{3}(\psi_3-\psi_1) - \frac{1}{4}(\psi_4-\psi_1) + \frac{0.125}{3}(\psi_5-\psi_1) + \frac{1.25}{3}(\psi_0-\psi_1) + O(\delta y^6\psi^{\mathrm{VI}}) \tag{2.7}$$

is recommended.

(ii) Neumann and Mixed Boundary Conditions

In this case $\partial\psi/\partial y$ is a constant on the boundary or else $\partial\psi/\partial y$ is given as a function of ψ. In the latter case calculate $\partial\psi_0/\partial y$ from the boundary condition and then, for both cases, use

$$\pm\delta y\,\frac{\partial\psi_1}{\partial y} = \frac{8.5}{9}(\psi_1-\psi_0) - \frac{1}{2}(\psi_1-\psi_2) + \frac{1}{18}(\psi_1-\psi_3) \mp \frac{1}{3}\delta y\,\frac{\partial\psi_0}{\partial y} + O(\delta y^5\psi^{\mathrm{V}}) \tag{2.8}$$

for a first derivative and

$$\frac{\delta y^2}{2}\frac{\partial^2\psi_1}{\partial y^2} = \frac{3.5}{4}(\psi_2-\psi_1) - \frac{1}{9}(\psi_3-\psi_1) + \frac{0.0625}{6}(\psi_4-\psi_1) + \frac{8.03125}{9}(\psi_0-\psi_1) \pm \frac{0.625}{3}\delta y\,\frac{\partial\psi_0}{\partial y} + O(\delta y^6\psi^{\mathrm{VI}}) \tag{2.9}$$

for a second derivative. The appropriate $\pm$ sign is chosen in the same way as in (i) above.

Also the appropriate form for $\partial^2\psi_0/\partial y^2$ is given by

$$\frac{\delta y^2}{2}\frac{\partial^2\psi_0}{\partial y^2} = 4\left(\psi_1 - \psi_0 \mp \delta y\frac{\partial\psi_0}{\partial y}\right) - 1.5\left(\psi_2 - \psi_0 \mp 2\delta y\frac{\partial\psi_0}{\partial y}\right)$$
$$+\frac{4}{9}\left(\psi_3 - \psi_0 \mp 3\delta y\frac{\partial\psi_0}{\partial y}\right) - \frac{1}{16}\left(\psi_4 - \psi_0 \mp 4\delta y\frac{\partial\psi_0}{\partial y}\right)$$
$$+ O(\delta y^6\psi^{\mathrm{VI}}). \tag{2.10}$$

In addition to first and second derivatives, formulas for higher derivatives may be found if required. For example, in the case of the Neumann boundary condition, $\partial^3\psi_1/\partial y^3$ can be determined by solving the equations

$$\psi_{n+1} - \psi_1 = nh\psi_1^{\mathrm{I}} + \frac{(nh)^2}{2}\psi_1^{\mathrm{II}} + \frac{(nh)^3}{3!}\psi_1^{\mathrm{III}} + \frac{(nh)^4}{4!}\psi_1^{\mathrm{IV}}$$
$$+\frac{(nh)^5}{5!}\psi_1^{\mathrm{V}} \qquad (n = -1, 1, 2, 3),$$
$$\frac{h\partial\psi_0}{\partial y} = h\psi_1^{\mathrm{I}} - h^2\psi_1^{\mathrm{II}} + \frac{h^3}{2}\psi_1^{\mathrm{III}} - \frac{h^4}{3!}\psi_1^{\mathrm{IV}} + \frac{h^5}{4!}\psi_1^{\mathrm{V}},$$

for ψ_1^{III} in terms of ψ_0, ψ_1, ψ_2, ψ_3, ψ_4 and $\partial\psi_0/\partial y$. Note that the required formula can be found conveniently by computer matrix inversion. In the above formulas h is written in place of ∂y.

3. Stability and Convergence of MOL

In part A of this section Hadamard's example of the Cauchy problem for the Laplace equation in a rectangle is discussed. This example shows that we may expect MOL to be inherently unstable.

A closer analysis of MOL, using the scheme (2.1), for the Laplace equation in a rectangle is made in part B. This analysis shows that the general solution by MOL is comprised of two parts. The first of these is an unwanted solution which is negligible for sufficiently small x (the continuous variable) or when using a sufficiently large finite-difference y increment but which otherwise grows large. The second part of the general MOL solution is the required solution which tends to the exact solution as the y increment tends to zero.

Finally in part C the stability and convergence of MOL is illustrated with a linear example. It will be seen that good accuracy (4 or 5 significant figures) is obtained with a suitable choice of both finite-difference y increment and integration step size δx.

A. *Hadamard's Example*

Hadamard [11] investigates the solution of Laplace's equation and shows that, subject to Cauchy data of a certain type, the solution is not well behaved since it will oscillate between very large positive and negative values when the correct solution, in the limit of vanishing Cauchy data, should be zero. Hadamard poses the example

$$\psi_{xx} + \psi_{yy} = 0 \tag{3.1}$$

with Cauchy data given at the line $x = 0$,

$$\begin{aligned} \psi(0, y) &= 0, \\ \psi_x(0, y) &= A_n \sin ny, \end{aligned} \tag{3.2}$$

where n is large and A_n is a function of n which grows small as n grows large (e.g., n^{-p}, $p > 0$). The solution to this problem is

$$\psi(x, y) = (A_n/n) \sin ny \sinh nx. \tag{3.3}$$

The sinh nx factor is large because of the growth of e^{nx}. The sin ny factor causes oscillation of the function with varying y. Hence however close to zero we choose to make the Cauchy data (i.e., n or p large) the solution $\psi(x, y)$ will not be zero but will oscillate between large positive and negative values. Since zero is the solution of (3.1) with vanishing Cauchy data ($A_n = 0$) we conclude that for Laplace's equation the dependence of the solution on the initial data is not in general continuous [12].

Garabedian [12] concludes also that the above problem is not correctly set or well posed. He defines a boundary-value problem for a partial differential equation, or for a system of partial differential equations, to be correctly set in the sense of Hadamard if and only if its solution exists, is unique, and depends continuously on the data assigned.

Consider now Hadamard's example in the context of MOL. We may proceed with MOL by estimating $\psi_x(0, y)$ and using this estimate integrate (3.1) numerically away from $x = 0$. After iteration we arrive at a numerical solution of $\psi_x(0, y)$. Suppose the exact solution to the problem is zero, i.e., $\psi_x(0, y) = 0$, but that due to discretization and round-off errors the value of $\psi_x(0, y)$ is of order 10^{-10}. Then the situation is similar to n and p being large in (3.2) in the sense that A_n is not quite zero. As we integrate numerically in MOL away from $x = 0$ the solution will be in a form similar to (3.3) and will thus become large and oscillatory for sufficiently large x. Thus we cannot obtain a good approximation to the exact solution unless x is small.

