AD-A122 197 IMPROVED SECOND ORDER METHODS FOR PARABOLIC PARTIAL DIFFERENTIAL EQUATION..(U) LEHIGH UNIV BETHLEHEM PA DEPT OF MECHANICAL ENGINEERING AND M.. W C LEE ET AL. 1/2

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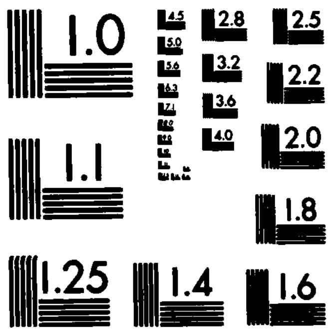

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IMPROVED SECOND ORDER METHODS FOR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

by

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Technical Report FM-82-2

April 1982

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REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER AFOSR-TR- 82-1034	2. GOVT ACCESSION NO. AD-A122 297	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) IMPROVED SECOND ORDER METHODS FOR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS		5. TYPE OF REPORT & PERIOD COVERED INTERIM 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) W.C. LEE J.D.A. WALKER		8. CONTRACT OR GRANT NUMBER(s) F49620-78-C-0071
9. PERFORMING ORGANIZATION NAME AND ADDRESS LEHIGH UNIVERSITY DEPT. OF MECHANICAL ENGINEERING & MECHANICS BETHLEHEM, PA 18015		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 61102F 2307/A2
11. CONTROLLING OFFICE NAME AND ADDRESS AIR FORCE OFFICE OF SCIENTIFIC RESEARCH/NA BOLLING AIR FORCE BASE, DC 20332		12. REPORT DATE APRIL '82 13. NUMBER OF PAGES 88
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

NUMERICAL METHODS
FINITE DIFFERENCES
PARABOLIC EQUATIONS

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Two new finite-difference ~~methods are developed~~ for the calculation of parabolic partial differential equations. The leading truncation error terms are derived and detailed comparisons are made with the errors associated with existing methods, namely the Crank-Nicolson method and Keller Box scheme. A number of examples of both linear and non-linear parabolic problems are computed with both the new and also the existing methods. The accuracy of all four methods are compared; ~~based on the computational experiments~~

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered) and a comparison of the magnitudes of the leading truncation errors, it is concluded that the improved methods are to be preferred over the existing methods.

ACKNOWLEDGEMENTS

The authors wish to thank the Air Force Office of Scientific Research for providing financial support for this study under contract no. F49620-78-C-0071. The present investigation is a small portion of a larger overall program "Theoretical and Experimental Investigation of Coherent Structure in the Turbulent Boundary Layer". The investigation described here is a preliminary study directed toward the development of improved numerical techniques for the prediction of turbulent boundary layers. One of us (W.-C. Lee) wishes to thank the Department of Mechanical Engineering, Lehigh University, for financial support as a teaching assistant during this investigation.

Abstract

Two new finite-difference methods are developed for the calculation of parabolic partial differential equations. The leading truncation error terms are derived and detailed comparisons are made with the errors associated with existing methods, namely the Crank-Nicolson method and Keller Box scheme. A number of examples for both linear and non-linear parabolic problems are computed with both the new and also the existing methods. The accuracy of all four methods are compared; based on the computational experiments and a comparison of the magnitudes of the leading truncation errors, it is concluded that the improved methods are to be preferred over the existing methods.

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I. INTRODUCTION

Parabolic partial differential equations arise frequently in engineering applications particularly in problems involving boundary-layer flows, heat conduction and mass diffusion. Finite-difference methods are frequently used to solve such equations numerically, especially in situations where an analytical solution is not readily available. Finite-difference techniques for parabolic equations may be divided into two categories, namely explicit and implicit methods. Both types of techniques are discussed by Smith (1978) in the context of the unsteady one-dimensional heat conduction equation and in this case the following results apply:

(1) Explicit methods lead to relatively simple computational algorithms but in order to obtain an accurate and stable numerical scheme, severe restrictions on the mesh sizes are usually necessary.

(2) These restrictions can often require very small mesh sizes and this can lead to excessively long computation times.

(3) Implicit methods normally do not suffer from stability problems and mesh size restrictions are not necessary to achieve numerical stability.

(4) Of the implicit schemes considered by Smith (1978), the Crank-Nicolson method, which is based upon approximating the heat conduction equation at the midpoint of two successive time planes, is preferred since it is second order accurate in both time and space.

Although these results apply strictly only to the one-dimensional unsteady heat conduction equation, experience suggests that they are representative of parabolic problems in general and in particular carry over to the non-linear case. For example, Raetz (1953), and Wu (1962) have considered the application of explicit methods for the laminar boundary layer equations and find that mesh size restrictions are necessary for the numerical scheme to be stable. Implicit methods have performed very well in the non-linear case and many modern laminar boundary-layer prediction methods, for example, use difference equations based on the Crank-Nicolson approach.

Another finite-difference technique has recently been suggested by Keller (1970) for parabolic differential equations. In general, for parabolic equations, there is a spatial direction in which the boundary conditions are assigned and a marching direction in which the solution is constructed in a step-by-step manner. In the so-called 'Keller Box' method, the governing equations are written as a system of first order equations and central difference approximations are made at points midway between the spatial mesh points. One major advantage of this technique is that unlike the Crank-Nicolson method non-uniform mesh sizes in the spatial direction may be used. This method and the Crank-Nicolson method will be described in detail in Chapter 2.

The Crank-Nicolson scheme and Keller Box scheme may easily be used with non-linear parabolic partial differential equations. The main difference in the non-linear case is that once the difference approximations are made, the difference equations are non-linear and cannot, in general, be solved immediately by direct elimination methods. In order to overcome this difficulty the difference equations must be linearized in some manner at each stage in a general iterative procedure and at each station in the marching direction; there are at least two ways in which this can be carried out. In Picard iteration, the non-linear terms are linearized by guessing selected terms from either the solution at the previous station or from the solution at the last iteration. This method is relatively easy to implement and if the terms being linearized are chosen carefully, then convergence will normally result. However, the rate of convergence may be slow and can often be accelerated by an alternative linearization technique known as Newton linearization; in this procedure, the solution at any step is rewritten as a combination of the unknown exact solution plus a perturbation quantity. Upon substitution into the non-linear difference equations and neglect of the terms which are quadratic in the perturbation, a set of linear difference equations is obtained; these equations may then be solved by a direct method such as Thomas Algorithm. In practice, an estimate of the exact solution is obtained by using the solution at the previous step or from last iteration. This method is more difficult to implement than Picard iteration but has the ultimate advantage that the convergence rate at each station is quadratic.

The principle difference between the Crank-Nicolson method, the Keller Box method and the two other approaches developed here is associated with the method of spatial differencing. In the Crank-Nicolson method, the spatial difference approximations are based on the classical central difference approximations for ordinary differential equations of boundary value type (see for example Fox, 1957); on the other hand, the Keller Box method is based on an alternative differencing scheme given by Keller (1969) for ordinary differential equations of the boundary value type. In a recent paper Walker and Weigand (1979) have described a simple finite-difference technique for ordinary differential equations which is shown to produce more accurate results than either the classical method or the Keller (1969) method. The objective of the present investigation is to adapt the spatial differencing scheme of Walker and Weigand (1979) to solve parabolic partial difference equations. The plan of this report is as follows. In Chapter 2, the Crank-Nicolson method and Keller Box method are discussed in connection with linear parabolic partial differential equations; modifications of these schemes for the non-linear case are also discussed in Chapter 5. Two new methods are developed in Chapter 3 for linear problems and the modifications for non-linear equations are discussed in Chapter 5. In Chapters 4 and 5 the various methods for the linear and non-linear cases respectively, are compared by using various mesh lengths for a number of example problems. Based on the truncation error terms given in Chapter 2, 3 and the computational experiments of Chapters 4 and 5, it is concluded that the present methods are to be preferred over the existing methods.

2. EXISTING METHODS

2.1 The Crank-Nicolson Method

Parabolic second order partial differential equations are usually of the form,

$$Q \frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial y^2} + P \frac{\partial u}{\partial y} + Ru + F , \qquad (2.1)$$

where x and y are two independent variables. The equation is linear when the coefficients Q,P,R, and F are constant or functions of x and y only. If the coefficients are functions of x,y, u, $\frac{\partial u}{\partial x}$, $\frac{\partial u}{\partial y}$, the equation is non-linear but is usually described as being quasi-linear since the non-linearity is not associated with the most highly differentiated terms.

There are two popular methods currently available to solve equation (2.1). The first of these is the Crank-Nicolson method and the application of this technique for linear equations will be discussed here; note that this method may only be used with a uniform mesh in the y-direction. The conditions usually associated with equation (2.1) are: (1) an initial condition specified at some initial station, say x = 0, according to u(0,y) = f(y) and (2) boundary conditions at two y locations, say y = a and b. Here a and b may be finite or infinite and normally either u, $\frac{\partial u}{\partial y}$ or a linear combination of both are given as specified functions of x. Here the simplest case where

$$u(x,a) = g_1(x) \ , \ u(x,b) = g_2(x) \qquad (2.2)$$

is assumed. Derivative boundary conditions may be treated through obvious modifications of the present development (see Appendix I).

The interval (a,b) in the y direction is split into N equal parts of mesh length h as indicated as in figure (2.1); the subscript j denotes a typical point in the mesh. Assuming that the solution is known at $x = x_{i-1}$, the object is to construct the solution at $x = x_i = x_{i-1} + k$; here k is the step length in the x-direction which may be varied as the integration proceeds. For simplicity and to avoid double scripting, define $x^* = x_{i-1}$ and $x^{**} = x_{i-1} + \frac{k}{2}$; the convention is then adopted that all quantities evaluated at x^*, x^{**} and x are denoted by a single asterick, a double asterisk and no asterisk, respectively. Quantities at the station x^* are known and the object is to evaluate the unknown quantities at x.

In the Crank-Nicolson method, the partial differential equation (2.1) is approximated at the point labelled C in figure (2.1) which is located mid-way between the (i) and (i-1) mesh lines and on the jth mesh line. Simple averages in the x direction and central difference approximations for the derivatives are used; both approximations are second order accurate

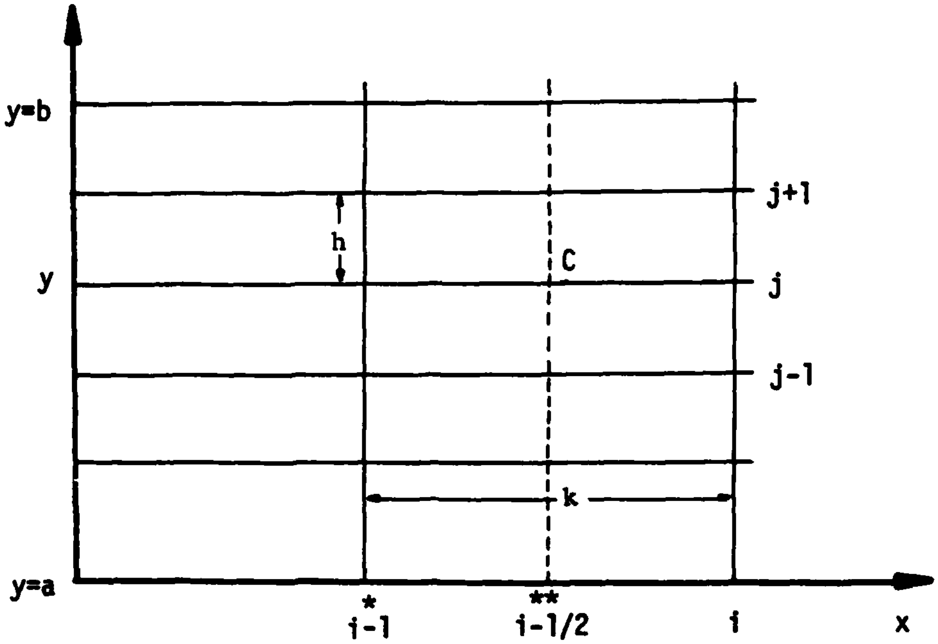

Figure 2.1. Grid configuration for the Crank-Nicolson method

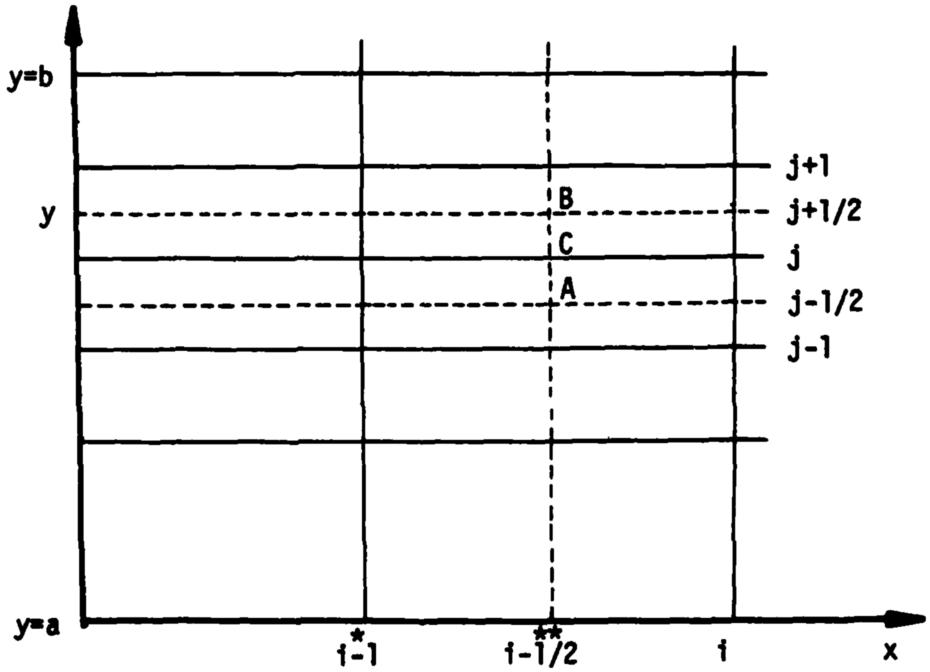

Figure 2.2. Grid configuration for the Keller Box method

and the following difference equations result at the typical jth mesh line:

$$Q_j^{**}\left(\frac{u_j-u_j^*}{k}\right) = 1/2\left(\frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} + \frac{u_{j+1}^* - 2u_j^* + u_{j-1}^*}{h^2}\right)$$

$$+ \frac{P_j^{**}}{2}\left(\frac{u_{j+1} - u_{j-1}}{2h} + \frac{u_{j+1}^* - u_{j-1}^*}{2h}\right) + R_j^{**}\left(\frac{u_j + u_j^*}{2}\right) + F_j^{**}$$

$$+ 0(h^2) + 0(k^2) \ . \tag{2.3}$$

Here j = 1,2,3...N-1 where N is the total number of mesh points in the y direction. Equation (2.3) may be rewritten in the tri-diagonal form

$$B_ju_{j+1} + A_ju_j + C_ju_{j-1} = D_j + h^2E_j \ , \tag{2.4}$$

where,

$$A_j = -2 + h^2R_j^{**} - \frac{2h^2}{k}Q_j^{**} \ , \tag{2.5a}$$

$$B_j = 1 + \frac{h}{2}P_j^{**} \ , \tag{2.5b}$$

$$C_j = 1 - \frac{h}{2}P_j^{**} \ , \tag{2.5c}$$

$$D_j = -2h^2F_j^{**} - u_{j+1}^*\left(1 + \frac{h}{2}P_j^{**}\right) - u_{j-1}^*\left(1 - \frac{h}{2}P_j^{**}\right)$$

$$- u_j^*\left(-2 + h^2R_j^{**} + \frac{2h^2}{k}Q_j^{**}\right). \tag{2.5d}$$

It is possible to write the leading order terms in the truncation error E_j in two different but equivalent ways. In the first method, the error is expressed in terms of the partial derivatives of the dependent variable u; here and in the subsequent methods discussed in this study, the point at which these derivatives are evaluated will be standardized at the point on the jth mesh line ($y = y_j$), midway between the current and previous solution plane. It may be shown through the use of Taylor series expansions at the point (x^{**}, y_j) that

$$E_j = \frac{k^2 Q_j^{**}}{12} \frac{\partial^3 u}{\partial x^3}\bigg|_j^{**} + \frac{k^2}{8} \left(\frac{\partial^2 Q}{\partial x^2} \frac{\partial u}{\partial x} + 2 \frac{\partial Q}{\partial x} \frac{\partial^2 u}{\partial x^2}\right)\bigg|_j^{**}$$

$$+ \frac{h^2}{12} \frac{\partial^4 u}{\partial y^4}\bigg|_j^{**} + \frac{h^2}{6} P_j^* \frac{\partial^3 u}{\partial y^3}\bigg|_j^{**} + \dots \quad . \tag{2.6}$$

A second form of the truncation error is in terms of central difference operators according to,

$$E_j = \frac{Q_j^{**}}{12k} \mu_x \delta_x^3 u_j^{**} + \frac{1}{8k} \{(\delta_x^2 Q_j^{**})(\mu_x \delta_x u_j^{**}) + 2(\mu_x \delta_x Q_j^{**})(\delta_x^2 u_j^{**})\}$$

$$+ \frac{1}{12h^2} \delta_y^4 u_j^{**} + \frac{1}{6h} P_j^{**} \mu_y \delta_y^3 u_j^{**} + \dots \quad . \tag{2.7}$$

Here δ and μ are the usual central difference operators and the subscript indicates that the differences are to be taken in that particular direction. Upon neglecting the leading truncation term, the matrix associated with the system of equations (2.4) is tridiagonal and a number of direct methods of solution are available; a particularly efficient method is often referred to as the Thomas Algorithm (Appendix I). For linear problems, equations(2.4) can then be solved directly to give the solution at $x = x_i$; the algorithm may then be applied again to obtain the solution at x_{i+1} and the computation proceeds in the x-direction in a step-by-step manner.

