THE NUMERICAL SOLUTION OF THE THREE-DIMENSIONAL VISCOUS NAVIER-STOKES EQUATIONS

by

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None of the work contained in this thesis has been done in collaboration with any other person, nor has the work, or any part of it, been submitted for any other award.

D F ROSCOE

DEDICATION

To my Mother, without whose earlier sacrifices this work would not have been possible.

A C K N O W L E D G E M E N T

Firstly, I would like to(belatedly) thank Professor N Mullineux of the Mathematics Department at Aston, who drove to North Wales, on a typically foul North Walian day in a blind, but successful, search for me on the last day for Ph.D. registration, 1970. Secondly, I would like to thank Roy Hetherington and Malcolm Sylvester of Rolls Royce, for their patient supervision of the work presented here, and for provision of computing facilities at Rolls Royce. Finally, I would like to thank Christine, my wife, for her forebearance whilst this work has been done, and for her diligent typing of the final result.

D F ROSCOE

SUMMARY

The main aim of this thesis has been to develop a reliable method for the solution of the three-dimensional Navier-Stokes equations for internal viscous flows. In the sense that the methods developed have always yielded solutions to the problems so far attempted, then they are successful. At present, these results do not always compare well with experiment. The author is optimistic that the difficulties can be overcome by following the line of research indicated at the end of Chapter 6.

The present qualified success is due to two innovations. The first is a new method of deriving difference representations of ordinary and partial differential operators, and forms the bulk of this thesis. The second is the construction of two matrix theorems, and their subsequent use to derive and analyse stable difference forms for the pressure and continuity terms of the Navier-Stokes equations. These theorems appear to point the way to novel and 'better' difference forms for these pressure and continuity terms.

Arising from the main part of the work, the thesis considers the classification of certain difference operators into hyperbolic, elliptic or parabolic type. It is postulated that a strong connection exists between the stability of a difference representation to a differential equation, and the preservation of the hyperbolic, elliptic or parabolic properties of the differential equation, in the difference equation.

CONTENTS

CHAPTER 1

A DISCUSSION OF THE PROBLEM

1.1 Introduction

The main concern of this thesis is to provide a convenient and reliable numerical method for the solution of the three dimensional Navier-Stokes equations for viscous flows in curvilinear ducts. The original purpose was to derive such a method for compressible flows, but shortage of time allowed only the basic development to be completed for incompressible flows.

There is presented a quick, economical and reliable method for the solution of the three dimensional equations in curvilinear ducts using laminar viscosity models. The method is a finite difference prodadure operating on the primitive variable (pressure, velocity field) form of the Navier-Stokes equations. The method of solution in no way compromises its extension to compressible flows, as does the 'artificial compressibility method' of Chorin [1], or to the use of the quasi-laminar turbulent models, (ie. the kinematic viscosity expressed as some heuristic function of the velocity field and space). Its extension to time dependent flows is envisaged, and the possibility of using it to test turbulent models, eg. [2] is being considered.

1.2 Background of the Problem

The complete set of equations governing fluid flows are extremely intractable, see for example [3], and it is fortunate that, in many situations of practical importance, substantial approximations can be made without the introduction of an intolerable error. Perhaps the most common such approximation is that of two dimensionality. This assumption is widely used in boundary layer calculations, where the crucial argument is that the major changes in the flow occur normally and parallel to the flow. The consequent approximations reduce the equations to a set of parabolic type, and it becomes possible to apply 'marching' procedures to the solution of the equations, see for example [4], [5] or [6]. Other situations in which two dimensionality may be assumed include flows in deep, or wide, channels where again little change occurs in one of the spatial dimensions ([7], [8]). Two dimensionality can be invoked in an exact sense when a plane of symmetry exists in a three dimensional flow, eg. flow in a straight circular pipe [9].

If the two dimensional flows are considered to be incompressible and inviscid (a reasonable assumption in high Reynolds number flows where viscous effects are confined to the regions near the boundaries) then streamline curvature methods are often used, eg. [10]. On the other hand, if the momentum terms do not dominate the flow, then the two most widely tried methods are finite difference methods applied to the primitive variable form of the equations, eg. [11], or finite difference methods applied to the stream function, vorticity form of the equations. Stream function vorticity methods have the advantage that the pressure field does not occur explicitly in the equations, with consequent reduction in the number of dependent variables to solve for. The price paid for this advantage is that the order of the equations is raised. On the other hand, if numerical solution of the primitive variable form of the equations is attempted, then great difficulties can arise in trying to obtain the pressure field. Generally speaking, to date workers have preferred to use the stream function vorticity form of the two dimensional Navier-Stokes equations.

Situations that have been successfully modelled by two dimensional finite difference/primary variable techniques have generally been those in which viscous terms have dominated the flow, eg. slow convection problems [12], and creeping flow problems [13]. Similarly, stream function/vortex function methods have been most successful when applied to two dimensional flows in which viscous terms have dominated the flow [14], [15][16]. The apparent limitations of these methods to viscosity dominated flows is probably more due to inadequate finite difference approximations than to the intrinsic unsuitability of these methods to high Reynolds number flows. Flows treated in the literature include slow convection, liquid flows, and combinations of these [17], [18], [19].

The application of finite element methods to fluid flow problems is currently being energetically researched, but there exists at present little numerical information about these methods to provide a comparative basis with other methods.

1.3 Discussion of Available Methods

The available possibilities briefly introduced above are:

Finite Element methods (i)

Stream/vortex function methods (ii)

Streamline Curvature methods (iii)

Finite Differences methods (iv)

Each of these will now be discussed.

1.4 Finite Element Methods

The finite element method traditionally operates by minimising a certain function (the functional), and which function when minimised, completely characterises the physical situation under study. A first step in this procedure is to express the problem in some variational form, and for some systems, this is easily done. For instance, systems which are characterised by Laplaces equation are systems in which the potential energy is minimised subject to certain conditions (the boundary conditions). In general, this step is perhaps the most difficult to make. Indeed, many systems do not possess a variational principle, and amongst these are the Navier-Stokes equations [25]. However, if the Navier-Stokes equations are put in conservation form, and a suitable orthogonalisation technique is applied, finite element equations can be deduced without reference to any variational principle [26].

Two and three dimensional potential flow calculations have been carried out by Argyris et al [27], Doctors [28] and Baker [29], and Baker also gives a computational theory for the calculation of two dimensional compressible flows [30], and three dimensional boundary layer flows [31], all these using finite elements. Schecter [32] derives variational formulations for transport problems, and gives amongst other results, some results on two dimensional boundary layer calculations. Norris and de Vries [33] are currently preparing a book on the application of finite element techniques to fluid dynamics. This selection of references gives an indication of the amount of work being applied to the problem of the application of finite elements to fluid dynamics. However, in 1970 at the start of this thesis, the finite element approach seemed a long shot from the point of view of obtaining a numerical method within the three years, and the approach was thus discounted.

1.5 Stream/Vortex Function Methods

Stream function/vortex function methods have been very successful in a wide number of applications for two dimensional flows, and naturally workers have sought to carry this success into a three dimensional setting. The vector potential method of Aziz and Hellums [34] can be viewed as a generalisation of stream/vortex function methods, since it collapses into these methods when applied to two dimensional problems. They transform the complete Navier-Stokes equations from primary variables and pressure into a vorticity and a vector-potential,† and then apply a numerical method to the resulting equations. Unfortunately, unless the primitive variable boundary conditions are very simple, and the geometry Euclidean, then the boundary conditions for the vector-potential assume an extremely

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† In two dimensional flows, there is a vorticity and a scalar potential

complicated form - Hirasaki and Hellums [35] discuss the problem in some detail. For present purposes, because the basic method is in a very early stage of development, and because there is a great deal of uncertainty about the correct treatment of boundary conditions [34], vector potential methods were considered to be impractical.

1.6 Streamline Curvature Methods

Two dimensional inviscid streamline curvature approach has long been favoured by workers engaged in compressor and turbine design. It was first proposed, for the purpose of compressor/turbine design, by Wu and Wolfenstien [36] in 1950. Compressibility presents no difficulties, and the compressible formulation has been extended to three dimensional flows by Stuart [37]. At the beginning of this investigation the present author derived the viscous form of the streamline curvature equations and found them to be exceedingly complex, especially in the three dimensional form. Apart from the possibility of numerical difficulties in treating these viscous equations, there is, in a viscous flow, always the possibility of recirculation, see Fig. 1.6.1.

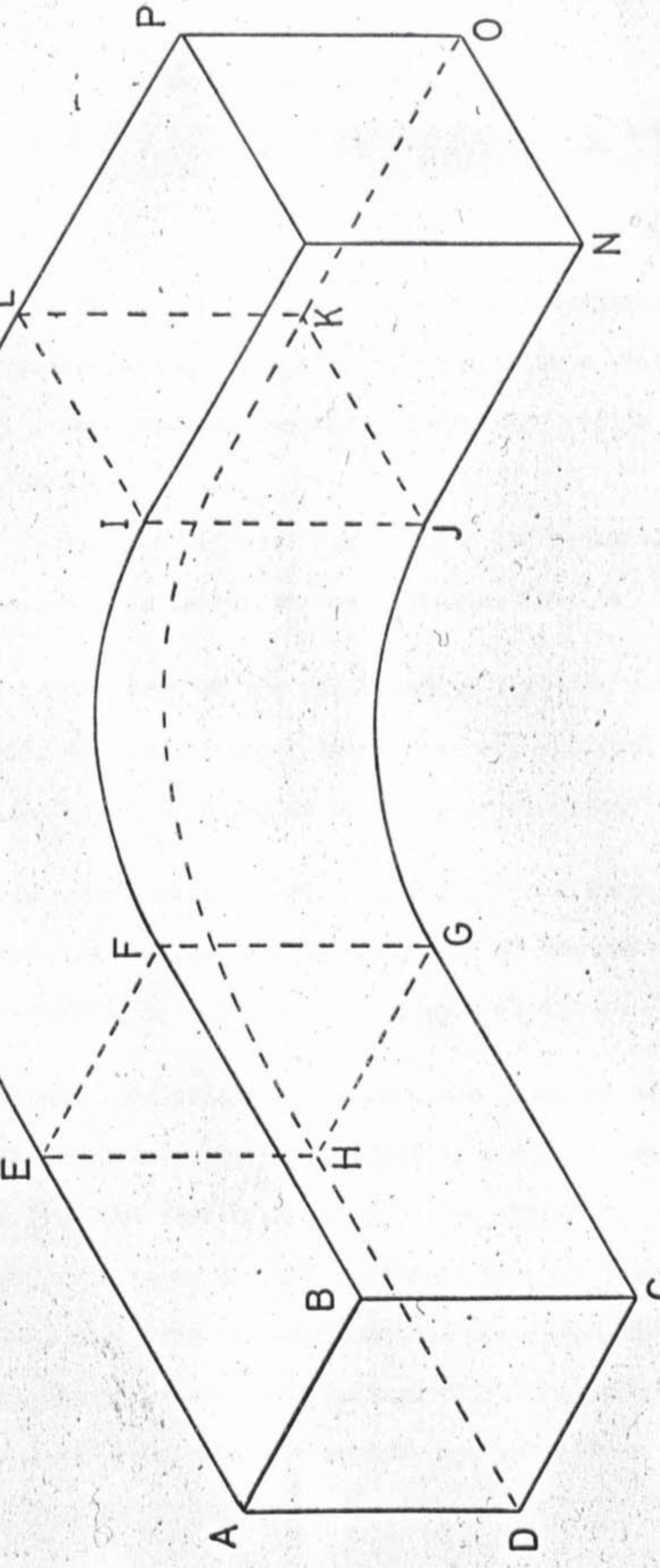
Figure 1.6.1

The streamline curvature method operates by effectively picking a streamline at the inlet plane, and tracing it through the flow. Clearly, there is no possibility of doing this for a closed streamline, like C in Fig. 1.6.1. Thus, the streamline curvature method in its present form is incapable of obtaining results within the contour C, moreover there is no facility in the method for transmitting information from within, and across C to the main flow. Thus, boundary information from the boundary adjacent to C cannot transmit to the main flow. Consequently, instability due to poor boundary data could result. It may be possible to resolve these difficulties, but it is certainly possible to say that streamline curvature will not readily adapt to the circumstance outlined above. For this reason, an extension of streamline curvature to three dimensional viscous flows was discounted. Further references are given at [21] and [22].

1.7 Finite Difference Methods

The finite difference technique has, in general, two main disadvantages. It is only well suited to orthogonal co-ordinate systems in which the boundaries of the problem are constant co-ordinate lines. There are two reasons for this, firstly that in co-ordinate systems where the angle between co-ordinate lines differs much from $\pi/2$ large truncation errors can arise, and secondly if boundaries are not co-ordinate lines, then some form of interpolation has to be resorted to in order to insert boundary conditions, and again large errors and instability can easily ensue [38], [39]. This disadvantage can always be removed since if an analytic orthogonal co-ordinate system cannot

Figure 1.7.1



CHAPTER 2

THE FINITE DIFFERENCE REPRESENTATIONS OF ORDINARY DIFFERENTIAL EQUATIONS

2.1

In this section, a brief discussion of the conventional finite difference representations is given, together with a criticism of their main failing. The three main methods of deriving finite difference representations are:

(i) The replacement of each term of the differential operator directly by a Taylor series approximation [44].

(ii) The integration of the differential equation over a finite difference block and the subsequent replacement of each term by a Taylor series approximation [45].

(iii) Formulation of the problem in variational form and the subsequent replacement of each term of the variational formulation by a Taylor series approximation, [46].

These methods, and related methods share a common defect, namely that the individual terms of the analytical operator are approximated in isolation from the remaining terms of the operator. Consequently, the interactions between the terms of operator are ignored.
It will be seen that this is a fundamental cause for the existence of instability in both ordinary and partial differential equations. In Appendix II it is shown that for method (i), conditions for stability require step lengths of the order τ ,

where $\tau = \text{Max}\,(\Delta x,\ \Delta y,\ \Delta z) \leq \dfrac{\nu}{\text{Max}\,(u,\ v,\ w)}$ (2.1.1)

where ν is the kinematic viscosity and u, v, w are the velocity components. For our application, ie. of air flowing subsonically in ducts, $\tau \simeq 10^{-7}$. Clearly, such a restriction is prohibitive. Similar conditions can be found to hold for the other representations.

2.2 Unified Finite Difference Representations

In this section it is shown how to derive representations which include term/term interactions of the differential operator. Such representations will be denoted the 'unified difference representations' (UDR).

The starting point is a homogenous, second order, ordinary, constant coefficient differential equation with arbitrary boundary conditions. It will be shown, how on an arbitrary mesh (non-constant spacing) it is possible to derive a difference equation whose solution is identical to that of the differential equation. Clearly, in this simple situation term/term interactions are included, and no possibility of instability can exist. The application to ordinary differential equations is of little practical interest, but it will be shown (Section 3.2 onward) that in their extension to second order partial operators the representations have many desirable properties, in particular that they preserve the ellipticity, or hyperbolicity of the original partial differential operator.†

Consider

$$\psi'' + f_1\,\psi' + f_2\,\psi = f_3(x) \qquad (2.2.1)$$

† For the form of parabolic equation considered, it is shown in appendix IV that the UDR is not uniquely determined.

where f_1 and f_2 are arbitrary constants. Assume that appropriate b.c's. are specified. The solution is

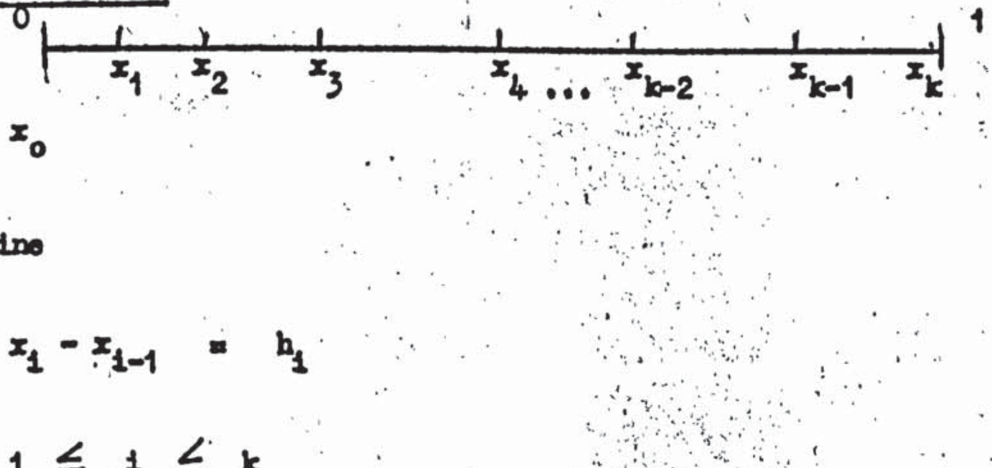
$$\psi(x) = A_0 e^{m_0 x} + A_1 e^{m_1(x)} + f_4(x) \qquad (2.2.2)$$

where A_0 and A_1 are arbitrary constants and $f_4(x)$ is a particular integral. m_0 and m_1 satisfy the auxiliary equation of (2.2.1). It is well-known that the stability of a difference equation is generally decided by its homogenous solution [48]. Accordingly, there is now constructed an homogenous difference equation whose solution is the homogenous solution of (2.2.1) ie.

$$\psi_1(x) = A_0 e^{m_0 x} + A_1 e^{m_1(x)} \qquad (2.2.3)$$

Suppose that it is wished to solve the difference equation on the non-uniform net in Fig. 2.2.1

Figure 2.2.1



Define

$$x_i - x_{i-1} = h_i \qquad (2.2.4)$$

$$1 \leq i \leq k$$

Thus, whenever $x = x_i$, $1 \leq i \leq k$, then

$$x = \sum_{s=1}^{i} h_s \qquad (2.2.5)$$

Thus, the difference form of (2.2.3) is given by

$$\psi_1 (x_i) = A_0 \exp (m_0 \sum_{s=1}^{i} h_s) + A_1 \exp (m_1 \sum_{s=1}^{i} h_s)$$

$$= A_0 \prod_{s=1}^{i} e^{m_0 h_s} + A_1 \prod_{s=1}^{i} e^{m_1 h_s} \qquad (2.2.6)$$

Thus, we require the difference equation whose solution is given by (2.2.6). Now, it is known, eg. Milne-Thomson [49], that a second order difference operator having as its solution space (u_i, v_i) is defined by the equation

$$\begin{vmatrix} \psi_{i-1} & U_{i-1} & V_{i-1} \\ \psi_i & U_i & V_i \\ \psi_{i+1} & U_{i+1} & V_{i+1} \end{vmatrix} = 0 \qquad (2.2.7)$$

Thus, setting

$$U_i = \prod_{s=1}^{i} e^{m_0 h_s}$$

$$V_i = \prod_{s=1}^{i} e^{m_1 h_s} \qquad (2.2.8)$$

and using (2.2.7) it is found upon simplification, that

$$\psi_{i+1} (e^{m_1 h_i} - e^{m_0 h_i}) - \psi_i (e^{m_1(h_{i+1} + h_i)} - e^{m_0(h_{i+1} + h_i)})$$

$$+ \psi_{i-1} e^{(m_0 + m_1) h_i} (e^{m_1 h_{i+1}} - e^{m_0 h_{i+1}}) = 0 \qquad (2.2.9)$$

is the required difference equation. Thus, if the boundary conditions of (2.2.9) are appropriately set, then (2.2.9) and (2.2.1) with $f_3(x) = 0$, have identical solutions. On a uniform grid of step h, (2.2.9) collapses to

$$\psi_{i+1} - \psi_i \left(e^{m_o h} + e^{m_1 h}\right) + \psi_{i-1} e^{(m_o + m_1)h} = 0 \qquad (2.2.10)$$

If the exponentials in (2.2.10) are expanded to the first three terms, then there is obtained the result:

$$\frac{(\psi_{i+1} - 2\psi_i + \psi_{i-1})}{h^2} + f_1 \frac{(\psi_i - \psi_{i-1})}{h} + f_2 \psi_{i-1}$$

$$= \frac{1}{2} (m_o^2 + m_1^2) (\psi_i - \psi_{i-1}) \qquad (2.2.11)$$

Alternatively, multiplying (2.2.10) through by $\exp[-(m_o + m_1)h]$, there follows the result:

$$\frac{(\psi_{i+1} - 2\psi_i + \psi_{i-1})}{h^2} + f_1 \frac{(\psi_{i+1} - \psi_i)}{h} + f_2 \psi_{i+1}$$

$$= \frac{1}{2} (m_o^2 + m_1^2) (\psi_i - \psi_{i+1}) \qquad (2.2.12)$$

Multiplying (2.2.10) through by $\exp\left[-\frac{(m_o + m_1)h}{2}\right]$ yields

$$\frac{(\psi_{i+1} - 2\psi_i + \psi_{i-1})}{h^2} + f_1 \frac{(\psi_{i+1} - \psi_{i-1})}{2h} + f_2 \psi_i$$

$$= \frac{f_1^2}{4} \left[\left(\frac{\psi_{i+1} + \psi_{i-1}}{2}\right) - \psi_i\right] \qquad (2.2.13)$$

The terms on the right of these equations represent the truncation errors arising from the truncation of the exponentials. It has thus been demonstrated how, to within a truncation error, the normal Taylor series forward, backward and central difference formulae may be obtained.