It may also be noted that in the general case when solving by MOL even an exact $\psi_x(0, y)$ cannot give a good solution for all x. The reason for this is that the x discretization error introduces an unwanted solution equivalent to $A_n \neq 0$ in the Hadamard example. Thus the instability is always present but its contribution may be insignificant for x sufficiently small.

The above observations of instability are analyzed more closely in the next part of this section. It will be confirmed that a reasonably accurate solution may be obtained if x is sufficiently small. It will also be shown that the instability is worse if the y increment is too small.

B. *Analysis of Stability and Convergence of MOL*

To illustrate the stability and convergence consider the problem of solving Laplace's equation

$$\psi_{xx} + \psi_{yy} = 0 \tag{3.4}$$

in a rectangular domain $0 \leqslant x \leqslant 1$, $-b \leqslant y \leqslant b$, with the following Dirichlet boundary conditions:

$$\psi(0, y) = \psi(1, y) = 0, \tag{3.5}$$

$$\psi(x, b) = \psi(x, -b) = \sin \pi x. \tag{3.6}$$

The exact solution for this problem is known to be

$$\psi(x, y) = \frac{\cosh \pi y \sin \pi x}{\cosh \pi b}. \tag{3.7}$$

We now consider the solution of this problem by MOL. Since the problem contains the two lines of symmetry $x = \frac{1}{2}$ and $y = 0$, we can reduce the region of interest to the upper left quadrant of the rectangle, $0 \leqslant x \leqslant \frac{1}{2}$, $0 \leqslant y \leqslant b$. $N - 1$ interior lines are drawn parallel to the x axis with equal spacing $h = b/N$, so that

$$y_n = nh = nb/N. \tag{3.8}$$

The symmetry conditions

$$\psi_x(\tfrac{1}{2}, y) = 0, \tag{3.9}$$

$$\psi(x, y) = \psi(x, -y), \tag{3.10}$$

are applied.

To get some insight into the stability and convergence of MOL the three-point formula (2.1) is used to approximate ψ_{yy} in (3.4) giving

$$\psi_n'' + (\psi_{n+1} - 2\psi_n + \psi_{n-1})/h^2 = 0 \qquad (n = 0, 1, 2, \ldots, N-1), \tag{3.11}$$

where $\psi_n(x)$ is the approximation for $\psi(x, y_n)$ and the primes indicate differentiation with respect to x. To the system (3.11) we add the appropriate boundary and symmetry conditions,

$$\psi_n(0) = 0, \tag{3.12}$$

$$\psi_n'(\tfrac{1}{2}) = 0, \tag{3.13}$$

$$\psi_N = \sin \pi x, \tag{3.14}$$

$$\psi_{-n}(x) = \psi_n(x), \qquad n = 0, 1, 2,..., N - 1. \tag{3.15}$$

It can be shown that the general solution of the system (3.11)–(3.15) is

$$\psi_n(x) = \sum_{m=1,3...}^{2N-1} T_n(\theta_m)(A_m e^{\mu_m x} + B_m e^{-\mu_m x}) + \frac{\cosh nz}{\cosh Nz} \sin \pi x, \tag{3.16}$$

where

$$\mu_m = (2N/b) \sin(m\pi/4N), \tag{3.17}$$

$$\theta_m = \cos(m\pi/2N), \tag{3.18}$$

$$z = \cosh^{-1}(1 + \tfrac{1}{2}(\pi b/N)^2) \tag{3.19}$$

and $T_n(\theta_m)$ is the Chebyshev polynomial of order n. The A_m and B_m are determined by applying the boundary conditions at $x = 0$ and $x = 1$. These conditions are, in our example, $\psi_n(0) = \psi_n(1) = 0$, hence in the exact solution we must have

$$A_m = B_m = 0 \qquad \text{for} \quad m = 1, 3,..., 2N - 1. \tag{3.20}$$

The particular solution is the term involving $\sin \pi x$, and it is of interest to compare it to the exact solution (3.7). This is accomplished by expanding the inverse hyperbolic function (3.19):

$$z = \frac{\pi b}{N}\left[1 - \frac{\pi^2 b^2}{24N^2} + O(N^{-4})\right]. \tag{3.21}$$

Using (3.21) in (3.16) gives (for $A_m = B_m = 0$)

$$\psi_n(x) = \frac{\cosh \pi y_n}{\cosh \pi b} \sin \pi x \left[1 + \left(\tanh \pi b - \frac{y_n}{b} \tanh \pi y_n\right) \cdot \left(\frac{\pi^3 b^3}{24N^2} + O(N^{-4})\right)\right]. \tag{3.22}$$

Thus we have shown that the analytic solution of the ordinary differential equations (3.11) resulting from MOL for this example consists of two parts. The first part is the complementary solution which vanishes for the boundary conditions of this example while the second part (3.22) converges to the exact solution (3.7) with error $O(N^{-2})$, i.e., as the y increment tends to zero.

At this stage it is interesting to note that, if A_m and B_m were not exactly zero but took on small values perhaps of order 10^{-10} and if N and x were sufficiently large, the first part of (3.16) and in particular the term for which $m = 2N - 1$ would dominate the solution. Thus an appreciable error would be obtained if either x was too large or N was too large.

In fact on integrating (3.11) numerically away from $x = 0$ even with $\psi_n(0) = 0$ and $\psi_n'(0)$ exactly correct $[= (\pi \cosh nz/\cosh Nz)]$ the solution would not be exact after the first step δx due to discretization error. The problem could now be considered as an initial-value problem with slightly incorrect initial conditions given at $x = \delta x$ and the exact solution given by (3.16). But now the unwanted first part of the solution is present and will grow larger as integration is carried out with respect to x. This phenomenon is called inherent instability and can arise in such a simple ordinary differential equation as $u' = u + x$ with initial condition $u(x_0 = 0) = -1$; the general solution is $u = -x - 1 + [1 + x_0 + u(x_0)]\, e^{-x_0} e^{x}$ but a reasonable approximation to the exact solution for the given initial condition can never be achieved numerically for x too large.

In summary the MOL system of ordinary differential Equations (3.11) is inherently unstable and the instability will be significant for x and/or N too large. To investigate the size of the unwanted solution for our example we now consider $\psi_n'(\frac{1}{2})$ which from (3.13) should be zero. We differentiate (3.16) with respect to x and consider the result.

Firstly $T_n(\theta_m)$ is bounded by unity so we ignore this part and consider only the growth of $\mu_m \exp(\frac{1}{2}\mu_m)$ for $m = 2N - 1$ which will dominate $\psi_n'(\frac{1}{2})$ for N sufficiently large. From (3.17) we have

$$\mu_{2N-1} = \frac{2N}{b} \sin\left(\frac{\pi}{2} - \frac{\pi}{4N}\right) \simeq \frac{2N}{b}$$

and

$$\mu_{2N-1} \exp(\tfrac{1}{2}\mu_{2N-1}) \simeq \frac{2N}{b} \exp\left(\frac{N}{b}\right). \tag{3.23}$$

Thus instead of $\psi_n'(\frac{1}{2})$ being zero we can see that it could be large if N is too large even though the factor A_{2N-1} may be small due to small discretization errors. The function (3.23) is tabulated in Table I for $N = 2, 3, 4, 5, 6, 9, 12$ using $b = 0.475$. Also in Table I are values of

$$\exp(4N^2/\pi b) \tag{3.24}$$

which is the equivalent error term arising from the method of integral relations (see Appendix A). Clearly instability of the method of integral relations is far more significant.