2.2 The Keller Box Scheme

The basis of this method is to introduce an auxiliary variable v and to rewrite equation (2.1) as the following set of first order equations:

$$v = \frac{\partial u}{\partial y} \quad , \tag{2.8}$$

$$Q \frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} + Pv + Ru + F \ . \tag{2.9}$$

Equations (2.8) and (2.9) are then approximated at point A of Figure (2.2), which is the center of the box formed by points (j-1,i), (j,i), (j,i-1) and (j-1,i-1); simple central differences are used for the derivatives and simple averages for v and u. Using the notation of the previous section, quantities evaluated at x_i^*, x_i^{**} and x_i are denoted by a single asterisk, a double asterisk and no asterisk, respectively. The results for equations (2.8) and (2.9) are

$$\frac{u_j^* + u_j}{2} = \frac{h}{4}\left(v_j^* + v_j + v_{j-1}^* + v_{j-1}\right) + \frac{u_{j-1}^* + u_{j-1}}{2}\,, \tag{2.10}$$

$$\begin{aligned}\frac{Q_{j-\frac{1}{2}}^{**}}{2k}\left(u_j + u_{j-1} - u_j^* - u_{j-1}^*\right) &= \frac{1}{2h}\left(v_j + v_j^* - v_{j-1} - v_{j-1}^*\right) \\ &+ \frac{P_{j-\frac{1}{2}}^{**}}{4}\left(v_j^*+v_j+v_{j-1}^*+v_{j-1}\right) + \frac{R_{j-\frac{1}{2}}^{**}}{4}\left(u_j^*+u_j+u_{j-1}^*+u_{j-1}\right) + F_{j-\frac{1}{2}}^{**}\,.\end{aligned} \tag{2.11}$$

A similar procedure is used to approximate (2.8) and (2.9) at the center of the upper box labelled B in Figure (2.2) and the results are ,

$$\frac{u_{j+1}^* + u_{j+1}}{2} = \frac{h}{4}\left(v_{j+1}^* + v_{j+1} + v_j^* + v_j\right) + \frac{u_j^* + u_j}{2}\,, \tag{2.12}$$

$$\begin{aligned}\frac{Q_{j+\frac{1}{2}}^{**}}{2k}\left(u_{j+1} + u_j - u_{j+1}^* - u_j^*\right) &= \frac{1}{2h}\left(v_{j+1} + v_{j+1}^* - v_j - v_j^*\right) \\ &+ \frac{P_{j+\frac{1}{2}}^{**}}{4}\left(v_{j+1}^*+v_{j+1}+v_j^*+v_j\right) + \frac{R_{j+\frac{1}{2}}^{**}}{4}\left(u_{j+1}^*+u_{j+1}+u_j^*+u_j\right) + F_{j+\frac{1}{2}}^{**}\,.\end{aligned} \tag{2.13}$$

It is worthwhile to note that this approach may be readily adopted for equations for which the use of a non-uniform mesh in the y direction is desirable; however, in what follows, only the uniform mesh case will be considered since this is the case of interest in this investigation. Keller (1970) prefers to solve the linear set of difference equations in the form of equations (2.10) and (2.11). However, following a procedure similar to the technique suggested by the work of Ackerberg and Phillips (1972), the set of difference equations may be written as a single tridiagonal matrix problem which may then be solved by a direct method. This procedure is more efficient than the procedure used by Keller (1970) and moreover for comparative purposes its convenient to perform the reduction to the tridiagonal form here. This reduction is carried out as follows. Equation (2.10) is used to eliminate the auxiliary variable v_{j-1} in equation (2.11); the resulting equation contains v_j, u_j and u_{j-1} and will be denoted as equation (A). A similar procedure is used to eliminate v_{j+1} in equation (2.13) using equation (2.12); the resulting equation is termed equation (B) and contains v_j, u_j and u_{j+1}. Equations (A) and (B) are then combined to completely eliminate the auxiliary variable v_j from the system; the result is:

$$B_j u_{j+1} + A_j u_j + C_j u_{j-1} = D_j + h^2 E_j \,, \tag{2.14}$$

where E_j is the truncation error. The coefficients in equation (2.14) are

$$A_j = -2 - \frac{h}{2}(P^{**}_{j+\frac{1}{2}} - P^{**}_{j-\frac{1}{2}}) + \frac{h^2}{4}(R^{**}_{j+\frac{1}{2}} + R^{**}_{j-\frac{1}{2}}) - \frac{h^2}{2k}(Q^{**}_{j+\frac{1}{2}} + Q^{**}_{j-\frac{1}{2}}) \,, \tag{2.15a}$$

$$B_j = 1 + \frac{h}{2} P^{**}_{j+\frac{1}{2}} + \frac{h^2}{4} R^{**}_{j+\frac{1}{2}} - \frac{h^2}{2k} Q^{**}_{j+\frac{1}{2}} \quad , \qquad (2.15b)$$

$$C_j = 1 - \frac{h}{2} P^{**}_{j-\frac{1}{2}} + \frac{h^2}{4} R^{**}_{j-\frac{1}{2}} - \frac{h^2}{2k} Q^{**}_{j-\frac{1}{2}} \quad ; \qquad (2.15c)$$

$$\begin{aligned} D_j = & -h^2 (F^{**}_{j+\frac{1}{2}} + F^{**}_{j-\frac{1}{2}}) - u^*_j\{-2 - \frac{h}{2} (P^{**}_{j+\frac{1}{2}} - P^{**}_{j-\frac{1}{2}}) \\ & + \frac{h^2}{4} (R^{**}_{j+\frac{1}{2}} + R^{**}_{j-\frac{1}{2}}) + \frac{h^2}{2k} (Q^{**}_{j+\frac{1}{2}} + Q^{**}_{j-\frac{1}{2}})\} \\ & - u^*_{j+1} \{1 + \frac{h}{2} P^{**}_{j+\frac{1}{2}} + \frac{h^2}{4} R^{**}_{j+\frac{1}{2}} + \frac{h^2}{2k} Q^{**}_{j+\frac{1}{2}}\} \qquad (2.15d) \\ & - u^*_{j-1} \{1 - \frac{h}{2} P^{**}_{j-\frac{1}{2}} + \frac{h^2}{4} R^{**}_{j-\frac{1}{2}} + \frac{h^2}{2k} Q^{**}_{j-\frac{1}{2}}\} \quad . \end{aligned}$$

It may be shown that the leading term in the truncation error in equation (2.14), related to the partial derivatives of u evaluated at the point (x^{**}, y_j), is

$$\begin{aligned} E_j = & -\frac{h^2 Q^{**}_j}{8} \frac{\partial^3 u}{\partial y^2 \partial x}\Big|^{**}_j + \frac{h^2}{8} \left(\frac{\partial^2 Q}{\partial y^2} \frac{\partial u}{\partial x} + \frac{\partial Q}{\partial y} \frac{\partial^2 u}{\partial x^2} + \frac{\partial Q}{\partial y} \frac{\partial^2 u}{\partial y \partial x}\right)\Big|^{**}_j \\ & + \frac{k^2 Q^{**}_j}{12} \frac{\partial^3 u}{\partial x^3}\Big|^{**}_j + \frac{k^2}{8} \left(\frac{\partial^2 Q}{\partial x^2} \frac{\partial u}{\partial x} + 2 \frac{\partial Q}{\partial x} \frac{\partial^2 u}{\partial x^2}\right)\Big|^{**}_j - \frac{h^2}{24} \frac{\partial^4 u}{\partial y^4}\Big|^{**}_j \\ & + \frac{h^2}{24} (\mu_y P^{**}_j) \frac{\partial^3 u}{\partial y^3}\Big|^{**}_j - \frac{h^2}{8} (\mu_y R^{**}_j) \frac{\partial^2 u}{\partial y^2}\Big|^{**}_j \ . \end{aligned} \qquad (2.16)$$

An alternative form for E_j in term of finite-difference operators is, to leading order,

$$E_j = -\frac{Q_j^{**}}{8k}\mu_x\delta_x(\delta_y^2 u_j^{**}) + \frac{1}{8k}(\delta_y^2 Q_j^{**})(\mu_x\delta_x u_j^{**})$$

$$+ \frac{h}{8k^2}(\mu_y\delta_y u_j^{**})(\delta_x^2 u_j^{**}) + \frac{1}{8k}(\mu_y\delta_y Q_j^{**})(\mu_y\delta_y(\mu_x\delta_x u_j^{**}))$$

$$+ \frac{Q_j^{**}}{12K}\mu_x\delta_x^3 u_j^{**} + \frac{1}{8k}\{(\delta_x^2 Q_j^{**})(\mu_x\delta_x u_j^{**}) + 2(\mu_x\delta_x Q_j^{**})(\delta_x^2 u_j^{**})\}$$

$$- \frac{1}{24h^2}\delta_y^4 u_j^{**} + \frac{1}{24h}(\mu_y P_j^{**})\mu_y\delta_y^3 u_j^{**} - \frac{1}{8}(\mu_y R_j^{**})\delta_y^2 u_j^{*} + \ldots. \tag{2.17}$$

Here δ and μ are the usual central difference operators and the subscript indicates that the differences are to be taken in that particular direction. Upon neglecting the leading truncation terms, the tridiagonal problem in (2.14) may be readily solved directly using, for example, the Thomas Algorithm.

The truncation errors associated with the classical Crank-Nicolson scheme and the Keller (1970) box scheme are compared in table (2.1) and (2.2). Referring to the x and y directions as the marching and spatial directions respectively, it is convenient to isolate the errors associated with the approximations in each direction. In table (2.1) the truncation errors which originate from the approximations in the marching direction are compared; such errors are defined to be those

Classical Method	$\frac{Q_j^{**} k^2}{12} \frac{\partial^3 u}{\partial x^3}\Big\vert_j^{**} + \frac{k^2}{8}\left(\frac{\partial^2 Q}{\partial x^2}\frac{\partial u}{\partial x} + 2\frac{\partial Q}{\partial x}\frac{\partial^3 u}{\partial x^3}\right)\Big\vert_j^{**}$	———
Keller Box Scheme	$\frac{Q_j^{**} k^2}{12} \frac{\partial^3 u}{\partial x^3}\Big\vert_j^{**} + \frac{k^2}{8}\left(\frac{\partial^2 Q}{\partial x^2}\frac{\partial u}{\partial x} + 2\frac{\partial Q}{\partial x}\frac{\partial^3 u}{\partial x^3}\right)\Big\vert_j^{**}$	$-\frac{Q_j^{**} h^2}{8} \frac{\partial^3 u}{\partial y^2 \partial x}\Big\vert_j^{**} + \frac{h^2}{8}\left(\frac{\partial^2 Q}{\partial y^2}\frac{\partial u}{\partial x} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial x^2} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial y \partial x}\right)\Big\vert_j^{**}$

Table 2.1. Comparison of the leading error terms arising from the approximations in the marching direction for the classical method and Keller Box scheme.

Classical Method	$+\frac{h^2}{12}\frac{\partial^4 u}{\partial y^4}\Big\vert_j^{**} + \dots$	$+\frac{h^2}{6} P_j^{**} \frac{\partial^3 u}{\partial y^3}\Big\vert_j^{**} + \dots$	———
Keller Box Scheme	$-\frac{h^2}{24}\frac{\partial^4 u}{\partial y^4}\Big\vert_j^{**} + \dots$	$+\frac{h^2}{24}(\mu_y P_j^{**}) \frac{\partial^3 u}{\partial y^3}\Big\vert_j^{**} + \dots$	$-\frac{h^2}{8}(\mu_y R_j^{**}) \frac{\partial^2 u}{\partial y^2}\Big\vert_j^{**} + \dots$

Table 2.2. Comparison of the leading error terms arising from the approximations in the spatial direction for the classical method and Keller Box scheme.

containing partial derivatives with respect to x. It may be observed that the first group of error terms are identical to leading order but that the Keller (1970) method contains an additional group of error terms $O(h^2)$. For this reason, the Crank-Nicholson method apparently has an advantage over the Keller scheme in regard to the accuracy of the approximation in the marching direction; this point will be reconsidered subsequently.

Consider now the leading order error terms arising from the approximations in the spatial direction which are compared in table (2.2); these same error terms arise in the approximation of the two-point boundary value problem,

$$\frac{d^2u}{dy^2} + P(y)\,\frac{du}{dy} + R(y)u + F = 0\,, \quad u(a)=A,\ u(b)=B\,, \qquad (2.18)$$

by either the classical method or the Keller method. This problem has been considered by Walker and Weigand (1979) who also derive an improved technique. Note that in table (2.2) the first and second error terms are smaller by a factor of one-half and one quarter, respectively, as compared to the corresponding terms for the Crank-Nicolson method; however, the Keller scheme contains an additional third error term $O(h^2)$. A general conclusion that may be inferred is that neither the Crank-Nicolson or the Keller method may be considered superior to the other insofar as the approximations in the spatial direction are concerned; this conclusion has been extensively verified for two point boundary value problems by Walker and Weigand (1979).

It is worthwhile to remark that the errors in table (2.1) and (2.2) are not independent. For example, for the ordinary diffusion equation,

$$\frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial y^2} \quad , \tag{2.19}$$

the additional error term in the Keller (1970) method in table (2.1) may be combined with the first term in table (2.2) and the total truncation error is

$$\frac{k^2}{12} \frac{\partial^3 u}{\partial x^3} \bigg|_j^{**} - \frac{h^2}{6} \frac{\partial^4 u}{\partial y^4} \bigg|_j^{**} + \dots \quad . \tag{2.20}$$

The corresponding error for the Crank-Nicolson method is

$$\frac{k^2}{12} \frac{\partial^3 u}{\partial x^3} \bigg|_j^{**} + \frac{h^2}{12} \frac{\partial^4 u}{\partial y^4} \bigg|_j^{**} + \dots \tag{2.21}$$

and it may be observed that the spatial error is smaller than for the Keller method but of opposite sign. The total error will in general depend on the particular problem under consideration and in particular on the sign of each of the error terms and how they combine.

At this stage, it appears that the total error term associated with the Crank-Nicolson scheme can be expected to be slightly smaller than for the Keller (1970) scheme because of the additional error terms associated with the latter scheme. However, a number of example problems will be considered in Chapter 4 and 5 to investigate this point since it appears at this stage that a general preference for the Crank-Nicolson method would be marginal at best.

3. TWO IMPROVED METHODS FOR PARABOLIC EQUATIONS

3.1 Method I

Consider the grid configuration of figure (2.2); at any fixed value of x (the marching direction) and at $y_\beta = y_j + \beta h$, the following expressions may be written for u, $\partial u/\partial y$ and $\partial^2 u/\partial y^2$ (Walker & Weigand, 1979):

$$u(x,y_\beta) = \{1 + \beta\mu_y\delta_y + \frac{\beta^2}{2}\delta_y^2 + \frac{\beta(\beta^2-1)}{6}\mu_y\delta_y^3 + \ldots\}u(x,y_j), \tag{3.1}$$

$$\left.\frac{\partial u}{\partial y}\right|_{x,y_\beta} = \frac{1}{h}\{\mu_y\delta_y+\beta\delta_y + \frac{(3\beta^2-1)}{6}\mu_y\delta_y^3 + \ldots\}u(x,y_j), \tag{3.2}$$

$$\left.\frac{\partial^2 u}{\partial y^2}\right|_{x,y_\beta} = \frac{1}{h^2}\{\delta_y^2 + \beta\mu_y\delta_y^3 + \frac{(6\beta^2-1)}{12}\delta_y^4 + \ldots\}u(x,y_j) . \tag{3.3}$$

Here δ_y and μ_y are the usual central difference operators and the subscript y denotes an operator in the y direction.

The general linear parabolic equation (2.1) may be rewritten according to

$$Q\,\frac{\partial u}{\partial t} = L(u) , \tag{3.4}$$

where the operator L(u) is defined by,

$$L(u) = \frac{\partial^2 u}{\partial x^2} + P\frac{\partial u}{\partial x} + Ru + F\ . \qquad (3.5)$$

Using the notation of the previous section, quantities evaluated at $\overset{*}{x_i}$, $\overset{**}{x_i}$ and x_i are denoted by a single asterisk, a double asterisk and no asterisk, respectively; equation (3.4) is then approximated at point B of figure (2.2) according to,

$$\overset{**}{Q}_{j+\frac{1}{2}} \left.\frac{\partial u}{\partial x}\right|^{**}_{j+\frac{1}{2}} = \frac{1}{2}\left[L(u)\Big|^{*}_{j+\frac{1}{2}} + L(u)\Big|_{j+\frac{1}{2}}\right] \ . \qquad (3.6)$$

Note that the error term has been omitted for the moment in equation (3.6); however, this term is associated only with the simple average on the right side and is $O(k^2)$. The principle difference between the two methods developed in this section lies in the approximation to the marching derivative $\partial u/\partial x$.

In method I, a central difference approximation is used along the line $y = y_{j+\frac{1}{2}}$ and this gives,

$$\left.\frac{\partial u}{\partial x}\right|^{**}_{j+\frac{1}{2}} = \frac{u_{j+\frac{1}{2}} - \overset{*}{u}_{j-\frac{1}{2}}}{k} \ . \qquad (3.7)$$

Equation (3.1) may now be used to relate $u_{j+\frac{1}{2}}$ and $\overset{*}{u}_{j+\frac{1}{2}}$ to values of u at points in the mesh. Using the first three terms in equation (3.1) leads to, for example,

$$u_{j+\frac{1}{2}} = \frac{3u_{j+1} + 6u_j - u_{j-1}}{8} \tag{3.8}$$

where the omitted error terms is $O(\mu_y \delta_y^3)$. Combining these approximations results in,

$$\begin{aligned}
&Q^{**}_{j+\frac{1}{2}}\left[\frac{3u_{j+1} + 6u_j - u_{j-1}}{8k} - \frac{3u^*_{j+1} + 6u^*_j - u^*_{j-1}}{8k}\right] \\
&= \tfrac{1}{2}\left[\frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} + \frac{u^*_{j+1} - 2u^*_j + u^*_{j-1}}{h^2}\right] \\
&+ \frac{P^{**}_{j+\frac{1}{2}}}{2}\left[\frac{u_{j+1} - u_j}{h}\right] + \frac{P^{**}_{j+\frac{1}{2}}}{2}\left[\frac{u^*_{j+1} - u^*_j}{h}\right] \\
&+ \frac{R^{**}_{j+\frac{1}{2}}}{16}(3u_{j+1} + 6u_j - u_{j-1}) \\
&+ \frac{R^{**}_{j-\frac{1}{2}}}{16}(3u^*_{j+1} + 6u^*_j - u^*_{j-1}) + F^{**}_{j+\frac{1}{2}} \;.
\end{aligned} \tag{3.9}$$

A similar procedure is applied to equation (3.4) in the lower box at point A of figure (2.2) to obtain

$$Q^{**}_{j-\frac{1}{2}} \left.\frac{\partial u}{\partial x}\right|^{**}_{j-\frac{1}{2}} = \tfrac{1}{2}\left\{L(u)\Big|^{*}_{j-\frac{1}{2}} + L(u)\Big|_{j-\frac{1}{2}}\right] \;. \tag{3.10}$$

Using a procedure analogous to that leading to the approximation (3.9), it may be shown that,

$$Q^{**}_{j-\frac{1}{2}}\left[\frac{-u_{j+1} + 6u_j + 3u_{j-1}}{8k} - \frac{-u^*_{j+1} + 6u^*_j + 3u^*_{j-1}}{8k}\right]$$

$$= \tfrac{1}{2}\left[\frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} - \frac{u^*_{j+1} - 2u^*_j + u^*_{j-1}}{h^2}\right] \tag{3.11}$$

$$+ \frac{P^{**}_{j-\frac{1}{2}}}{2}\left[\frac{u_j - u_{j-1}}{h}\right] + \frac{P^{**}_{j-\frac{1}{2}}}{2}\left[\frac{u^*_j - u^*_{j-1}}{h}\right]$$

$$+ \frac{R^{**}_{j-\frac{1}{2}}}{16}(-u_{j+1}+6u_j+3u_{j-1}) + \frac{R^{**}_{j-\frac{1}{2}}}{16}(-u^*_{j+1}+6u^*_j+3u^*_{j-1})+F^{**}_{j-\frac{1}{2}}.$$

Equations (3.9) and (3.11) may be combined to form a set of algebraic equations of the form,

$$B_j u_{j+1} + A_j u_j + C_j u_{j-1} = D_j + h^2 E_j \;, \tag{3.12}$$

where,

$$A_j = -2 - \frac{h}{2}(P^{**}_{j+\frac{1}{2}} - P^{**}_{j-\frac{1}{2}}) + \frac{3h^2}{8}(R^{**}_{j+\frac{1}{2}} + R^{**}_{j-\frac{1}{2}}) - \frac{3h^2}{4k}(Q^{**}_{j+\frac{1}{2}} + Q^{**}_{j-\frac{1}{2}}), \tag{3.13a}$$

$$B_j = 1 + \frac{h}{2}P^{**}_{j+\frac{1}{2}} + \frac{h^2}{16}(3R^{**}_{j+\frac{1}{2}} - R^{**}_{j-\frac{1}{2}}) - \frac{h^2}{8k}(3Q^{**}_{j+\frac{1}{2}} - Q^{**}_{j-\frac{1}{2}}), \tag{3.13b}$$

$$C_j = 1 - \frac{h}{2}P^{**}_{j-\frac{1}{2}} - \frac{h^2}{16}(R^{**}_{j+\frac{1}{2}} - 3R^{**}_{j-\frac{1}{2}}) + \frac{h^2}{8k}(Q^{**}_{j+\frac{1}{2}} - 3Q^{**}_{j-\frac{1}{2}}), \tag{3.13c}$$

$$D_j = -h^2(F^{**}_{j+\frac{1}{2}} + F^{**}_{j-\frac{1}{2}}) - u^*_j(-2 - \frac{h}{2}(P^{**}_{j+\frac{1}{2}} - P^{**}_{j-\frac{1}{2}})$$

$$+ \frac{3h^2}{8}(R^{**}_{j+\frac{1}{2}} + R^{**}_{j-\frac{1}{2}}) + \frac{3h^2}{4k}(Q^{**}_{j+\frac{1}{2}} + Q^{**}_{j-\frac{1}{2}}))$$

$$-u^{*}_{j+1}\left(1 + \frac{h}{2} P^{**}_{j+\frac{1}{2}} + \frac{h^2}{16}\left(3R^{**}_{j+\frac{1}{2}} - R^{**}_{j-\frac{1}{2}}\right) + \frac{h^2}{8k}\left(3Q^{**}_{j+\frac{1}{2}} - Q^{**}_{j-\frac{1}{2}}\right)\right)$$

$$-u^{*}_{j-1}\left(1 - \frac{h}{2} P^{**}_{j-\frac{1}{2}} - \frac{h^2}{16}\left(R^{**}_{j+\frac{1}{2}} - 3R^{**}_{j-\frac{1}{2}}\right) - \frac{h^2}{8k}\left(Q^{**}_{j+\frac{1}{2}} - 3Q^{**}_{j-\frac{1}{2}}\right)\right).$$