The non-uniform grid formulation is given because a non-uniform grid is often used in boundary layer calculations.

2.3 The Cases $f_3(x) \neq 0$, f_1, f_2 Non-Constant

(i) f_1 = constant, f_2 = constant, f_3 = constant (non-zero).

In this case, the solution of (2.2.1) is given by

$$\psi(x) = A_0 e^{m_0 x} + A_1 e^{m_1 x} + \frac{f_3}{f_2} \qquad (2.3.1)$$

where f_3/f_2 is constant.

If we suppose that (2.3.1), in its difference form is the solution of the modified (2.2.9)

$$B_0 (C_{i1} \psi_{i+1} - C_{i2} \psi_i + C_{i3} \psi_{i-1}) = f_3 \qquad (2.3.2)$$

where C_{i1}, C_{i2}, C_{i3} are the coefficients of ψ_{i-1}, ψ_i, ψ_{i+1} in (2.2.9), then we find upon substituting (2.3.1) into (2.3.2) that

$$B_0 = \frac{f_2}{C_{i1} - C_{i2} + C_{i3}} \qquad (2.3.3)$$

and, on a uniform grid

$$B_o = \frac{f_2}{1 + e^{(m_o + m_1)h} - e^{m_o h} - e^{m_1 h}} \qquad (2.3.4)$$

If $f_2 = 0$, then a similar caloulation yields

$$B_o = \frac{f_1}{h\,(1 - e^{-f_1 h})} \qquad (2.3.5)$$

(ii) f_1, f_2 and f_3 known functions of (ψ, x)

Consider the representation given at (2.3.2), where B_o is given at (2.3.3) and C_{1i}, C_{2i}, C_{3i} given at (2.2.9). The coefficients in (2.3.2) are functions of m_o and m_1 where m_o and m_1 satisfy

$$m_o = \frac{-f_1 + \sqrt{f_1^2 - 4 f_2}}{2}$$
$$m_1 = \frac{-f_1 - \sqrt{f_1^2 - 4 f_2}}{2} \qquad (2.3.6)$$

from the auxiliary equation of the differential equation (2.2.1).† If f_1 and f_2 are functions of (ψ, x) then in the difference representation acting at a pivotal point i, we evaluate m_o and m_1 at the pivotal point i and use these values in the representations given at (2.3.2). This procedure means that the difference representation does not have an homogenous solution which is identical to that of the original differential equation, but in a vanishingly small region about any point $x = ih$, for arbitrary h, the solutions of the homogenous difference equation behave exactly as the solutions of the corresponding differential

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† whenever $f_1^2 - 4 f_2 < 0$, the UDR's can be reformulated, and they then contain sine and cosine terms.

equation. This is opposed to the situation with Taylor series when solutions of the homogenous difference and differential equations only coincide for vanishingly small h. This property of the UDR's strongly suggests that they are inherently more stable than the corresponding Taylor schemes.

2.4 Boundary Conditions for 2nd Order Equations

In this section the possibility of improving the treatment of mixed end point conditions is discussed. For a linear differential equation (ordinary and partial), the boundary conditions are essentially statements about linear combinations of functions of the solution space of the differential equation at a point in the domain of the solution. However, when derivative conditions are specified at end points, or boundary points, it is common practice to treat these conditions as differential equations valid in a region about the end point, or boundary point, in the sense that the difference representations used to represent them are identical to those used for a similar differential equation valid over an arbitrary region. Intuitively, we can see that such an approach can only be reasonable when the solution and its first derivatives do not change rapidly in the region of the boundary. Quite clearly, the practice is at odds with the realities of the situation and unless the mesh size can be sufficiently reduced to limit the truncation error, large errors can ensue. A procedure will now be suggested based on the principles of previous sections, and to test the effectiveness of the above suggestion, a non-constant coefficient equation with mixed end point conditions is solved and comparisons are given with the standard procedure.

Consider equation (2.2.1) where f_1, f_2 and f_3 are all constant. The solution is given by

$$\psi(x) = A_o e^{m_o x} + A_1 e^{m_1 x} + \frac{f_3}{f_2} \qquad (2.4.1)$$

Suppose that the given conditions are

$$\frac{d\psi}{dx} + \varepsilon_o \psi = a_o, \qquad x = 0$$

$$\frac{d\psi}{dx} + \varepsilon_1 \psi = a_1, \qquad x = 1 \qquad (2.4.2)$$

and that (2.4.2) will uniquely specify $\psi(x)$ of (2.4.1). Let the discretisation of the interval [0, 1] be 0, x_1, x_2, ... x_{n-1}, x_n and of $\psi(x)$ on the interval of ψ_o, ψ_1, ψ_2, ... ψ_{n-1}, ψ_n. The question posed is 'Can linear combinations of ψ_o, ψ_1, and ψ_{n-1}, ψ_n be found which are equivalent to (2.4.2)?'

Apply the first of (2.4.2) to (2.4.1) and apply (2.4.1) at $x = 0$, $x = x_1$ respectively to obtain the three equations

$$A_o m_o + A_1 m_1 + \varepsilon_o \psi_o = a_o$$

$$A_o + A_1 + \frac{f_3}{f_2} - \psi_o = 0$$

$$A_o e^{m_o x_1} + A_1 e^{m_1 x_1} + \frac{f_3}{f_2} - \psi_1 = 0 \qquad (2.4.3)$$

If A_o and A_1 are eliminated between the three equations of (2.4.3) there is obtained the relationship

$$\psi_o + \lambda_o \psi_1 = b_o \tag{2.4.4}$$

where λ_o and b_o are known functions of m_o, m_1, ϵ_o, a_o, x_1, and f_3/f_2. In a similar fashion we may derive

$$\psi_n + \lambda_1 \psi_{n-1} = b_1 \tag{2.4.5}$$

In the situation of (2.2.1) having f_1, f_2, f_3 as constants and (2.4.2) as boundary conditions, then (2.4.4) and (2.4.5) together with the UDR will ensure that an identical solution is obtained. In the situation of f_1, f_2, f_3 being functions of (ψ, x) then an identical procedure to the constant case is followed, with the non-constant values being substituted at the end. Hence λ_o, λ_1, b_o and b_1 of (2.4.4) and (2.4.5) are functions of (ψ, x). The author finds it a satisfying result that if (2.2.1) is non-linear, and (2.4.2) are the specified conditions, then the derived equivalent conditions (2.4.4) and (2.4.5) are non-linear, (not convenient, but satisfying!)

2.5 A Numerical Example

The equation considered is

$$\frac{d^2\psi}{dx^2} - \epsilon\left(\frac{1}{2} - x\right)\frac{d\psi}{dx} = 0 \tag{2.5.1}$$

on the interval [0, 1]. If the conditions $\psi(o) = 0$, $\psi(1) = 1$ are specified then the analytical solution is

$$\psi(x) = \frac{\int_o^x e^{\frac{1}{2}\epsilon x(1-x)}\,dx}{\int_o^1 e^{\frac{1}{2}\epsilon x(1-x)}\,dx} \tag{2.5.2}$$

The equation (2.5.1) has been chosen, since on [0, 1], the ratio of the coefficients of the 1st and 2nd derivative terms changes sign, and this condition, for large value of ε, can be expected to cause trouble for conventional difference representations (see Appendix II). It is of interest to note that as $\varepsilon \to \infty$, then $\psi(x) \to H\left(x - \frac{1}{2}\right)$, the unit step function at $x = \frac{1}{2}$.

Results of two numerical experiments are given. In the first, the UDR will be compared against three standard difference representations for the simple form of the boundary conditions $\psi(o) = 0$, $\psi(1) = 1$. The second experiment compares standard Taylor series representations of derivative end conditions with representations derived according to the ideas of section 2.4.

For the experiment, the equation (2.5.1) is used with mixed end conditions contrived to yield the analytic solution

$$\psi(x) = \int_0^x e^{\frac{1}{2}\varepsilon x(1-x)} dx \qquad (2.5.3)$$

Appropriate end conditions are

$$\left(\frac{d\psi}{dx} + \psi\right)_{x=0} = 1$$

$$\left(\frac{d\psi}{dx}\right)_{x=1} = 1 \qquad (2.5.4)$$

This particular example is perhaps not the best for the purpose, since for moderate values of ε, the gradients of $\psi(x)$ in the region of the end points do not exhibit rapid changes - a circumstance in which it can be expected that Taylor representations become more inaccurate. Both of these experiments will be performed with several values of ε.

The First Experiment

Write h as the step length and

$$w(x) = \varepsilon\left(\tfrac{1}{2} - x\right) \qquad (2.5.5)$$

The four difference schemes considered are

The Unified Difference Representation (UDR)

$$\psi_{i+1} - (1 + e^{w(x)h})\,\psi_i + e^{w(x)h}\,\psi_{i-1} = 0 \qquad (2.5.6)$$

The Central Difference Representation (CDR)

$$(2 - w(x)\,h)\,\psi_{i+1} - 4\,\psi_i + (2 + w(x)\,h)\,\psi_{i-1} = 0 \qquad (2.5.7)$$

The Forward Difference Representation (FDR)

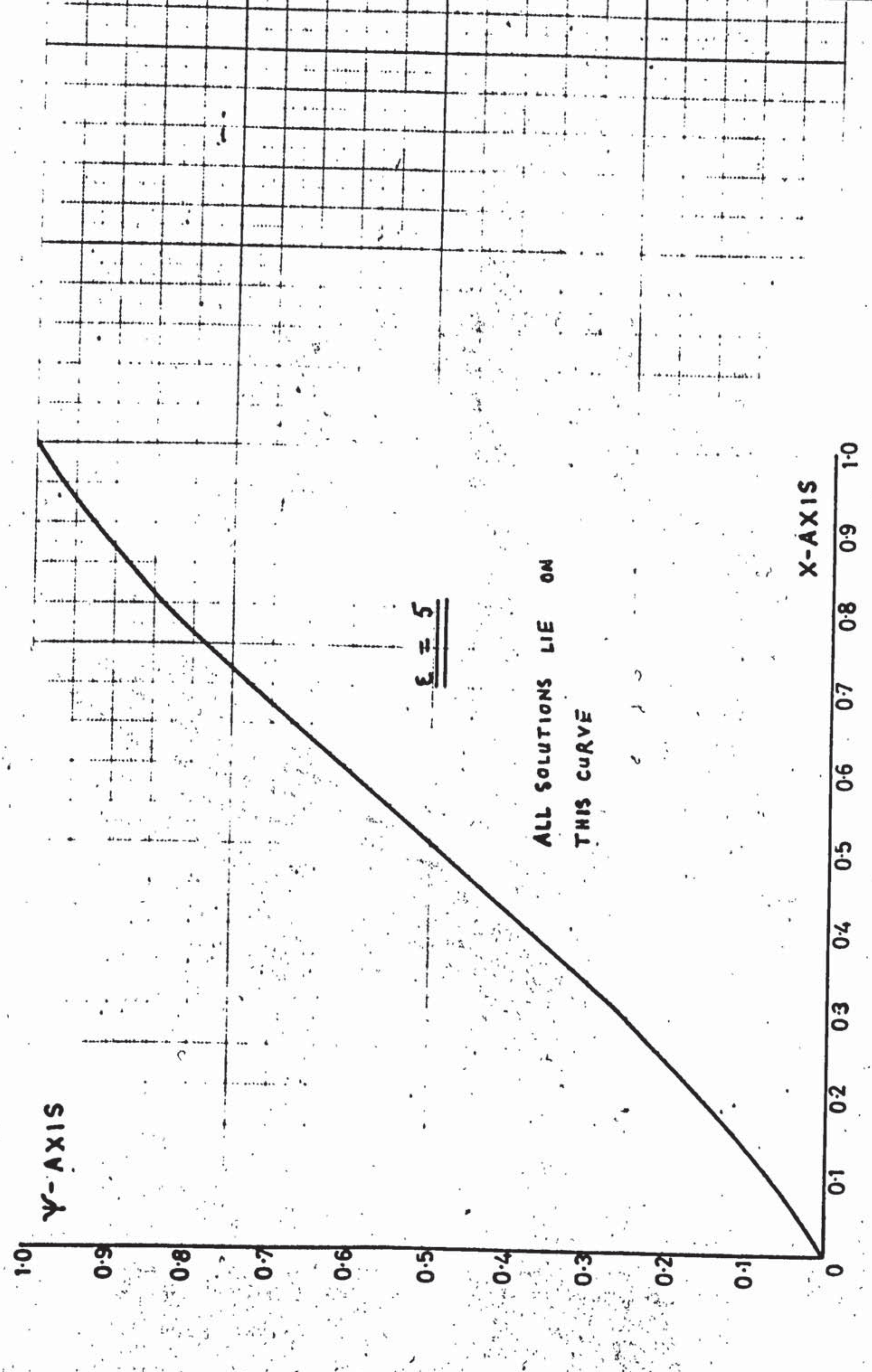
$$(1 - w(x)\,h)\,\psi_{i+1} - (2 - w(x)\,h)\,\psi_i + \psi_{i-1} = 0 \qquad (2.5.8)$$

The Backward Difference Representation (BDR)

$$\psi_{i+1} - (2 + w(x)\,h)\,\psi_i + (1 + w(x)\,h)\,\psi_{i-1} = 0 \qquad (2.5.9)$$

With $h = 0.1$, (2.5.1) was solved for integer values of ε for $0 \leq \varepsilon \leq 750$ using each of the four schemes above, with the simple boundary conditions $\psi(0) = 0$, $\psi(1) = 1$. The results are presented in Fig. 2.1 - 2.3 for $\varepsilon = 5, 100, 750$. For the case $\varepsilon = 0$, each of the

Figure 2.1


Y-AXIS
X-AXIS
ε = 5
ALL SOLUTIONS LIE ON
THIS CURVE
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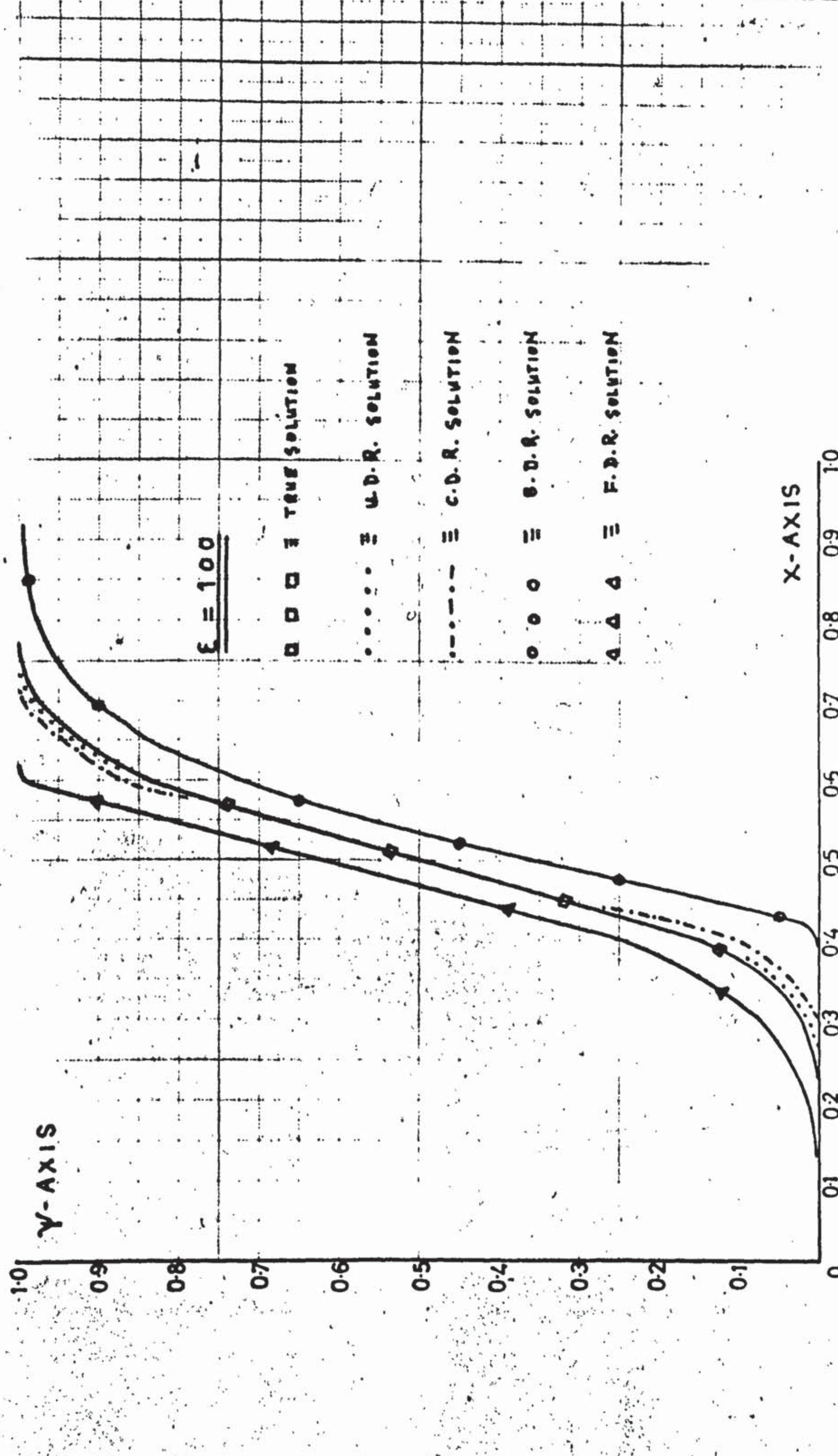
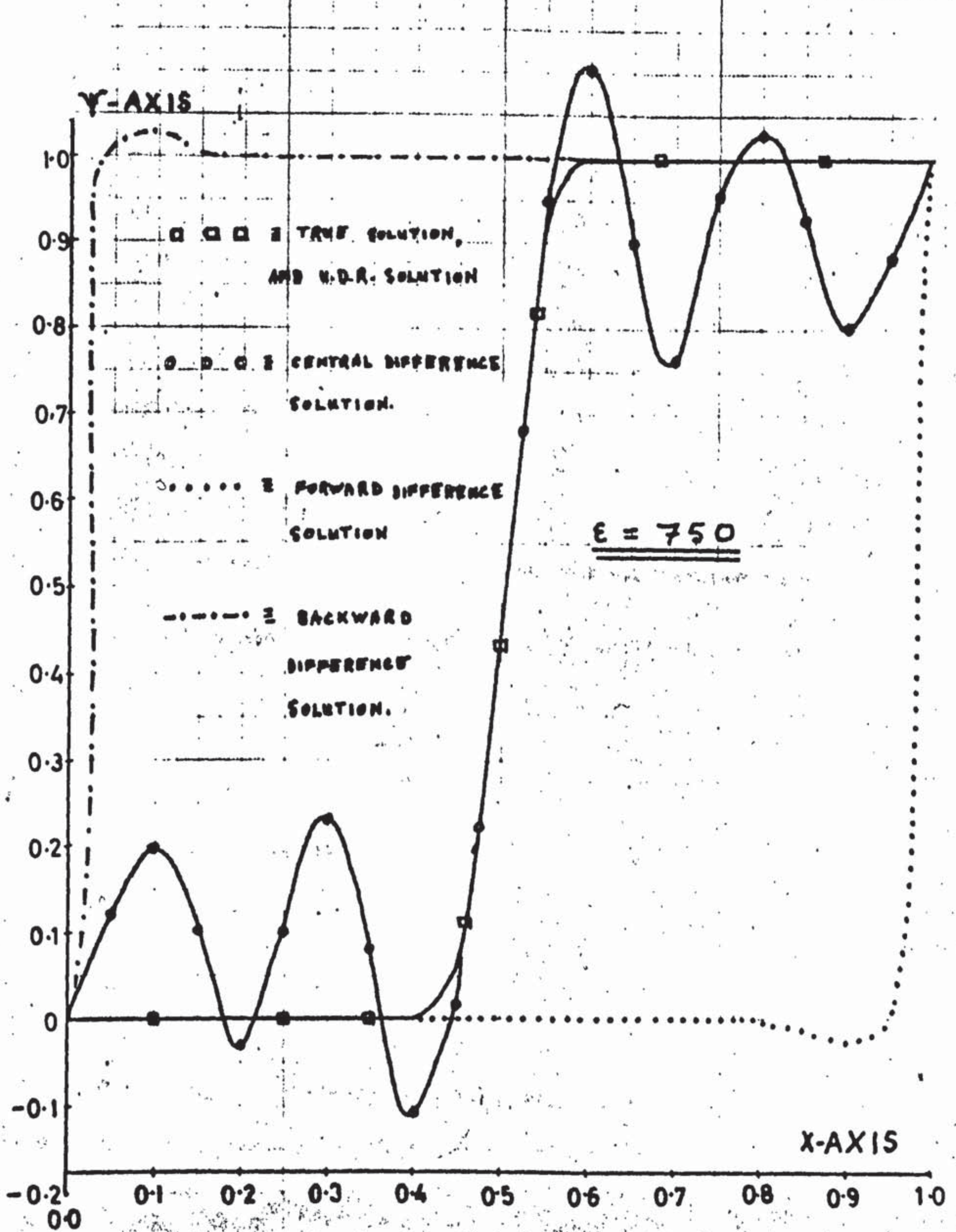
0·6
0·7
0·8
0·9
1·0