TABLE I

Table of the Functions (3.23) and (3.24) Using $b = 0.475$ to Illustrate the Instability of MOL and of the Method of Integral Relations for N too Large

N	(3.23)	(3.24)
2	5.7, 2	4.5, 4 ($\equiv 4.5 \times 10^4$)
3	7.0, 3	3.0, 10
4	7.6, 4	4.2, 18
5	7.8, 5	1.3, 29
6	7.7, 6	8.1, 41
9	6.4, 9	$>10^{75}$
12	4.7, 12	$>10^{75}$

The above analysis shows that it is desirable to use as few lines as possible to keep the instability insignificant but at the same time it is also desirable to use as many lines as possible so that the particular integral [the second part of (3.16)] adequately represents the exact solution. It is clear, therefore, that difference schemes for ψ_{yy}, and other y derivatives if they occur, which give a smaller truncation error than the 3-point scheme (2.1) are needed. For this reason the formulas (2.2) are recommended; it was shown in Section 2 that an order-of-magnitude fewer lines could be used with scheme (2.2).

Other schemes with smaller truncation errors for the y derivatives are given in Appendix B. Although these schemes cannot be used for general partial differential equations they may be useful for the Poisson equation or for a system of first-order partial differential equations of a certain type. These schemes have been used a great deal in the Soviet Union for application to the Poisson equation [1].

The analytical investigation carried out above is next illustrated by the numerical MOL solution of the problem given by (3.4) and the above boundary conditions. The schemes (2.1) and (2.2) are used to obtain the solution.

C. *A Linear Example* (Example 3.C)

This example illustrates the stability and convergence of MOL by solving numerically the problem given in part B of this section with $b = 0.475$.

The problem is to solve

$$\psi_{xx} + \psi_{yy} = 0 \tag{3.25}$$

with boundary conditions

$$\begin{aligned} \psi(0, y) &= 0, \\ \psi(x, 0.475) &= \sin \pi x, \end{aligned} \tag{3.26}$$

with symmetry about $x = 0.5$ and $y = 0$.

The exact solution is given in (3.7).

Lines are considered parallel to the x axis. The second derivative ψ_{yy} is replaced by differences [Eqs. (2.1) or (2.2)]. Image lines are considered outside $y = 0$ and the difference Equation (2.7) is used, if Eq. (2.2) is being used, for the line adjacent to $y = 0.475$. ψ_x is replaced by p, say, and the Equation (3.25) becomes a set of

TABLE II

Exact and MOL Values of ψ_x at $x = 0$ for Example 3.C Using Difference Scheme (2.1). Also Richardson Extrapolation from $N = 3$ and $N = 6$.

δx	$y \rightarrow$ / N	0	$\frac{0.475}{3}$	$\frac{2 \times 0.475}{3}$	$\sum p_i^2 \; (x = 0.5)$
	Exact →	1.3449	1.5147	2.0671	
$\frac{1}{4}$	3	1.3665	1.5317	2.0633	5, −18 ($\equiv 5 \times 10^{-18}$)
	6	1.3536	1.5199	2.0555	8, −14
	9	1.3512	1.5176	2.0540	5, −11
	12	1.3503	1.5168	2.0535	1, −9
	Extrapolated	1.3493	1.5160	2.0529	
$\frac{1}{8}$	3	1.3638	1.5323	2.0780	5, −16
	6	1.3502	1.5196	2.0693	8, −12
	9	1.3476	1.5173	2.0677	2, −8
	12	1.3508	1.5199	2.0691	8, −4
	Extrapolated	1.3457	1.5154	2.0664	
$\frac{1}{12}$	3	1.3633	1.5319	2.0791	1, −15
	6	1.3496	1.5192	2.0701	1, −11
	9	1.3470	1.5168	2.0685	1, −7
	12	1.4925	1.6428	2.1412	0.99
	Extrapolated	1.3450	1.5150	2.0671	
$\frac{1}{16}$	3	1.3632	1.5318	2.0793	6, −18
	6	1.3495	1.5191	2.0703	3, −11
	9	1.3475	1.5171	2.0688	1, −5
	12	0.2696	0.5813	1.5259	53.4
	Extrapolated	1.3449	1.5149	2.0673	
0[a]	3	1.3632	1.5318	2.0794	
	6	1.3495	1.5190	2.0702	
	9	1.3469	1.5166	2.0685	
	12	1.3460	1.5158	2.0679	
	54	1.3449	1.5148	2.0671	
	57	1.3449	1.5147	2.0671	

[a] Analytic solution of the MOL ordinary differential equations; see Eq. (3.16).

coupled first-order ordinary differential equations for ψ and p at each line. The values of p at $x = 0$ and at each line are then estimated so that the boundary condition at $y = 0.475$ is satisfied. In fact the function $p = \pi y/0.475$ was chosen and used at each line. One iteration of Powell's minimization procedure is then used to minimize $\sum p_i^2$ at $x = 0.5$, where p_i is the value of p at the i-th line (we require $p_i = 0$ at $x = 0.5$ because of the symmetry about $x = 0.5$). Note that only one iteration is needed since the problem is linear.

In order to illustrate the accuracy of MOL, Tables II and III give exact and MOL values of ψ_x at $x = 0$ for y values of 0, $\frac{1}{3}(0.475)$, $\frac{2}{3}(0.475)$.

TABLE III

Exact and MOL Values of ψ_x at $x = 0$ for Example 3.C Using Difference Scheme (2.2) with (2.7) Near the Dirichlet Boundary

$y \rightarrow$		0	$\frac{0.475}{3}$	$\frac{2 \times 0.475}{3}$	$\sum p_i^2$ $(x = 0.5)$
Exact $\rightarrow$		1.3449	1.5147	2.0671	
δx	N				
$\frac{1}{4}$	3	1.3497	1.5164	2.0532	4, −17 ($\equiv 4 \times 10^{-17}$)
	6	1.3492	1.5158	2.0528	8, −13
	9	1.3492	1.5158	2.0528	3, −10
	12	1.3493	1.5158	2.0529	4, −8
$\frac{1}{8}$	3	1.3461	1.5161	2.0671	2, −16
	6	1.3455	1.5153	2.0664	9, −11
	9	1.3457	1.5155	2.0664	1, −6
	12	1.4234	1.5829	2.1055	0.28
$\frac{1}{12}$	3	1.3455	1.5156	2.0681	4, −16
	6	1.3449	1.5148	2.0671	2, −10
	9	1.3473	1.5169	2.0683	2, −4
	12	0.0964	0.4335	1.4430	71.7
$\frac{1}{16}$	3	1.3455	1.5155	2.0682	3, −15
	6	1.3449	1.5147	2.0672	2, −10
	9	1.3593	1.5272	2.0744	7, −3
	12	0.5573	0.7942	1.6072	90.1
0[a]	3	1.3446	1.5145	2.0669	
	6	1.3449	1.5147	2.0671	
	9	1.3449	1.5147	2.0671	
	12	1.3449	1.5147	2.0671	

[a] Analytic solution of MOL tridiagonal scheme; see Eqs. (3.16) and (B6).