(3.13d)

In equation (3.12), E_j is the total error term associated with the difference approximations. After some algebra it may be shown using Taylor series expansions that the leading truncation error terms in equation (3.12), related to partial derivatives of the dependent variable at the point (x^{**}, y_j), are

$$E_j = \frac{k^2 Q^{**}_j}{12} \left.\frac{\partial^3 u}{\partial x^3}\right|^{**}_j + \frac{h^2}{8}\left.\left(\frac{\partial^2 Q}{\partial y^2}\frac{\partial u}{\partial x} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial x^2} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial y \partial x}\right)\right|^{**}_j$$

$$+ \frac{k^2}{8}\left.\left(\frac{\partial^2 Q}{\partial x^2}\frac{\partial u}{\partial x} + 2\frac{\partial Q}{\partial x}\frac{\partial^2 u}{\partial x^2}\right)\right|^{**}_j$$

$$- \frac{h^2}{24}\left.\frac{\partial^4 u}{\partial y^4}\right|^{**}_j + \frac{h^2}{24}\left(\mu_y P^{**}_j\right)\left.\frac{\partial^3 u}{\partial y^3}\right|^{**}_j + \frac{h^3}{32}\left(\delta_y R^{**}_j\right)\left.\frac{\partial^3 u}{\partial y^3}\right|^{**}_j.$$

(3.14)

A second form of the truncation error is in terms of central difference operators according to,

$$E_j = \frac{Q^{**}_j}{12k}\mu_x \delta^3_x u^{**}_j + \frac{1}{8k}\left(\delta^2_y Q^{**}_j\right)\left(\mu_x \delta_x u^{**}_j\right) + \frac{h}{8k^2}\left(\mu_y \delta_y u^{**}_j\right)\left(\delta^2_x u^{**}_j\right)$$

$$+ \frac{1}{8k}\left(\mu_y \delta_y Q^{**}_j\right)\left(\mu_y \delta_y\left(\mu_x \delta_x u^{**}_j\right)\right)$$

$$+ \frac{1}{8k}\left(\left(\delta^2_x Q^{**}_j\right)\left(\mu_x \delta_x u^{**}_j\right) + 2\left(\mu_x \delta_x Q^{**}_j\right)\left(\delta^2_x u^{**}_j\right)\right)$$

$$- \frac{1}{24h^2} \delta_y^4 u_j^{**} + \frac{1}{24h} (\mu_y P_j^{**}) \mu_y \delta_y^3 u_j^{**} + \frac{1}{32} (\delta_y R_j^{**}) \mu_y \delta_y^3 u_j^{**} \; . \tag{3.15}$$

Upon neglecting the leading truncation terms, the tridiagonal problem in equation (3.12) may be readily solved directly.

In situations where P,R,F and Q are not analytic but numerical functions, the required values at the midway points must be obtained with interpolation formulae. For the present method this situation may be treated by replacing values of P, R, F and Q at $y_{j+\frac{1}{2}}$ and $y_{j-\frac{1}{2}}$ when they appear in the development leading to equations (3.13), by the first three terms of equation (3.1); this procedure leads to an alternative form of equations (3.13) which is ,

$$A_j = -2 - \frac{h}{4}(P_{j+1}^{**} - P_{j-1}^{**}) + \frac{3h^2}{32} (R_{j+1}^{**} + 6R_j^{**} + R_{j-1}^{**})$$
$$- \frac{3h^2}{16k} (Q_{j+1}^{**} + 6Q_j^{**} + Q_{j-1}^{**}) \; , \tag{3-16a}$$

$$B_j = 1 + \frac{h}{16} (3P_{j+1}^{**} + 6P_j^{**} - P_{j-1}^{**}) + \frac{h^2}{64} (5R_{j+1}^{**} + 6R_j^{**} - 3R_{j-1}^{**})$$
$$- \frac{h^2}{32k} (5Q_{j+1}^{**} + 6Q_j^{**} - 3Q_{j-1}^{**}) \; , \tag{3-16b}$$

$$C_j = 1 + \frac{h}{16} (P_{j+1}^{**} - 6P_j^{**} - 3P_{j-1}^{**}) - \frac{h^2}{64} (3R_{j+1}^{**} - 6R_j^{**} - 5R_{j-1}^{**})$$
$$+ \frac{h^2}{32k} (3Q_{j+1}^{**} - 6Q_j^{**} - 5Q_{j-1}^{**}), \tag{3-16c}$$

$$D_j = -\frac{h^2}{4}(F^{**}_{j+1} + 6F^{**}_j + F^{**}_{j-1}) - u^*_j\Big[-2 - \frac{h}{4}(P^{**}_{j+1} - P^{**}_{j-1})$$

$$+ \frac{3h^2}{32}(R^{**}_{j+1} - 6R^{**}_j + R^{**}_{j-1}) + \frac{3h^2}{16k}(Q^{**}_{j+1} + 6Q^{**}_j + Q^{**}_{j-1})\Big]$$

$$- u^*_{j+1}\Big[1 + \frac{h}{16}(3P^{**}_{j+1} + 6P^{**}_j - P^{**}_{j-1}) + \frac{h^2}{64}(5R^{**}_{j+1} + 6R^{**}_j - 3R^{**}_{j-1})$$

$$+ \frac{h^2}{32k}(5Q^{**}_{j+1} + 6Q^{**}_j - 3Q^{**}_{j-1})\Big] - u^*_{j-1}\Big[1 + \frac{h}{16}(P^{**}_{j+1} - 6P^{**}_j - 3P^{**}_{j-1})$$

$$- \frac{h^2}{64}(3R^{**}_{j+1} - 6R^{**}_j - 5R^{**}_{j-1}) - \frac{h^2}{32k}(3Q^{**}_{j+1} - 6Q^{**}_j - 5Q^{**}_{j-1})\Big]. \qquad (3.16d)$$

Note that the functions in equations (3.16) evaluated at x^{**} may be evaluated at the points in the current and previous time plane through use of the simple average. For example,

$$P^{**}_j = \frac{1}{2}(P_j + P^*_j) \quad . \qquad (3.17)$$

3.2 Method II (Slant Scheme)

An alternative approach to method I may be considered where the approximation of the derivative in marching direction is modified. The basis of the method II is to approximate the differential equation at the point $x = x^{**}$ and $y = y_j$ which is the same location as for the Crank-Nicolson method. A central difference approximation along the line $y = y_j$ is used for the x derivative as in the Crank-Nicolson method; the new feature is that the operator L(u) is averaged along a diagonal line intersecting the midpoints of the mesh at x^* and x as illustrated in figure (3.1). This procedure results in the two approximations,

$$Q_j^{**}\left[\frac{u_j-u_j^*}{k}\right] = 1/2\left[L(u)\Big|_{j+\frac{1}{2}}^{*} + L(u)\Big|_{j-\frac{1}{2}}\right], \tag{3.18a}$$

and

$$Q_j^{**}\left[\frac{u_j-u_j^*}{k}\right] = 1/2\left[L(u)\Big|_{j-\frac{1}{2}}^{*} + L(u)\Big|_{j+\frac{1}{2}}\right], \tag{3.18b}$$

where the omitted error terms are $O(h^2,k^2)$. Equations (3.18a) and (3.18b) are now combined into a single equation

$$2Q_j^{**}\left[\frac{u_j-u_j^*}{k}\right] = \tfrac{1}{2}\left[L(u)\Big|_{j+\frac{1}{2}}^{*} + L(u)\Big|_{j-\frac{1}{2}}^{*} + L(u)\Big|_{j+\frac{1}{2}} + L(u)\Big|_{j-\frac{1}{2}}\right]. \tag{3.19}$$

Finite difference approximations in the spatial direction are used which are identical to method I of the previous section. The approximation in the marching direction is simpler and potentially more accurate since no errors in the spatial direction are incurred.

Writing equation (3.19) in finite difference form, the following tridiagonal problem is obtained,

$$A_j u_j + B_j u_{j+1} + C_j u_{j-1} = D_j + h^2 E_j\ , \tag{3.20}$$

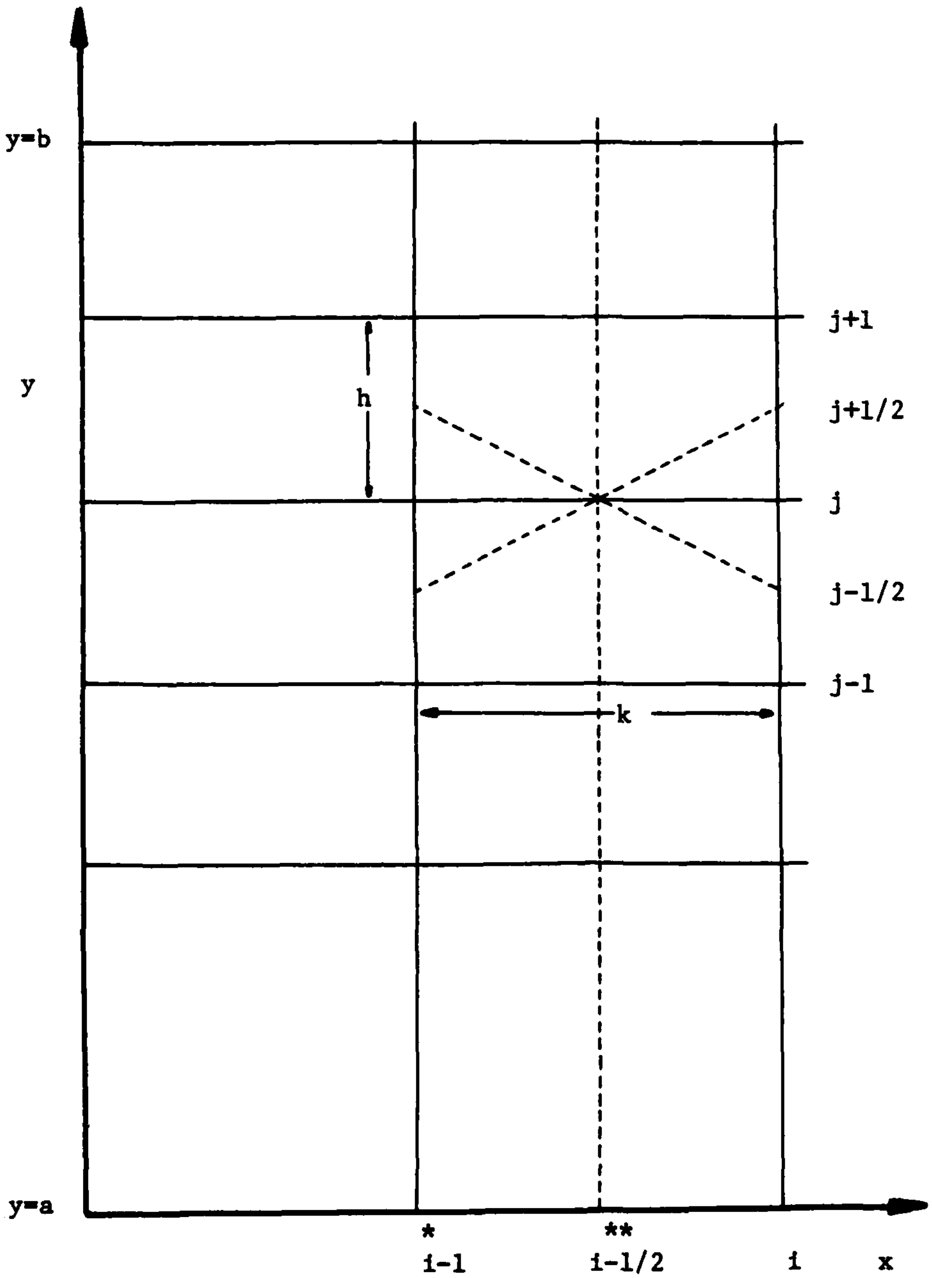

Figure 3.1. Grid configuration for the Slant Scheme(method II).

where,

$$A_j = -2 - \frac{h}{2}(P^{**}_{j+\frac{1}{2}} - P^{**}_{j-\frac{1}{2}}) + \frac{3h^2}{8}(R^{**}_{j+\frac{1}{2}} + R^{**}_{j-\frac{1}{2}}) - \frac{2h^2}{k} Q^{**}_j, \tag{3.21a}$$

$$B_j = 1 + \frac{h}{2} P^{**}_{j+\frac{1}{2}} + \frac{h^2}{16}(3R^{**}_{j+\frac{1}{2}} - R^{**}_{j-\frac{1}{2}}), \tag{3.21b}$$

$$C_j = 1 - \frac{h}{2} P^{**}_{j-\frac{1}{2}} - \frac{h^2}{16}(R^{**}_{j+\frac{1}{2}} - 3R^{**}_{j-\frac{1}{2}}), \tag{3.21c}$$

$$\begin{aligned} D_j = &- h^2 (F^{**}_{j+\frac{1}{2}} + F^{**}_{j-\frac{1}{2}}) \\ &-u^*_j\left[-2 - \frac{h}{2}(P^{**}_{j+\frac{1}{2}} - P^{**}_{j-\frac{1}{2}}) + \frac{3h^2}{8}(R^{**}_{j+\frac{1}{2}} + R^{**}_{j-\frac{1}{2}}) + \frac{2h^2}{k} Q^{**}_j\right] \\ &-u^*_{j+1}\left[1 + \frac{h}{2} P^{**}_{j+\frac{1}{2}} + \frac{h^2}{16}(3R^{**}_{j+\frac{1}{2}} - R^{**}_{j-\frac{1}{2}})\right] \\ &-u^*_{j-1}\left[1 - \frac{h}{2} P^{**}_{j-\frac{1}{2}} - \frac{h^2}{16}(R^{**}_{j+\frac{1}{2}} - 3R^{**}_{j-\frac{1}{2}})\right]. \end{aligned} \tag{3.21d}$$

It may be shown through the use of Taylor series expansions, that the leading truncation error terms in equation (3.20) related to derivatives of u at the point (x^{**}, y_j) is,

$$\begin{aligned} E_j = &\frac{h^2 Q^{**}_j}{8} \frac{\partial^3 u}{\partial y^2 \partial x}\bigg|^{**}_j + \frac{k^2}{8}\left(\frac{\partial^2 Q}{\partial x^2}\frac{\partial u}{\partial x} + 2\frac{\partial Q}{\partial x}\frac{\partial^2 u}{\partial x^2}\right)\bigg|^{**}_j + \ldots + \frac{k^2 Q^{**}_j}{12}\frac{\partial^3 u}{\partial x^3}\bigg|^{**}_j \\ &+ \frac{h^2}{8}\left(\frac{\partial^2 Q}{\partial y^2}\frac{\partial u}{\partial x} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial x^2} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial y \partial x}\right)\bigg|^{**}_j + \ldots - \frac{h^2}{24}\frac{\partial^4 u}{\partial y^4}\bigg|^{**}_j \\ &+ \frac{h^2}{24}(\mu_y P^{**}_j)\frac{\partial^3 u}{\partial y^3}\bigg|^{**}_j + \frac{h^3}{32}(\delta_y R^{**}_j)\frac{\partial^3 u}{\partial y^3}\bigg|^{**}_j. \end{aligned} \tag{3.22}$$

A second form of the truncation error is in terms of central difference operators according to,

$$E_j = \frac{Q_j^{**}}{8k}\mu_x\delta_x(\delta_y^2 u_j^{**}) + \frac{1}{8k}(\delta_y^2 Q_j^{**})(\mu_x\delta_x u_j^{**}) + \frac{h}{8k^2}(\mu_y\delta_y u_j^{**})(\delta_x^2 u_j^{**})$$

$$+ \frac{1}{8k}(\mu_y\delta_y Q_j^{**})(\mu_y\delta_y(\mu_x\delta_x u_j^{**}))$$

$$+ \frac{Q_j^{**}}{12k}\mu_x\delta_x^3 u_j^{**} + \frac{1}{8k}\{(\delta_x^2 Q_j^{**})(\mu_x\delta_x u_j^{**}) + 2(\mu_x\delta_x Q_j^{**})(\delta^2{}_x u_j^{**})\}$$

$$- \frac{1}{24h^2}\delta_y^4 u_j^{**} + \dots + \frac{1}{24h}(\mu_y P_j^{**})\mu_y\delta_y^3 u_j^{**} + \dots + \frac{1}{32}(\delta_y R_j^{**})\mu_y\delta_y^3 u_j^{**}. \tag{3.23}$$

Upon neglecting the leading truncation terms the tridiagonal problem in equation (3.20) may be readily solved directly.

In situations where P,R,F and Q are not analytic but numerical functions, the required values at the midway points must be obtained with interpolation formulae. For the present method this situation may be treated by replacing values of P,R,F and Q at $y_{j+\frac{1}{2}}$ and $y_{j-\frac{1}{2}}$ when they appear in the development leading to equations (3.21), by the first three terms of equation (3.1); this procedure leads to an alternative form of equations (3.21) which is,

$$A_j = -2 - \frac{h}{4}(P_{j+1}^{**} - P_{j-1}^{**}) + \frac{3h^2}{32}(R_{j+1}^{**} + 6R_j^{**} + R_{j-1}^{**}) - \frac{2h^2}{k}Q_j^{**}, \tag{3.24a}$$

$$B_j = 1 + \frac{h}{16}(3P^{**}_{j+1}+6P^{**}_j-P^{**}_j) + \frac{h^2}{64}(5R^{**}_{j+1}+6R^{**}_j-3R^{**}_{j-1}), \quad (3.24b)$$

$$C_j = 1 + \frac{h}{16}(P^{**}_{j+1}-6P^{**}_j-3P^{**}_{j-1}) - \frac{h^2}{64}(3R^{**}_{j+1}-6R^{*}_j-5R^{**}_{j-1}), \quad (3.24c)$$

$$\begin{aligned} D_j = &- \frac{h^2}{4}(F^{**}_{j+1} + 6F^{**}_j + F^{**}_{j-1}) \\ &-u^*_j\left[(-2- \frac{h}{4}(P^{**}_{j+1}-P^{**}_{j-1}) + \frac{3h^2}{32}(R^{**}_{j+1}-6R^{**}_j+R^{**}_{j-1}) + \frac{2h^2}{k} Q^{**}_j\right] \\ &-u^*_{j+1}\left[1 + \frac{h}{16}(3P^{**}_{j+1}+6P^{**}_j-P^{**}_{j-1}) + \frac{h^2}{64}(5R^{**}_{j+1}+6R^{**}_j-3R^{**}_{j-1})\right] \\ &-u^*_{j-1}\left[1 + \frac{h}{16}(P^{**}_{j+1}-6P^{**}_j-3P^{**}_{j-1}) - \frac{h^2}{64}(3R^{**}_{j+1}-6R^{**}_j-5R^{**}_{j-1})\right]. \end{aligned}$$

$$(3.24d)$$

Again equation (3.17) may be used to relate values of P, Q, R, F at x^{**} to values at x and x^*.