Figure 2.2



Y-AXIS
X-AXIS
ε = 100
≡ TRUE SOLUTION
≡ U.D.R. SOLUTION
≡ C.D.R. SOLUTION
≡ B.D.R. SOLUTION
≡ F.D.R. SOLUTION
0
0·1
0·2
0·3
0·4
0·5
0·6
0·7
0·8
0·9
1·0

Figure 2.3



Y-AXIS
1·0
0·9
0·8
0·7
0·6
0·5
0·4
0·3
0·2
0·1
0
-0·1
-0·2
0·0
0·1
0·2
0·3
0·4
0·5
0·6
0·7
0·8
0·9
1·0
X-AXIS
TRUE SOLUTION, AND N.D.R. SOLUTION
CENTRAL DIFFERENCE SOLUTION.
FORWARD DIFFERENCE SOLUTION
BACKWARD DIFFERENCE SOLUTION.
E = 750

schemes collapse into the same representation, and gives a straight line solution.

For $\varepsilon = 5$, it can be seen that there is not a great deal of discrepancy between the schemes, the error in each scheme being about the same over the whole interval [0, 1]. For $\varepsilon = 750$, it can be seen that the UDR is very accurate over the whole interval [0, 1], The CDR exhibits a Gibbs type oscillation (although not shown, this feature increases dramatically as ε increases) on both 'legs' of the step function. The BDR is good on (0,0.5) and very bad on (0.5,1). The FDR is very bad on (0,0.5) and very good on (0.5,1). For $\varepsilon = 100$, the results are midway between the two extreme cases.

These results are to be expected from the quantative analysis of Appendix II.

<u>The Second Experiment</u>

(i) <u>Equivalent Boundary Conditions for (2.5.3)</u>

Write equation (2.5.1) as

$$\frac{d^2\psi}{dx^2} - w(x)\frac{d\psi}{dx} = 0 \qquad (2.5.10)$$

If we solve (2.5.10) in a small region about $x = 0$ say $0 \leq x \leq h$, and assume that $w(x) \simeq w(h/2)$ in this region, we get

$$\psi(x) \simeq A_0 + A_1 e^{w(h/2)x} \qquad (2.5.11)$$

for $0 \leq x \leq h$. Suppose that this small region contains x_1, the first point in the discretisation of [0, 1] then (2.5.11) gives

$$A_0 + A_1 e^{w(h/2)x_1} - \psi_1 = 0$$

$$A_0 + A_1 - \psi_0 = 0 \qquad (2.5.12)$$

If the first of (2.5.4) is applied with (2.5.11), then the equation

$$A_1 w(h/2) + (A_0 + A_1) = 1 \qquad (2.5.13)$$

is obtained. Eliminating A_0 and A_1 between (2.5.11), (2.5.12) and (2.5.13) the relationship

$$\psi_0 (e^{x_1 w(h/2)} - w(h/2) - 1) + \psi_1 w(h/2) = e^{x_1 w(h/2)} - 1 \qquad (2.5.14)$$

is obtained. A similar calculation in a small region about $x = 1$ yields the relationship

$$\psi_n (2 - w - 2e^{-hw}) + w \psi_{n-1} = 1 - e^{-hw} \qquad (2.5.15)$$

where $w = w(1 - h/2)$

Relationships (2.5.14) and (2.5.15) are considered to be the finite difference equivalents of conditions (2.5.4).

(ii) Taylor Series Boundary Conditions for (2.5.3)

Forward and backward differences for $d\psi/dx$ at $x = 0,1$ are used to give

$$\left.\frac{\psi_1 - \psi_0}{h} + \psi_1 = 1 \right\} \qquad (2.5.16)$$

and

$$\left.\frac{\psi_n - \psi_{n-1}}{h} = 1 \right\} \qquad (2.5.16)$$

and central differences for $d\psi/dx$ at $x = 0,1$ are used to give

$$\frac{\psi_1 - \psi_{-1}}{2h} + \psi_o = 1$$

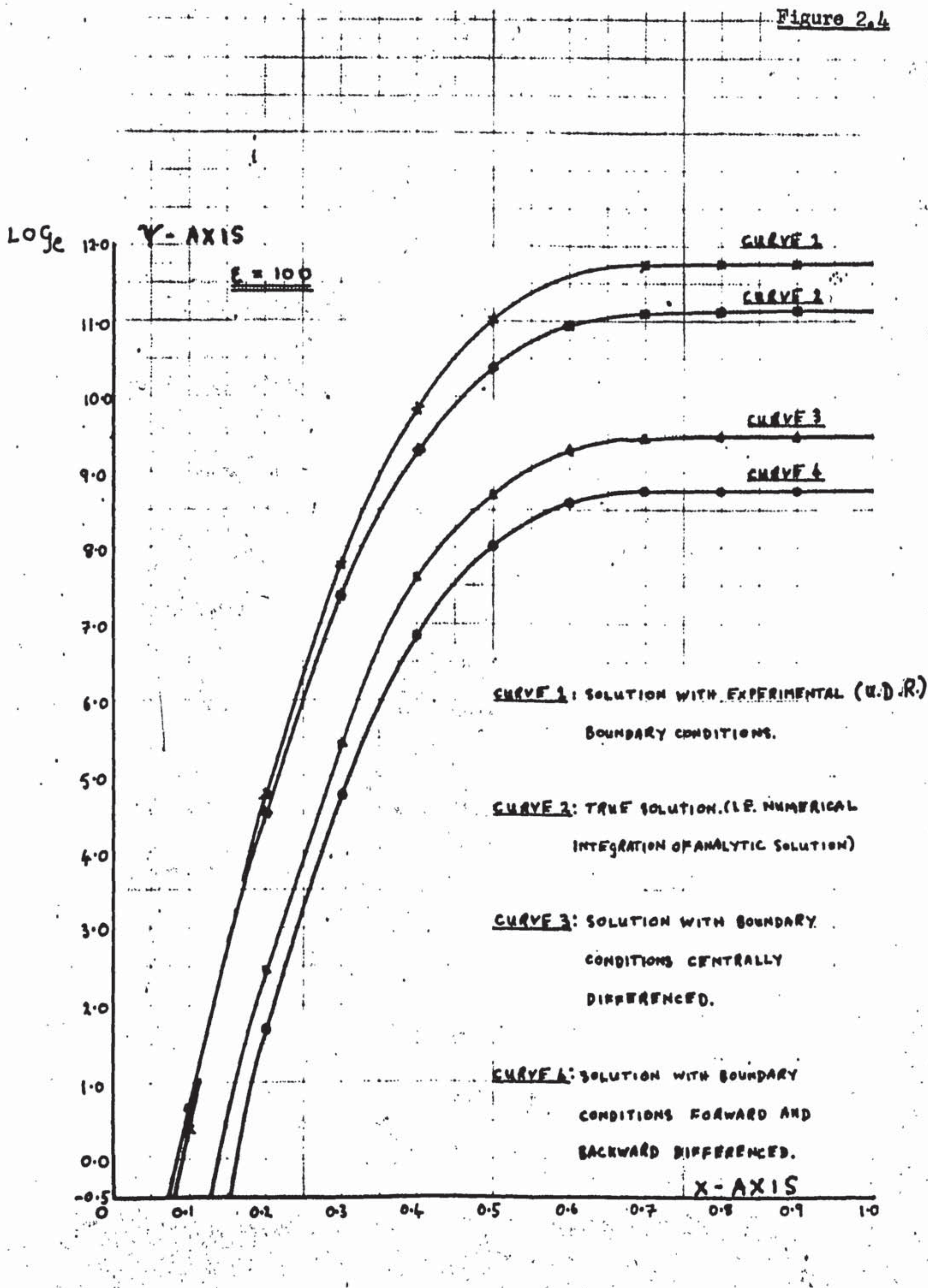
and

$$\frac{\psi_{n+1} - \psi_{n-1}}{2h} = 1 \qquad (2.5.17)$$

The numerical experiment was performed for $\varepsilon = (1, 2, 3, 5, 10, 20, 50, 100)$. In Fig. 2.4, the results for $\varepsilon = 100$ are depicted. A $\log_e$ scale has been used. Clearly, the new end point conditions give much better answers than the Taylor conditions. The forward/backward forms for the end conditions were consistently poor for all values of ε, whilst the central difference forms for these conditions were very good for $1 \leq \varepsilon \leq 10$, but for increasing values of ε, the central difference forms grow progressively worse.

Although in later chapters, the applications of the UDR's will be extended and shown to be very effective, no more will be said on these ideas for boundary condition formulations, mainly because for the applications that are contemplated in this thesis the boundary conditions are very simple. Whilst nothing conclusive has been demonstrated, the boundary condition examples cited suggest that the ideas might be worth investigating further.

Figure 2.4



LOGe Y-AXIS
E = 100
CURVE 1
CURVE 2
CURVE 3
CURVE 4
12·0
11·0
10·0
9·0
8·0
7·0
6·0
5·0
4·0
3·0
2·0
1·0
0·0
-0·5
0
0·1
0·2
0·3
0·4
0·5
0·6
0·7
0·8
0·9
1·0
X-AXIS
CURVE 1: SOLUTION WITH EXPERIMENTAL (U.D.R.) BOUNDARY CONDITIONS.
CURVE 2: TRUE SOLUTION. (I.E. NUMERICAL INTEGRATION OF ANALYTIC SOLUTION)
CURVE 3: SOLUTION WITH BOUNDARY CONDITIONS CENTRALLY DIFFERENCED.
CURVE 4: SOLUTION WITH BOUNDARY CONDITIONS FORWARD AND BACKWARD DIFFERENCED.

2.6 Local Truncation Error of UDR

The local truncation error is of order h^2, as will now be shown for a constant mesh.

The differential operator of (2.2.1) may be written

$$T = D^2 + f_1 D + f_2 \qquad (2.6.1)$$

The constant mesh UDR operator is

$$\hat{T}_i = \frac{f_{2i}\left(E - (e^{m_{0i}h} + e^{m_{1i}h}) + E^{-1} e^{(m_{0i} + m_{1i})h}\right)}{\left(1 + e^{(m_{0i} + m_{1i})h} - e^{m_{0i}h} - e^{m_{1i}h}\right)} \qquad (2.6.2)$$

where E is the forward shift operator ($Eg_k = g_{k+1}$)
Using the relationship $E = e^{hD}$ in (2.6.2) yields

$$\hat{T}_i = \frac{f_{2i}\left(e^{hD} - (e^{m_{0i}h} + e^{m_{1i}h}) + e^{-hD} e^{(m_{0i} + m_{1i})h}\right)}{1 + e^{(m_{0i} + m_{1i})h} - e^{m_{0i}h} - e^{m_{1i}h}} \qquad (2.6.3)$$

Note the relationships, for the auxiliary equation of (2.6.1)

$$\begin{aligned} m_{0i} + m_{1i} &= -f_{1i} \\ m_{0i}\, m_{1i} &= f_{2i} \end{aligned} \qquad (2.6.4)$$

Expand the exponential terms of (2.6.3) to obtain

$$\hat{T}_i = f_{2i}\,(1 + hD + \frac{h^2D^2}{2!} + \ldots)$$

$$- (2 + m_{0i}h + m_{1i}h + \frac{m_o^2h^2}{2!} + \frac{m_1^2h^2}{2!} + \ldots) +$$

$$(1 - hD + \frac{h^2D^2}{2!} + \ldots)\,(1 + \overline{m_{0i} + m_{1i}}\,h + \frac{\overline{m_{0i} + m_{1i}}^{\,2}}{2!}\,h^2 + \ldots))\,/$$

$$(1 + 1 + \overline{m_{0i} + m_{1i}}\;h + \overline{m_{0i} + m_{1i}}^{\,2}\,\frac{h^2}{2!} + \ldots - 1 - 1 - m_{0i}h - m_{1i}h$$

$$- m_{0i}^2\,\frac{h^2}{2!} - m_{1i}^2\,\frac{h^2}{2!} \quad \ldots) \tag{2.6.5}$$

If we neglect terms of higher order than h^4, and collect terms, then (2.6.5) becomes

$$\hat{T}_i \simeq \frac{h^2\,f_{2i}\,(D^2 + f_{1i}\,D + f_{2i})\,(1 - f_{1i}\,h/2) + 0\,(h^4)}{h^2\,f_{2i}\,(1 - f_{1i}\,h/2) + 0\,(h^4)}$$

$$= D^2 + f_{1i}\,D + f_{2i} + 0\,(h^2) \tag{2.6.6}$$

$$\therefore \quad T \simeq \hat{T}_i + 0\,(h^2) \tag{2.6.7}$$

and the result is proved. The result is also true for the variable mesh.

CHAPTER 3

THE PARTIAL DIFFERENTIAL EQUATION AND THE UNIFIED DIFFERENCE REPRESENTATIONS

3.1 The Problem

Consider the partial differential equation with constant coefficients

$$a \frac{\partial^2 \psi}{\partial x^2} + b \frac{\partial \psi}{\partial x} + c \frac{\partial^2 \psi}{\partial y^2} + d \frac{\partial \psi}{\partial y} + f\psi = g \qquad (3.1.1)$$

with ψ (boundary) specified. The possibility of mixed derivatives is ignored, since they do not fall naturally into what follows, and they do not normally arise in the situations that are to be considered. Furthermore, if they do arise, they can always be transformed away by a suitable co-ordinate transformation. The solution of a linear ordinary differential equation is a linear combination of a finite number of independent functions, (eg. $Ae^{m_0 x} + Be^{m_1 x}$ for a second order constant coefficient ordinary differential equation), and it is precisely this property which allows the explicit construction of a difference operator with an identical solution. However, the solution of (3.1.1) is generally a linear combination of an infinite number of independent functions, and it is thus by no means clear that the technique of Chapter 2 (ie. the direct formation of the auxiliary equation of the required difference equation from the known solution) can be applied to (3.1.1) to obtain a UDR whose solution is identical to that of (3.1.1). However, in the particular case of (3.1.1) being elliptic, it is shown in Appendix IV that a polynomial difference representation (one with a finite number of terms) does not exist.

A certain approach, necessary for elliptic equations, is developed and the ramifications of the approach applied to elliptic, parabolic and hyperbolic equations is studied.

Write (3.1.1) as

$$T_x \psi + T_y \psi = g \dagger \qquad (3.1.2)$$

It is proposed to derive the representations for T_x and T_y independently of each other and then to assume that these are additive to obtain the representation for $T_x + T_y$. This representation will be termed the UDR of (3.1.1).

In a sense this is a retrogressive approach, since the equation is split into distinct components which are to be treated independently, and this approach, in a more extreme form has been criticised earlier. However, it is one step removed from previous practice and as will be seen in later Sections of this Chapter it is sufficiently refined to guarantee a large measure of stability in the representations.

Having said this, the question arises, 'How should the term $f\psi$ of (3.1.1) be split between T_x and T_y?' To attempt an answer of this question, suppose that given ψ (boundary) = 0 a solution of (3.1.1) can be written as

$$\psi(x, y) = \sum_{i=1} F_i(x)\, G_i(y) + \text{Particular Integral} \qquad (3.1.3)$$

---

† T_x and T_y are the x and y differential operators respectively in (3.1.1).

where $F_i(x)\ G_i(y)$ is a separable solution of (3.1.1). Putting $\psi_i = F_i\ G_i$ in (3.1.1) and performing the usual algebra yields

$$a\frac{d^2\psi_i}{dx^2} + b\frac{d\psi_i}{dx} + (f - \lambda_i)\psi_i = 0 \qquad (3.1.4)$$

$$c\frac{d^2\psi_i}{dy^2} + d\frac{d\psi_i}{dy} + \lambda_i\psi_i = 0$$

these give

$$\left(a\frac{\partial^2\psi_i}{\partial x^2} + b\frac{\partial\psi_i}{\partial x} + (f - \lambda_i)\psi_i\right) + \left(c\frac{\partial^2\psi_i}{\partial y^2} + d\frac{\partial\psi_i}{\partial y} + \lambda_i\psi_i\right) = 0 \qquad (3.1.5)$$

Thus we see the solution $\psi(x, y)$ is a linear combination of components $F_i\ G_i$, each of which is associated by (3.1.5) with a particular splitting of $f\psi$ between T_x and T_y. Thus, in general it is not possible to attach any particular significance to a particular splitting of $f\psi$ between T_x and T_y, consequently the term '$f\psi$' is treated independently of $T_x\psi$ and $T_y\psi$. Accordingly, (3.1.1) is written as

$$T_x\psi + T_y\psi + f\psi = g$$

where

$$T_x = a\,\partial^2/\partial x^2 + b\,\partial/\partial x \qquad (3.1.6)$$

and

$$T_y = c\,\partial^2/\partial y^2 + d\,\partial/\partial y$$

To derive the UDR of (3.1.6) T_x and T_y are treated as ordinary differential operators and the procedure of Chapter 2 is applied. Thus, the homogenous solutions of

$$\left.\begin{aligned} T_x \psi &= 0 \\ T_y \psi &= 0 \end{aligned}\right\} \qquad (3.1.7)$$

are given by $A + Be^{-bx/a}$ and $C + De^{-dy/c}$ respectively. Thus the representations of (3.1.7) are found to be

$$\psi_{i+1j} - \psi_{ij}(1 + e_1) + \psi_{i-1j}\, e_1 = 0$$

where

$$e_1 = e^{-bh/a};\; h = x_i - x_{i-1} \qquad (3.1.8)$$

and

$$\psi_{ij+1} - \psi_{ij}(1 + e_2) + \psi_{ij-1}\, e_2 = 0$$

where

$$e_2 = e^{-dk/c};\; k = y_j - y_{j-1}$$

The UDR of (3.1.6) is now defined as

$$\lambda_1 (\psi_{i+1j} - \psi_{ij}(1 + e_1) + \psi_{i-1j}\, e_1)$$
$$+ \lambda_2 (\psi_{ij+1} - \psi_{ij}(1 + e_2) + \psi_{ij-1}\, e_2)$$
$$+ \lambda_3 f\, \psi_{ij} = g \qquad (3.1.9)$$

where λ_1, λ_2 and λ_3 are chosen according to certain criteria. Details are given in Appendix I, and they are found to be given by

$$\left.\begin{aligned} \lambda_1 &= \frac{b}{h(1 - e_1)} \\ \lambda_2 &= \frac{d}{k(1 - e_2)} \\ \lambda_3 &= 1 \end{aligned}\right\} \qquad (3.1.10)$$

A uniform mesh has been assumed. For notational simplicity, the (i, j) suffices have been omitted from a, b, c, d, f and g.