The results given in Table II were obtained by using the finite-difference Equation (2.1) for ψ_{yy} while those of Table III were obtained by using Eq. (2.2). Table II also lists the value of $p = \psi_x$ obtained by Richardson extrapolation from the $N = 3$ and $N = 6$ results, i.e.,

$$p(\text{extrapolated}) = \tfrac{4}{3}p(N = 6) - \tfrac{1}{3}p(N = 3)$$

and also contains the analytic solution of the MOL ordinary differential equations given by Eq. (3.16) with $A_m = B_m = 0$. The MOL values tabulated show the effect of increasing the number of lines N and of decreasing the Hamming predictor-modifier-corrector and Runge–Kutta step length, δx.

Observing Tables II and III it can be seen that the predictions of parts A and B of this section are confirmed, i.e., the instability of the MOL ordinary differential equations becomes significant as the number of lines N is increased and indeed the results are quite meaningless for $N = 12$ with $\delta x = 1/12$ and $1/16$. The last column in Tables II and III gives $\sum p_i^2$ at $x = 0.5$ and it can be seen that this value indicates instability when it does not approach zero.

For $N = 12$ with $\delta x = \frac{1}{4}$ and $\frac{1}{8}$ fairly reasonable results appear to be obtained even though one would still expect a significant instability. The reason for this is that the large exponentials in Eq. (3.16) are grossly underestimated by the numerical integration procedure when the product of the step size δx and the eigenvalue μ_m exceeds about 2. For example, the fourth-order Runge–Kutta method, after k steps, approximates $\exp(\mu_{2N-1} k\, \delta x)$ by E^k, where

$$E = 1 + \Delta + \frac{\Delta^2}{2!} + \frac{\Delta^3}{3!} + \frac{\Delta^4}{4!} \tag{3.27}$$

and

$$\Delta = \mu_{2N-1}\, \delta x. \tag{3.28}$$

The error grows in the numerical integration like E^k rather than $\exp(k\Delta)$; E^k is always less than $\exp(k\Delta)$ for $\Delta > 0$ and the ratio $E^k/\exp(k\Delta)$ shrinks rapidly with increasing Δ. For example when $\delta x = \frac{1}{4}$ (i.e., $k = 2$) $E^k/\exp(k\Delta)$ is about 10^{-4} for $N = 12$.

So much for the stability when N is large. The other aspects brought out in Table III are firstly that an accuracy of better than 1 % is obtained even with the most coarse finite-difference and integration step size ($N = 3$ with $\delta x = 0.25$) and secondly that convergence to 4- or 5-figure accuracy is obtained when $N = 6$ with $\delta x = 1/12$ or $1/16$.

The important points of this section are summarized as follows:

1. The error due to the instability of the MOL ordinary differential equations may be expected to grow large proportionally to $\exp(Nx)$ where x is the distance integrated and N is the number of lines.

2. Accurate solutions may be obtained with the five-point difference scheme (2.2) provided N and x are not too large.

As an aside it may be noted that the complete solutions for Table II took 25 sec and for Table III 28 sec on an IBM 360/67.

In the next section nonlinear examples are discussed. In these examples the instability is not mentioned since it is assumed that sufficiently few lines are used and that the integration distance is not too large. Comparisons of results, however, are made with other theories.

4. Nonlinear Examples

Since the above example is linear, only one iteration of Powell's scheme is required to attain the minimum from a fairly crude estimate. For nonlinear equations, the situation is not so simple and the authors have found, as is often the case when solving nonlinear equations, that a reasonably good estimate is necessary to obtain a solution. However, the authors have found that this limitation is not severe for two reasons. The first reason is that a nonlinear problem can often be made linear by a suitable choice of a parameter in the problem. This linear problem can then be solved with a fairly crude estimate and then the parameter can be varied in discrete steps. To obtain each solution a good initial estimate is available by extrapolation from previous results. An example of this is in first setting the Mach number to be near zero for compressible flow problems and then increasing the Mach number. The second reason is that a parameter in the problem can often be chosen so that a solution is already known at that value, and estimates for each solution are then obtained by extrapolation as above. An example of this is in first setting the angle of incidence to be zero in the conical flow calculations of Example C below; this has the effect, for the circular cone, of making the flow axisymmetric and solutions in this case are well known.

A. *Minimal Surface Equation*

This is a well known problem which Concus [13, 14] has solved by a grid finite-difference approach. The problem is to solve

$$(1 + \psi_y^2)\,\psi_{xx} - 2\psi_x\psi_y\psi_{xy} + (1 + \psi_x^2)\,\psi_{yy} = 0$$

subject to

$$\psi = 0 \text{ on } x = 0 \quad \text{and} \quad y = 1,$$
$$\psi = K\sin(\pi x/2) \text{ on } y = 0,$$

and

$$x = 1 \text{ is a line of symmetry.}$$

The solution is required for various values of K up to 10, say (Concus obtains solutions up to $K = 5$).

To apply MOL, lines were considered parallel to the y axis. Difference equations of the type (2.2), (2.6) and (2.7) were used for x derivatives. Integration was made from $y = 1$ to $y = 0$ by first estimating $p = \psi_y$ at $y = 1$. This estimate was made by increasing K gradually from zero since clearly at $K = 0$ the solution is $p = \psi_y = 0$ at $y = 1$. Solutions for successive values of K were then started by estimating p at $y = 1$ from the previous solutions. This problem has the feature that it is practically linear if K is small and becomes highly nonlinear for K large [13].

Seven lines were considered, including those at $x = 0$ and 1, parallel to the y axis and a step length $\delta y = -0.1$ was chosen for the Runge–Kutta fourth-order integration. Solutions for $K = 0.05, 0.1, 0.2, 0.3, 0.5, 0.7, 0.8$, and 1 were obtained in about 20 sec of IBM 360/67 computer time. The solutions when $K = 0.5$ and 1 are compared with those of Concus in Table IV. The table lists the angle which the surface profile ψ along $x = 1$ makes with the vertical at $y = 0$. Concus' solutions were obtained by extrapolation to a zero mesh size from mesh sizes of 1/10, 1/20 and 1/40.