The truncation errors associated with both improved methods are compared in table (3.1) and (3.2). In table (3.1) the truncation errors which originate from approximations in the marching direction are compared; such errors are considered to be those containing partial derivatives with respect to x. It may be observed that for method I the first group of error terms is identical to the corresponding term of the method II. The second group of error terms for method I appear to be smaller than for method II because method II contains an additional term of $O(h^2)$.

METHOD I	$\frac{k^2 Q_j^{**}}{12} \frac{\partial^3 u}{\partial x^3}\Big\|_j^{**} + \frac{k^2}{8}\left(\frac{\partial^2 Q}{\partial x^2}\frac{\partial u}{\partial x} + 2\frac{\partial Q}{\partial x}\frac{\partial^2 u}{\partial x^2}\right)\Big\|_j^{**}$	$+ \frac{h^2}{8}\left(\frac{\partial^2 Q}{\partial y^2}\frac{\partial u}{\partial x} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial x^2} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial x^2}\right)\Big\|_j^{**}$
METHOD II	$\frac{k^2 Q_j^{**}}{12} \frac{\partial^3 u}{\partial x^3}\Big\|_j^{**} + \frac{k^2}{8}\left(\frac{\partial^2 Q}{\partial x^2}\frac{\partial u}{\partial x} + 2\frac{\partial Q}{\partial x}\frac{\partial^2 u}{\partial x^2}\right)\Big\|_j^{**}$	$+ \frac{h^2 Q_j^{**}}{8}\frac{\partial^3 u}{\partial y^2 \partial x}\Big\|_j^{**} + \frac{h^2}{8}\left(\frac{\partial^2 Q}{\partial y^2}\frac{\partial u}{\partial x} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial x^2} + \frac{\partial Q}{\partial y}\frac{\partial^2 u}{\partial x^2}\right)\Big\|_j^{**}$

Table 3.1. Comparison of the leading error terms arising from the approximations in the marching direction for Method I and Method II.

METHOD I	$-\frac{h^2}{24}\frac{\partial^4 u}{\partial y^4}\Big\|_j^{**} + \ldots$	$+\frac{h^2}{24}(\mu_y P_j^{**})\frac{\partial^3 u}{\partial y^3}\Big\|_j^{**} + \ldots$	$+\frac{h^3}{32}(\delta_y R_j^{**})\frac{\partial^3 u}{\partial y^3}\Big\|_j^{**}$
METHOD II	$-\frac{h^2}{24}\frac{\partial^4 u}{\partial y^4}\Big\|_j^{**} + \ldots$	$+\frac{h^2}{24}(\mu_y P_j^{**})\frac{\partial^3 u}{\partial y^3}\Big\|_j^{**} + \ldots$	$+\frac{h^2}{32}(\delta_y R_j^{**})\frac{\partial^3 u}{\partial y^3}\Big\|_j^{**}$

Table 3.2. Comparison of the leading error terms arising from the approximations in the spatial direction for Method I and Method II.

The leading order terms arising from the approximation in the spatial direction are listed in table (3.2); these same error terms arise in the approximation of the two-point boundary value problem

$$\frac{d^2u}{dy^2} + P(y)\frac{du}{dy} + R(y)u + F(y) = 0,$$

$$u(a) = A, \quad u(b) = B \quad . \qquad (3.25)$$

This problem has been considered by Walker and Weigand (1979). Since both method I and method II use the same scheme in the spatial direction approximations, the spatial error terms are identical.

It is also of interest to compare the error of the present methods to that associated with the Crank-Nicolson and Keller methods. First consider the error associated with approximations in the marching direction. Referring to table (2.1) and (3.1), the first group of error terms for all four methods may be observed to be identical. The improved methods and the Keller Box Scheme have an additional second group of error terms not present in the Crank-Nicolson method. For this reason, the Crank-Nicolson method appears to have some advantage over the improved methods in regard to the accuracy of the approximation in the marching direction. Note also for improved Method I that if Q term is a constant the second group error terms associated with method I will vanish; however, method II and the Keller's method will still contain a term $O(\hbar^2)$; note that the sign of this remaining term is of opposite sign in method II and the Keller method.

In regard to the approximation in the spatial direction Walker and Weigand (1979) have shown that the improved technique is more accurate than the existing methods. Note that in table (2.2) and (3.2) the first and second terms of the improved methods are one-half and a quarter, respectively, of the corresponding terms for the classical method. In comparison to the Keller Box method, the first two terms are identical; however, the third term in Keller's method is an order of magnitude larger than for the improved methods. For this reason, it is expected that the improved methods will, in general, produce more accurate results than either the Keller or classical method insofar as the approximation associated with spatial direction is concerned.

On the basis of the error terms listed in tables (2.1), (2.2), (3.1), and (3.2) as well as the results given by Walker and Weigand (1979) for two point boundary value problems, the improved methods appear to offer improved accuracy over the Keller (1970) method and possibly over the Crank-Nicolson method. However, the situation is complicated in the general case by the fact that, although a given method may have smaller individual error terms, it may not produce more accurate results on a specific problem. This is because in a particular problem, the error terms may combine through differences in sign between individual errors in each error term to produce a smaller overall error. For this reason it is important to consider a number of test cases and this is carried out in the next section.

4. LINEAR EXAMPLE PROBLEMS

4.1 Linear Examples

Three linear example problems are considered here to compare the accuracy of the four methods discussed in the previous two chapters; the three example problems are listed in table (4.1). For all four methods, the truncation terms were neglected and solutions were calculated with a uniform spatial mesh size, h, and uniform marching mesh size, k (the particular mesh values are listed in table 4.1). The exact solution for example 1 is not known, and to produce an 'exact' solution as a basis of comparison, example 1 was solved by the Crank-Nicolson method with a set of extremely small mesh sizes. The accuracy comparison for both examples 2 and 3 are based on the quoted exact solution in table (4.1).

4.2 Calculated Results

In figure (4.1), the root-mean square errors (defined as the square root of the sum of the squares of the error at each mesh point divided by the total number of mesh points at a given time station) for example 1, are plotted; method I and method II give better results than both existing methods as time increases. However, method II (the Slant Scheme) performed slightly better than method I. According to the error terms

	DIFFERENTIAL EQUATION	SOLUTION	MESH SIZE
1	$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + 2x \frac{\partial u}{\partial x} + 2u$ $u(0,t) = 1,\ u(\infty,t) = 0,\ u(x,0) = e^{-3x}$	——	$h = .05$ $k = .05$
2	$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r}$ $u(1,t)=1,\ \frac{\partial u(0,t)}{\partial r} = 0,\ u(r,0) = 0$	$u = \frac{1}{r}\sum_{n=0}^{\infty} (\mathrm{erfc}\,\frac{(2n+1)-r}{2\sqrt{t}}$ $- \mathrm{erfc}\,\frac{(2n+1)+r}{2\sqrt{t}})$ $u_c = \frac{1}{\sqrt{\pi t}} \sum_{n=0}^{\infty} e^{-(2n+1)^2/4t}$ *	$h = .05$ $k = .05$
3	$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$ $u(1,t) = 0,\ u(0,t) = 0,\ u(x,0)=\sin \pi x$	$u = \sum_{n=1}^{\infty} \sin n\pi x\ e^{-n^2\pi^2 t}$	$h = .1$ $k = .1$

Table 4.1 Differential equations, exact solutions and mesh sizes for the linear example problems.

*Here u_c denotes the center value $u(0,t)$.

given in chapter 3, method II appears to have an extra leading error term when compared to method I. In general, method II might be expected to under-perform method I; however, the situation is somewhat more complicated than this. It appears that the reason method II gave a more accurate solution in example 1 is that the error terms combine through differences in sign with the extra error term, namely, $\frac{h^2Q_j^{**}}{8} \left.\frac{\partial^3 u}{\partial y^2 \partial x}\right|_j^{**}$, to produce a smaller overall error.

In example 2 (refering to figure (4.2)) method II produces a better solution than the other methods; method I and Crank-Nicolson method are about even but both under-perform method II; again, the Keller Box scheme produces the least accurate results. Example 3 is a simple unsteady heat conduction equation; for this equation method II reduces to the Crank-Nicolson method. The root-mean-square error is computed and plotted on figure (4.3); the results for this problem shows that Crank-Nicolson method performs slightly better than both method I and Keller Box scheme.

For the three linear examples considered, both improved methods are always clearly superior to the Keller Box scheme. These results are generally representative of a number of other linear problems with various values of the mesh lengths which were considered but not reported here. Method II appears to give superior results but it appears that a general preference for Method II over either Method I or the Crank-Nicolson method is still not conclusively clear. In the next section, the various methods will be compared for some nonlinear problems.

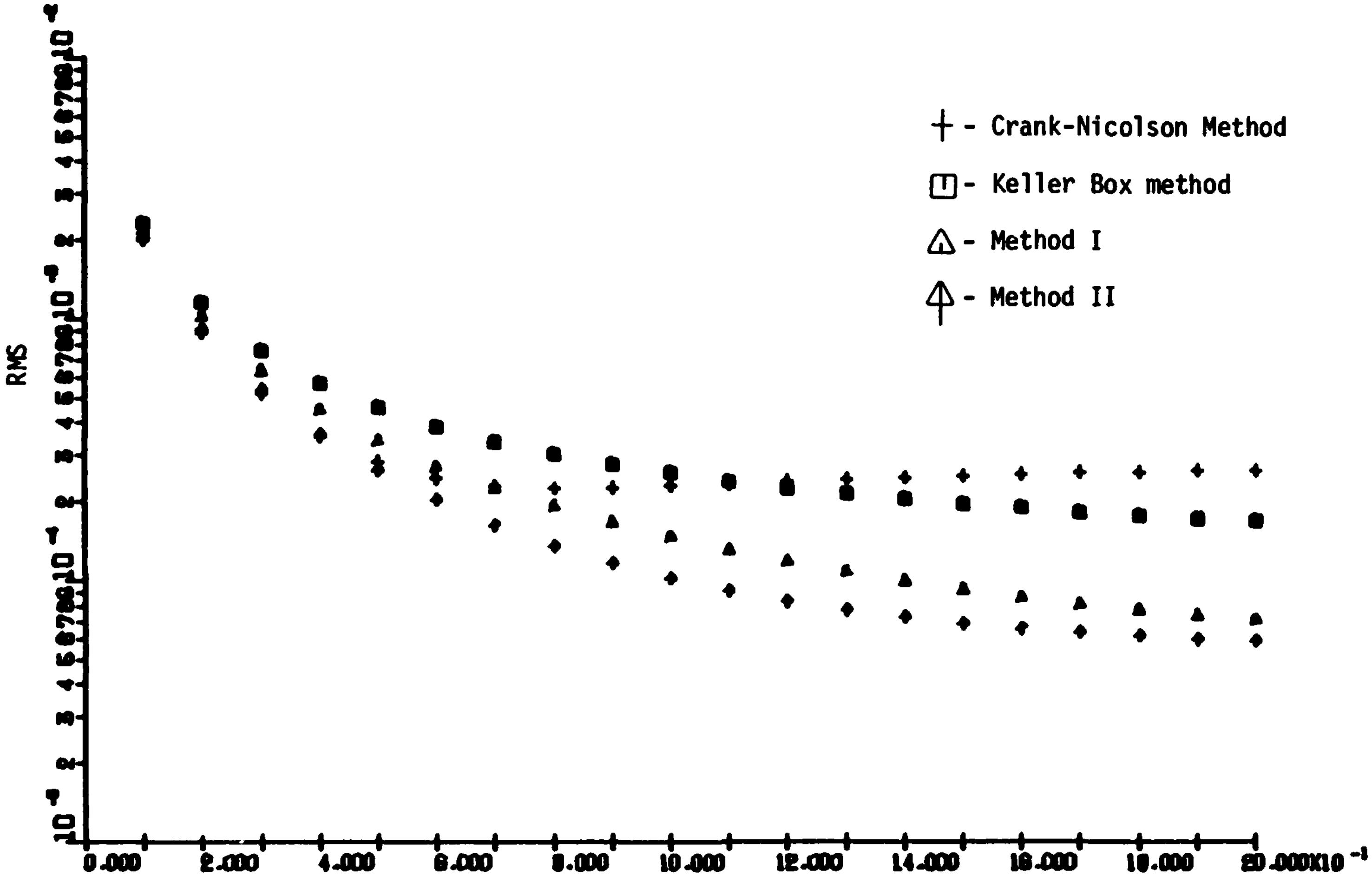

Figure 4.1. Comparison of RMS error for linear test problem 1.

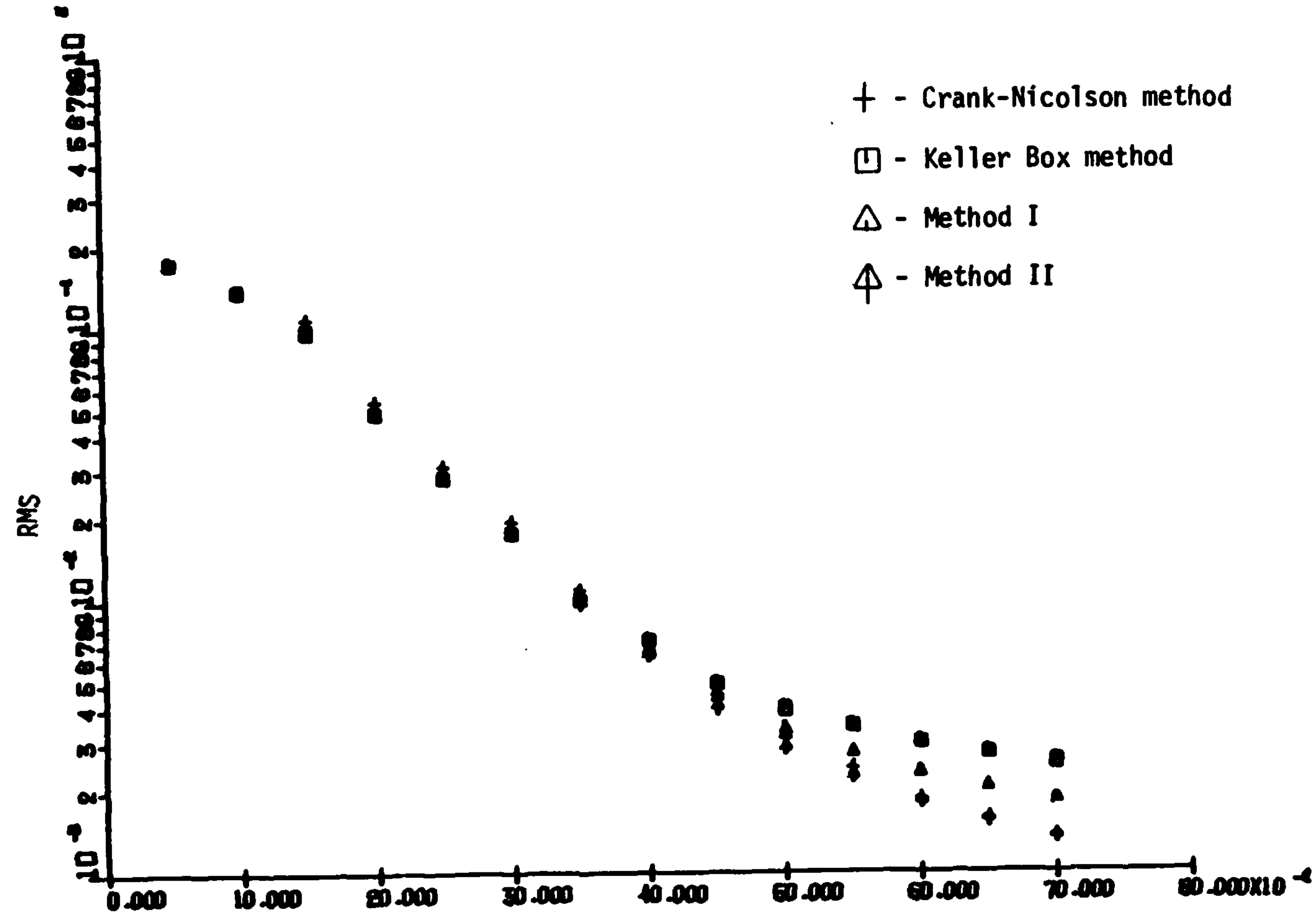

Figure 4.2. Comparison of RMS error for linear test problem 2.

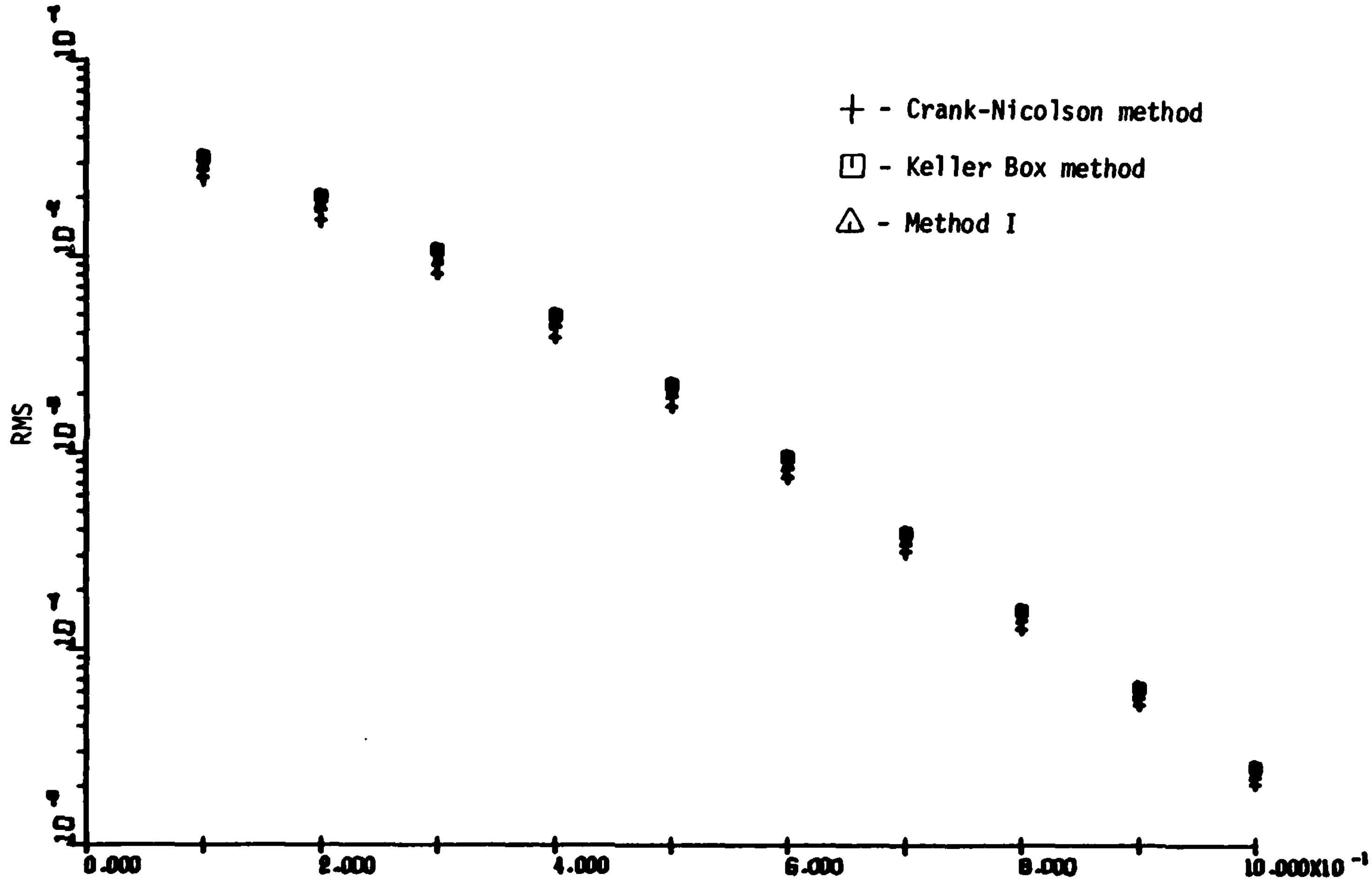

Figure 4.3. Comparison of RMS error for linear test problem 3.