At this juncture, an interesting observation may be made about (3.1.9), with (λ_i) defined at (3.1.10). Suppose that $\pm$ b/a becomes large and positive, then

$$\lim_{\frac{b}{a}\to\infty} [\lambda_1 (\psi_{i+1j} - \psi_{ij} (1 + e_1) + \psi_{i-1j} e_1] = \frac{b}{h} (\psi_{i+1j} - \psi_{ij})$$

and

$$\lim_{\frac{-b}{a}\to\infty} [\lambda_1 (\psi_{i+1j} - \psi_{ij} (1 + e_1) + \psi_{i-1j} e_1] = \frac{b}{h} (\psi_{ij} - \psi_{i-1j}) \qquad (3.1.11)$$

ie. as $b/a \to +\infty$, forward difference schemes result, and as $b/a \to -\infty$, backward difference schemes result. Thus, in limiting situations, the UDR's as defined, contain the mixed forward/backward difference representations first proposed by Lelevier [50], in 1953, and others since.

The representation given at (3.1.9) forms the basis for our approximations of the velocity terms in the Navier-Stokes momentum equations.

3.2 Properties of the Unified Difference Representations

Property 1 The transformation from the second order partial differential operator to its UDR leaves invariant the hyperbolic [illegible] or elliptic nature of the operator, in that it satisfies the necessary condition (A3.2.7) for hyperbolicity or the sufficient condition for ellipticity, (A3.2.8), as the original operator is hyperbolic or elliptic respectively.†

It is plausible to assume that the invariance of operator type under the transformation to finite difference form is a necessary condition for the stability of the difference representation. With this assumption, Property 1 is a very useful property. As a counter example, consider the hyperbolic equation

$$\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi}{\partial y^2} - \lambda \frac{\partial \psi}{\partial y} = 0 \qquad (3.2.1)$$

this can be represented in Taylor series form as

$$\frac{(\psi_{i+1j} - 2\psi_{ij} + \psi_{i-1j})}{h^2} - \frac{(\psi_{ij+1} - 2\psi_{ij} + \psi_{ij-1})}{k^2} - \lambda \frac{(\psi_{ij} - \psi_{ij-1})}{k} = 0 \qquad (3.2.2)$$

The notation is self-explanatory. In order to classify the difference equation (3.2.2), (see Appendix III), it is re-arranged in the form

$$a\,\delta_i^{\,2}\,\psi_{ij} + c\,\delta_j^{\,2}\,\psi_{ij} + G(\psi_{ij}) = 0 \qquad (3.2.3)$$

where δ_i and δ_j are first order central difference operators a and c are coefficients, and G is a certain function of first order differences. Hence (3.2.2) is written as

† Parabolic equations are not considered since as shown in Appendix III their UDR's are not uniquely defined.

$$\frac{\psi_{i+1j} - 2\psi_{ij} + \psi_{i-1j}}{h^2} - (1 - \lambda k/2)\frac{\psi_{ij+1} - 2\psi_{ij} + \psi_{ij-1}}{k^2}$$

$$- \frac{\lambda}{2k}\left[(\psi_{ij+1} - \psi_{i-1j}) + (\psi_{i-1j} - \psi_{ij-1})\right] = 0 \qquad (3.2.4)$$

Thus defining

$$\delta_i U_i = \frac{U_{i+\frac{1}{2}} - U_{i-\frac{1}{2}}}{h} \qquad (3.2.5)$$

etc. then (3.2.4) may be written as

$$\delta_i^2 \psi_{ij} + (\frac{\lambda k}{2} - 1)\, \delta_j^2 \psi_{ij} = g[(\psi_{ij+1} - \psi_{i-1j}), (\psi_{i-1j} - \psi_{ij-1})] \qquad (3.2.6)$$

which is the required form. Thus, using the classifications given in Appendix III, (3.2.6) is hyperbolic if

$$(\frac{\lambda k}{2} - 1) < 0 \qquad (3.2.7)$$

and elliptic if

$$(\frac{\lambda k}{2} - 1) > 0 \qquad (3.2.8)$$

Thus, with the assumption of the previous page, (3.2.7) is a necessary condition for the stability of the hyperbolic equation.

Property 2 If the differential operator has Dirichlet boundary conditions and is negative-definite,† then all of the eigenvalues of the UDR lie in the left hand half complex plane. Thus, for any negative-definite differential operator, we are assured unconditional

† $f \leq 0$ in equation (3.1.1), with $a > 0$, $c > 0$.

Before discussing the second property of the UDR, it is necessary to expand on the nature of the operator in (3.1.1).

Assume that the set of all eigenfunctions (ψ_i) of the operator of (3.1.1) that are zero on the boundary of a region $(x, y) = [0, 1] \times [0, 1]$ together with a scalar product defined by

$$\langle \phi, \psi \rangle = \int_0^1 \int_0^1 \phi \, \bar{\psi} \, dx \, dy \quad \text{for } \phi, \psi \in \mathcal{H} \tag{3.2.8a}$$

is a Hilbert space, $\mathcal{H}$ say.

Then if, in (3.1.1), $a > 0$, $c > 0$ and $f < 0$ (a, b, c, d, f all constants) then the operator of (3.1.1) over $\mathcal{H}$ is the sum of a negative definite operator and a skew-adjoint operator.

<u>Proof</u>

In (3.1.1) let

$$\left.\begin{aligned} L_1 + L_2 \equiv L &\equiv \left(a\frac{\partial^2}{\partial x^2} + c\frac{\partial^2}{\partial y^2} + f\right) + \left(b\frac{\partial}{\partial x} + d\frac{\partial}{\partial y}\right) \\ \text{where} \quad & \\ L_1 &\equiv a\frac{\partial^2}{\partial x^2} + c\frac{\partial^2}{\partial y^2} + f \\ L_2 &\equiv b\frac{\partial}{\partial x} + d\frac{\partial}{\partial y} \end{aligned}\right\} \tag{3.2.8b}$$

If L_1 is negative definite then it is also self-adjoint and so $L_1 + L_2$ is the sum of self-adjoint and skew-adjoint operators if

$$\langle (L_1 + L_2)\, \phi,\ \psi \rangle = \langle \phi,\ (L_1 - L_2)\, \psi \rangle . \tag{3.2.8c}$$

L_1 over $\mathcal{H}$ is well-known to be negative definite and hence self-adjoint, thus we only need to prove that

$$\langle L_2\, \phi,\ \psi \rangle = - \langle \phi,\ L_2\, \psi \rangle \tag{3.2.8d}$$

we have

$$\begin{aligned}
\langle L_2\, \phi,\ \psi \rangle &= \int_0^1 \int_0^1 \psi \left(b \frac{\partial \phi}{\partial x} + d \frac{\partial \phi}{\partial y} \right) dx\, dy \\
&= \int_0^1 \left\{ \int_0^1 \psi\, b \frac{\partial \phi}{dx}\, dx \right\} dy + \\
&\quad \int_0^1 \left\{ \int_0^1 \psi\, d \frac{\partial \phi}{dy}\, dy \right\} dx \\
&= \int_0^1 \left\{ (b\, \psi\, \phi)_0^1 - \int_0^1 b\, \phi \frac{\partial \psi}{\partial x}\, dx \right\} dy + \\
&\quad \int_0^1 \left\{ (d\, \psi\, \phi)_0^1 - \right. \\
&\quad \left. \int_0^1 b\, \phi \frac{\partial \psi}{\partial y}\, dy \right\} dx \\
&= - \int_0^1 \int_0^1 \phi \left(b \frac{\partial \psi}{\partial y} + d \frac{\partial \psi}{\partial y} \right) dx\, dy \\
&= - \langle \phi,\ L_2\, \psi \rangle
\end{aligned} \tag{3.2.8e}$$

and thus L_2 is skew-adjoint.

Hence $L = L_1 + L_2$ is the sum of positive definite and skew-adjoint operators. This leads to the main result that

Theorem

Every eigenvalue of L lies in the left hand complex plane.

Proof

Let λ be an eigenvalue of L and let ψ be a corresponding eigenfunction, then

$$(L_1 + L_2)\,\psi = \lambda\,\psi \tag{3.2.8f}$$

therefore

$$\langle (L_1 + L_2)\,\psi,\ \psi \rangle = \langle \lambda\,\psi,\ \psi \rangle \tag{3.2.8g}$$

therefore $\langle L_1\,\psi,\ \psi \rangle + \langle L_2\,\psi,\ \psi \rangle = \lambda \langle \psi,\ \psi \rangle$ (3.2.8h)

Since L_1 is negative definite, then $\langle L_1\,\psi,\ \psi \rangle = -\,\omega^2$ for some real ω, and since L_2 is skew-adjoint then $\langle L_2\,\psi,\ \psi \rangle = jx$ for some real x thus, (3.2.8h) can be written as

$$-\,\omega^2 + jx = \lambda \langle \psi,\ \psi \rangle \tag{3.2.8i}$$

therefore $\text{Real}\,(\lambda) = \dfrac{-\,\omega^2}{\langle \psi,\ \psi \rangle} < 0$ (3.2.8j)

the result is therefore proven.

Property 2

The matrix of the UDR of (3.1.1) for Dirichlet boundary conditions; and for $a > 0$, $c > 0$, $f < 0$ has all of its eigenvalues in the left hand complex plane, as they are for L. This property holds for all step lengths and all values of b and d. Such a property is highly desirable from a numerical viewpoint, since it virtually assures us that the numerical problem will be well conditioned.

Proof of Property 1

Consider the differential equation

$$a \frac{\partial^2 \psi}{\partial x^2} + b \frac{\partial \psi}{\partial x} + c \frac{\partial^2 \psi}{\partial y^2} + d \frac{\partial \psi}{\partial y} + g \psi = f \qquad (3.2.10)$$

where $a \neq 0$, $c \neq 0$.

The UDR representation of (3.2.10) is

$$\begin{aligned} & r_1 \left(\psi_{i+1j} - \psi_{ij} (r_2 + 1) + \psi_{i-1j} r_2\right) \\ & + s_1 \left(\psi_{ij+1} - \psi_{ij} (s_2 + 1) + \psi_{ij-1} s_2\right) \\ & + g \psi_{ij} = f \end{aligned} \qquad (3.2.11)$$

where

$$\left.\begin{aligned} r_2 (h_i, h_{i+1}, a, b) &= \frac{\exp(-b (h_i + h_{i+1})/a) - 1}{\exp(-bh_i/a) - 1} \\ r_1 (h_i, h_{i+1}, a, b) &= \frac{b}{(h_{i+1} - h_i r_2)} \\ \text{and} \quad s_2 &= r_2 (k_j, k_{j+1}, d, c) \\ s_1 &= r_1 (k_j, k_{j+1}, d, c) \end{aligned}\right\} \qquad (3.2.12)$$

For notational simplicity, the (i, j) suffices on a, b, c, d, r_1, r_2, s_1 and s_2 are left out. Details of the derivations are given in Appendix I. To classify (3.2.11) according to the method of Appendix III, write (3.2.11) in the form of (A3.7.5).

To this end, notice that

$$\begin{aligned} & \psi_{i+1j} - \psi_{ij} (1 + r_2) + r_2 \psi_{i-1j} \\ & = \frac{(1 + r_2)}{2} (\psi_{i+1j} - 2 \psi_{ij} + \psi_{i-1j}) + \frac{(1 - r_2)}{2} (\psi_{i+1j} - \psi_{i-1j}) \end{aligned} \qquad (3.2.13)$$

Thus, equation (3.2.11) may be written

$$r_1 \frac{(1 + r_2)}{2} (\psi_{i+1j} - 2\psi_{ij} + \psi_{i-1j}) + S_1 \frac{(1 + s_2)}{2} (\psi_{ij+1} - 2\psi_{ij} + \psi_{ij-1})$$

$$= f - g\psi_{ij} - r_1 \frac{(1 - r_2)}{2} (\psi_{i+1j} - \psi_{i-1j}) - S_1 \frac{(1 - S_2)}{2} (\psi_{ij+1} - \psi_{ij-1}) \qquad (3.2.14)$$

Hence

$$r_1 \frac{(1 + r_2)}{2} \delta_i^2 \psi_{ij} + S_1 \frac{(1 + S_2)}{2} \delta_j^2 \psi_{ij}$$

$$= h\,[(\psi_{i+1j} - \psi_{i-1j}), (\psi_{ij+1} - \psi_{ij-1})] \qquad (3.2.15)$$

δ_i and δ_j are central difference operators.† (3.2.15) is now in the required form.

Following the procedure of A3.2, if

$$\left.\begin{aligned} \hat{a} &= r_1 \frac{(1 + r_2)}{2} \\ &\text{and} \\ \hat{c} &= S_1 \frac{(1 + S_2)}{2} \end{aligned}\right\} \qquad (3.2.16)$$

then to prove the result, it is sufficient to prove that when

$$\left.\begin{aligned} \hat{a}\hat{c} > 0 \text{ then } ac > 0 \\ \hat{a}\hat{c} < 0 \text{ then } ac < 0 \end{aligned}\right\} \qquad (3.2.17)$$

It is sufficient to prove that iff $a \gtrless 0$ then $\hat{a} \gtrless 0$, since if this is true then because c is similar to a, it is also true that iff

† The difference operators δ_i and δ_j are now defined by $\delta_i \psi_i = \psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}$ and by $\delta_j \psi_j = \psi_{j+\frac{1}{2}} - \psi_{j-\frac{1}{2}}$.

$c \gtrless 0$ implies $\hat{c} \gtrless 0$ and hence (3.2.17) follows. By (3.2.12) $r_2 > 0$, for all a and b, hence by (3.2.16), it is possible to work in terms of r_1 rather than $\hat{a}$. Consider then

$$\lambda = r_1 = b/[h_{i+1} - h_i e^{-bh_i/a} \left(\frac{e^{-bh_{i+1}/a} - 1}{e^{-bh_i/a} - 1}\right)] \tag{3.2.18}$$

where $a \neq 0$.

It is to be proved that

$$\text{Sign}(\lambda) = \text{Sign}(a) \tag{3.2.19}$$

For simplicity write $-b/a = c$, where the subscripts are implied. Then if $B(c)$ is defined as the denominator of (3.2.18) then

$$\lambda = \frac{b}{B(c)} \tag{3.2.20}$$

or

$$\lambda = -a\frac{c}{B(c)} \tag{3.2.21}$$

The proof of (3.2.19) will have the structure

(i) Prove that $B(c)$ has a zero at $c = 0$

(ii) Prove that $B(c)$ is monotonic in c and therefore that $c = 0$ is the only zero of $B(c)$

(iii) Note from (ii) that $c/B(c)$ must be single signed, and then prove that the sign is negative

(iv) Hence (3.2.19) will follow

(i) $B(c) = 0$

<u>Proof</u> $$\lim_{c\to 0} B(c) = \lim_{c\to 0}\left\{h_{i+1} - h_i\, e^{+ch_i}\left(\frac{e^{+ch_{i+1}} - 1}{e^{+ch_i} - 1}\right)\right\} \qquad (3.2.22)$$

$$= h_{i+1} - h_i\left(\frac{h_{i+1}}{h_i}\right) = 0 \qquad (3.2.23)$$

by L'Hopitals rule. Hence

$$\lim_{c\to 0} B(c) = 0 \qquad (3.2.24)$$

Thus (i) is proved.

(ii) B(c) is monotonic in c

<u>Proof</u> The result is immediate if $h_1 = h_2 = h_3 = \dots$

Now B(c) is monotonic in c if $\widetilde{B}(c)$ defined by

$$\widetilde{B}(c) = -\left(\frac{B(c) - h_{i+1}}{h_i}\right) + 1 \qquad (3.2.25)$$

is monotonic in c. It is found convenient to consider the monotonic nature of $\widetilde{B}(c)$. From (3.2.25)

$$\widetilde{B}(c) = \frac{e^{+c(h_i + h_{i+1})} - 1}{e^{+ch_i} - 1} \qquad (3.2.26)$$

write $k = h_i + h_{i+1}$ and $k_1 = h_i$, then

$$\widetilde{B}(c) = \frac{e^{+ck} - 1}{e^{+ck_1} - 1}\ ;\ k > k_1 > 0 \qquad (3.2.27)$$

$\widetilde{B}(c)$ may be considered as the quotient of two positive functions, since the numerator and denominator are positive and negative together.

Use is now made of the following result:

If L_1 and L_2 are positive functions, and δL_1 and δL_2 are positive increments, then

$$\frac{L_1 + \delta L_1}{L_2 + \delta L_2} \geq \frac{L_1}{L_2} \quad \text{iff} \quad \frac{\delta L_1}{\delta L_2} \geq \frac{L_1}{L_2} \qquad (3.2.28)$$

This is easily verified. It follows from (3.2.28) and (3.2.27) that

$$\widetilde{B}(c + \delta c) \geq \widetilde{B}(c), \qquad \delta c \geq 0 \qquad (3.2.29)$$

iff

$$\frac{k\, e^{ck}\, \delta c}{k_1\, e^{ck_1}\, \delta c} \geq \frac{e^{ck} - 1}{e^{ck_1} - 1} \qquad (3.2.30)$$

(3.2.30) reduces to the requirement that

$$\frac{1}{k_1}\, (1 - e^{-ck_1}) \geq \frac{1}{k}\, (1 - e^{-ck}), \qquad c \geq 0$$

and

$$\frac{1}{k_1}\, (e^{-ck_1} - 1) \geq \frac{1}{k}\, (e^{-ck} - 1), \quad c < 0 \qquad (3.2.31)$$

It suffices to prove the first of (3.2.31).

Certainly, equality holds when $k = k_1$.

As $k \to \infty$, then the inequality certainly holds, since $k > k_1$.

Thus, if the RHS of the inequality is monotonic in k, then the inequality is true for all $k > k_1$, and hence since $c \geq 0$ is arbitrary, for all $c \geq 0$.

To prove monotonicity of

$$A(k) = \frac{1}{k}(1 - e^{-ck}) \tag{3.2.32}$$

$$\frac{dA}{dK} = \frac{1}{k^2}\ k(c\,e^{-ck}) - (1 - e^{-ck})$$

$$= \frac{1}{k^2}\left\{\frac{1 + ck}{e^{ck}} - 1\right\} \tag{3.2.33}$$

therefore, since $\frac{1 + ck}{e^{ck}} < 1$ for $c > 0$, then

$$\frac{dA}{dk} < 0 \tag{3.2.34}$$

for all $k > k_1$. Similarly, the second of (3.2.31) can be proven. Hence $B(c)$ is monotonic in c.

(iii) It follows from (i), (ii) and (iii) that $c/B(c)$ must be single signed. It will now be proved that

$$\frac{c}{B(c)} < 0 \tag{3.2.35}$$

It suffices to demonstrate the truth of (3.2.35) for one value of c. Thus, consider

$$\lim_{c \to -\infty} \frac{c}{B(c)} = \lim_{c \to -\infty} \frac{c}{h_{i+1}} < 0 \tag{3.2.36}$$

using definition of $B(c)$ given at (3.2.22).

Hence (3.2.35) is true, and from (3.2.21) there follows

$$\text{Sign}(\lambda) = \text{Sign}(a) \tag{3.2.38}$$

and (3.2.19) has been proved. Thus, the conditions of (3.2.13) are satisfied and therefore Property 1 is established.