TABLE IV

Angle which Profile of ψ along $x = 1$ Makes with the Vertical at $y = 0$ for the Minimal Surface Problem

	$K = 0.5$	$K = 1$	$K = 5$
MOL (4 lines)	44.4°	15.41°	0.044°
MOL (7 lines)	44.4°	15.34°	see text
Concus (grid finite difference)	44°	16°	$< 0.2°$

Solutions for $K > 1$ were difficult to obtain with the parameters of 7 lines and $\delta y = -0.1$. This is to be expected since K increasing is similar to the eigenvalue μ_m [Eq. (3.17)] increasing. To obtain further solutions, the authors had to accept less accuracy and used 4 lines with $\delta y = -0.25$. Using these parameters solutions were obtained up to $K = 10$. Comparisons with Concus using these parameters are made in Table IV. These solutions by MOL required only one iteration of Powell's procedure for small values of K and no more than three iterations for larger values. The total computer time for 25 values of K between 0 and 10 was 14 sec on an IBM 360/67. It can be seen from Table IV that results of good accuracy are obtained even with such coarse finite-difference and integration step size.

B. *Transonic Flow*

One of the most interesting aerodynamic problems at the present time is that of solving the equations for subsonic, compressible, inviscid, irrotational flow about two-dimensional lifting airfoils. In this example, we consider the flow about bodies which are related but which are more of academic interest such as circular and elliptic cylinders without lift.

Consider polar coordinates (r, θ) with the free stream coming from infinity at $\theta = 0$. Then $\theta = 0$ and $\theta = 90^\circ$ are lines of symmetry and a quadrant of the full flow field can be considered.

The equations of motion can be written

$$\left(1 - \frac{u^2}{a^2}\right) u_r + \frac{1}{r}\left(1 - \frac{v^2}{a^2}\right)(v_\theta + u) - \frac{2uv}{a^2} v_r = 0,$$

$$v_r = \frac{1}{r} u_\theta - \frac{v}{r},$$

$$u^2 + v^2 + \frac{2a^2}{\gamma - 1} = V_\infty{}^2 + \frac{2a_\infty{}^2}{\gamma - 1},$$

where u, v are the velocities in the r, θ directions, a is the local speed of sound, γ is the ratio of specific heats ($= 1.4$ for air) and V_∞, a_∞ are constants representing the free stream velocity and speed of sound, respectively. Subscripts r and θ denote partial differentiation.

The boundary conditions are

$$r \to \infty: \qquad u \to -V_\infty \cos \theta \qquad v \to V_\infty \sin \theta,$$

while on the body given by $r = G(\theta)$ the normal velocity is zero, i.e.,

$$u = (1/G)(dG/d\theta)v.$$

The transformation

$$\xi = \left(\frac{G(\theta)}{r}\right)^2 \qquad \phi = \theta$$

transforms the region of integration into

$$0 \leqslant \xi \leqslant 1 \qquad 0 \leqslant \phi \leqslant \pi/2.$$

The authors solved the equations for the dependent variables given by $U = u + V_\infty \cos \theta$ and $V = v - V_\infty \sin \theta$. On making these transformations of dependent and independent variables the problem becomes that of solving

$$\left(1 - \frac{u^2}{a^2}\right)(-2\xi)\, U_\xi + \left(1 - \frac{v^2}{a^2}\right)\left(2\frac{G'}{G}\xi V_\xi + V_\phi + U\right) + \frac{4uv}{a^2}\xi V_\xi = 0, \quad (4.2)$$

$$-2\xi V_\xi = 2\frac{G'}{G}\xi U_\xi + U_\phi - V, \quad (4.3)$$

$$u^2 + v^2 + \frac{2a^2}{\gamma - 1} = V_\infty{}^2 + \frac{2a_\infty{}^2}{\gamma - 1}, \quad (4.4)$$

subject to

$$\xi = 0: \quad U = V = 0,$$
$$\xi = 1: \quad U - V_\infty \cos\theta = \frac{G'}{G}(V + V_\infty \sin\theta).$$

To apply MOL, lines $\theta = \text{const}$ were taken and an estimate was made of V at $\xi = 1$ at each of the lines. U was then found from the boundary condition at $\xi = 1$. Image lines were introduced outside the boundaries at $\phi = 0$ and $\pi/2$ in order that symmetry be conserved. The difference formula (2.2) was used for the derivatives $\partial/\partial\phi$ and integration of the resulting ordinary differential equations was made from $\xi = 1$ to $\xi = 0.1$ in steps $\delta\xi = -0.1$, using Runge–Kutta followed by Hamming's predictor-modifier-corrector method. The predictor only was used to integrate from $\xi = 0.1$ to $\xi = 0$ because of the form of Eqs. (4.2) and (4.3) when $\xi = 0$. Examination of the residuals of U and V at $\xi = 0$ then enabled iteration by Powell's method of minimization.

A systematic method of estimating V at $\xi = 1$ was made by first considering the body to be in incompressible flow [Mach number zero, $1/a = 0$ and leave out (4.4)]. The estimate $V = V_\infty \sin\theta$ (the known circular cylinder solution) at $\xi = 1$ then gave convergence in one iteration since the problem is linear. The Mach number was then increased by discrete amounts and estimates of V at $\xi = 1$ for each Mach number were made by extrapolation from previous lower Mach-number results.

It was found that good results were obtained for circular cylinders and for elliptic cylinders whose ratio of semimajor to semiminor axes (a/b) was < 2 (major axis parallel to the free stream). To obtain results for higher values of a/b the authors found it necessary to use elliptic coordinates (ζ, η) [15] given in terms of Cartesian coordinates x, y by

$$\frac{x^2}{c^2 \cosh^2 \zeta} + \frac{y^2}{c^2 \sinh^2 \zeta} = 1,$$
$$\frac{x}{c^2 \cos^2 \eta} - \frac{y^2}{c^2 \sin^2 \eta} = 1,$$

where $c^2 = a^2 - b^2$.

Some circular and elliptic cylinder results are given in Tables V and VI. All results quoted are for Mach numbers high enough that the local flow on and near the body is supersonic in a maximum velocity region. The finite difference increment for ϕ was 10°. Just how accurate are the results for these supercritical cases is difficult to assess but it can be seen, from Table V, that excellent agreement with series solutions [16] is obtained in the case of the circular cylinder with Mach number of 0.4. Results were also obtained by MOL for the circular cylinder at Mach number 0.45 when the maximum surface Mach number was 1.495.

TABLE V

$(u^2 + v^2)^{\frac{1}{2}}/V_\infty$ on Surface of Circular Cylinder at Mach Number 0.4, Series Solutions and MOL Solution

θ	Lush and Cherry	Imai	Simasaki	Wang	Linearized	MOL
10	0.3280	0.323	0.3231	0.319	0.319	0.3230
20	0.6464	0.644	0.6433	0.635	0.635	0.6431
30	0.9536	0.959	0.9575	0.941	0.957	0.9571
40	1.2537	1.266	1.2625	1.247	1.260	1.2620
50	1.5560	1.561	1.5546	1.552	1.571	1.5526
60	1.8340	1.836	1.8288	1.845	1.836	1.8237
70	2.1075	2.068	2.0704	2.097	2.070	2.0632
80	2.2492	2.227	2.2454	2.271	2.229	2.2526
90	2.3102	2.284	2.3106	2.335	2.285	2.3350

TABLE VI

Elliptic Cylinder $a/b = 2$. $(u^2 + v^2)^{\frac{1}{2}}/V_\infty$ at the Surface for Mach Number, M, Zero (Incompressible) and for a Supercritical Mach Number 0.5

ϕ	Exact ($M = 0$)	MOL ($M = 0$)	MOL ($M = 0.5$)
10	0.865	0.866	0.813
20	1.236	1.236	1.241
30	1.377	1.377	1.441
40	1.438	1.438	1.546
50	1.468	1.468	1.601
60	1.485	1.486	1.638
70	1.494	1.494	1.655
80	1.499	1.500	1.669
90	1.500	1.500	1.669

C. *Conical Flow Problems*

The examples given in this section are those for which the authors first developed and adapted MOL in its present form.