5. NON-LINEAR PROBLEMS

5.1 Introduction

In this chapter the most common type of non-linear parabolic problem will be considered; this is the quasi-linear parabolic equation which is of the form of equation (2.1) but for which the coefficients Q,P,R and F also depend on u and $\partial u/\partial y$. For all of the four methods considered thus far, the method of approximating the non-linear differential equation is similar to the linear problem; the distinguishing feature from the linear case is that the finite difference equations are now non-linear. For this reason, the solution must be obtained iteratively at any x station; this is carried out by first estimating values of u at the current station to linearize the finite difference equations and thereby produce new estimates for u; these values are used to re-estimate the non-linear terms in the finite difference equations. This iterative process continues until convergence is obtained. Another common procedure for handling the non-linear difference equations is to use Newton linearization; this approach generally accelerates convergence of the iterative scheme at any x-station at the expense of increased algebraic complexity in deriving the difference equations.

The application of the new methods developed in this study to the non-linear type of problem is best illustrated by example. In the next two sections two non-linear example problems are considered and the performance of the methods compared.

5.2 The Howarth Boundary Layer Problem

The steady incompressible boundary layer equations for two-dimensional steady flow are (see for example, Schlichting, 1968, p. 121),

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = -\frac{dp}{dx} + \mu \frac{\partial^2 u}{\partial y^2} , \tag{5.1}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad . \tag{5.2}$$

It is convenient to introduce the Levy-Lees variables ξ,η (see for example, Blottner, 1975) given by

$$d\xi = \mu\rho U dx , \tag{5.3}$$

$$d\eta = \rho U (2\xi)^{-\frac{1}{2}} dy , \tag{5.4}$$

and a stream function

$$\psi = \sqrt{2\xi}\; f(\xi,\eta) \quad . \tag{5.5}$$

Here U is the mainstream velocity outside the boundary layer and ρ,μ are the fluid density and absolute viscosity. Upon substitution of these transformations equations (5.1) become,

$$\frac{\partial^3 f}{\partial \eta^3} + f \frac{\partial^2 f}{\partial \eta^2} + \beta\left[1 - \left(\frac{\partial f}{\partial \eta}\right)^2\right] = 2\xi\left[\frac{\partial f}{\partial \eta}\frac{\partial^2 f}{\partial \xi \partial \eta} - \frac{\partial^2 f}{\partial \eta^2}\frac{\partial f}{\partial \xi}\right] , \tag{5.6}$$

where the function $\beta(\xi) = \frac{2\xi}{U}\frac{dU}{d\xi}$ describes the pressure variation in the mainstream flow outside the boundary layer. The boundary conditions are,

$$f(\xi,0) = \left.\frac{\partial f}{\partial \eta}\right|_{\xi,0} = 0 \ , \quad \left.\frac{\partial f}{\partial \eta}\right|_{\xi,\infty} = 1, \tag{5.7}$$

which express the impermeable wall and no slip condition at the wall, in addition to the condition that the velocity approach the free stream velocity at the edge of the boundary layer.

In this section,the two improved methods are applied to the Howarth (1938) boundary-layer problem and the performance of the improved methods are compared with existing methods. This problem describes the development of a boundary layer in the presence of an adverse pressure gradient and is selected here as a particularly challenging test case. Historically this example flow also has been used previously by Keller and Cebeci (1971) and Blottner (1975) as a test case.

For the Howarth (1938) linearly retarded flow, the mainstream velocity distribution is,

$$U = 1 - \frac{x}{8} \ , \tag{5.8}$$

and in this case ,

$$\beta = \frac{\xi}{\xi - 4} \ . \tag{5.9}$$

It is convenient to rewrite equation (5.6) as a second order system of equations according to ,

$$2\xi u \frac{\partial u}{\partial \xi} = \frac{\partial^2 u}{\partial \eta^2} + (f + 2\xi \frac{\partial f}{\partial \xi}) \frac{\partial u}{\partial \eta} - \beta u^2 + \beta, \tag{5.10}$$

$$\frac{\partial f}{\partial \eta} = u,$$

with the boundary conditions,

$$f(\xi,0) = u(\xi,0) = 0 \ , \quad u(\xi,\infty) \to 1 \ . \tag{5.11}$$

In equation (5.10), ξ is the marching direction and η is the spatial direction. At $\xi \to 0$ equations (5.10) reduce to the ordinary differential equations,

$$\frac{d^2u}{d\eta^2} + f \frac{du}{d\eta} = 0 \ , \quad \frac{df}{d\eta} = u, \tag{5.12}$$

which is the Blasius equation describing the boundary layer flow on a semi-infinite flat plate; the numerical solution of this equation provides the initial condition for the equations (5.10).

For all four methods to be described here, a uniform mesh in the η direction was used with h being the mesh size. Let N-1 be the total number of internal mesh points in the boundary layer; the value of η, where the mainstream boundary conditions in equation (5.7) were applied as an approximation is denoted by $\ell = Nh$. In practice a value of $\ell = 8$ was found to be large enough to ensure no change in the solution. The systems of equations (5.10) and (5.12) are non-linear; at any stage in an iterative procedure at each ξ station, once an estimate of u is available, the second of equations (5.10) or (5.12) was integrated using a trapezoidal calculation according to

$$f_j = f_{j-1} + \frac{h}{2}(u_j + u_{j-1}), \qquad (5.13)$$

for $j = 1,2,3,\ldots,N$. The differences in the four methods described here are associated with the approximations to the first of equations (5.10) and (5.12) and these will now be described.

Crank-Nicolson Method

In this method, to calculate the initial profile, central difference approximations at each internal mesh point $\eta_j = jh$ are made; this classical technique (Walker and Weigand, 1979) leads to the tridiagonal matrix problem,

$$B_j\, u_{j+1} + A_j\, u_j + C_j\, u_{j-1} = D_j\ , \qquad (5.14)$$

where

$$A_j = -2,\ B_j = 1 + \frac{h}{2} f_j,\ C_j = 1 - \frac{h}{2} f_j,\ D_j = 0\ . \qquad (5.15)$$

In equations (5.15), the f_j are evaluated either from an initial guess or from a previous iterate. At any stage the tridiagonal problem for u in equation (5.14) is solved by the Thomas algorithm and the f_j are then obtained from equation (5.13). The iteration was continued until two successive iterates agreed to within five significant figures at each internal mesh point. After a converged solution is obtained at $\xi = 0$, the marching procedure may be initiated to advance the solution to $\xi = k$ and thence to $\xi = ik$, $i = 2,3,4...$; here k denotes the marching step.

The first of equations (5.10) is approximated at $\xi=\xi^{**}=\xi_{i-1} + k/2$ and at $\eta = \eta_j$; using the approximations described in section (2.1), the first of equations (5.10) may be written in finite difference form as a tridiagonal problem of the form (5.14) where now,

$$B_j = 1 + \frac{h}{4}(f_j+f_j^*) + \frac{h}{k}\xi^{**}(f_j-f_j^*) , \tag{5.16a}$$

$$C_j = 1 - \frac{h}{4}(f_j+f_j^*) - \frac{h}{k}\xi^{**}(f_j-f_j^*) , \tag{5.16b}$$

$$A_j = -2 - \frac{h^2}{2}\beta^{**}(u_j+u_j^*) - \frac{2h^2}{k}\xi^{**}u_j , \tag{5.16c}$$

$$\begin{aligned} D_j = &-u_{j+1}^*\left[1 + \frac{h}{4}(f_j+f_j^*) + \frac{h}{k}\beta^{**}(f_j-f_j^*)\right] \\ &- u_j^*\left[-2 - \frac{h^2}{2}\beta^{**}u_j^* + \frac{2h^2}{k}\xi^{**}u_j^*\right] \\ &- u_{j-1}^*\left[1 - \frac{h}{4}(f_j+f_j^*) - \frac{h}{k}\xi^{**}(f_j-f_j^*)\right] -2h^2\beta^{**}. \end{aligned} \tag{5.16d}$$

Here the u_j and f_j (on the right sides of equations (5.16)) are evaluated initially from the solution at the previous step or from the last iterate, as the iteration procedes at each ξ station.

The iteration method just described is relatively slow and the rate of convergence can be enhanced by using a standard procedure of Newton linearization which is described in Appendix IV. This is merely an alternate form of the difference equations associated with the Crank-Nicolson method which may be written (after some algebra) in the form,

$$A_j u_j + B_j u_{j+1} + C_j u_{j-1} + G_j f_j + H_j f_{j+1} + M_j f_{j-1} = D_j, \tag{5.17}$$

where,

$$B_j = \frac{1}{2} + \frac{h}{8} f_j + \frac{h}{8} f_j^* + \frac{h}{2k} \xi^{**} f_j - \frac{h}{2k} \xi^{**} f_j^* , \tag{5.18a}$$

$$A_j = -1 - \frac{h^2}{2} \beta^{**} u_j - \frac{h^2}{2} \beta^{**} u_j^* - \frac{2h^2}{k} \xi^{**} u_j , \tag{5.18b}$$

$$C_j = \frac{1}{2} - \frac{h}{8} f_j - \frac{h}{8} f_j^* - \frac{h}{2k} \xi^{**} f_j + \frac{h}{2k} \xi^{**} f_j^* , \tag{5.18c}$$

$$G_j = \frac{h}{8} u_{j+1} + \frac{h}{2k} \xi^{**} u_{j+1} - \frac{h}{8} u_{j-1} - \frac{h}{2k} \xi^{**} u_{j-1} \tag{5.18d}$$

$$+ \frac{h}{8} u_{j+1}^* + \frac{h}{2k} \xi^{**} u_{j+1}^* - \frac{h}{8} u_{j-1}^* - \frac{h}{2k} \xi^{**} u_{j-1}^* ,$$

$$H_j = 0 , \tag{5.18e}$$

$$M_j = 0 \ , \tag{5.18f}$$

$$\begin{aligned} D_j = {} & u_{j+1} f_j \left(\frac{h}{8} + \frac{h}{2k}\, \xi^{**}\right) - u_{j-1} f_j \left(- \frac{h}{8} + \frac{h}{2k}\, \xi^{**}\right) \\ & - u_j^2 \left(\frac{h^2}{4}\, \beta^{**} + \frac{h^2}{k}\, \xi^{**}\right) - u_j^* \left(-1 - \frac{h^2}{4}\, \beta^{**} u_j^* + \frac{h^2}{k}\, \xi^{**} u_j^*\right) \\ & - u_{j+1}^* \left(\frac{1}{2} + \frac{h}{8}\, f_j^* - \frac{h}{2k}\, \xi^{**} f_j^*\right) - u_{j-1}^* \left(- \frac{1}{2} - \frac{h}{8} f_j^* + \frac{h}{2k}\, \xi^{**} f_j^*\right) \\ & - \beta^{**} h^2 \ . \end{aligned} \tag{5.18g}$$

Again u_{j-1}, u_j, u_{j+1} and f_{j-1}, f_j, f_{j-1} are evaluated from the previous iterate at any ξ station. Equation (5.17) then can be solved by an elimination method described by Ackerberg and Phillips (1972) which is given in Appendix III. Iteration at each ξ station procedes as previously described and convergence is decided by the same criterion; typically the number of iterations was reduced from 8-9 at each ξ station to 3-4 with the Newton linearization.

Keller Box Scheme

This method was originally described by Keller (1970) and later applied by Keller and Cebeci (1971) to the solution of boundary-layer flow problems. To implement the method, equations (5.12) and (5.10) are rewritten as a system of first order differential equations according to,

$$\frac{df}{d\eta} = u \ , \quad \frac{du}{d\eta} = v \ , \quad \frac{df}{d\eta} = -fv \ , \tag{5.19}$$

and

$$\frac{\partial f}{\partial \eta} = u \ , \quad \frac{\partial u}{\partial \eta} = v \ , \tag{5.20}$$

$$\frac{\partial v}{\partial \eta} = -(f + 2\xi \frac{\partial f}{\partial \xi})\ v + 2\xi u \frac{\partial u}{\partial \xi} - \beta u^2 + \beta \ .$$

To compute the initial profile, equations (5.19) are approximated at points $\eta_{j+\frac{1}{2}}$ and $\eta_{j-\frac{1}{2}}$ on either side of the typical mesh point η_j as described by Walker and Weigand (1979); the two sets of approximations are then combined to form algebraic equations of the form of equation (5.14), where now,

$$A_j = -2 - \frac{h}{4}(f_{j+1} - f_{j-1}) \ , \tag{5.21a}$$

$$B_j = 1 + \frac{h}{4}(f_{j+1} + f_j) \ , \tag{5.21b}$$

$$C_j = 1 - \frac{h}{4}(f_j + f_{j-1}) \ , \tag{5.21c}$$

$$D_j = 0 \ . \tag{5.21d}$$

In equations (5.21), the f_j are evaluated either from an initial guess or from a previous iterate. At any stage the tridiagonal problem for u in equation (5.14) is solved by Thomas algorithm and the f_j are then obtained from equation (5.13). The iteration was continued until two successive iterates agreed to within five significant figures at each internal mesh point. After a converged solution is obtained at $\xi = 0$, the marching procedure may be initiated to advance the solution to $\xi = k$ and from there to $\xi = ik$, $i = 1,2,3,4,\ldots$; here k denotes the marching step.

For equation (5.20), the approximations are made at both $\eta = \eta_{j+\frac{1}{2}}$ and $\eta = \eta_{j-\frac{1}{2}}$ using the technique described in section (2.2). Using Newton linearization, it may be shown (after a considerable amount of algebra) that the last two of equations (5.20) may be written in the form of equation (5.17), where now,

$$A_j = (\frac{h^2}{4}\beta^{**} + \frac{h^2}{k}\xi^{**})(u_{j+1} + 2u_j + u_{j-1}) + \frac{h^2}{4}\beta^{**}(u^*_{j+1} + 2u^*_j + u^*_{j-1}) + (\frac{h}{4} + \frac{h}{k}\xi^{**})(f_{j+1}-f_{j-1}) + (\frac{h}{4} - \frac{h}{k}\xi^{**})(f^*_{j+1}-f^*_{j-1})+4, \tag{5.22a}$$

$$B_j = (\frac{h^2}{4}\beta^{**} + \frac{h^2}{k}\xi^{**})(u_j+u_{j+1}) + \frac{h^2}{4}\beta^{**}(u^*_j + u^*_{j+1}) -(\frac{h}{4} + \frac{h}{k}\xi^{**})(f_j+f_{j+1}) - (\frac{h}{4} - \frac{h}{k}\xi^{**})(f^*_j+f^*_{j+1})-2, \tag{5.22b}$$

$$C_j = (\frac{h^2}{4}\beta^{**} + \frac{h^2}{k}\xi^{**})(u_j+u_{j-1}) + \frac{h^2}{4}\beta^{**}(u^*_{j-1} + u^*_j) +(\frac{h}{4} + \frac{h}{k}\xi^{**})(f_j+f_{j-1}) + (\frac{h}{4} - \frac{h}{k}\xi^{**})(f^*_j+f^*_{j-1})-2, \tag{5.22c}$$

$$H_j = -(\frac{h}{4} + \frac{h}{k}\,\xi^{**})(u_{j+1} - u_j + u^*_{j+1} - u^*_j) \,, \qquad (5.22d)$$

$$G_j = -(\frac{h}{4} + \frac{h}{k}\,\xi^{**})(u_{j+1} - u_{j-1} + u^*_{j+1} - u^*_{j-1}) \,, \qquad (5.22e)$$

$$M_j = -(\frac{h}{4} + \frac{h}{k}\,\xi^{**})(u_j - u_{j-1} + u^*_j - u^*_{j-1}) \,, \qquad (5.22f)$$

$$\begin{aligned}
D_j = {} & 2(u^*_{j+1} - 2u^*_j + u^*_{j-1}) + 4h^2\beta^{**} \\
& -(\frac{h}{4} + \frac{h}{k}\,\xi^{**}) \Big[(f_j+f_{j-1})(u_j-u_{j-1}) + (f_{j+1}+f_j)(u_{j+1}-u_j)\Big] \\
& + (\frac{h}{4} - \frac{h}{k}\,\xi^{**}) \Big[(f^*_j+f^*_{j-1})(u^*_j-u^*_{j-1}) + (f^*_{j+1}+f^*_j)(u^*_{j+1}-u^*_j)\Big] \\
& + (\frac{h^2}{8}\,\beta^{**} + \frac{h^2}{2k}\,\xi^{**}) \Big[(u_j+u_{j-1})^2 + (u_{j+1} + u_j)^2\Big] \\
& -(\frac{h^2}{8}\,\beta^{**} - \frac{h^2}{2k}\,\xi^{**}) \Big[(u^*_j + u^*_{j-1})^2 + (u^*_j + u^*_{j+1})^2\Big] \,. \qquad (5.22g)
\end{aligned}$$

Equation (5.17) is readily solved by the Ackerberg and Phillips (1972) technique coupled with trapezoidal rule of integration given by equation (5.13). At each time step iteration is required and the calculation proceeds in the ξ direction in a manner similar to the Crank-Nicolson method.

Improved Method I

To compute the initial profile, equation (5.12) is approximated at points $\eta_{j+\frac{1}{2}}$ and $\eta_{j-\frac{1}{2}}$ on either side of the typical mesh point η_j as described by Walker and Weigand (1979); the two sets of approximation are then combined to form algebraic equations in the form of equation (5.14), where now,

$$A_j = -2 - \frac{h}{4}(f_{j+1} - f_{j-1}) , \quad (5.23a)$$

$$B_j = 1 + \frac{h}{16}(3f_{j+1} + 6f_j - f_{j-1}) , \quad (5.23b)$$

$$C_j = 1 + \frac{h}{16}(f_{j+1} - 6f_j - 3f_{j-1}) , \quad (5.23c)$$

$$D_j = 0 . \quad (5.23d)$$

In equations (5.23), the f_j are evaluated either from an initial guess or from a previous iterate. At any stage, the tridiagonal problem for u in equation (5.14) is solved by the Thomas Algorithm and the f_j are then obtained from equation (5.13). The iteration continued until two successive iterates agreed to within five significant figures at each internal mesh point. The calculation may then be advanced in the $+\xi$ direction as previously indicated for the other methods.