Proof of Property 2

If the differential equation has the general form

$$a\frac{\partial^2 \psi}{\partial x^2} + b\frac{\partial \psi}{\partial x} + c\frac{\partial^2 \psi}{\partial y^2} + d\frac{\partial \psi}{\partial y} - f\psi = 0 \tag{3.2.39}$$

where $a > 0$, $c > 0$, and $f > 0$ with ψ specified on the boundary, then it is negative-definite. To prove Property 2, it is sufficient to prove that the matrix of the UDR is strictly or irreducibly diagonally dominant and that every diagonal element has the same sign. The UDR of (3.2.39) is, from (3.2.11)

$$r_1\left(\psi_{i+1j} - \psi_{ij}(r_2+1) + \psi_{i-1j}\, r_2\right)$$

$$+ S_1\left(\psi_{ij+1} - \psi_{ij}(S_2+1) + \psi_{ij-1}\, S_2\right) - f\psi_{ij} = 0 \tag{3.2.40}$$

where, since $a > 0$, $c > 0$ using (3.2.19)

$$\left.\begin{aligned} r_1 &> 0 \\ S_1 &> 0 \end{aligned}\right\} \tag{3.2.41}$$

also

$$r_2 = e^{-b\,h_i/a}\left\{\frac{e^{-b\,h_{i+1}/a} - 1}{e^{-b\,h_i/a} - 1}\right\} \tag{3.2.42}$$

S_2 is defined in a similar fashion. Clearly r_2, and thus S_2, is positive.

The sum of the diagonal terms is, from (3.2.40), given by

$$S_D = -(r_1(1 + r_2) + S_1(1 + S_2) + f) \tag{3.2.43}$$

and of the off-diagonal terms by

$$S_{OD} = r_1 + r_1 r_2 + S_1 + S_1 S_2 \tag{3.2.44}$$

Now either $f = 0$ or $f > 0$. In the case $f = 0$, we have

$$S_D = -S_{OD} \tag{3.2.45}$$

for all matrix rows corresponding to points not adjoining a boundary, and

$$S_D > -S_{OD} \tag{3.2.46}$$

for all matrix rows corresponding to points adjacent to a boundary.

Thus, the matrix is diagonally dominant with all the diagonal elements negative, and all off-diagonal elements positive, and with strict diagonal dominance in at least one row. The matrix is irreducible since it represents an elliptic operator. The matrix is therefore irreducibly diagonally dominant.

If f $>$ 0, the strict diagonal dominance of the matrix is immediate. Thus, the matrix of the UDR of (3.2.39) has all of its eigenvalues with non-zero positive real parts. Property 2 is proven.

CHAPTER 4

THE NAVIER-STOKES EQUATIONS, THEIR DIFFERENCE REPRESENTATIONS AND THE STABILITY OF THESE REPRESENTATIONS

4.1 Cartesian Equations

The equations considered represent the three dimensional equations with a laminar viscous model. Initially, the Cartesian form on an orthogonal box will be considered. These are given by

$$\begin{pmatrix} T & 0 & 0 & +\partial/\partial x \\ 0 & T & 0 & +\partial/\partial y \\ 0 & 0 & T & +\partial/\partial z \\ +\partial/\partial x & +\partial/\partial y & +\partial/\partial z & 0 \end{pmatrix} \begin{pmatrix} u \\ v \\ w \\ p \end{pmatrix} = 0 \qquad (4.1.1)$$

where

$$T = -\frac{\mu}{\rho}\nabla^2 + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z} \qquad (4.1.2)$$

(notation is explained in the Glossary, but unless stated in the text, standard notations have been used).

Dirichlet conditions on u, v and w are assumed. The equations will be discretised on a uniform mesh so that $(x, y, z) \rightarrow (i\,\Delta x, j\,\Delta y, k\,\Delta z)$. The representation of T is the UDR derived in Appendix I. In the case of the Navier-Stokes equations, the coefficients of the first derivatives of the velocities are also velocities, and are therefore unknown. Thus, the coefficients in the difference equations will also be unknown functions of velocities. In the iterative solution procedure to be described in Chapter 5, these functions will be assumed known from the previous iteration. Let the representation of T be $\hat{T}$.

Thus, $\hat{T}$ is defined by

$$\hat{T}\,\psi_{ijk} = \frac{+\,\rho\, u_{ijk}}{\Delta x\,(1 - h\,(u_{ijk}, \Delta x))} \Big\{ \psi_{i+1ij} - \psi_{ijk}\,(1 + h\,(U_{ijk}, \Delta x))$$

$$+ \psi_{i-1jk}\, h\,(U_{ijk}, \Delta x)\Big\} + \frac{V_{ijk}}{\Delta y\,(1 - h\,(V_{ijk}, \Delta y))}\cdot$$

$$\Big\{\psi_{ij+1k} - \psi_{ijk}\,(1 + h\,(V_{ijk}, \Delta y)) + \psi_{ij-1k}\, h\,(V_{ijk}, \Delta y)\Big\}$$

$$+ \frac{W_{ijk}}{\Delta z\,(1 - h\,(W_{ijk}, \Delta z))}\cdot$$

$$\Big\{\psi_{ijk+1} - \psi_{ijk}\,(1 + h\,(W_{ijk}, \Delta z)) + \psi_{ijk-1}\, h\,(W_{ijk}, \Delta z)\Big\}$$

where $h\,(a, b) = \exp\,(\rho\, ab/\nu\,)$ (4.1.3)

It is known, from the form of (4.1.2) and from Property 2 of Chapter 3, that the matrix corresponding to T will be strictly diagonally dominant for all μ , ρ , Δx, Δy and Δz. $(\nu = \mu/\rho)$

The question now arises 'How are the operators $\partial/\partial x$, $\partial/\partial y$ and $\partial/\partial z$ corresponding to the pressure derivatives and continuity equation to be represented?' Suppose that central differences defined by

$$\frac{\partial}{\partial x}\,\psi_i \simeq \frac{\psi_{i+1} - \psi_{i-1}}{2\Delta x} \qquad (4.1.4)$$

are appropriate for use in (4.1.1). Their use will subsequently be justified. Let

$$H_1 \psi_{ijk} = \frac{\psi_{i+1jk} - \psi_{i-1jk}}{2\Delta x}$$

$$H_2 \psi_{ijk} = \frac{\psi_{ij+1k} - \psi_{ij-1k}}{2\Delta y}$$

$$H_3 \psi_{ijk} = \frac{\psi_{ijk+1} - \psi_{ijk-1}}{2\Delta z} \qquad (4.1.5)$$

then if $\hat{\underline{I}}$, $\underline{H}_1$, $\underline{H}_2$, $\underline{H}_3$ are the matrices of the difference operators then the representation of (4.1.1) becomes

$$\begin{pmatrix} \hat{\underline{T}} & 0 & 0 & \underline{H}_1 \\ 0 & \hat{\underline{T}} & 0 & \underline{H}_2 \\ 0 & 0 & \hat{\underline{T}} & \underline{H}_3 \\ \underline{H}_1 & \underline{H}_2 & \underline{H}_3 & 0 \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{v} \\ \underline{w} \\ \underline{p} \end{pmatrix}_{ijk} = \begin{pmatrix} \underline{h}_u \\ \underline{h}_v \\ \underline{h}_w \\ \underline{h}_c \end{pmatrix}_{\text{boundary}} \qquad (4.1.6)$$

where $\underline{T}$ is defined at (4.1.3), and 0 indicates an empty matrix. In what follows it will be assumed that the right hand side of (4.1.6) is known. This is not entirely true of p on the boundary since although the velocity field entirely determines the pressure field (to within a constant), pressure is not known on the boundaries until the full solution has been obtained.

4.2 Stability of the Representations of the Navier-Stokes Equations

The linearised system (4.1.6) is stable, if the eigenvalues of the matrix of (4.1.6) all lie in the right hand ½ complex plane. It will be shown in Chapter 5 that (4.1.6), with $\hat{\underline{T}}$ defined at (4.1.3), is satisfactory from the point of view of obtaining numerical solutions.

Unfortunately, the present author has not been able to make any categorical statements about the stability of (4.1.6) with $\hat{T}$ defined at (4.1.3). However, by slightly modifying the definition of $\hat{T}$, it has been possible to assert that the subsequently modified version of (4.1.6) is unconditionally stable† (given the stated assumptions of linearisation, and of p (boundary) known).

Two results are required.

Theorem 4.2.1

If a matrix A is such that

(i) $\qquad a_{ij} \leq 0$ all $i \neq j$

(ii) $\qquad a_{ii} \geq -\frac{1}{2}\sum_{\substack{j=1 \\ j\neq i}}^{n} (a_{ij} + a_{ji})$

then A may be written as $A_{sy} + A_{sk}$, where A_{sy} is a positive semi-definite symmetric matrix, and A_{sk} is some skew-symmetric matrix.

Proof

Any matrix can be written as the sum of a symmetric and a skew-symmetric matrix, therefore write

$$A = A_{sy} + A_{sk} \tag{4.2.1}$$

It follows that

$$A^{*} = A_{sy} - A_{sk} \tag{4.2.2}$$

---

† In the sense that every eigenvalue of the new matrix has a positive real part.

Equations (4.2.1) and (4.2.2) give

$$A_{sy} = \frac{1}{2}(A + A^{*}) \tag{4.2.3}$$

Since $a_{ij} \leq 0$, $i \neq j$ by condition (i), then the sum of the moduli of the off-diagonal elements of A_{sy} of the i-th row is given by

$$S = -\frac{1}{2} \sum_{\substack{j=1 \\ i \neq j}}^{n} (a_{ij} + a_{ji}) \tag{4.2.4}$$

The i-th diagonal element of A_{sy} is a_{ii}, and therefore by condition (ii), the matrix A_{sy} is diagonally dominant. By (i) and (ii), $a_{ij} \leq 0$ for all $i \neq j$ and $a_{ii} \geq 0$ for all i. Hence A_{sy} is positive semi-definite.

Corollary

If A of the previous theorem is

(i) such that $a_{ij} \neq 0$ if and only if $a_{ji} \neq 0$ for $i \neq j$ (ie is symmetric wrt. the displacement of its off-diagonal elements)

(ii) irreducible

(iii) such that the strict inequality of condition (ii) of the previous theorem holds at least once,

then A_{sy} is irreducibly diagonally dominant. It will then follow that A_{sy} is positive definite.

Let $A = (a_{ij})$, $A_{sy} = (\hat{a}_{ij})$, $A_{sk} = (\tilde{a}_{ij})$, $G(B) \equiv$ the directed graph of a matrix B, [46].

The proof will then have the following structure

(a) prove that $\hat{a}_{ij} \neq 0$ if and only if $a_{ij} \neq 0$ for $i \neq j$

(b) hence $G(A_{sy}) \equiv G(A)$

(c) note that since A is irreducible, then G (A) is strongly connected, and therefore $G(A_{sy})$ is also strongly connected, and therefore, A_{sy} is irreducible, [46]. By condition (iii), A_{sy} is then irreducibly diagonally dominant, and ∴ positive definite.

Proof

(a) From the previous theorem

$$a_{ij} = \hat{a}_{ij} + \tilde{a}_{ij} \tag{4.2.5}$$

Suppose that $a_{ij} = 0$ for $i \neq j$, then by statement of the corollary $a_{ji} = 0$. Thus, by (4.2.5)

$$\hat{a}_{ij} + \tilde{a}_{ij} = 0 \quad , \quad i \neq j \tag{4.2.6}$$

and

$$\hat{a}_{ij} - \tilde{a}_{ij} = 0 \quad . \quad i \neq j \tag{4.2.7}$$

(this last comes from $a_{ji} = \hat{a}_{ji} + \tilde{a}_{ji} = \hat{a}_{ij} - \tilde{a}_{ij}$)

Equations (4.2.6) and (4.2.7) give $\hat{a}_{ij} = 0 = \tilde{a}_{ij}$. Thus, if $a_{ij} = 0$, then $\hat{a}_{ij} = 0$ for $i \neq j$.

Now consider $\hat{a}_{ij} = 0$ for $i \neq j$. Symmetry of A_{sy} gives $\hat{a}_{ji} = 0$. Equation (4.2.5) then gives

$$a_{ij} - \tilde{a}_{ij} = 0 \quad i \neq j \tag{4.2.8}$$

and

$$a_{ji} + \tilde{a}_{ij} = 0 \quad i \neq j \tag{4.2.9}$$

Hence

$$a_{ij} + a_{ji} = 0 \quad i \neq j \tag{4.2.10}$$

Since A is such that $a_{ij} \leq 0$, $i \neq j$ (from the conditions of theorem 4.2.1), then (4.2.10) gives $a_{ij} = 0$ if $\hat{a}_{ij} = 0$. Thus, we have obtained that $\hat{a}_{ij} = 0$ if and only if $a_{ij} = 0$ for $i \neq j$, which is equivalent to $\hat{a}_{ij} \neq 0$ if and only if $a_{ij} \neq 0$ for $i \neq j$.

The result now follows from (b) and (c) of the proof structure.

Theorem 4.2.2

If P_1 is an nxn positive/definite symmetric matrix and P is a kxk (k>n) matrix having the form $\begin{pmatrix} P_1 & 0 \\ 0 & 0 \end{pmatrix}$ and S is a kxk skew-symmetric matrix having the form $\begin{pmatrix} 0 & S_1 \\ -S_1^* & 0 \end{pmatrix}$ (note that S_1 is not necessarily square), such that P + S is non-singular, then every eigenvalue of P + S has a positive real part.

Proof

Suppose that $\underline{x}^* = (\underline{x}_1^*, \underline{x}_2^*)$ is a normalised eigenvector of P + S with corresponding eigenvalue $\lambda + jw$. Then

$$\lambda + jw = \underline{x}^* (P + S) \underline{x}$$

$$= \underline{x}_1^* P_1 \underline{x}_1 + \underline{x}^* S \underline{x} \tag{4.2.11}$$

Thus,

$$\left.\begin{aligned} \lambda &= \underline{x}_1^* \; P_1 \, \underline{x}_1 \\ jw &= \underline{x}^* \; S \; \underline{x} \end{aligned}\right\} \qquad (4.2.12)$$

For $\lambda > 0$, we require only that $\underline{x}_1 \neq 0$, since P_1 is positive definite. But, if $\underline{x}_1 = 0$, then $jw = 0$ since

$$\begin{aligned} jw &= \underline{x}^* \; S \, \underline{x} = -\underline{x}_2^* \; S_1 \; \underline{x}_1 + \underline{x}_1^* \; S_1 \, \underline{x}_2 \\ &= 0 \text{ if } \underline{x}_1 = 0 \end{aligned} \qquad (4.2.13)$$

Thus, since (P + S) is non-singular, all eigenvalues are non-zero and therefore $\underline{x}_1 \neq 0$ giving

$$\lambda = \underline{x}_1^* \; P_1 \, \underline{x}_1 > 0 \qquad (4.2.14)$$

to establish the result.

Having established these two results, it is possible to consider the stability of a modified form of (4.1.6). From (4.1.3), with an obvious notation, it is possible to write

$$\begin{aligned} \hat{T} \, \psi_{ijk} = \; & f_i \, \psi_{i+1jk} - (f_i + f_i \, g_i) \, \psi_{ijk} + f_i \, g_i \, \psi_{i-1jk} \\ & + \text{(Similar terms for j, k differences)} \end{aligned} \qquad (4.2.15)$$

$\hat{T}$ is modified to $\tilde{T}$, where $\tilde{T}$ is defined by

$$\begin{aligned} \tilde{T} \, \psi_{ijk} = \; & f_{i+1} \, \psi_{i+1jk} - \tfrac{1}{2} (f_{i+1} + f_i + f_i \, g_i + f_{i-1} \, g_{i-1}) \, \psi_{ijk} \\ & + f_{i-1} \, g_{i-1} \, \psi_{i-1jk} \\ & + \text{(Similar terms)} \end{aligned} \qquad (4.2.16)$$

Intuitively, $\tilde{T}$ is not an unreasonable redefinition of $\hat{T}$.

Now split $\tilde{T}$ into the three matrices corresponding to x, y and z derivatives respectively.

Thus

$$\tilde{T} = \tilde{T}_i + \tilde{T}_j + \tilde{T}_k \qquad (4.2.17)$$

Each of these is a tri-diagonal matrix, and in Fig 4.2.1 a section of $\tilde{T}_i$ is illustrated. From the definitions of f_i, g_i and from (3.2.41) of Property 2 in Chapter 3, it is known that condition (i) of Theorem 4.2.1 is satisfied. Consideration of Fig 4.2.1 shows that condition (ii) of Theorem 4.2.1 is also satisfied. By symmetry, these conditions are also satisfied by $\tilde{T}_j$ and $\tilde{T}_k$.† Thus, by Theorem 4.2.1 and its corollary it is possible to write

$$\tilde{T} = \tilde{T}_{sy} + \tilde{T}_{sk} \qquad (4.2.18)$$

where $\tilde{T}_{sy}$ is positive definite. The modified matrix of (4.1.6) can thus be written

$$\begin{bmatrix} \underline{\tilde{T}}_{sy} & 0 & 0 & 0 \\ 0 & \underline{\tilde{T}}_{sy} & 0 & 0 \\ 0 & 0 & \underline{\tilde{T}}_{sy} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} \underline{\tilde{T}}_{sk} & 0 & 0 & 0 \\ 0 & \underline{\tilde{T}}_{sk} & 0 & 0 \\ 0 & 0 & \underline{\tilde{T}}_{sk} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & \underline{H}_1 \\ 0 & 0 & 0 & \underline{H}_2 \\ 0 & 0 & 0 & \underline{H}_3 \\ \underline{H}_1 & \underline{H}_2 & \underline{H}_3 & 0 \end{bmatrix} \qquad (4.2.19)$$

But since $\underline{H}_1$, $\underline{H}_2$ and $\underline{H}_3$ are skew-symmetric by definition (see (4.1.5))

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† Also since $\tilde{T}$ represents an elliptic differential operator, it is irreducible. $\tilde{T}$ satisfies condition (iii) of the corollary at a boundary point. This can be seen from figure 4.2.1.

A TYPICAL BAND OF $\widetilde{T}_i$ (ALSO TYPIFIES $\widetilde{T}_j$, $\widetilde{T}_k$)

Lower Diagonal	Main Diagonal	Upper Diagonal
$f_{i-2}\, g_{i-2}$	$-\frac{1}{2}(f_i + f_{i-2}\, g_{i-2} + f_{i-1} + f_{i-1}\, g_{i-1})$	f_i
$f_{i-1}\, g_{i-1}$	$-\frac{1}{2}(f_{i+1} + f_{i-1}\, g_{i-1} + f_i + f_i\, g_i)$	f_{i+1}
$f_i\, g_i$	$-\frac{1}{2}(f_{i+2} + f_i\, g_i + f_{i+1} + f_{i+1}\, g_{i+1})$	f_{i+2}

Figure 4.2.1

then the third matrix of (4.2.19) is also skew-symmetric. This is easily seen by writing down a few elements of this matrix. Thus (4.2.19) has the general form

$$P \; + \; S \qquad (4.2.20)$$

where P is a symmetric positive semi-definite matrix, and S is a skew-symmetric matrix, each having the form of P and S in Theorem 4.2.2. Thus, (P + S) has all of its eigenvalues lying wholly in the right hand complex plane. Thus, the modified equations

$$\begin{pmatrix} \underline{\tilde{T}} & 0 & 0 & \underline{H}_1 \\ 0 & \underline{\tilde{T}} & 0 & \underline{H}_2 \\ 0 & 0 & \underline{\tilde{T}} & \underline{H}_3 \\ \underline{H}_1 & \underline{H}_2 & \underline{H}_3 & 0 \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{v} \\ \underline{w} \\ \underline{p} \end{pmatrix}_{ijk} = \begin{pmatrix} \underline{h}_u \\ \underline{h}_v \\ \underline{h}_w \\ \underline{h}_o \end{pmatrix} \qquad (4.2.21)$$

are unconditionally stable, subject to the assumption of linearisation, and that boundary pressures are explicitly known.

4.3 Generalised Orthogonal Co-ordinates Systems

It will be shown how a proper treatment of the Navier-Stokes equations leads to a difference representation which can be expressed as the sum of positive definite and skew-symmetric matrices. By Section 4.2, such a representation is unconditionally stable.

(a) Treatment of the Momentum Terms for Orthogonal Co-ordinate Systems.