The elliptic equations describing the supersonic flow about conical bodies with attached shock waves had not previously been solved numerically with sufficient accuracy. Jones [17] used MOL mainly for circular and elliptic cones while South and Klunker [18] used the method also for solving the flow about delta wings of flat, circular arc and parabolic arc cross sections.

Jones uses the finite-difference representation (2.2) to approximate the derivatives for use in MOL while South and Klunker fit a fourth-degree polynomial to five adjacent points in order to get the derivative at the midpoint. Either method appears to be equally successful and results are practically identical for the two approaches. One other difference between the Jones and the South–Klunker approach is that Jones uses Powell's method of minimization to iterate on the required boundary condition but South and Klunker use Newton's method and an important simplification of that method [4].

The equations defining the motion are too lengthy to describe here but they are fully reported in Ref. [17] and [18]. Here we describe briefly the equations for flow about a conical body.

The problem is that of finding the shock wave shape and the flow field variables between a conical body in supersonic flow and its attached shock wave. A cylindrical coordinate system (z, r, θ) is adopted with the z axis along the axis of the conical body (which may for example be a circular cone).

The equation of the given body can be written in the form, $r = zG(\theta)$ say, and we let the equation of the unknown attached shock wave be $r = zF(\theta)$. The full three-dimensional equations of motion (momentum, continuity and energy conservation) can be written in matrix form as

$$A' \frac{\partial X}{\partial z} + B' \frac{\partial X}{\partial r} + C' \frac{\partial X}{\partial \theta} + D' = 0, \tag{4.5}$$

where $A'B'C'$ are (5×5) matrices, D' is a column vector and X is also a column vector given by

$$X = \begin{pmatrix} u \\ v \\ w \\ p \\ \rho \end{pmatrix},$$

where u, v, w, are the velocity components in the (z, r, θ) directions, respectively, p is the pressure and ρ the density. The matrices and the vector D' consist of elements which are functions of u, v, w, p, and ρ; their exact form can be found in Ref. [17]. A cross section ($z =$ const) of the flow field is shown in Fig. 1a, here the flow and body are assumed to be symmetrical about $\theta = 0$, π as is usually the case. The boundary conditions to be satisfied are the Rankine–Hugoniot relations at the shock wave which can be written in the form

$$X = f(\alpha, \gamma, M_\infty, \theta, F, F'), \tag{4.6}$$

where f is a column vector whose elements are functions of the listed arguments. The first three arguments in (4.6) are α the angle of incidence which is the angle that the direction of the free stream makes with the z axis, γ the ratio of specific heats and M_∞ the free-stream Mach number. Since these three arguments are known for a given problem it follows that the elements of X are known at the shock once the equation of the shock $r = zF(\theta)$ is known.

On the body the normal velocity should be zero and can be written

$$uG - v + (1/G)(dG/d\theta)w = 0. \tag{4.7}$$

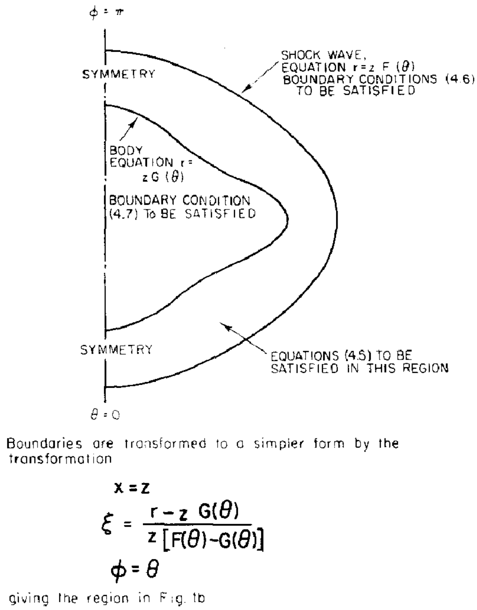

FIG. 1a. Cross section z = const of the flow field; flow field for Example 4.C.

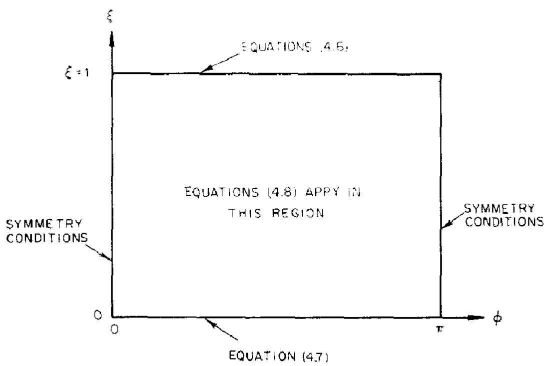

FIGURE 1b.

Now it is known that the equations of motion (4.5) can be reduced to two dimensions since the flow is conical. A suitable transformation to do this and also one which makes the boundaries easier to handle is given by

$$\begin{aligned} x &= z, \\ \xi &= [r - zG(\theta)]/z[F(\theta) - G(\theta)], \\ \phi &= \theta. \end{aligned}$$

It is seen now that the body $r = zG(\theta)$ and shock wave $r = zF(\theta)$ are transformed to the lines $\xi = 0$ and $\xi = 1$, respectively, see Fig. 1. The equations of motion (4.5) are transformed to

$$B(\partial X/\partial \xi) + C(\partial X/\partial \phi) + D = 0, \tag{4.8}$$

where B, C are (5×5) matrices and D is a column vector. The term $\partial X/\partial x$ is omitted from the above equation since the flow is conical and $\partial X/\partial x$ is zero. Now we can consider the equations at unit distance $x = z = 1$. Hence the problem is reduced to that of finding solutions of (4.8) in the region $0 \leqslant \xi \leqslant 1$, $0 \leqslant \phi \leqslant \pi$ (assuming symmetry) subject to boundary conditions (4.6) at $\xi = 1$ and (4.7) at $\xi = 0$.