For equation (5.10), the approximations are made at both $\eta = \eta_{j+\frac{1}{2}}$ and $\eta = \eta_{j-\frac{1}{2}}$ using the technique described in section (3.1). Using Newton linearization, it may be shown (after a considerable amount of algebra) that the approximations to equation (5.10) can be written in the form of (5.17), where now,

$$A_j = -4+\left(-\frac{h}{4} + \frac{h}{k}\xi^{**}\right)(f^*_{j+1}-f^*_{j-1}) - \left(\frac{h}{4} + \frac{h}{k}\xi^{**}\right)(f_{j+1}-f_{j-1})$$

$$- \frac{3h^2}{16}\beta^{**}(u^*_{j+1} + u^*_{j-1} + 6u^*_j) - \left(\frac{3h^2}{16}\beta^{**} + \frac{3h^2}{4k}\xi^{**}\right)(u_{j+1}+u_{j-1})$$

$$- \left(\frac{9h^2}{8}\beta^{**} + \frac{9h^2}{2k}\xi^{**}\right)u_j \, , \tag{5.24a}$$

$$B_j = 2+\left(\frac{h}{4} - \frac{h}{k}\xi^{**}\right)\left(\frac{3}{4}f^*_{j+1} + \frac{3}{2}f^*_j - \frac{1}{4}f^*_{j-1}\right)$$

$$- \frac{h^2}{32}\beta^{**}(5u^*_{j+1} + 6u^*_j - 3u^*_{j-1})$$

$$+ \left(\frac{h}{4} + \frac{h}{k}\xi^{**}\right)\left(\frac{3}{2}f_j + \frac{3}{4}f_{j+1} - \frac{1}{4}f_{j-1}\right)$$

$$- \left(\frac{5h^2}{32}\beta^{**} + \frac{h^2}{8k}\xi^{**}\right)u_{j+1} + \left(\frac{3h^2}{32}\beta^{**} - \frac{h^2}{8k}\xi^{**}\right)u_{j-1}$$

$$- \left(\frac{3h^2}{16}\beta^{**} + \frac{3h^2}{4k}\xi^{**}\right)u_j \, , \tag{5.24b}$$

$$C_j = 2+\left(\frac{h}{4} - \frac{h}{k}\xi^{**}\right)\left(\frac{1}{4}f^*_{j+1} - \frac{3}{2}f^*_j - \frac{3}{4}f^*_{j-1}\right)$$

$$+ \frac{h^2}{32}\beta^{**}(3u^*_{j+1}-6u^*_j-5u^*_{j-1}) + \left(\frac{h}{4} + \frac{h}{k}\xi^{**}\right)\left(\frac{1}{4}f_{j+1} - \frac{3}{2}f_j - \frac{3}{4}f_{j-1}\right)$$

$$+ \left(\frac{3h^2}{32}\beta^{**} - \frac{h^2}{8k}\xi^{**}\right)u_{j+1} - \left(\frac{3h^2}{16}\beta^{**} + \frac{3h^2}{4k}\xi^{**}\right)u_j$$

$$- \left(\frac{5h^2}{32}\beta^{**} + \frac{h^2}{8k}\xi^{**}\right)u_{j-1} \, , \tag{5.24c}$$

$$G_j = \left(\frac{3h}{8} + \frac{3h}{2k}\xi^{**}\right)(u_{j+1} - u_{j-1} + u^*_{j+1} - u^*_{j-1}) \, , \tag{5.24d}$$

$$H_j = \left(\frac{h}{4} + \frac{h}{k}\xi^{**}\right)\left[\frac{3}{4}(u_{j+1}+u^*_{j+1})-(u_j+u^*_j) + \frac{1}{4}(u_{j-1}+u_{j-1}{}^*)\right], \tag{5.24e}$$

$$M_j = -\left(\frac{h}{4} + \frac{h}{k}\xi^{**}\right)\left[\frac{1}{4}(u_{j+1}+u^*_{j+1})-(u_j+u^*_j) + \frac{3}{4}(u_{j-1}+u^*_{j-1})\right], \tag{5.24f}$$

$$\begin{aligned} D_j = {} & 4u^*_j - 2u^*_{j+1} - 2u^*_{j-1} - 4h^2\beta^{**}+\left(\frac{h}{16} + \frac{h}{4k}\xi^{**}\right)\Big[-4u_j(f_{j+1} \\ & - f_{j-1})+u_{j+1}(3f_{j+1}+6f_j-f_{j-1}) + u_{j-1}(f_{j+1}-6f_j-3f_{j-1})\Big] \\ & + \left(\frac{h}{16} - \frac{h}{4k}\xi^{**}\right)\Big[4u^*_j(f^*_{j+1}-f^*_{j-1})-u^*_{j+1}(3f^*_{j+1}+6f^*_j-f^*_{j-1}) \\ & - u^*_{j-1}(f^*_{j+1}-6f^*_j-3f^*_{j-1})\Big] + \frac{h^2}{16}\beta^{**}\Big[3(u^*_j(u^*_{j+1}+u^*_{j-1}) \\ & - u_j(u_{j+1}+u_{j-1})) + \frac{3}{2}(u_{j-1}u_{j+1} - u^*_{j+1}u^*_{j-1}) \\ & + \frac{5}{4}(u^*_{j+1}u^*_{j+1} + u^*_{j-1}u^*_{j-1} - u^2_{j+1} - u^2_{j-1}) + 9(u^*_ju^*_j-u_j{}^2)\Big] \\ & - \frac{h^2}{16k}\xi^{**}\Big[(u_{j+1}+6u_j+u_{j-1})^2 + (u^*_{j+1}+6u^*_j+u^*_{j-1})^2\Big] . \end{aligned} \tag{5.24g}$$

Equation (5.17) is readily solved by the Ackerberg and Phillips (1972) technique coupled with the trapezoidal rule of integration given by equation (5.13). At each time step, iteration is required and the calculation proceeds in the ξ direction in a manner similar to the Crank-Nicolson method.

Improved Method II (Slant Scheme)

This is a similar but alternative approach to method I, with the basic difference being in the approximation made in the marching direction (as discussed in Chapter 3). For this method, the initial profile is computed with the identical finite difference approximation and computational procedure as method I. For equation (5.10), the approximations are made at both $\eta = \eta_{j+\frac{1}{2}}$ and $\eta = \eta_{j-\frac{1}{2}}$ using the technique described in section (3.2). Using Newton linearization, it may be shown that approximations to equation (5.10) are of the form of equation (5.17), where now,

$$A_j = -4 + \left(-\frac{h}{4} + \frac{h}{k}\xi^{**}\right)(f^*_{j+1} - f^*_{j-1}) - \left(\frac{h}{4} + \frac{h}{k}\xi^{**}\right)(f_{j+1} - f_{j-1})$$
$$- \frac{3h^2}{16}\beta^{**}(u^*_{j+1} + u^*_{j-1} + 6u^*_j) - \frac{3h^2}{16}\beta^{**}(u_{j+1} + u_{j-1})$$
$$- \left(\frac{9h^2}{8}\beta^{**} + \frac{8h^2}{k}\xi^{**}\right)u_j \,, \tag{5.25a}$$

$$B_j = 2 + \left(\frac{h}{4} - \frac{h}{k}\xi^{**}\right)\left(\frac{3}{4}f^*_{j+1} + \frac{3}{2}f^*_j - \frac{1}{4}f^*_{j-1}\right) - \frac{h^2}{32}\beta^{**}(5u^*_{j+1}$$
$$+ 6u^*_j - 3u^*_{j-1}) + \left(\frac{h}{4} + \frac{h}{4}\xi^{**}\right)\left(\frac{3}{2}f_j + \frac{3}{4}f_{j+1} - \frac{1}{4}f_{j-1}\right)$$
$$- \frac{5h^2}{32}\beta^{**}u_{j+1} - \frac{3h^2}{16}\xi^{**}u_j + \frac{3h^2}{32}\beta^{**}u_{j-1} \,, \tag{5.25b}$$

$$C_j = 2+\left(\frac{h}{4} - \frac{h}{k}\,\xi^{**}\right)\left(\frac{1}{4}\,f^*_{j+1} - \frac{3}{2}\,f^*_j - \frac{3}{4}\,f^*_{j-1}\right)$$

$$+ \frac{h^2}{32}\,\beta^{**}(3u^*_{j+1} - 6u^*_j - 5u^*_{j-1}) + \left(\frac{h}{4} + \frac{h}{k}\,\xi^{**}\right)\left(\frac{1}{4}\,f_{j+1} - \frac{3}{2}\,f_j\right.$$

$$\left.- \frac{3}{4}\,f_{j-1}\right) + \frac{3h^2}{32}\,\beta^{**}u_{j+1} - \frac{3h^2}{16}\,\beta^{**}u_j - \frac{5h^2}{32}\,\beta^{**}u_{j-1}\ , \tag{5.25c}$$

$$G_j = \left(\frac{3h}{8} + \frac{3h}{2k}\,\xi^{**}\right)(u_{j+1} - u_{j-1} + u^*_{j+1} - u^*_{j-1})\ , \tag{5.25d}$$

$$H_j = \left(\frac{h}{4} + \frac{h}{k}\,\xi^{**}\right)\left[\frac{3}{4}(u_{j+1}+u^*_{j+1})-(u_j+u^*_j)+\frac{1}{4}(u_{j-1}+u^*_{j-1})\right]\ , \tag{5.25e}$$

$$M_j = -\left(\frac{h}{4} + \frac{h}{k}\,\xi^{**}\right)\left[\frac{1}{4}(u_{j+1}+u^*_{j+1})-(u_j+u^*_j) + \frac{3}{4}(u_{j-1}+u^*_{j-1})\right]\ , \tag{5.25f}$$

$$D_j = 4u^*_j - 2u^*_{j+1} - 2u^*_{j-1} - 4h^2\beta^{**} + \left(\frac{h}{16} + \frac{h}{4k}\,\xi^{**}\right)\left[-4u_j(f_{j+1}\right.$$

$$\left.- f_{j-1})+u_{j+1}(3f_{j+1}+6f_j-f_{j-1})+u_{j-1}(f_{j+1}-6f_j-3f_{j-1})\right]$$

$$+ \left(\frac{h}{16} - \frac{h}{4k}\,\xi^{**}\right)\left[4u^*_j(f^*_{j+1}-f^*_{j-1})-u^*_{j+1}(3f^*_{j+1}+6f^*_j-f^*_{j-1})\right.$$

$$\left.-u^*_{j-1}(f^*_{j+1}-6f^*_j-3f_{j-1})\right] + \frac{h^2}{16}\,\beta^{**}\left[3(u^*_j(u^*_{j+1}+u^*_{j-1})\right.$$

$$-u_j(u_{j+1}+u_{j-1})) + \frac{3}{2}(u_{j-1}u_{j+1}-u^*_{j+1}u^*_{j-1}) + \frac{5}{4}(u^*_{j+1}u^*_{j+1}$$

$$\left.+ u^*_{j-1}u^*_{j-1}-u^2_{j+1}-u^2_{j-1})+9(u^*_ju^*_j-u_j{}^2)\right] - \frac{4h^2}{k}\,\xi^{**}(u^2_j+u^*_ju^*_j)\ . \tag{5.25g}$$

The computational and marching procedure is carried out in the same manner as method I.

5.3 Calculated Results for the Howarth Flow

The results of the calculations of the incompressible boundary layer equation for the Howarth flow are described in this section for all four schemes. There is no known analytical solution to the problem and in order to produce an 'exact' solution, as a basis of comparison, equations (5.12) and (5.10) were solved by using very fine mesh sizes in the η direction and a decreasing non-uniform mesh in ξ direction until five significant figures of accuracy were obtained. The mesh size, h, in the η direction is uniform throughout; however, a non-uniform mesh size, k, is used in ξ direction; in particular, k is uniform and equal to k_0, say, from $\xi = 0$ to $\xi = .8$; from $\xi = .8$ to $\xi = .85$, k is reduced by a quarter; between $\xi = .85$ and $\xi = .9$, k is reduced by half.

The root mean square error (defined as the square root of the sum of the squares of the error at each mesh point divided by total number of mesh points for a given ξ station) for the four methods were computed for various mesh sizes, this RMS error is summarized in table (5.1), and the results are plotted on figures (5.1). According to the results for this test problem, the improved schemes produced more accurate results than either the Keller Box Scheme or the Crank-Nicolson method; note that the Keller Box Scheme performs better than the Crank-Nicolson method for this problem. Referring to figures (5.1),

MESH SIZE h	k_o	NUMBER OF GRID POINTS IN η DIRECTION	NUMBER OF GRID POINTS IN ξ DIRECTION	CORRESPONDING FIGURE
.05	.025	161	45	5-1a
.1	.05	81	23	5-1b
.2	.1	41	12	5-1c

Table 5.1. Mesh sizes and related number of grid points (k_o is the initial mesh size in the ξ direction which decreases as $\xi \rightarrow 0.9$; see text for details).

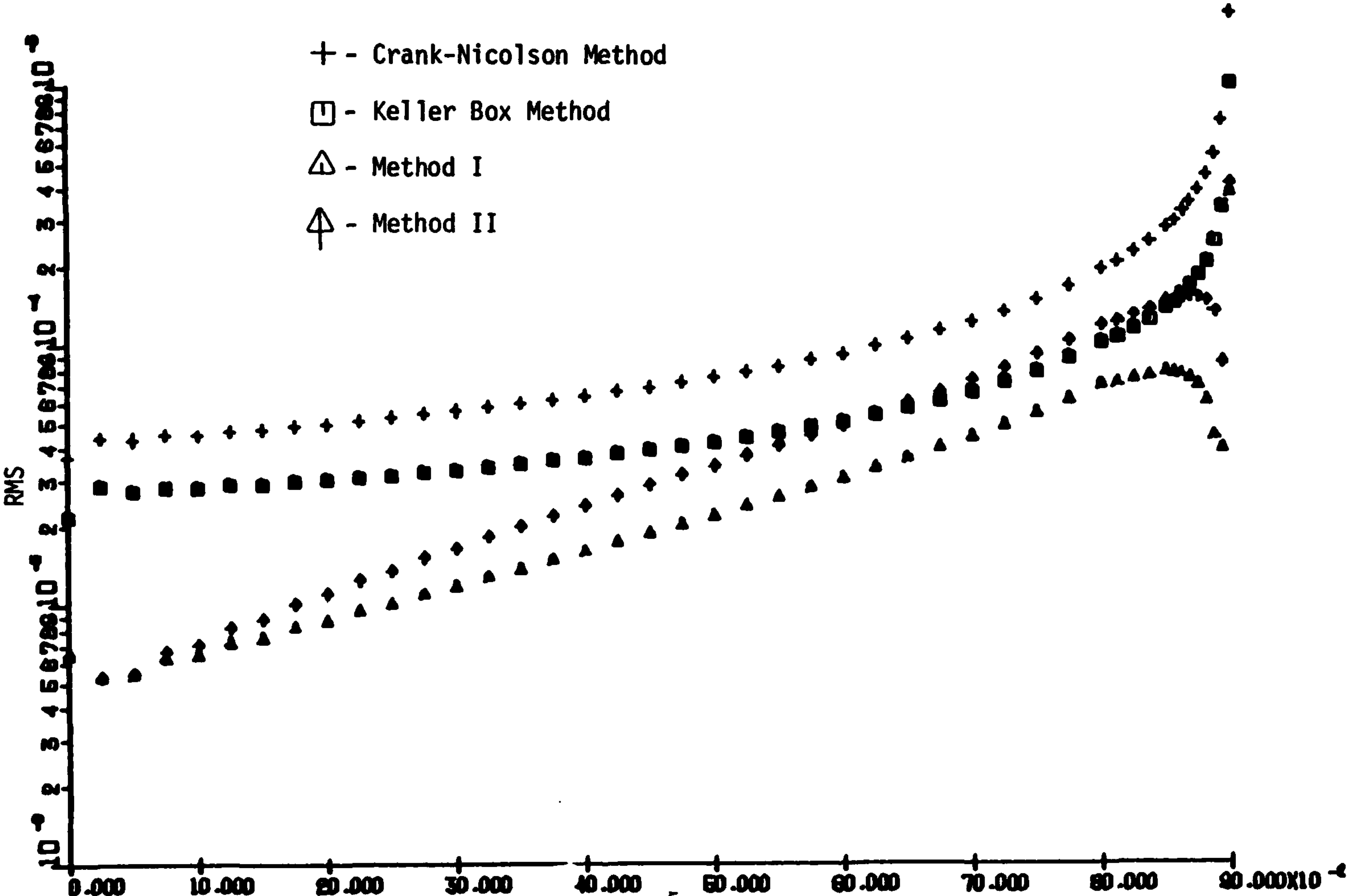

Fig. 5.1a. Comparison of RMS error for the Howarth flow problem for mesh sizes listed in table 5.1.

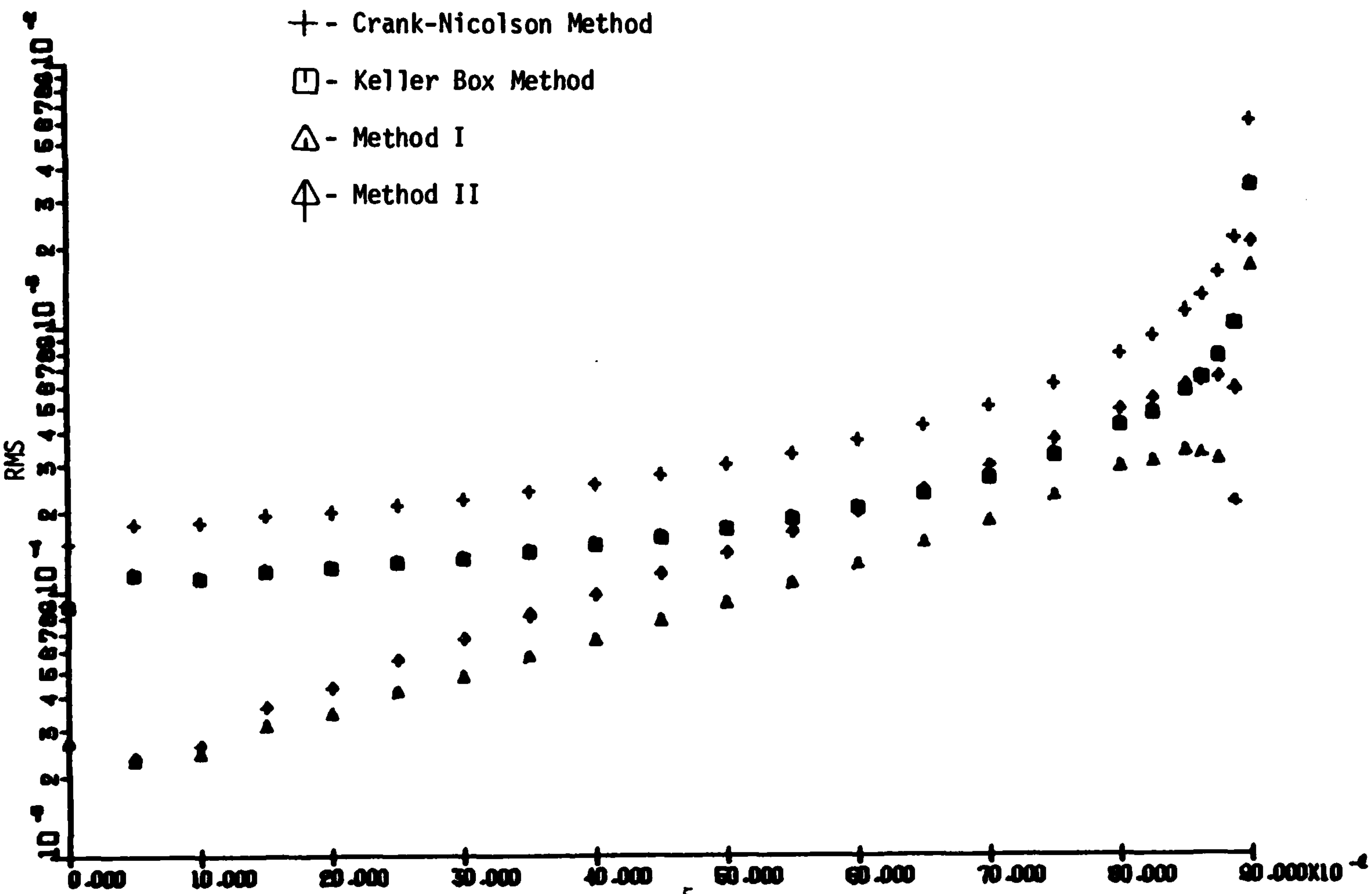

Fig. 5.1b. Comparison of RMS error for the Howarth flow problem for mesh sizes listed in table 5.1.