Let g_{ij} be the components of the metric tensor, and (x_s) be curvilinear coordinates and (y_t) be cartesian coordinates. Defining

$$h_{st} = \frac{\partial y_t}{\partial x_s} \qquad h^{st} = \frac{\partial x_s}{\partial y_t} \tag{4.3.1}$$

then the incompressible Navier-Stokes momentum equations in general orthogonal coordinates are

$$v_i \frac{\partial}{\partial x_i} (h_{st} v_s) - \frac{\nu}{\sqrt{g}} \frac{\partial}{\partial x_i} \left(\sqrt{g}\, g^{ij} \frac{\partial}{\partial x_j} (h_{st} v_s)\right) + \frac{h^{st}}{\rho} \frac{\partial p}{\partial x_s} = 0 \tag{4.3.2}$$

The summation convention is applied to i, j, and s. In orthogonal systems, $g^{ij} = 0$ for $i \neq j$, and so mixed derivatives do not appear. In this situation, the velocity terms of (4.3.2) have the general form

$$A_i \frac{\partial^2}{\partial x_i^2} (h_{st} v_s) + B_i \frac{\partial}{\partial x_i} (h_{st} v_s) \tag{4.3.3}$$

where the A_i are negative functions of geometry and physical parameters, and the B_i are functions of geometry and velocity components. Thus if the operand of (4.3.3) is considered to be $h_{st} v_s$, then for Dirichlet boundary conditions on velocity, Property 2 of Chapter 3 assures us that the matrix representation of the UDR of (4.3.3) is diagonally dominant.

This is not necessarily the case if the operand is chosen to be v_s, for then (4.3.3) becomes

$$A_i \, h_{st} \frac{\partial^2 v_s}{\partial x_i^2} + (2 A_i \frac{\partial h_{st}}{\partial x_i} + B_i \, h_{st}) + B_i \frac{\partial h_{st}}{\partial x_i} v_s \qquad (4.3.4)$$

Thus, whenever $\frac{B_i}{h_{st}} \frac{\partial h_{st}}{\partial x_i}$ becomes negative then the UDR of (4.3.4) is not diagonally dominant.

(b) Treatment of Pressure Derivatives and the Continuity Equation

It is shown how to treat the pressure terms and the continuity equation to ensure that the matrix representation corresponding to these terms is skew-symmetric, as it is for the Caretesian case. The conservative form of the continuity equation is given by

$$\frac{\partial}{\partial x_i} (\sqrt{g} \, v_i) \equiv \frac{\partial}{\partial x_i} (\sqrt{g} \, h^{it} \, h_{st} \, v_s) = 0 \qquad (4.3.5)$$

The identity $v_i \equiv h^{it} \, h_{st} \, v_s$ is employed for convenience, as will soon become clear. From (4.3.2) and (4.3.5) define †

$$T \equiv \sqrt{g} \, \rho \, v_i \frac{\partial \cdot}{\partial x_i} - \mu \frac{\partial}{\partial x_i} (\sqrt{g} \, g^{ij} \frac{\partial \cdot}{\partial x_j})$$

$$\left. \begin{array}{l} \overline{D}_t \equiv h^{st} \sqrt{g} \dfrac{\partial \cdot}{\partial x_s} \\ D_t \equiv \dfrac{\partial}{\partial x_s} (h^{st} \sqrt{g} \, \cdot) \end{array} \right\} t = 1, 2, 3 \qquad (4.3.6)$$

† The second of (4.3.6) is from the pressure term of (4.3.2) and the third is from the continuity equation (4.3.5).

Then (4.3.2) and (4.3.5) may be written as

$$\begin{pmatrix} T & 0 & 0 & \bar{D}_1 \\ 0 & T & 0 & \bar{D}_2 \\ 0 & 0 & T & \bar{D}_3 \\ D_1 & D_2 & D_3 & 0 \end{pmatrix} \begin{pmatrix} h_{i1} \cdot v_i \\ h_{i2} \cdot v_i \\ h_{i3} \cdot v_i \\ p \end{pmatrix} = 0 \qquad (4.3.7)$$

we now observe that $-D_s^*$ is the adjoint operator of $\bar{D}_s$ for $s = 1, 2, 3.$† (The '$*$' superfix indicates the adjoint). Consequently if

$$\Delta = \begin{pmatrix} 0 & 0 & 0 & \bar{D}_1 \\ 0 & 0 & 0 & \bar{D}_2 \\ 0 & 0 & 0 & \bar{D}_3 \\ D_1 & D_2 & D_3 & 0 \end{pmatrix} \qquad (4.3.8)$$

then

$$\Delta = -\Delta^* \qquad (4.3.9)$$

To see this transpose (4.3.8), and take the adjoints of the separate elements. It is therefore possible to find a difference representation of Δ which is skew-symmetric. Suppose that this representation is given by

$$\hat{\Delta} = \begin{pmatrix} 0 & 0 & 0 & \bar{H}_1 \\ 0 & 0 & 0 & \bar{H}_2 \\ 0 & 0 & 0 & \bar{H}_3 \\ H_1 & H_2 & H_3 & \bar{0} \end{pmatrix} \qquad (4.3.10)$$

---

† For given s, this is easily proven by considering functions $\psi_1(X_s)$, $\psi_2(X_s)$ s.t. $\psi_1(0) = \psi_2(0) = 0 = \psi_1(1) = \psi_2(1)$ and showing that

$$\int_0^1 \psi_1 \bar{D}_s \psi_2 \, d x_s = -\int_0^1 \psi_2 D_s \psi_1 \, d x_s$$

with the obvious correspondence between D_i, $\bar{D}_i$ and H_j, $\bar{H}_j$.
then, by definition

$$\hat{\Delta} = -\hat{\Delta}^{*} \qquad (4.3.11)$$

(c) <u>The Complete Representation</u>

In section 4.3 (a), it was shown how to write the general orthogonal curvilinear momentum operator T, so that its UDR, $\hat{T}$, is diagonally dominant. The general form is given at (4.2.15). If the modified UDR, $\tilde{T}$ defined at (4.2.16), is used then $\tilde{T}$ can be expressed as a sum of a positive definite, and skew-symmetric matrices.

From the definitions of H_i and $\bar{H}_i$, it follows that the matrix of the complete representation

$$\begin{pmatrix} \tilde{T} & 0 & 0 & \bar{H}_1 \\ 0 & \tilde{T} & 0 & \bar{H}_2 \\ 0 & 0 & \tilde{T} & \bar{H}_3 \\ H_1 & H_2 & H_3 & 0 \end{pmatrix} \begin{pmatrix} h_{i1}\underline{v}_i \\ h_{i2}\underline{v}_i \\ h_{i3}\underline{v}_i \\ \underline{p} \end{pmatrix} = \begin{pmatrix} \underline{b}_1 \\ \underline{b}_2 \\ \underline{b}_3 \\ \underline{b}_4 \end{pmatrix} \qquad (4.3.12)$$

(where $\underline{b}_i$ are boundary conditions) can be expressed as a sum of positive semi-definite and skew-symmetric matrices, and therefore by Theorem 4.2.2, every eigenvalue of the matrix lies in the right hand half complex plane, and the representation is therefore unconditionally stable, subject to the boundary pressures being considered as explicitly known.

4.4 The Finite Difference Forms used for the Pressure Derivatives and the Continuity Equation

We are concerned with representations for D_t and $\bar{D}_t$ defined by

$$\left.\begin{aligned} D_t &= h^{st}\frac{\partial .}{\partial x_s} \\ \bar{D}_t &= \frac{\partial}{\partial x_s}(h^{st} .) \end{aligned}\right\} \quad t = 1, 2, 3 \qquad (4.4.1)$$

Suppose that central differences are used for D_t and $\bar{D}_t$ so that if $x_1 = i\Delta_1$, $x_2 = j\Delta_2$, and $x_3 = k\Delta_3$ and if E_1, E_2 and E_3 are forward shift operators in the i, j and k directions respectively then typically

$$\left.\begin{aligned} h^{1t}\frac{\partial .}{\partial x_1} &= \bar{H}_1 \equiv h^{1t}_{ijk}\left(\frac{E_1 - E_1^{-1}}{2\Delta_1}\right) \\ \frac{\partial}{\partial x_1}(h^{1t} .) &= H_1 \equiv \frac{h^{1t}_{i+1jk}E_1 - h^{1t}_{i-1jk}E_1^{-1}}{2\Delta_1} \end{aligned}\right\} \qquad (4.4.2)$$

The approximations of $h^{2t}\frac{\partial .}{\partial x_2}$, $h^{3t}\frac{\partial .}{\partial x_3}$, $\frac{\partial}{\partial x_2}(h^{2t} .)$ and $\frac{\partial}{\partial x_3}(h^{3t} .)$ are similarly defined giving $\bar{H}_2$, $\bar{H}_3$, H_2 and H_3 respectively. From fig. 4.4.1-a and fig. 4.4.1-b it is clear that $H_1 = -\bar{H}_1^*$ and so $H_2 = -\bar{H}_2^*$ and $H_3 = -\bar{H}_3^*$. It follows that

$$\Delta = \begin{pmatrix} 0 & 0 & 0 & \bar{H}_1 \\ 0 & 0 & 0 & \bar{H}_2 \\ 0 & 0 & 0 & \bar{H}_3 \\ H_1 & H_2 & H_3 & 0 \end{pmatrix} \qquad (4.4.3)$$

is skew-symmetric.

4.4 The Finite Difference Forms used for the Pressure Derivatives and the Continuity Equation

We are concerned with representations for D_t and $\bar{D}_t$ defined by

$$\left.\begin{aligned} D_t &= h^{st}\frac{\partial .}{\partial x_s} \\ \bar{D}_t &= \frac{\partial}{\partial x_s}(h^{st}.) \end{aligned}\right\} \quad t = 1, 2, 3 \qquad (4.4.1)$$

Suppose that central differences are used for D_t and $\bar{D}_t$ so that if $x_1 = i\Delta_1$, $x_2 = j\Delta_2$, and $x_3 = k\Delta_3$ and if E_1, E_2 and E_3 are forward shift operators in the i, j and k directions respectively then typically

$$\left.\begin{aligned} h^{1t}\frac{\partial .}{\partial x_1} &= \bar{H}_1 \equiv h^{1t}_{ijk}\left(\frac{E_1 - E_1^{-1}}{2\Delta_1}\right) \\ \frac{\partial}{\partial x_1}(h^{1t}.) &= H_1 \equiv \frac{h^{1t}_{i+1jk}E_1 - h^{1t}_{i-1jk}E_1^{-1}}{2\Delta_1} \end{aligned}\right\} \qquad (4.4.2)$$

The approximations of $h^{2t}\frac{\partial .}{\partial x_2}$, $h^{3t}\frac{\partial .}{\partial x_3}$, $\frac{\partial}{\partial x_2}(h^{2t}.)$ and $\frac{\partial}{\partial x_3}(h^{3t}.)$ are similarly defined giving $\bar{H}_2$, $\bar{H}_3$, H_2 and H_3 respectively. From fig. 4.4.1-a and fig. 4.4.1-b it is clear that $H_1 = -\bar{H}_1^*$ and so $H_2 = -\bar{H}_2^*$ and $H_3 = -\bar{H}_3^*$. It follows that

$$\Delta = \begin{pmatrix} 0 & 0 & 0 & \bar{H}_1 \\ 0 & 0 & 0 & \bar{H}_2 \\ 0 & 0 & 0 & \bar{H}_3 \\ H_1 & H_2 & H_3 & 0 \end{pmatrix} \qquad (4.4.3)$$

is skew-symmetric.

Figure 4.4.1-a

Main diagonal

$$\begin{matrix} -h^{1t}_{i-1jk} & 0 & h^{1t}_{i-1jk} & 0 & 0 \\ 0 & -h^{1t}_{ijk} & 0 & h^{1t}_{ijk} & 0 \\ 0 & 0 & -h^{1t}_{i+1jk} & 0 & h^{1t}_{i+1jk} \end{matrix}$$

Matrix representation of $\bar{\bar{H}}_1$

Figure 4.4.1-b

Main diagonal

$$\begin{matrix} -h^{1t}_{i-2jk} & 0 & h^{1t}_{ijk} & 0 & 0 \\ 0 & -h^{1t}_{i-1jk} & 0 & h^{1t}_{i+1jk} & 0 \\ 0 & 0 & -h^{1t}_{ijk} & 0 & h^{1t}_{i+2jk} \end{matrix}$$

Matrix representation of H_1

CHAPTER 5

THE METHOD OF SOLUTION OF THE DIFFERENCE EQUATIONS

5.1 Summary

In any orthogonal co-ordinate system, the matrix representation of the Navier-Stokes equations has the form

$$\begin{pmatrix} \underline{\tilde{T}} & 0 & 0 & +\underline{\tilde{H}}_1 \\ 0 & \underline{\tilde{T}} & 0 & +\underline{\bar{H}}_2 \\ 0 & 0 & \underline{\tilde{T}} & +\underline{\bar{H}}_3 \\ +\underline{H}_1 & +\underline{H}_2 & +\underline{H}_3 & 0 \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{v} \\ \underline{w} \\ \underline{p} \end{pmatrix} = \begin{pmatrix} \underline{h}_u \\ \underline{h}_v \\ \underline{h}_w \\ -\underline{h}_c \end{pmatrix} \qquad (5.1.1)$$

where $\underline{h}_u$, $\underline{h}_v$, $\underline{h}_w$ and $\underline{h}_c$ are the vectors of boundary conditions for the u-momentum, v-momentum, w-momentum and continuity equations respectively. $\underline{\tilde{T}}$, $\underline{H}_i$ and $\underline{\bar{H}}_i$ are the matrix representations of the difference operators $\tilde{T}$, H_i and $\bar{H}_i$ defined in Chapter 4. If $\tilde{T}$ is the modified form of the momentum difference operator defined at (4.2.16), then it is known, from the previous chapter that the eigenvalues of the matrix of (5.1.1) all lie in the right hand half complex plane. It follows, that given $\tilde{T}$ fixed, and a suitable treatment of boundary pressures then (5.1.1) is amenable to an SOR (successive over-relaxation) type of solution procedure. The equations of (5.1.1) are manipulated, and an iterative procedure is applied to the resulting equations.

5.2 The General Method

Consider a member of the first equation of (5.1.1) at a point i, j, k written for an SOR solution procedure.

$$u_{ijk}^{n+1} = u_{ijk}^{n} + \varepsilon_{ijk} (\tilde{T} u_{ijk}^{n} + \bar{H}_1 p_{ijk}^{n+1}) \tag{5.2.1}$$

where ε_{ijk} is a space dependent positive relaxation parameter.[†] The reason for expressing p_{ijk} at the (n + 1)th iteration will clarify soon. Define a vector $\hat{u}_{ijk}$ by

$$\hat{u}_{ijk}^{n+1} = u_{ijk}^{n} + \varepsilon_{ijk} \tilde{T} u_{ijk}^{n} \tag{5.2.2}$$

Equations (5.2.1) and (5.2.2) give

$$u_{ijk}^{n+1} = \hat{u}_{ijk}^{n+1} + \varepsilon_{ijk} \bar{H}_1 p_{ijk}^{n+1} \tag{5.2.3}$$

Similarly, if

$$\begin{aligned} \hat{v}_{ijk}^{n+1} &= v_{ijk}^{n} + \varepsilon_{ijk} \tilde{T} v_{ijk}^{n} \\ \text{and} \quad \hat{w}_{ijk}^{n+1} &= w_{ijk}^{n} + \varepsilon_{ijk} \tilde{T} w_{ijk}^{n} \end{aligned} \tag{5.2.4}$$

---

† A precise definition of ε_{ijk} is given in Appendix V.

then

$$\left.\begin{aligned} v_{ijk}^{n+1} &= \hat{v}_{ijk}^{n+1} + \varepsilon_{ijk}\,\tilde{H}_2\,p_{ijk}^{n+1} \\ \text{and} \qquad & \\ w_{ijk}^{n+1} &= \hat{w}_{ijk}^{n+1} + \varepsilon_{ijk}\,\bar{H}_3\,p_{ijk}^{n+1} \end{aligned}\right] \qquad (5.2.5)$$

From (5.1.1) the representation of the continuity equation is

$$H_1\,u_{ijk}^{n+1} + H_2\,v_{ijk}^{n+1} + H_3\,w_{ijk}^{n+1} = 0 \qquad (5.2.6)$$

Substitution from (5.2.3) and (5.2.5) for u_{ijk}, v_{ijk} and w_{ijk} into (5.2.6) yields

$$-(H_1\,\varepsilon_{ijk}\,\bar{H}_1 + H_2\,\varepsilon_{ijk}\,\bar{H}_2 + H_3\,\varepsilon_{ijk}\,\bar{H}_3)\,p_{ijk}^{n+1}$$
$$= H_1\,\hat{u}_{ijk}^{n+1} + H_2\,\hat{v}_{ijk}^{n+1} + H_3\,\hat{w}_{ijk}^{n+1} \qquad (5.2.7)$$

This is an equation, in terms of p_{ijk}, derived from and equivalent to the continuity equation. Chorin [18] makes use of a similar device for time dependent problems.

It follows that given $\hat{u}_{ijk}^{n+1}$, $\hat{v}_{ijk}^{n+1}$ and $\hat{w}_{ijk}^{n+1}$ then (5.2.7) may be solved exactly for p_{ijk}^{n+1}. If u_{ijk}^{n+1}, v_{ijk}^{n+1} and w_{ijk}^{n+1} are then found using (5.2.3) and (5.2.5), then the new velocity field $\underline{u}^{n+1}$, $\underline{v}^{n+1}$ and $\underline{w}^{n+1}$ satisfies the continuity equation exactly. Thus, in essence, the solution procedure is as follows

(i) Set $\underline{u}^o$, $\underline{v}^o$, $\underline{w}^o$.

(ii) Calculate $\hat{\underline{u}}^1$, $\hat{\underline{v}}^1$, $\hat{\underline{w}}^1$ from (5.2.2) and (5.2.4).

(iii) Calculate $\underline{p}^1$ from (5.2.7).

(iv) Calculate $\underline{u}^1$, $\underline{v}^1$, $\underline{w}^1$ from (5.2.3) and (5.2.5). The continuity equation is exactly satisfied.

Repeat steps (ii), (iii) and (iv) until convergence, in some sense, is obtained.

5.3 Treatment of Boundary Conditions

The boundary conditions on the velocities required to close the momentum equations present no difficulties since either velocities, or gradients are specified on all boundaries. The treatment of the pressure field at a boundary poses a more difficult problem since because the velocity field determines the pressure field at all points, including the boundaries, to within an arbitrary constant, then no independent pressure information is available. Therefore suitable conditions to close the pressure equation (5.2.7) have to be deduced from the momentum equations. To simplify the discussion, the equations will be considered defined on a two dimensional rectangular region. The three dimensional problem and its solution is identical.