The method of lines is applied in the (ξ, ϕ) plane; symmetry conditions at $\phi = 0$ and at $\phi = \pi$ are satisfied by introducing image lines in the usual manner. An estimate for $F(\phi)$ at each of the lines is made, $F'(\phi)$ is obtained from (2.2) and substitution in (4.6) gives $X(\xi = 1)$. Equations (4.8) are next reduced to ordinary differential equations by writing $\partial X/\partial \phi$ at each line in the finite-difference form (2.2). Integration of these ordinary differential equations is then made from $\xi = 1$ to $\xi = 0$ where Eq. (4.7) must be satisfied at each dividing line. The shock shape, i.e., $F(\phi)$ is changed by iteration so that conditions (4.7) are satisfied to a required accuracy. It was found convenient in this example to represent $F(\phi)$ by a cosine Fourier series $\sum_{i=0}^{m} F_i \cos i\phi$, say, where m is 1 or 2 for the circular cone at small angles of incidence; by this representation the work involved in (2.3) and (2.4) is greatly reduced.

It is important in this example to have a good estimate of the shock shape $F(\phi)$. To be always sure of a good estimate, a situation is first considered for that of a circular cone $r = G(\phi) = \text{const}$ which is at incidence $\alpha = 0$ deg. For this case the flow is axisymmetric and the problem is easily solved. A situation is next considered which has a small perturbation from the circular cone at zero incidence [either a small change to the body shape $G(\phi)$ or a small change in incidence may be considered]. In this case the estimate for $F(\phi)$ is taken to be that obtained for the first case of the circular cone at zero incidence. The solution for this small perturbation is then found by the method of lines. Next a larger perturbation of body shape or incidence, which is proportional to the first perturbation, is considered and $F(\phi)$ is estimated by extrapolation from the two previous results. And so the technique can be continued for larger proportional perturbations and always a good estimate for $F(\phi)$ is available by extrapolation from previous results at the smaller perturbations. For example, to find solutions at incidence for the circular cone whose semi-apex angle is θ_c, a solution is first found for $\alpha = 0$ deg, then successively for $\alpha/\theta_c = 0.01, 0.1, 0.2, 0.3, \ldots$.

By the method of lines it was possible to generate solutions for the circular cone for relative incidence α/θ_c as high as 1.4 in some cases, which is higher than relative incidences at which any other theoretical solutions are available. The only other methods available which give solutions at relative incidences greater than unity (up to about 1.2) are methods which solve the full hyperbolic equations (4.5) [19, 20] and these methods are 50–100 times less efficient than the method of lines.

The quality of the results can be seen in Table VII which compares pressures on a circular cone obtained by MOL with $\delta\phi = 22.5°$ and $\delta\xi = 0.1$ and by the method of Babenko et al. [19] with $\delta\phi = 11.25$ and $\delta\xi = 0.05$, which solves the full hyperbolic equations (4.5).

TABLE VII

Comparison of Surface Pressure on a Circular Cone at Mach Number 7, Half Cone Angle 15° and Angle of Incidence 10°
(MOL Solution and Babenko's [19])

Circumferential angle	0	22.5	45	67.5	90	112.5	135	157.5	180
Babenko	1.0798	1.0179	0.8544	0.6433	0.4426	0.2899	0.1974	0.1615	0.1560
MOL	1.0795	1.0178	0.8542	0.6435	0.4426	0.2901	0.1972	0.1615	0.1562

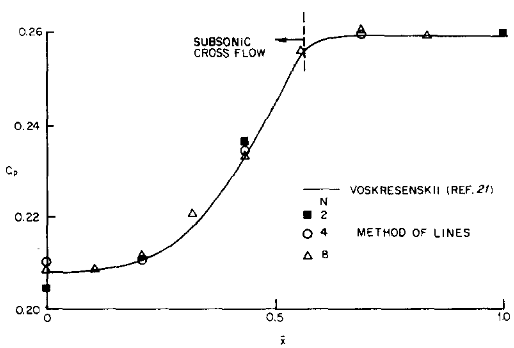

FIG. 2. Surface pressure on flat delta wing, $M_\infty = 4.0$, $\Lambda = 50°$, $\alpha = 15°$; MOL and finite-difference hyperbolic solutions.

A typical surface pressure result of South and Klunker [18] for the delta wing problem (compression side) is given in Fig. 2. In this problem, the cross section [illegible] also along the leading edges which are swept back 50°. The total velocity is everywhere supersonic, but in this problem the conical cross flow is also supersonic in a region adjacent to the leading edge ($\bar{x} = 1$ on Fig. 2). It is interesting that MOL can be used without difficulty in this case, since the conical equations are of mixed type; MOL gives an excellent prediction of the constant pressure which occurs in the hyperbolic region (for the flat wing) as well as in the elliptic region near the wing center line ($\bar{x} = 0$ on Fig. 2), where the cross flow is conically subsonic. In Fig. 2 the MOL results are compared with those of Voskresenskii [21], who used the three-dimensional, fully hyperbolic, finite-difference method. It can be seen that the two methods agree well, and that remarkable accuracy is obtained by MOL with only one intermediate line between the wing center line and leading edge (i.e., $N = 2$). Further MOL results for delta wing problems are given in Ref. [4] and [18], including comparisons with experiment and other calculative methods.

It may be noted in Fig. 2 that South and Klunker, in applying MOL to the delta wing problem, did not use constant strip widths but took more lines in the region where there is more variation in quantities, i.e., near $\bar{x} = 0$ in Fig. 2. This is possible in their case since they approximate derivatives by fitting a fourth-order polynomial to five adjacent points near to the point at which the derivative is required.

5. Conclusions

The preceding examples have illustrated the power of the method of lines for solving elliptic partial differential equations. The method was illustrated by one linear example and by three nonlinear examples which would be difficult to solve by other means.

The two areas which need careful attention when applying MOL are, in the authors' opinion,

(i) Too many lines cause nonconvergence. It is recommended that a few lines only be used with the scheme (2.2) and schemes of the type (2.6)–(2.10) on and adjacent to boundary lines. Alternatively a fifth-order polynomial could be used for approximating derivatives.

(ii) A good initial estimate of the missing boundary condition (or conditions) on the initial line is usually needed. In the authors' experience one can usually use a poor estimate in linear problems since convergence is assured after one iteration of the iterative procedure. But for nonlinear problems one should try to set some parameter of the problem (angle of incidence or Mach number or geometry for example) to a value such that either a solution is known or else the problem becomes linear. Having obtained solutions with the parameter close to its first value, further solutions can be obtained by altering the parameter and extrapolating the estimate of the missing boundary condition.

APPENDIX A: THE METHOD OF INTEGRAL RELATIONS

As mentioned in the Introduction, there is another semidiscrete method which has been widely used in aerodynamic problems, called the method of integral relations (MIR). Reference [3] reviews the aerodynamic applications of the method, but theoretical treatments or studies of asymptotic convergence are rare.

The method is usually applied to systems of first-order partial differential equations. As in MOL, the region is considered to be divided into strips which are parallel to one coordinate, x say. The equations are partially integrated with respect to the other coordinate, y, to obtain an approximate system of ordinary differential equations. The partial integration is performed explicitly by assuming an appropriate y dependence of the integrands. Most applications have used for this purpose a polynomial whose degree increases proportionally to the number of strips. The algebraic development required for this procedure becomes very cumbersome for $N > 2$, so several investigators have used a linear y dependence from one line to the next in order to obtain a simple recursive form for system of ordinary differential equations. We will consider the application of the latter procedure to the example of Section 3.C, since an explicit solution can then be found.