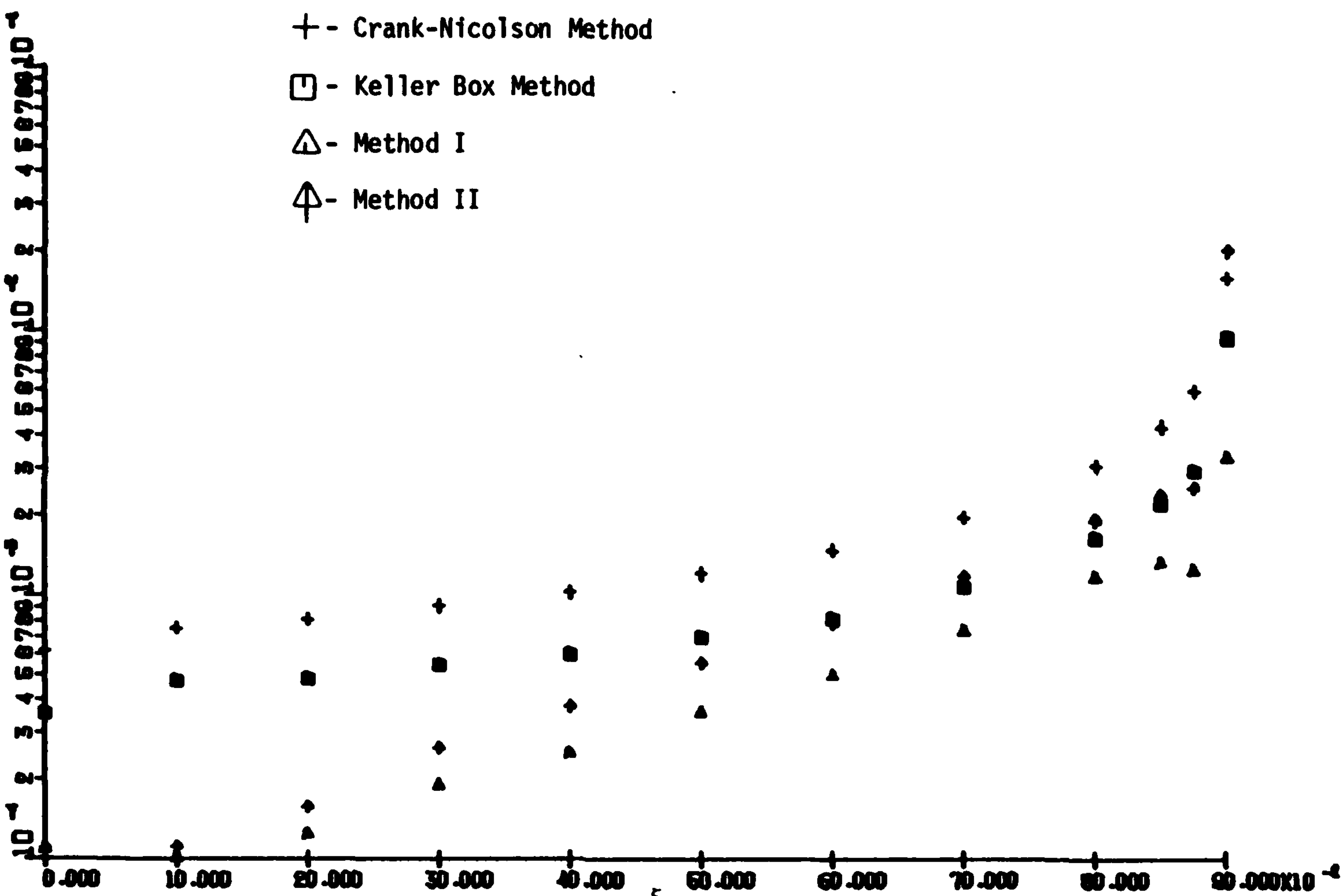

Fig. 5.1c. Comparison of RMS error for the Howarth flow problem for mesh sizes listed in table 5.1.

the root mean square plots indicate Method I has the lowest overall error of all, while the level accuracy of Method II lies between the Keller Box Scheme and Method I. Note that the root mean square error increases substantially for all methods as $\xi \rightarrow .9$; this is because a point of zero skin friction occurs at $\xi_0 = .9008694$ which suggests a flow separation occurs there. In fact, with the mainstream velocity constrained to be of the form equation (5.8), equation (5.6) contains an irregular behavior of the form $(\xi-\xi_0)^{\frac{1}{2}}$ which is usually referred to as the Goldsten singularity (1948). For this reason the truncation error will become large as $\xi \rightarrow \xi_0$ for all methods.

It is known that the improved method of Walker and Weigand (1979) produces more accurate results than either of the existing methods for solution of the initial equation (5.12) and the question naturally arises as to whether the apparent better performance of the two improved parabolic methods is simply a result of the more accurate initial condition. To investigate this point, all four methods were re-run but this time using 'exact' solution at the initial station (based on the solution of equation (5.10) with a very small η mesh size); in this way the error associated with the initial condition is eliminated, and the accuracy of each parabolic scheme can be isolated. The root mean square errors (RMS) for one set of computations are plotted in figure (5.2); note that the mesh sizes are the same as was used to figure 5.1a (see table 5.1). It may be observed that similar conclusions as discussed in connection with figures (5.1) can be drawn from these computations.

The velocity gradient at wall (u') and number of iterations for selected ξ stations for all four methods and for the three sets of mesh sizes considered are presented in tables (5.2) through (5.4) respectively; in addition, a comparison is made with the 'exact' result. The absolute magnitude of the error for the test problem at two different ξ stations for grid sizes $h = .1$ and $k = .05$ are plotted on figures (5.3). It may be observed that the improved methods have smaller errors than either the Crank-Nicolson or the Keller Box method; furthermore, method I gives slightly better results than method II.

For this example, both improved methods give an accurate solution for the boundary-layer equations. In the next section, another non-linear problem will be examined.

5.4 An MHD Problem

The second non-linear example considered here is associated with the problem of boundary layer for flow past a cylinder with an applied radial magnetic field (see, for example, Crisalli and Walker, 1976). The equations governing the flow in the

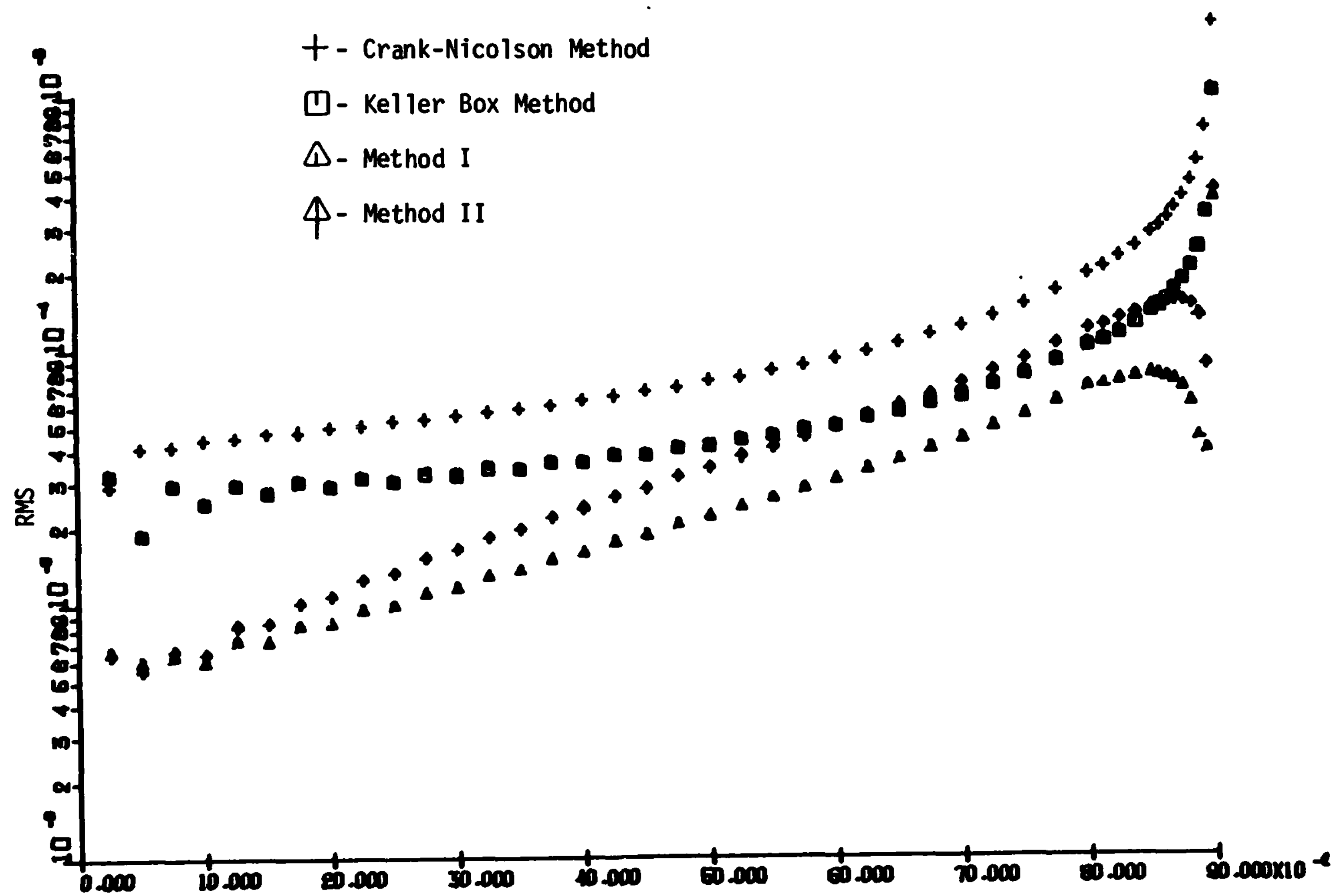

Fig. 5.2. Comparison of the RMS error for the Howarth flow problem starting with an 'exact' initial profile at $\xi=0$; mesh sizes are the same as for figure 5.1a.

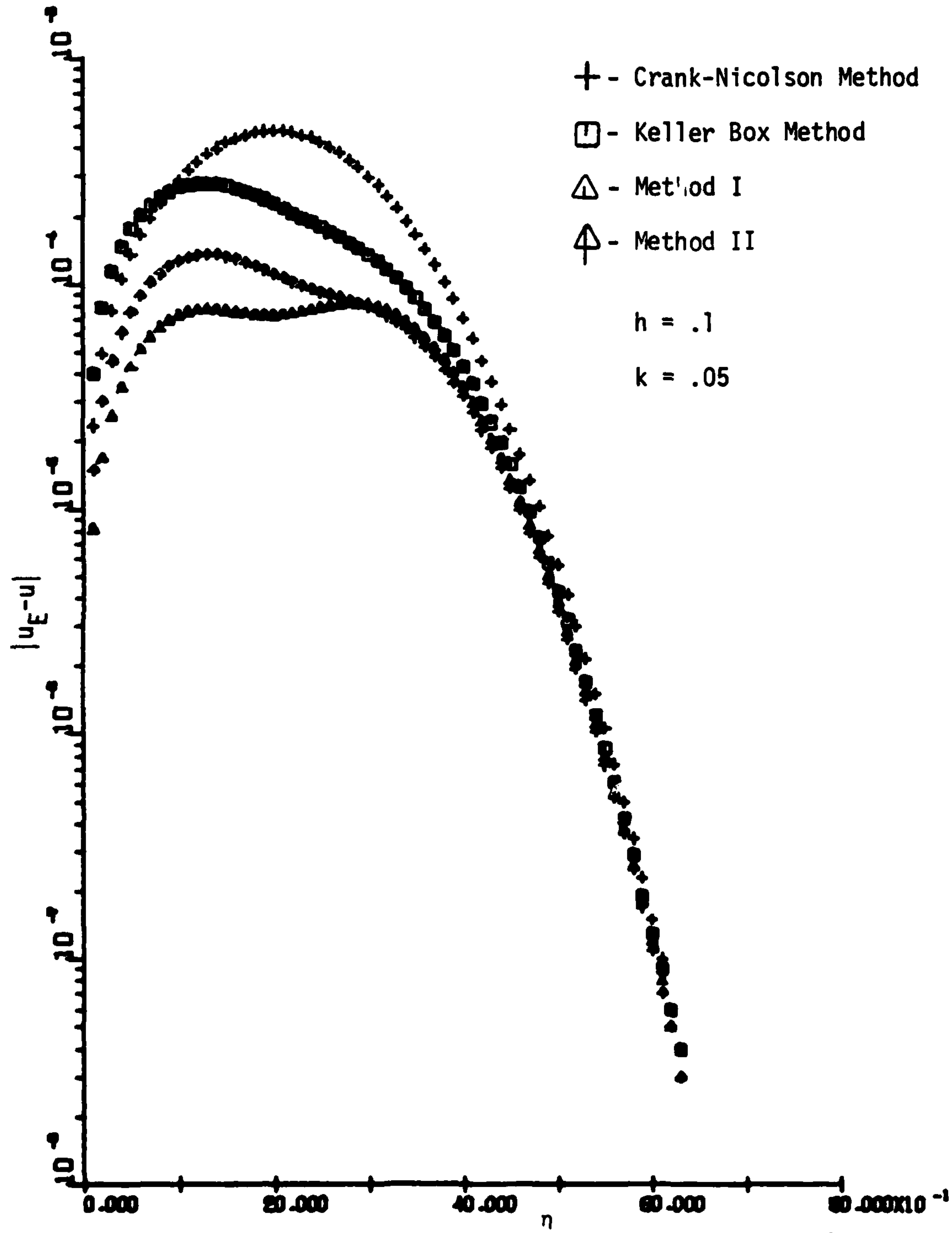

Fig. 5.3a. Magnitude of the error for Howarth flow problem at ξ = .3.

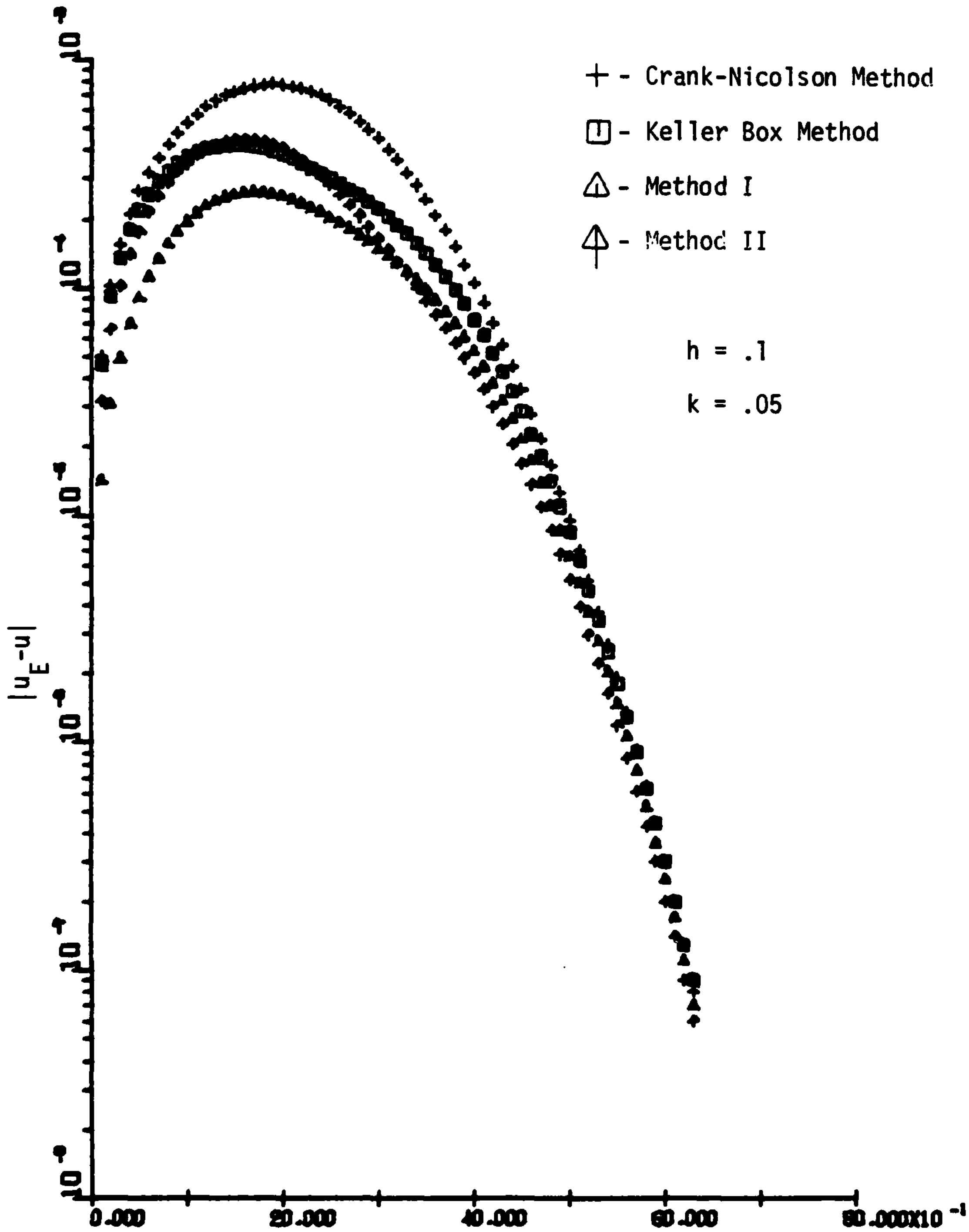

Fig. 5.3b. Magnitude of the error for Howarth flow problem at ξ = .6.

	Method I		Method II		KBS		CN		Exact
ξ	u'	ITER	u'	ITER	u'	ITER	u'	ITER	u'
.2	.41409	3	.41426	3	.41508	3	.41416	3	.41349
.4	.34662	3	.34701	3	.34760	3	.34708	3	.34597
.6	.26145	4	.26217	4	.26262	4	.26273	4	.26079
.8	.14016	4	.14143	4	.14217	4	.14381	4	.13927

Table 5.2. Velocity gradient at wall and number of iterations at selected ξ locations (grid sizes are $h = .2$, $k_o = .1$)

	Method I		Method II		KBS		CN		Exact
ξ	u'	ITER	u'	ITER	u'	ITER	u'	ITER	u'
.2	.41355	3	.41359	3	.41389	3	.41366	3	.41349
.4	.34606	3	.34616	3	.34638	3	.34625	3	.34597
.6	.26092	3	.26109	3	.26125	3	.26128	3	.26079
.8	.13950	4	.13981	4	.14000	4	.14042	4	.13927

Table 5.3. Velocity gradient at wall and number of iterations at selected ξ location (grid sizes are $h=.1$, $k_0=.05$)

	Method I		Method II		KBS		CN		Exact
ξ	u'	ITER	u'	ITER	u'	ITER	u'	ITER	u'
.2	.41350	3	.41351	3	.41358	3	.41353	3	.41349
.4	.34599	3	.34601	3	.34607	3	.34603	3	.34597
.6	.26082	3	.26087	3	.26090	3	.26091	3	.26079
.8	.13932	4	.13940	4	.13945	4	.13955	4	.13927

Table 5.4. Velocity gradient at wall and number of iterations at selected ξ location (grid sizes are $h = .05$, $k_o = .025$)

vicinity of the rear stagnation point of the cylinder are (Leibovich, 1967; Buckmaster, 1969, 1971; Walker and Stewartson, 1972)

$$\frac{\partial^2 u}{\partial y^2} - F\frac{\partial u}{\partial y} + (u-m)\,u + m-1 = \frac{\partial u}{\partial t}\,,$$

$$\frac{\partial F}{\partial y} = u\,, \tag{5.26}$$

with boundary conditions

$$\frac{\partial u}{\partial y} = F = 0 \quad \text{at} \quad y = 0,\; u \to 1 \quad \text{as} \quad y \to \infty\,. \tag{5.27}$$

Here m is a parameter which is proportional to the magnetic field strength. In addition, y measures distance normal to the wall, u is the velocity tangential to the wall in the boundary layer, F is a stream function and t is the time.

The time dependent problem considered here corresponds to that for which the cylinder is impulsively started from rest and from this initial condition, the solution of equations (5.26) describes the time-dependent development of the boundary layer near the rear stagnation point of the cylinder. For small times it is convenient to introduce Rayleigh variables f, η given by,

$$\eta = y/2\sqrt{t}\quad,\quad f = F/2\sqrt{t}\,. \tag{5.28}$$

Upon substitution of these transformations, equations (5.26) become,

$$\frac{\partial^2 u}{\partial \eta^2} + (2\eta - 4tf)\frac{\partial u}{\partial \eta} + 4t(u-m)u + 4t(m-1) = 4t\frac{\partial u}{\partial t},$$

$$\frac{\partial f}{\partial \eta} = u \quad . \tag{5.29}$$

The initial condition for equation (5.29) is obtained by taking the limit as $t \to 0$ and the solution satisfying the boundary conditions in equation (5.27) is

$$u = \mathrm{erf}\eta \quad . \tag{5.30}$$

In this section, the improved methods are applied to equations (5.29) and (5.26) and the performance of the improved methods are compared with the Crank-Nicolson method. A value of $m = 3$ is selected for this test case. As time increases and the boundary layer develops, the variables given in equation (5.28), which were introduced in connection with the impulsive start, are no longer appropriate and it is convenient to switch back to the original (y,t) variables; this was carried out at $t = .5$ in all cases. A brief description of each method follows.