From (5.2.7) the equation to be considered is

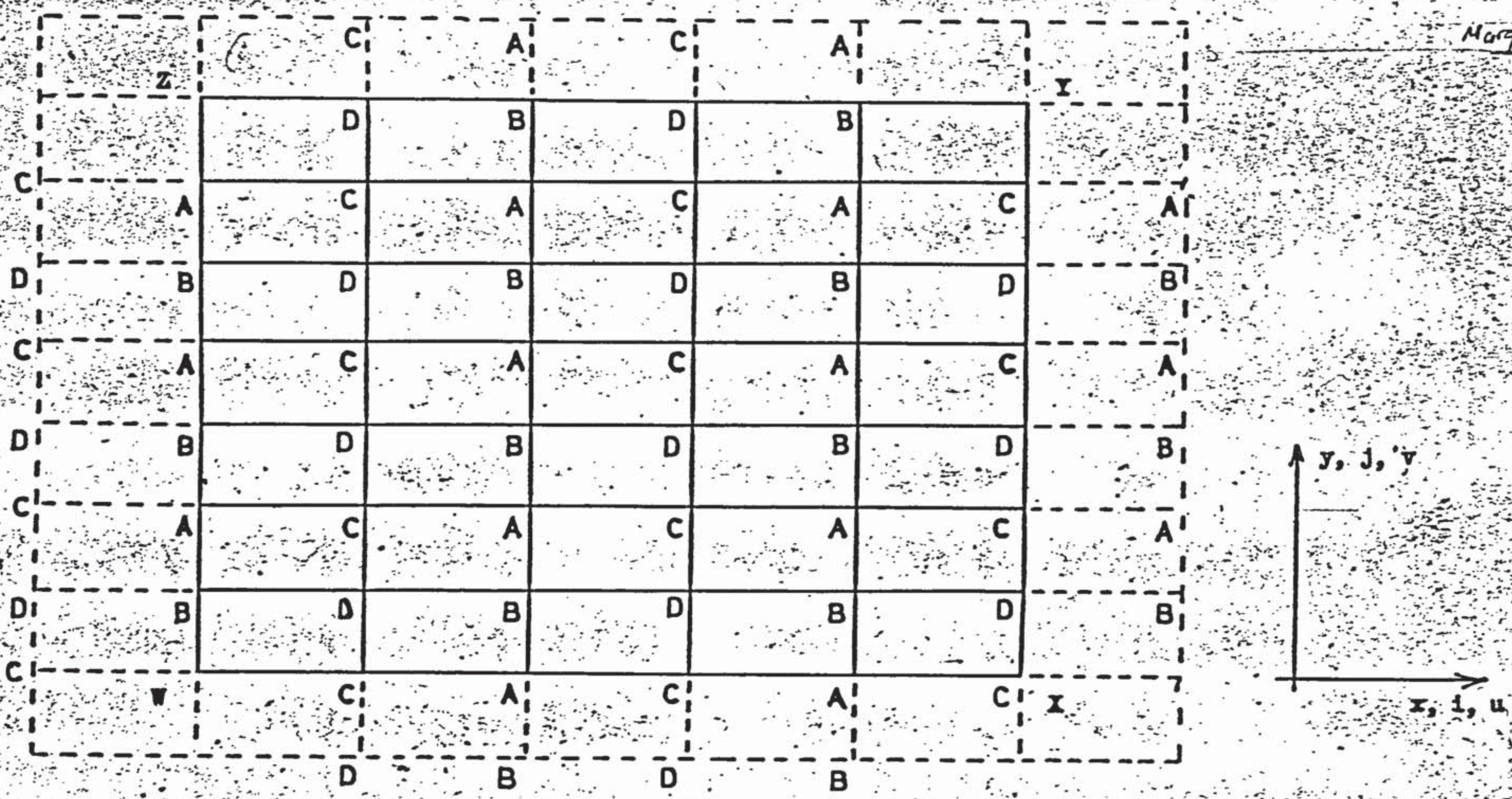
$$\frac{\varepsilon_{i+1j}\,(p_{i+2j} - p_{ij}) - \varepsilon_{i-1j}\,(p_{ij} - p_{i-2})}{4\,\Delta x^2}$$

$$+ \frac{\varepsilon_{ij+1}\,(p_{ij+2} - p_{ij}) = \varepsilon_{ij-1}\,(p_{ij} - p_{ij-2})}{4\,\Delta y^2}$$

$$= \frac{-\,(u_{i+1j} - u_{i-1j})}{2\,\Delta x} - \frac{(v_{ij+1} - v_{ij-1})}{2\,\Delta y} \qquad (5.3.1)$$

In Figure 5.3.1, it can be seen that the eq$\underline{^n}$ (5.3.1) connects all the points A independently of B, C and D points, all B points independently of A, C and D points, all C points independently of A, B and D points, and all D points independently of A, B and C points. Thus, (5.3.1) over the region may be considered as representing four independent sets of second order difference equations. In three dimensions, there will be eight sets of independent equations. Suppose that in Fig 5.3.1, the set connecting the A-points is considered. Let the solid boundary W X Y Z be the physical boundary of the problem, and let the dotted boundary exterior to W X Y Z represent a fictitious boundary. To close (5.3.1) on the A-points, it can be seen that on Z W and W X either pressures on Z W and W X are required or pressure differences between points on Z W and W X and interior points are required, whilst on X Y and Y Z either pressure differences <u>across</u> points on X Y and Y Z or pressures on the exterior boundaries to X Y and Y Z are required. Applying similar arguments to close (5.3.1) on all A, B, C and D points, then there are obtained the following possibilities for the close of (5.3.1) on all points.

Figure 5.3.1



The rectangular 2-dimensional grid of the pressure equation showing the four independent grids on points marked A, B, C and D respectively.

W X Y Z represent the physical boundary.

<u>Case (i)</u> Pressure differences prescribed between W X Y Z points and interior points, and pressure differences prescribed across † W X Y Z points between fictitious points and interior points.

<u>Case (ii)</u> Pressures prescribed on W X Y Z with pressure differences prescribed <u>across</u> W X Y Z between fictitious points and internal points.

<u>Case (iii)</u> Pressures prescribed on the fictitious boundary and pressures prescribed on W X Y Z points.

<u>Case (iv)</u> Pressures prescribed on the fictitious boundary and pressure differences prescribed between W X Y Z points and interior points.

<u>Case (v)</u> Combinations of the previous four cases.

Each case will be briefly discussed.

<u>Case (i)</u> This is the case used in practice for the numerical experiments of Chapter 6. The discussion is continued in a general geometry. Diagrams are represented in a Cartesian geometry, but

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† With Poisson equation $\nabla^2\psi = k$, with $\delta\psi/\delta n$ specified on the boundary it is required that $\int_c \frac{\delta\psi}{\delta n}\, ds = \int k dS$, and a similar condition holds with the difference equation (5.3.1) when differences are prescribed over all the boundary, as in Case (i). It will later be shown that the conditions derived for Case (i) are consistent with the equation (5.3.1).

curvilinear goemetries are implied.

(A) Pressure differences between fictitious and internal points

Consider Fig 5.3.2. The pressure difference

$$\Delta p_E \;=\; p_H - p_B \qquad (5.3.2)$$

is required. Applying the normal momentum equation to D E F at the point E gives

$$p_H - p_B \;=\; G\,(u_H,\, u_E,\, u_B,\, u_D,\, u_F,\, v_E) \qquad (5.3.3)$$

where u and v are the curvilinear velocity components. Of the quantities on the rhs of (5.3.3), u_D, u_E, u_F, and v_E are given as boundary data and u_H can be obtained from the internal flow via independent equations. u_B is the only unknown.

Applying the continuity equation at E gives

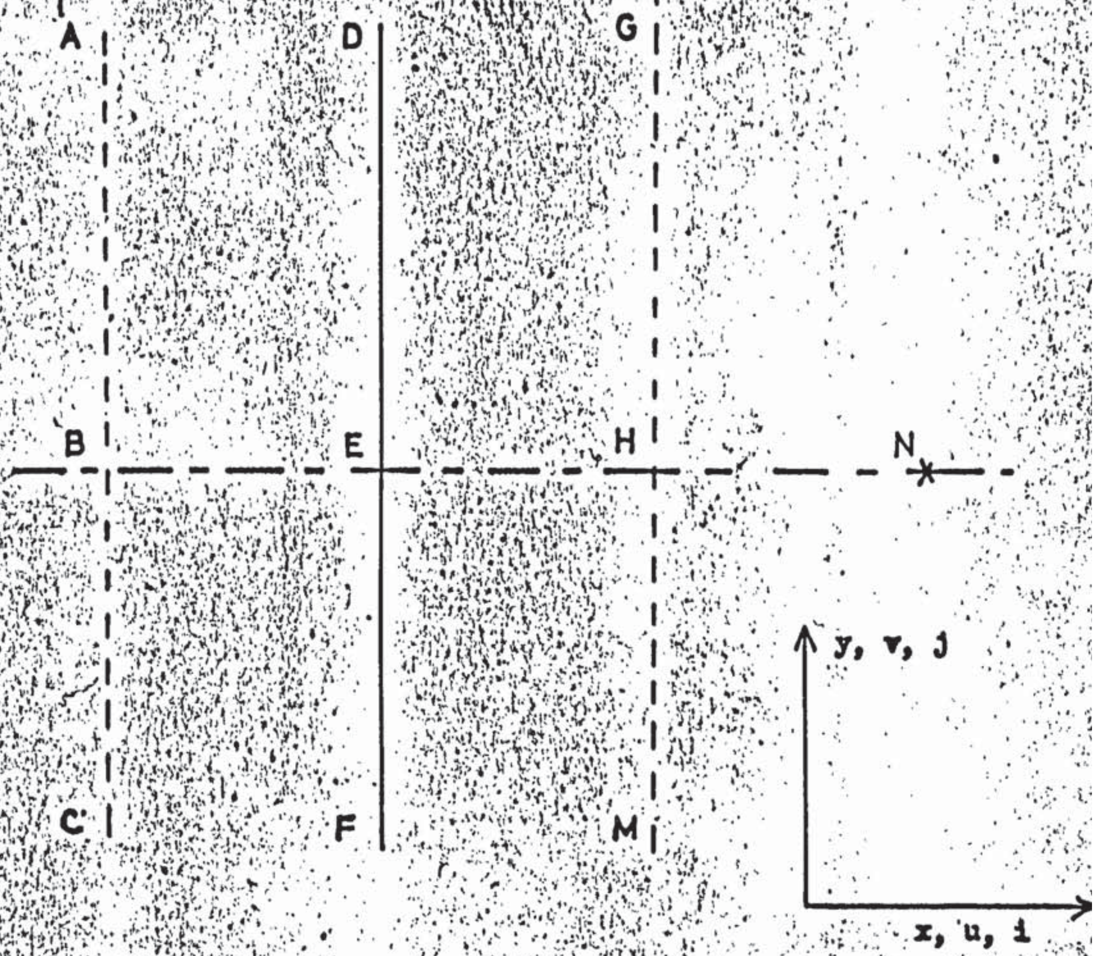
$$\frac{\sqrt{g_H}\,u_H - \sqrt{g_B}\,u_B}{2\,\Delta x_1} + \frac{\sqrt{g_D}\,v_D - \sqrt{g_F}\,v_F}{2\,\Delta x_2} \;=\; 0 ^{\dagger} \qquad (5.3.4)$$

This equation determines u_B. Repeated application of (5.3.3) and (5.3.4) all around the boundary provides the required information.

---

† This is the discretised form of (4.3.11). In (5.1.1) this conservative form is used. The symbol 'g' is $|g_{ij}|$ where g_{ij} are components of the metric element.

Figure 5.3.2



ABC = FICTITIOUS BOUNDARY

DEF = PHYSICAL BOUNDARY

GHM = LINE INTERNAL TO FLOW

N + AN INTERNAL POINT

(B) The pressure difference between W X Y Z points and internal points

This quantity is used to ensure the conservation of total mass within the flow.

Consider Fig 5.3.3, then at every point (i,j) on AD, the form of the continuity equation used is

$$\frac{\sqrt{g}_{i+1j}\, u_{i+1j} - \sqrt{g}_{i-1j}\, u_{i-1j}}{2\,\Delta x_1} + \frac{\sqrt{g}_{ij+1}\, v_{ij+1} - \sqrt{g}_{ij-1}\, v_{ij-1}}{2\,\Delta x_2} = 0 \qquad (5.3.5)$$

and it is known that satisfaction of this equation everywhere is not sufficient to guarantee conservation of mass. A condition will be derived, which together with (5.3.5) everywhere will ensure the total conservation of mass. Define the notation $U_{ij} = \sqrt{g}_{ij}\, u_{ij}$ and $V_{ij} = \sqrt{g}_{ij}\, v_{ij}$. Summation of (5.3.5) over $2 \leq j \leq J-1$ ($j = 1, J$ are points on the physical boundaries) yields

$$(V_{iJ} + V_{iJ-1}) - (V_{i1} + V_{i2}) = -\frac{\Delta x_2}{\Delta x_1} \sum_{j=2}^{J-1} (U_{i+1j} - U_{i-1j}) \qquad (5.3.6)$$

The trapezium rule interpretation of the statement that the total mass flow from M N P Q M in Fig 5.3.3 is zero is that

$$\frac{\Delta x_2}{2}\left(U_{i+11} + 2\sum_{j=2}^{J-1} U_{i+1j} + U_{i+1J}\right)$$

$$-\frac{\Delta x_2}{2}\left(U_{i-11} + 2\sum_{j=2}^{J-1} U_{i-1j} + U_{i-1J}\right)$$

$$+ \frac{\Delta x_1}{2} (V_{i+1J} + 2 V_{iJ} + V_{i-1J})$$

$$- \frac{\Delta x_1}{2} (V_{i+11} + 2 V_{i1} + V_{i-11}) = 0 \qquad (5.3.7)$$

This rearranges into

$$\sum_{j=2}^{J-1} (U_{i+1j} - U_{i-1j}) = -(U_{i+11} - U_{i-11})$$

$$- (U_{i+1J} - U_{i-1J}) + \frac{\Delta x_1}{2\Delta x_2} (V_{i+11} + 2 V_{i1} + V_{i-11})$$

$$- \frac{\Delta x_1}{2\Delta x_2} (V_{i+1J} + 2 V_{iJ} + V_{i-1J}) \qquad (5.3.8)$$

Substitution of the lhs of (5.3.8) into the rhs of (5.3.6) yields, with some manipulation

$$\left[\frac{2 V_{i2} - (V_{i+11} + V_{i-11})}{2 \Delta x_2} + \frac{U_{i+11} - U_{i-11}}{2 \Delta x_1} \right]$$

$$= - \left[\frac{(V_{i+1J} + V_{i-1J}) - 2 V_{iJ-1}}{2 \Delta x_2} + \frac{U_{i+1J} - U_{i-1J}}{2 \Delta x_1} \right] \qquad (5.3.9)$$

Clearly, as $\Delta x_1, \Delta x_2 \to 0$, then the lhs of (5.3.9) tends to the continuity equation at $(i,1)$ and the rhs tends to the continuity equation at (i,J). We can therefore write from (5.3.9)

$$\frac{2 V_{i2} - (V_{i+11} + V_{i-11})}{2 \Delta x_2} + \frac{U_{i+11} - U_{i-11}}{2 \Delta x_1} = 0$$

and

$$\frac{(V_{i+1J} + V_{i-1J}) - 2 V_{iJ-1}}{2 \Delta x_2} + \frac{U_{i+1J} - U_{i-1J}}{2 \Delta x_1} = 0 \qquad (5.3.10)$$

Upon writing $U_{ij} = \sqrt{g_{ij}}\, u_{ij}$ and $V_{ij} = \sqrt{g_{ij}}\, v_{ij}$ these yield

$$v_{i2} = f \text{ (wall velocities)}$$

and

$$v_{iJ-1} = g \text{ (wall velocities)} \qquad (5.3.11)$$

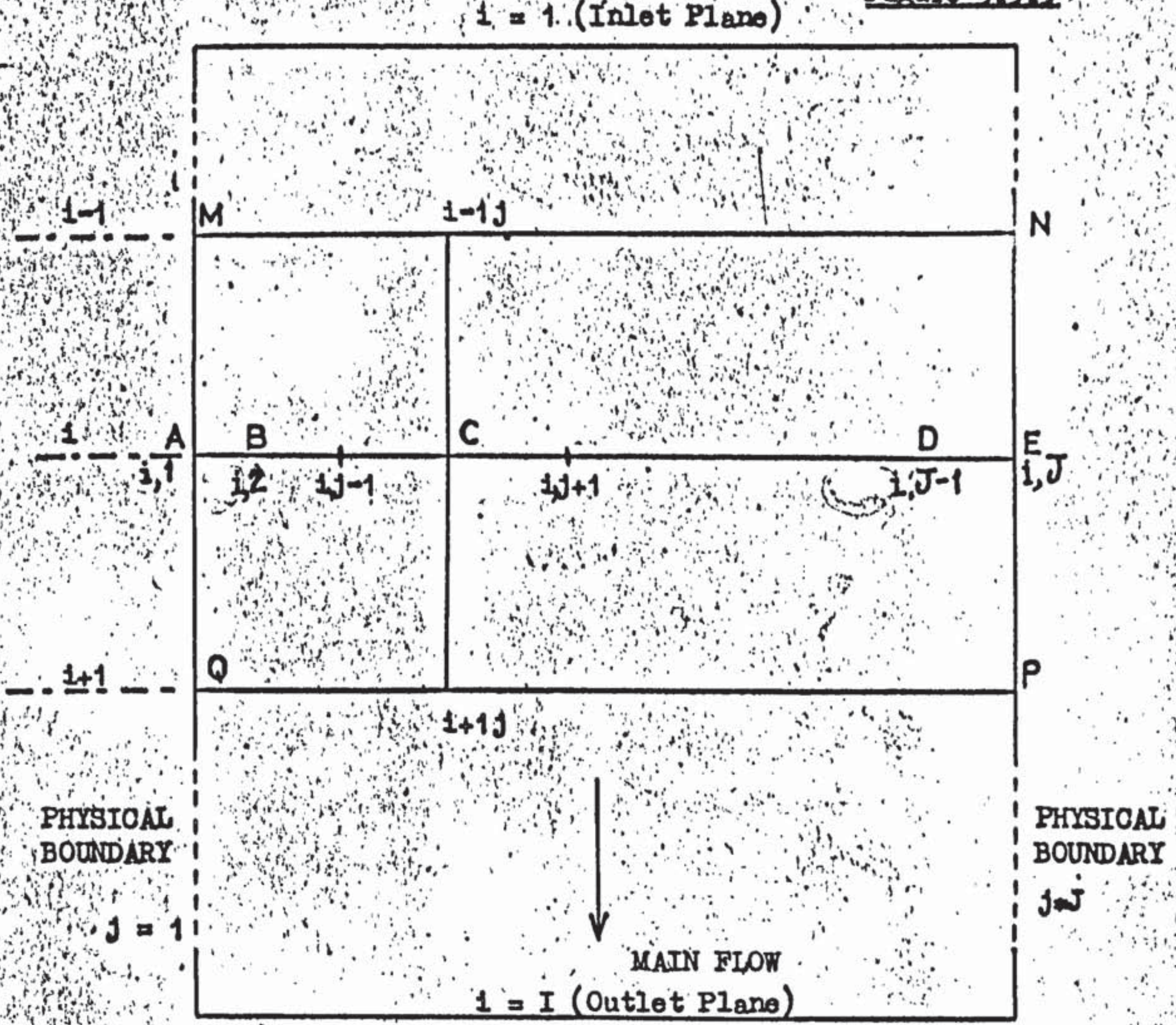
The equations (5.3.11) are the conditions, which together with the continuity equation (5.3.5) everywhere, guarantee the conservation of mass in the region M N P Q M of Fig 5.3.3. If equations (5.3.11) are used to calculate v_{i2} and v_{iJ-1}, then the v - momentum equations at the points $(i,2)$ and $(i, J-1)$ may be used to calculate

$$\Delta p_{i2} = p_{i3} - p_{i1}$$

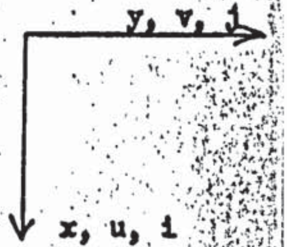
$$\Delta p_{iJ-1} = p_{iJ} - p_{iJ-2} \qquad (5.3.12)$$

By following a similar procedure over all the boundary for all i, j then total mass conservation is ensured for all blocks similar to M N P Q M bounded by $j = 1$ and $j = J$, and all blocks similar to M N P Q M bounded by $i = 1$ and $i = I$.

Figure 5.3.3



The continuity equation is summed over the line AD to obtain an expression between U-velocities on MN and QP and V-velocities at A, B, D and E. The application of the trapezium rule for mass conservation over MNPQM then eliminates all internal velocities except for V_B and V_D. Conditions are then obtained on V_B and V_D which, together with continuity everywhere on AE, ensure mass conservation over MNPQM.



In three dimensions, an identical argument is followed, with more involved algebra to derive conditions which ensure that between any pair of alternate parallel planes, taken from boundary to boundary total mass flow is conserved.

Case (ii)

(A) Pressure difference between fictitious and internal points

The procedure for Case (i)(A) may be followed.

(B) Pressures on W X Y Z

The suggestion is to integrate the tangential momentum equation along the physical boundaries to determine a suitable pressure distribution. The Cartesian tangential momentum equation at D of Fig 5.3.3 is

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \frac{1}{\rho} \frac{\partial p}{\partial x} = \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \qquad (5.3.13)$$

It is clear that the term $\partial^2 u / \partial y^2$ will require u_C, u_D and u_E for its approximation. But E is a fictitious point, and although it is possible to estimate v_E at E by applying the continuity equation at D, a similar procedure is not available for calculating u_E. The only possibility is to guess a value of u_E†, for instance, $u_E = -u_C$, and hope that numerical results support such an arbitrary procedure. Harlow and Welch [17] have used precisely this condition at a no-slip wall and have obtained for their dam-bursting problems reasonable results, from a quantative viewpoint. It may be that in detailed calculations of small regions,

†

eg boundary layer calculations such a procedure would prove inadequate.