First the substitution $\psi_x = u$, $\psi_y = -v$ is made in Eq. (3.25) to obtain the Cauchy–Riemann equations

$$u_x - v_y = 0; \qquad v_x + u_y = 0. \tag{A1}$$

With the polygon approximation for the y dependence, the partial integration with respect to y yields

$$\tfrac{1}{2}(u'_{n+1} + u_n') - \frac{v_{n+1} - v_n}{h} = 0, \tag{A2}$$

$$\tfrac{1}{2}(v_n' + v'_{n+1}) + \frac{u_{n+1} - u_n}{h} = 0, \tag{A3}$$

where the notation is similar to that introduced in Eqs. (3.8) and (3.11). Differentiation of (A2) with respect to x and manipulation yields:

$$\tfrac{1}{4}(u''_{n+1} + 2u''_n + u''_{n-1}) + \frac{1}{h^2}(u_{n+1} - 2u_n + u_{n-1}) = 0, \tag{A4}$$

producing a tridiagonal system for the x derivatives.

The solution of the above system is in the identical form of Eqs. (3.16)–(3.19), except that

$$\mu_m = (2N/b)\tan(m\pi/4N), \tag{A5}$$

$$\cosh z = \left(1 + \frac{\pi^2 b^2}{4N^2}\right)\Big/\left(1 - \frac{\pi^2 b^2}{4N^2}\right). \tag{A6}$$

From Eq. (A5) we see that the largest eigenvalue is

$$\mu_{2N-1} \approx 8N^2/\pi b, \tag{A7}$$

giving Eq. (3.24) for the instability factor in $\psi_n'(\tfrac{1}{2}) \equiv u_n(\tfrac{1}{2})$. Expansion of the hyperbolic cosine function as in Eq. (3.21) shows that the MIR discretization error is $O(N^{-2})$; but MIR is clearly inferior to MOL from the viewpoint of the size of the eigenvalues μ_m. That is, the MOL eigenvalues grow linearly with N, while the MIR eigenvalues are quadratic in N. Further, the extra complication of the tridiagonal system for the x derivatives has been added without gaining the benefit of decreased y-truncation error, contrary to the scheme of Appendix B.

APPENDIX B: A Tridiagonal MOL System with Accuracy $O(N^{-4})$

As an alternative to the five-point difference schemes (2.2) we present here a scheme with the same accuracy $O(N^{-4})$ which involves only three adjacent lines. The schemes are not general but can be derived in certain cases as follows.

Poisson Equation

We have in the notation of this paper from Taylor-series expansions

$$\psi_{n+1} - 2\psi_n + \psi_{n-1} = h^2 \frac{\partial^2 \psi_n}{\partial y^2} + \frac{h^4}{12}\frac{\partial^4 \psi_n}{\partial y^4} + O(h^6) \tag{B1}$$

and also

$$\frac{\partial^2 \psi_{n+1}}{\partial y^2} - 2\frac{\partial^2 \psi_n}{\partial y^2} + \frac{\partial^2 \psi_{n-1}}{\partial y^2} = h^2 \frac{\partial^4 \psi_n}{\partial y^4} + O(h^4). \tag{B2}$$

On eliminating $\partial^4\psi_n/\partial y^4$ from (B1) and (B2) and substituting

$$\frac{\partial^2\psi_k}{\partial y^2} = -\frac{\partial^2\psi_k}{\partial x^2} + f(x, y_k) \qquad (k = n-1, n, n-1) \tag{B3}$$

from Poisson's equation, we obtain

$$\frac{1}{12}(\psi''_{n+1} + 10\psi''_n + \psi''_{n-1}) + h^{-2}(\psi_{n+1} - 2\psi_n + \psi_{n-1})$$
$$= \frac{1}{12}(f(x, y_{n+1}) + 10f(x, y_n) + f(x, y_{n-1})), \tag{B4}$$

giving a tridiagonal system of equations with accuracy $O(h^4)$ i.e., $O(N^{-4})$.

In fact the system (B4) can be solved analytically in certain cases and in particular we refer to Example 3.C [$f(x, y) \equiv 0$] and obtain the solution. It can be shown that this solution is identical to (3.16)–(3.19) except that (3.17) and (3.19) become

$$\mu_m = \frac{2N}{b}\sin\frac{m\pi}{4N}\cdot\left(1 - \frac{1}{3}\sin^2\frac{m\pi}{4N}\right)^{-1/2} \tag{B5}$$

and

$$\cosh z = \left(1 + \frac{5}{12}\frac{\pi^2 b^2}{N^2}\right)\Big/\left(1 - \frac{\pi^2 b^2}{12N^2}\right). \tag{B6}$$

With this scheme the y-truncation error is reduced by two orders of magnitude compared to (2.1) while the largest eigenvalue μ_{2N-1} is increased only by a constant factor of about $\sqrt{(1.5)}$. We may expect to obtain results of accuracy comparable to the five-point scheme (2.2) which is verified in Table III, where the solutions [numerical using (2.2) while the analytic solution is given for the tridiagonal scheme] by both methods are listed for various N.

First-Order Equations

Consider the first-order equations

$$\frac{\partial P_i}{\partial x} + \frac{\partial Q_i}{\partial y} + R_i = 0 \tag{B7}$$

$i = 1, 2,..., m$, where P_i, Q_i and R_i are linear or nonlinear functions of the independent and dependent variables, e.g., $P_i = P_i(x, y, u_1, u_2, ..., u_m)$. For instance the governing equations for two-dimensional flow can be written in the above form [3].

Dropping the i subscript and using Q_n to denote the value of Q on the n-th line for any one of the i values in Eq. (B7) we have from Taylor-series expansions

$$\frac{Q_{n+1} - Q_{n-1}}{2h} = \frac{\partial Q_n}{\partial y} + \frac{h^2}{6} \frac{\partial^3 Q_n}{\partial y^3} + O(h^4) \tag{B8}$$

and also

$$\frac{\partial Q_{n+1}}{\partial y} - 2 \frac{\partial Q_n}{\partial y} + \frac{\partial Q_{n-1}}{\partial y} = h \frac{\partial^3 Q_n}{\partial y^3} + O(h^4). \tag{B9}$$

Eliminating $\partial^3 Q_n / \partial y^3$ from (B8) and (B9) and substituting

$$(\partial Q_k / \partial y) = -R_k - (\partial P_k / \partial x) \qquad (k = n-1, n, n+1) \tag{B10}$$

gives

$$\tfrac{1}{6}(P'_{n+1} + 4P_n{}' + P'_{n-1}) + \frac{Q_{n+1} - Q_{n-1}}{2h} + \tfrac{1}{6}(R_{n+1} + 4R_n + R_{n-1}) = 0, \tag{B11}$$

where $P_k' \equiv dP_k/dx$. Hence a tridiagonal system for the x derivatives is obtained which has error of order h^4, i.e., $O(N^{-4})$.

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