Method I

According to the new method described in section (3.1), the first of equations (5.29) is reduced to a set of non-linear algebraic equations of the form of equation (3.12) with associated equations (3.13); for this test example,

$$Q_j^{**} = 4t_j^{**} \quad , \tag{5.31a}$$

$$P_j^{**} = 2\eta_j^{**} - 2t_j^{**}(f_j + f_j^{*}) \quad , \tag{5.31b}$$

$$R_j^{**} = 2t_j^{**}(u_j + u_j^{*}) - 4t_j^{**}m \ , \tag{5.31c}$$

$$F_j^{**} = 4t_j^{**}(m-1) \ . \tag{5.31d}$$

Equation (3.12) may then be solved by the Thomas Algorithm in a general iterative procedure at each time step; in this procedure, values of u_j in equations (5.31) are replaced by the values at previous iteration and values f_j may be determined by the Simpson rule of integration (see Appendix II). Iteration continues until a converged solution is obtained to five significant figures; the solution is then advanced to the next time step.

For larger values of time ($t > 0.5$) a switch back to principle plane (y,t) is made and in this case the first of equations (5.26) must be solved; it is reduced to the same form as equations (3.12) and (3.13), where now,

$$Q_j^{**} = 1 \quad , \tag{5.32a}$$

$$P_j^{**} = (F_j + F_j^{*})/2 \ , \tag{5.32b}$$

$$R_j^{**} = (u_j + u_j^{*})/2 - m \ , \tag{5.32c}$$

$$F_j^{**} = m-1 \quad . \tag{5.32d}$$

Following the same type of procedure as described for the small time solution, the integration may be advanced to successively larger times.

Method II (slant scheme)

Referring to the method described in section (3.2), the first equation of both (5.29) and (5.26) may be reduced to the form of equation (3.20) with associated equations (3.21); here the coefficients Q,P,R and F are identical to equations (5.31) and (5.32) for the small time and large time solutions, respectively. The computational procedure is analogous to that previously described for Method I.

Crank-Nicolson Method

According to the method described in section (2.1), the first equations of both (5.29) and (5.26) may be reduced to the form of equation (2.4) with associated equations (2.5). Again the coefficients Q,P,R, and F are identical to the two previous cases and the computational procedure is similar.

5.5 Calculated Results for the MHD Problem

There is no known analytical solution to the example problem and in order to produce an 'exact' solution, as a basis of comparison, equations (5.29) and (5.26) were solved by using a very fine mesh sizes in the ξ and η directions until five significant figures of accuracy were obtained. The root mean square error (RMS) for the three methods were computed for a mesh size of $h = 0.05$ and a time step of $k = 0.1$; the results are plotted in figures (5.4). According to the results from this test problem, the improved methods performed better than the Crank-Nicolson method; however, Method I solution is somewhat more accurate than Method II. This conclusion is similar to that reached for the Howarth flow problem.

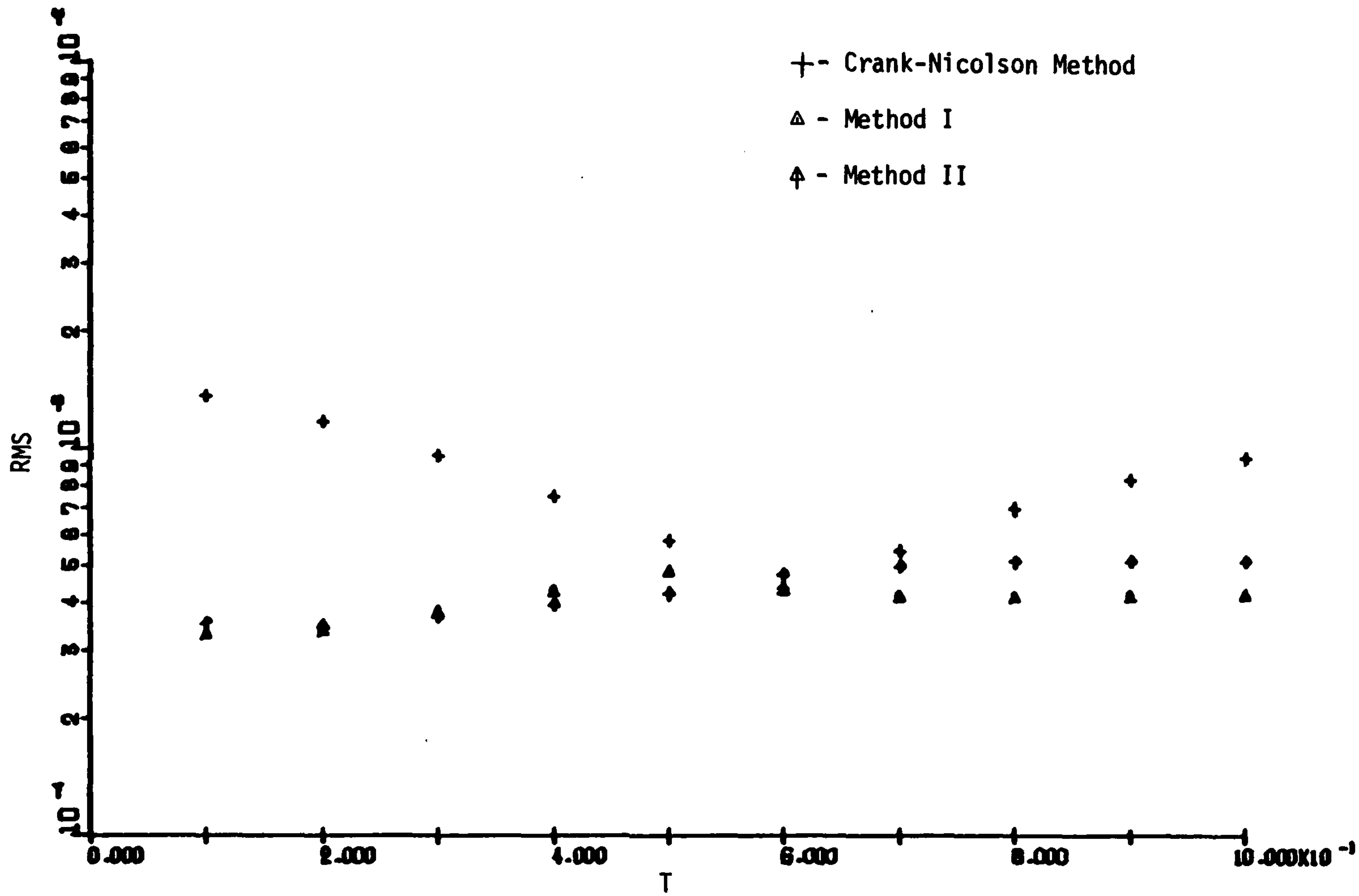

Fig. 5.4. Comparison of the root-mean-square error for the MHD problem.

6. SUMMARY AND CONCLUSIONS

In this study, second order finite difference methods for parabolic partial differential equation have been studied. Two improved methods have been introduced. The leading truncation error terms are discussed and the new methods have been compared to two existing methods, namely, the Crank-Nicolson method and Keller Box scheme. Examples of both linear and non-linear problems for all four methods have been considered. In general, the new methods give more accurate solutions than the existing methods. However, in some special cases, Crank-Nicolson may perform somewhat better than the improved methods. This is due to the fact that for some problems the error terms may happen to combine through differences in sign between individual errors in each error term to produce a small overall error. In addition, computational results consistantly showed that improved methods were superior to the Keller Box scheme and often by a substantial margin. Based on the leading order truncation term comparisons in chapter 2 and 3, and the computational results, it is concluded that the improved methods and particularly method I are preferred for the calculation of parabolic equations.

REFERENCES

1. Ackerberg, R.C. & Phillips, J.H. 1972 "The Unsteady Laminar Boundary Layer on a Semi-Infinite Flat Plate due to Small Fluctuations in the Magnitude of the Free Stream Velocity", J. Fluid Mech. 51, 137-157.

2. Blottner, F.G. 1975 "Investigation of Some Finite-Difference Techniques for Solving the Boundary Layer Equations", Computer Methods in Applied Mechanics and Engineering, 6, 1-30.

3. Buckmaster, J. 1969 "Separation and Magnetohydrodynamics", J. Fluid Mech. 38, 481.

4. Buckmaster, J. 1971 "Boundary Layer Structure at a Magnetohydrodynamics Near Stagnation Point", Q.J. Mech. Appl. Math. 24, 373.

5. Fox, L. 1957 The Numerical Solution of Two-Point Boundary Value Problems. Oxford Press.

6. Goldstein, S. 1948 "On Laminar Boundary Layer Flow Near a Position of Separation", Quarterly J. Mech. and App. Math. 1, 43-69.

7. Howarth, L. 1938 "On the Solution of the Laminar Boundary Layer Equations", Proc. Roy. Soc., London, A164, 547-579.

8. Keller, H.B. 1969 "Accurate Difference Methods for Linear Ordinary Differential Systems Subject to Linear Constraints", SIAM J. Numer. Anal. 6, 8-30.

9. Keller, H.B. 1970 "A New Difference Scheme for Parabolic Problems", in J. Bramble (ed.), Numerical solution of partial differential equation 2. Academic Press.

10. Keller, H.B. & T. Cebeci 1971 "Accurate Numerical Methods for Boundary Layer Flows Part 1. Two Dimensional Laminar Flows", Proceedings of Second International Conference on Numerical Methods in Fluid Dynamics. Springer-Verlag.

11. Leibovich, S. 1967 "Magnetohydrodynamic Flow at a Rear Stagnation Point", J. Fluid Mech. 29, 401.

12. Raetz, G.S. 1953 "A Method of Calculating the Incompressible Laminar Boundary Layer on Infinitely-Long Swept Suction Wings, Adaptable to Small-Capacity Automatic Computer", Northrop Aircraft Co. Rept. BLC-11.

13. Smith, G.D. 1978 Numerical Solution of Partial Differential Equation. Oxford Press.

14. Walker, J.D.A. and Stewartson 1972 "The Flow Past a Circular Cylinder in a Rotating Frame", Z. Angew. Math. Phys. 23, 745.

15. Walker, J.D.A. & Weigand G.G. 1979 "An Accurate Method for Two-Point Boundary Value Problems", International Journal for Numerical Methods in Engineering, 14, 1335-1346.

16. Crisalli, A.J. and Walker, J.D.A. 1976 "Nonlinear Effects for the Taylor Column for a Hemisphere", the Physics of Fluids, 19, 1661-1668.

17. Wu, J.C. 1962 "The Solution of the Laminar Boundary Layer Equation by the Finite Difference Method", Proceeding of the 1961 Heat Transfer and Fluid Mechanics Institute. Stanford University Press.

APPENDIX I

SOLUTION OF THE DIFFERENCE EQUATIONS

1. The Thomas Algorithm

In chapters 2 and 3, the finite difference approximations for the existing methods and the new methods, lead to a tri-diagonal matrix problem of the form,

$$B_j u_{j+1} + A_j u_j + C_j u_{j+1} = D_j \quad . \tag{A.1.1}$$

Here $j = 1,2,3,\ldots,n-1$ and equation (A.1.1) holds at each internal mesh point. In the simplest case where the boundary conditions are given by equation (2.2), the values of u are given at the boundary according to

$$u_o = g_1(x) \quad , \qquad u_n = g_2(x) \quad . \tag{A.1.2}$$

For all methods A_j, B_j, C_j and D_j are known.

The solution of equations (A.1.2) may be obtained directly through use of a solver generally referred to as the Thomas algorithm. The procedure is as follows. Define two arrays, δ and F according to

$$F_o = 0 \quad , \quad F_{n+1} = \frac{-B_{n+1}}{A_{n+1}+C_{n+1}\,F_n} \quad , \tag{A.1.3}$$

$$\delta_o = u_o \quad , \quad \delta_{n+1} = \frac{D_{n+1} - C_{n+1}\delta_n}{A_{n+1} + C_{n+1} F_n} \quad . \tag{A.1.4}$$

The solution to equation (A.1.1) is then obtained by back substitution in

$$u_j = F_j u_{j+1} + \delta_j , \tag{A.1.5}$$

with $j = n-1, n-2, \ldots, 1$ since u_n is known.

2. Derivative Boundary Conditions

When one of the boundary conditions involves a derivative condition, the above procedure must be modified. Suppose that

$$\frac{\partial u}{\partial y} = g_3(x) \quad \text{at} \quad y = b \ , \tag{A.1.6}$$

instead of the second of equation (A.1.2). There are a number of methods available for the approximation of equation (A.1.6); the method which is believed to be the most satisfactory and which preserves the overall second order accuracy in h, is to approximate the derivative in equation (A.1.6) with a sloping difference according to,

$$\frac{\partial u}{\partial y} = \frac{11u_n - 18u_{n-1} + 9u_{n-2} - 2u_{n-3}}{6h} + O(h^3) \ . \tag{A.1.7}$$

Substitution in (A.1.6) leads to ,

$$11u_n - 18u_{n-1} + 9u_{n-2} - 2u_{n-3} = 6hg_3(x) \quad \text{(A.1.8)}$$

This relation may be combined with equations (A.1.3) to (A.1.5) to compute the value of u at y=b according to ,

$$u_n = \frac{6hg_3(x) - (\delta_{n-1}(-18+9F_{n-2}-2F_{n-2}F_{n-3}) + \delta_{n-3}(9-2F_{n-3}) - 2\delta_{n-3})}{11-18F_{n-1}+9F_{n-1}F_{n-2}-2F_{n-1}F_{n-2}F_{n-3}} . \quad \text{(A.1.9)}$$

This value may then be used to initiate the back substitution in equation (A.1.5).

APPENDIX II

SIMPSONS RULE FOR INTEGRATION OF INDEFINITE INTEGRALS

In the solution of the boundary-layer problems considered in chapter 5, it is necessary to evaluate an indefinite integral of the form,

$$f(y_i) = \int_{y_o}^{y_i} u(y)dy \quad . \qquad \text{(A.2.1)}$$

This can be accomplished with good accuracy $O(h^5)$ through the use of Simpson's rule. To calculate an integral over the first step, the starting formula is,

$$f_1 = \int_{y_o}^{y_1} u\,dy = \frac{h}{24}\{9u_o + 19u_1 - 5u_2 + u_3\} , \qquad \text{(A.2.2)}$$

and successive values of f are calculated according to

$$f_{i+1} = f_{i-1} + \frac{h}{3}\{u_{i+1} + 4u_i + u_{i-1}\} , \qquad \text{(A.2.3)}$$

for $i = 1,2,3,\ldots$.

APPENDIX III

THE ACKERBERG AND PHILLIPS (1972) ELIMINATION METHOD

Consider a system equations of the form,

$$A_j u_{j+1} + B_j u_j + C_j u_{j-1} + G_j f_{j+1} + H_j f_j + M_j f_{j-1} = D_j , \tag{A.3.1}$$

with the additional relation,

$$f_{j+1} = f_j + \frac{h}{2}(u_j + u_{j+1}) , \tag{A.3.2}$$

where $j = 1,2,3,\ldots,n-1$. This system may be solved directly by the following algorithm described by Ackerberg and Phillips (1972). Assume the following relation,

$$u_{j+1} = \alpha_{j+1} + \beta_{j+1} u_j + \gamma_{j+1} f_j , \tag{A.3.3}$$

and substitute equations (A.3.3) and (A.3.2) into (A.3.1); this procedure results in an equation of the form,

$$u_j = \alpha_j + \beta_j u_{j-1} + \gamma_j f_{j-1} , \tag{A.3.4}$$

where the following recurrence relations are obtained:

$$\alpha_j = (D_j - A_j\alpha_{j+1} - \frac{h}{2} G_j\alpha_{j+1})/(A_j\beta_{j+1} + B_j + hG_j + \frac{h}{2}H_j + \frac{h}{2}A_j\gamma_{j+1}$$
$$+ \frac{h}{2} G_j\beta_{j+1} + \frac{h^2}{4} G_j\gamma_{j+1}) , \tag{A.3.5}$$

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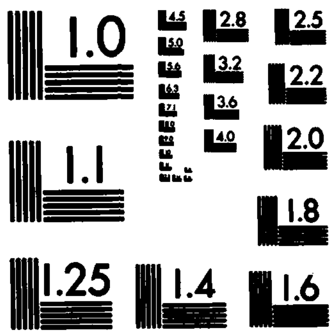

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$$\beta_j = -\left(C_j + \frac{h}{2}G_j + \frac{h}{2}H_j + \frac{h}{2}A_j\gamma_{j+1} + \frac{h^2}{4}G_j\gamma_{j+1}\right) / \left(A_j\beta_{j+1} + B_j + hG_j + \frac{h}{2} H_j + \frac{h}{2}A_j\gamma_{j+1} + \frac{h}{2}G_j\gamma_{j+1} + \frac{h^2}{4}G_j\gamma_{j+1}\right) , \tag{A.3.6}$$

$$\gamma_j = -\left(G_j + H_j + M_j + A_j\gamma_{j+1} + \frac{h}{2}G_j\gamma_{j+1}\right) / \left(A_j\beta_{j+1} + B_j + hG_j + \frac{h}{2}H_j + \frac{h}{2}A_j\gamma_{j+1} + \frac{h}{2}G_j\beta_{j+1} + \frac{h^2}{4} G_j\gamma_{j+1}\right) . \tag{A.3.7}$$

The values of A_j, B_j, C_j, and D_j are known. In addition, the values of u at the boundaries are known, and the boundary conditions given by equation (2.1) may be expressed as,

$$u_o = g_1(x) \quad \text{and} \quad u_n = g_2(x) . \tag{A.3.8}$$

At $y = y_n$ a comparison of equation (A.3.3) and the last of equations (A.3.8) gives,

$$\alpha_n = g_2(x) , \ \beta_n = 0 \ \text{ and } \ \gamma_n = 0 . \tag{A.3.9}$$

These relations may be used to initiate the calculation of α_n, β_n and γ_n, through the use of the recurrence relations (A.3.5) to (A.3.7). The solution of equations (A.3.1) and (A.3.2) is then obtained by substitution in equation (A.3.4) with $j=1,2,3,\ldots$.

APPENDIX IV

NEWTON ITERATION

When the difference equations are non-linear, they cannot be solved directly at each time step and iteration is required. Convergence may be accelerated through use of Newton iteration which is implemented as follows. Suppose the unknown variables are f and u which can be expressed as,

$$f_m = \bar{f}_m + \delta f_m \quad , \tag{A.4.1}$$

$$u_m = \bar{u}_m + \delta u_m \quad . \tag{A.4.2}$$

The superbars denote the results of a previous iteration or the solution of the previous marching step in the case of the first iteration. Suppose that a non-linear term of the form,

$$f_m u_m = (\bar{f}_m + \delta f_m)(\bar{u}_m + \delta u_m) \quad , \tag{A.4.3}$$

arises in the difference equations. Carrying out the multiplication gives

$$f_m u_m = \bar{f}_m \bar{u}_m + \bar{f}_m\,(\delta u_m) + \bar{u}_m(\delta f_m) + O(\delta^2) \quad . \tag{A.4.4}$$

The terms $O(\delta^2)$ are neglected and substitution for δu_m and δf_m from equations (A.4.1) and (A.4.2) yields,

$$f_m u_m = \bar{f}_m \bar{u}_m + \bar{f}_m (u_m - \bar{u}_m) + \bar{u}_m (f_m - \bar{f}_m), \qquad \text{(A.4.5)}$$

or

$$f_m u_m = \bar{f}_m u_m + \bar{u}_m f_m - \bar{f}_m \bar{u}_m \quad . \qquad \text{(A.4.6)}$$

This is the basis of Newton process for linearization of the difference equations.