Case (iii) The comments of Case (ii) (B) are applicable.

Case (iv)

(A) Pressure differences between W X Y Z points and interior points

The comments of Case (i) (B) are applicable.

(B) Pressures on fictitious points

The comments of Case (ii) (B) are applicable.

Case (v) The comments of the previous four cases apply.

5.4 Consistency of the Case (i) Boundary Conditions with the Pressure Equation

In the numerical experiments of Chapter 6, use is made of the Case (i) boundary conditions, and it is necessary to prove their consistency with the pressure equation (5.2.7). The situation to be discussed is directly analogous to the following:

Given

$$\frac{(\psi_{i+1j} - 2\psi_{ij} + \psi_{i-1j})}{\Delta x^2} + \frac{(\psi_{ij+1} - 2\psi_{ij} + \psi_{ij-1})}{\Delta y^2} = k \tag{5.4.1}$$

with the boundary conditions

$$
\begin{aligned}
\psi_{2j} - \psi_{1j} &= \lambda_{1j} \\
\psi_{Ij} - \psi_{I-1j} &= \lambda_{Ij}
\end{aligned}
\qquad 2 \leq j \leq J - 1
$$

and

$$
\begin{aligned}
\psi_{i2} - \psi_{i1} &= \lambda_{i1} \\
\psi_{iJ} - \psi_{iJ-1} &= \lambda_{iJ}
\end{aligned}
\qquad 2 \leq i \leq I - 1
\tag{5.4.2}
$$

What conditions must apply to make λ_{1j}, λ_{Ij}, λ_{i1} and λ_{iJ} consistent with (5.4.1)?

Summation of (5.4.1) over $2 \leq i \leq I - 1$, $2 \leq j \leq J - 1$ yields

$$
\frac{1}{\Delta x^2} \sum_{j=2}^{J-1} (\psi_{1j} - \psi_{2j} + \psi_{Ij} - \psi_{I-1j}) + \frac{1}{\Delta x^2} \sum_{i=2}^{I-1} (\psi_{i1} - \psi_{i2} + \psi_{iJ} - \psi_{iJ-1})
$$

$$
= \quad (I - 2)(J - 2)\, k \tag{5.4.3}
$$

Substitution from (5.4.2) into (5.4.3) yields

$$
\frac{1}{\Delta x^2} \sum_{j=2}^{J-1} (\lambda_{Ij} - \lambda_{1j}) + \frac{1}{\Delta y^2} \sum_{i=2}^{I-1} (\lambda_{iJ} - \lambda_{i1}) = (I - 2)(J - 2)\, k \tag{5.4.4}
$$

This equation is the condition that the boundary conditions (5.4.2) must satisfy to be consistent with (5.4.1). The pressure equation is

$$
-(H_1\, \varepsilon_{ijk} \overline{H}_1 + H_2\, \varepsilon_{ijk} \overline{H}_2 + H_3\, \varepsilon_{ijk} \overline{H}_3)\, p_{ijk}^{n+1}
$$

$$
= H_1\, \hat{u}_{ijk}^{n+1} + H_2\, \hat{v}_{ijk}^{n+1}\, H_3\, \hat{w}_{ijk}^{n+1} \tag{5.4.5}
$$

with boundary conditions

over all values of i, j, k

$$\left.\begin{aligned} \bar{H}_1 \, p^{n+1}_{tjk} &= \tilde{T} \, u^{n}_{tjk} \; ; \; t = 1, 2, I-1, I \\ \bar{H}_2 \, p^{n+1}_{itk} &= \tilde{T} \, v^{n}_{itk} \; ; \; t = 1, 2, J-1, J \\ \bar{H}_3 \, p^{n+1}_{ijt} &= \tilde{T} \, w^{n}_{ijt} \; ; \; t = 1, 2, K-1, K \end{aligned}\right\} \qquad (5.4.6)$$

The conditions above are just the momentum equations applied at the appropriate points. The velocities u_{tjk}, v_{itk} and w_{ijt} given in (5.4.6) are assumed found by the application of the conditions derived in Section 5.3 to ensure mass conservation over all boundary to boundary blocks.

The operators H_1, H_2 and H_3 of (5.4.5) are conservatively defined at equation (4.4.2), and therefore may be summed over $2 \leq i \leq I-1$, $2 \leq j \leq J-1$, $2 \leq k \leq K-1$ to obtain a relationship between $\varepsilon_{ijk} \bar{H}_t p_{ijk}$, $(t = 1, 2, 3)$ and $(\hat{u}_{ijk}, \hat{v}_{ijk}, \hat{w}_{ijk})$ at the points (1, j, k), (2, j, k), (I-1, j, k), (I, j, k), (i, 1, k), (i, 2, k), (i, J-1, k), (i, J, k), (i, j, 1), (i, j, 2), (i, j, K-1) and (i, j, K) for all i, j, k over the range of summation.

For example, suppose that H is defined by

$$H \psi_i = \psi_{i+1} - \psi_{i-1} \qquad (5.4.7)$$

then

$$\sum_{i=2}^{I-1} H \psi_i = \psi_I + \psi_{I-1} - \psi_2 - \psi_1 \qquad (5.4.8)$$

The intention is to sum (5.4.5) over i, j, k. To this end define, for an arbitrary ψ_{ijk}

$$\left.\begin{aligned}\sum_i \sum_j \sum_k H_1 \; \psi_{ijk} &= L_1 (\psi_{ijk}) \\ \sum_i \sum_j \sum_k H_2 \; \psi_{ijk} &= L_2 (\psi_{ijk}) \\ \sum_i \sum_j \sum_k H_3 \; \psi_{ijk} &= L_3 (\psi_{ijk}) \\ 2 \leq i \leq I-1; \; 2 \leq j \leq J-1&; \; 2 \leq k \leq K-1 \end{aligned}\right\} \qquad (5.4.8)$$

and since H_1, H_2, H_3 are conservatively defined, then typically

$$L_1 (\psi_{ijk}) = \sum_{t=1,2,I,I-1} (a_t \, \psi_{tjk}) + \sum_{t=1,2,J,J-1} (b_t \, \psi_{itk}) + \sum_{t=1,2,K,K-1} (c_t \, \psi_{ijt}) \qquad (5.4.9)$$

thus, only values of ψ_{ijk} on boundaries, and adjacent to boundaries occur. With this notation, summation of (5.4.5) over i, j, k yields

$$-\left(L_1 (\varepsilon_{ijk} \bar{H}_1 \, p^{n+1}_{ijk}) + L_2 (\varepsilon_{ijk} \bar{H}_2 \, p^{n+1}_{ijk}) + L_3 (\varepsilon_{ijk} \bar{H}_3 \, p^{n+1}_{ijk})\right)$$

$$= L_1 (\hat{u}^{n+1}_{ijk}) + L_2 (\hat{v}^{n+1}_{ijk}) + L_3 (\hat{w}^{n+1}_{ijk}) \qquad (5.4.10)$$

This equation represents the consistency condition to be satisfied by the boundary conditions (5.4.6). The continuity equation is

$$H_1 \, u^n_{ijk} + H_2 \, v^n_{ijk} + H_3 \, w^n_{ijk} = 0 \qquad (5.4.11)$$

Summing over (5.4.11) yields

$$L_1 (u^n_{ijk}) + L_2 (v^n_{ijk}) + L_3 (w^n_{ijk}) = 0 \qquad (5.4.12)$$

Adding (5.4.12) to (5.4.10) and using the linearity of L_1, L_2 and L_3 gives an equivalent consistency condition

$$L_1 (\varepsilon_{ijk} \bar{H}_1 \overset{n+1}{p_{ijk}} + \overset{\wedge n+1}{u_{ijk}} - \overset{n}{u_{ijk}})$$

$$+ L_2 (\varepsilon_{ijk} \bar{H}_2 \overset{n+1}{p_{ijk}} + \overset{\wedge n+1}{v_{ijk}} - \overset{n}{v_{ijk}})$$

$$+ L_3 (\varepsilon_{ijk} \bar{H}_3 \overset{n+1}{p_{ijk}} + \overset{\wedge n+1}{w_{ijk}} - \overset{n}{w_{ijk}}) = 0 \qquad (5.4.13)$$

It will be shown that (5.4.13) is identically satisfied by (5.4.6). Consider in particular the first boundary condition of (5.4.6) multiplied through by ε_{ijk}

$$\therefore \quad \varepsilon_{ijk} \bar{H}_1 \overset{n+1}{p_{ijk}} = \varepsilon_{ijk} \tilde{T} \overset{n}{u_{ijk}}$$

from (5.2.2)

$$= -\overset{\wedge n+1}{u_{ijk}} + \overset{n}{u_{ijk}} \qquad (5.4.14)$$

$$\therefore \quad \varepsilon_{ijk} \bar{H}_1 \overset{n+1}{p_{ijk}} + \overset{\wedge n+1}{u_{ijk}} - \overset{n}{u_{ijk}} = 0 \qquad (5.4.15)$$

((5.4.15) assumes that u_{ijk} is iterated, but this is irrelevant). A similar result holds for the remaining eleven conditions of (5.4.6). Now notice that the lhs of (5.4.13) is merely a linear combination of the twelve equations similar to (5.4.15) derived from (5.4.6), and thus the condition (5.4.13) is identically satisfied, and thus the boundary conditions (5.4.6) are consistent with the pressure equation (5.4.5).

CHAPTER 6

NUMERICAL RESULTS

6.1 Summary

Three problems are presented:

(a) For $\nu = 1$, there is an analytic solution available for a two dimensional rectangular geometry. Comparisons are given between solutions obtained by the presented method, and the analytic results on a two dimensional region.

(b) Comparisons are given for a three dimensional test problem between the presented method and a method based on the vector potential as developed by Aregbosola [52]. This test problem has a Reynolds number of unity and a rectangular geometry with a step function inlet profile and a Poisson solution outlet profile.

(c) Comparisons are given between the present method, and a physical experiment performed by Joy [51]. The Reynolds number is of the order 5×10^5. The geometry is the complex one of Fig 6.4.1.

6.2 The Two Dimensional Problem: Comparisons between an Analytic Solution and Roscoe

The two dimensional Navier-Stokes equations are

$$\left.\begin{aligned} uu_x + vu_y + \frac{1}{\rho} p_x &= \nu (u_{xx} + u_{yy}) \\ u v_x + vv_y + \frac{1}{\rho} p_y &= \nu (v_{xx} + v_{yy}) \\ u_x + v_y &= 0 \end{aligned}\right\} \quad (6.2.1)$$

For $\nu = 1$, a solution is given by

$$\left.\begin{aligned} u &= - \operatorname{Cos} x \operatorname{Sin} y \\ v &= \operatorname{Sin} x \operatorname{Cos} y \end{aligned}\right\} \quad (6.2.2)$$

Following Chapter 4, the finite difference representation of (6.2.1) is given by

$$\left.\begin{aligned} Tu_{ij} + H_1 p_{ij} &= 0 \\ Tv_{ij} + H_2 p_{ij} &= 0 \\ H_1 u_{ij} + H_2 v_{ij} &= 0 \end{aligned}\right\} \quad (6.2.3)$$

where T, H_1 and H_2 are difference operators defined by

$$\left.\begin{aligned} T &= \frac{\rho u_{ij}}{\Delta x (1 - e_u)} \left[E_i - (1 + e_u) + e_u E_i^{-1}\right] \\ &+ \frac{\rho v_{ij}}{\Delta y (1 - e_v)} \left[E_j - (1 + e_v) + e_v E_j^{-1}\right] \\ \text{where} \quad e_u &= \exp(\rho u_{ij} \Delta x/\nu) \\ e_v &= \exp(\rho v_{ij} \Delta y/\nu) \end{aligned}\right\} \quad (6.2.4)$$

$$\left.\begin{aligned} H_1 &= (E_i - E_i^{-1}) / (2 \Delta x) \\ H_2 &= (E_j - E_j^{-1}) / (2 \Delta y) \end{aligned}\right\} \quad (6.2.4)$$

E_i and E_j are the normally defined forward shift operators in the i and j directions respectively. Note that the stability analysis of Chapter 4 used the modified momentum difference operator of (4.2.16). In practice it was discovered that the simpler original form of (4.2.15) is effective. T, defined above, has this simple original form.

The problem was solved on the region

$$\left.\begin{aligned} 0.1 &\leq x \leq 0.35 \\ 0.1 &\leq y \leq 0.35 \end{aligned}\right\} \quad (6.2.5)$$

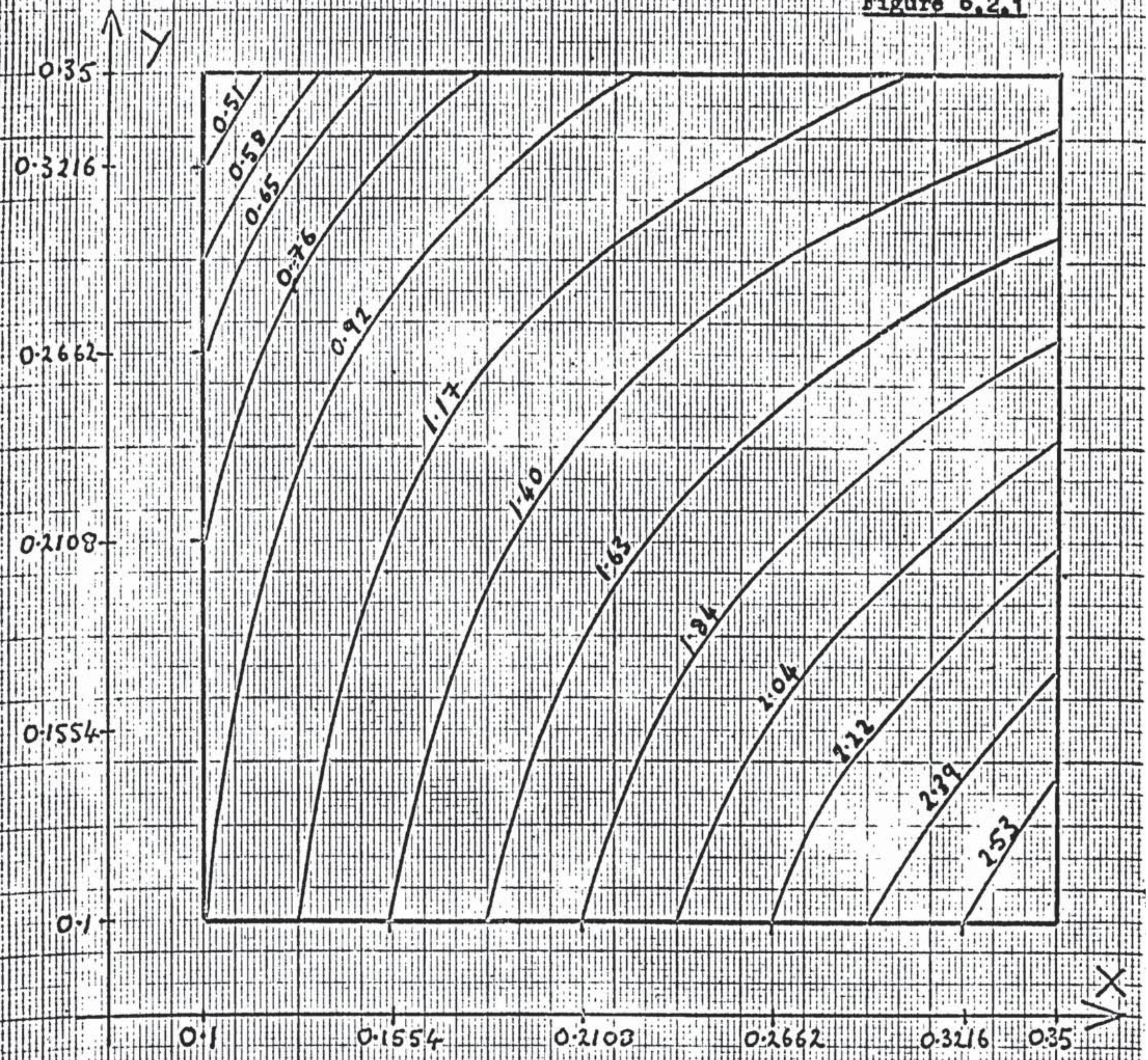
and boundary velocities at the boundaries of this region are specified by the application of (6.2.2) there. A 10 x 10 mesh was used. The boundary conditions on pressure are those discussed in Case (i), Chapter 5.

Results

Figure 6.2.1 gives equi-velocity contours for u (x, y). as predicted by the present method. On the scale used, there is no visual discrepancy between these results and the analytic results, hence only the single diagram is presented.

Figures 6.2.2 and 6.2.3 give tabulated values for u (x, y) on the

Figure 6.2.1



Axes give spatial co-ordinates, and the curves are equi-velocity contour plots.

Figure 6.2.2

TABLE 1, y = 0.1554		
x	u (analytic)	u (numerical)
0.1000	0.857	0.857
0.1277	1.084	1.089
0.1554	1.302	1.322
0.1831	1.511	1.518
0.2108	1.708	1.715
0.2385	1.892	1.888
0.2662	2.061	2.059
0.2939	2.215	2.203
0.3216	2.352	2.345
0.3500	2.472	2.472

TABLE 2, y = 0.2108		
x	u (analytic)	u (numerical)
0.1000	0.765	0.765
0.1277	0.967	0.978
0.1831	1.348	1.362
0.2108	1.524	1.531
0.2385	1.688	1.684
0.2662	1.840	1.829
0.2939	1.977	1.959
0.3216	2.099	2.090
0.3500	2.206	2.206

Figure 6.2.3

TABLE 3, y = 0.2662		
x	u (analytic)	u (numerical)
0.1000	0.650	0.650
0.1277	0.821	0.828
0.1554	0.987	0.996
0.1831	1.145	1.157
0.2108	1.294	1.294
0.2385	1.434	1.436
0.2662	1.562	1.552
0.2939	1.679	1.670
0.3216	1.783	1.780
0.3500	1.873	1.873

TABLE 4, y = 0.3216		
x	u (analytic)	u (numerical)
0.1000	0.514	0.514
0.1277	0.651	0.643
0.1554	0.782	0.748
0.1831	0.907	0.912
0.2108	1.025	1.013
0.2385	1.135	1.152
0.2662	1.237	1.234
0.2939	1.330	1.366
0.3216	1.412	1.423
0.3500	1.483	1.483

constant lines y = 0.1554, y = 0.2108, y = 0.2662 and y = 0.3216. The largest error is 2 per cent.

6.3 A Test Problem in a Simple Three Dimensional Geometry: Comparisons between Aregbesola and Roscoe

The geometry is shown in Fig 6.3.1 and represents a straight duct of square cross section, and of dimensions 1 x 1 x 2.5. The equations are the three dimensional form of (6.2.1), and their representations the three dimensional generalisations of (6.2.3) and (6.2.4).

The inlet profile is the step input defined by

$$\left.\begin{aligned} u(x, y, 0) &= 1;\ 0 \le x \le 0.5,\ 0 \le y \le 1 \\ u(x, y, 0) &= 2;\ 0.5 \le x \le 1.0,\ 0 \le y \le 1 \\ u(x, y, 0) &= 0 \text{ on } x = 0, 1:\ y = 0, 1 \\ v(x, y, 0) &= 0;\ 0 \le x \le 1 \\ w(x, y, 0) &= 0;\ 0 \le y \le 1 \end{aligned}\right\} \qquad (6.3.1)$$

On Z = 2.5 the Poisson solution was specified (ie. the equivalent of Poiseuille flow in a two dimensional straight channel).

Both the present author and Aregbesola used a 14 x 14 x 16 mesh for the problem. Direct comparisons were difficult because Aregbesola defines his physical boundaries half way between boundary mesh points and adjacent internal mesh points, whilst the present author defines his physical boundaries to coincide with mesh points. Apart from the

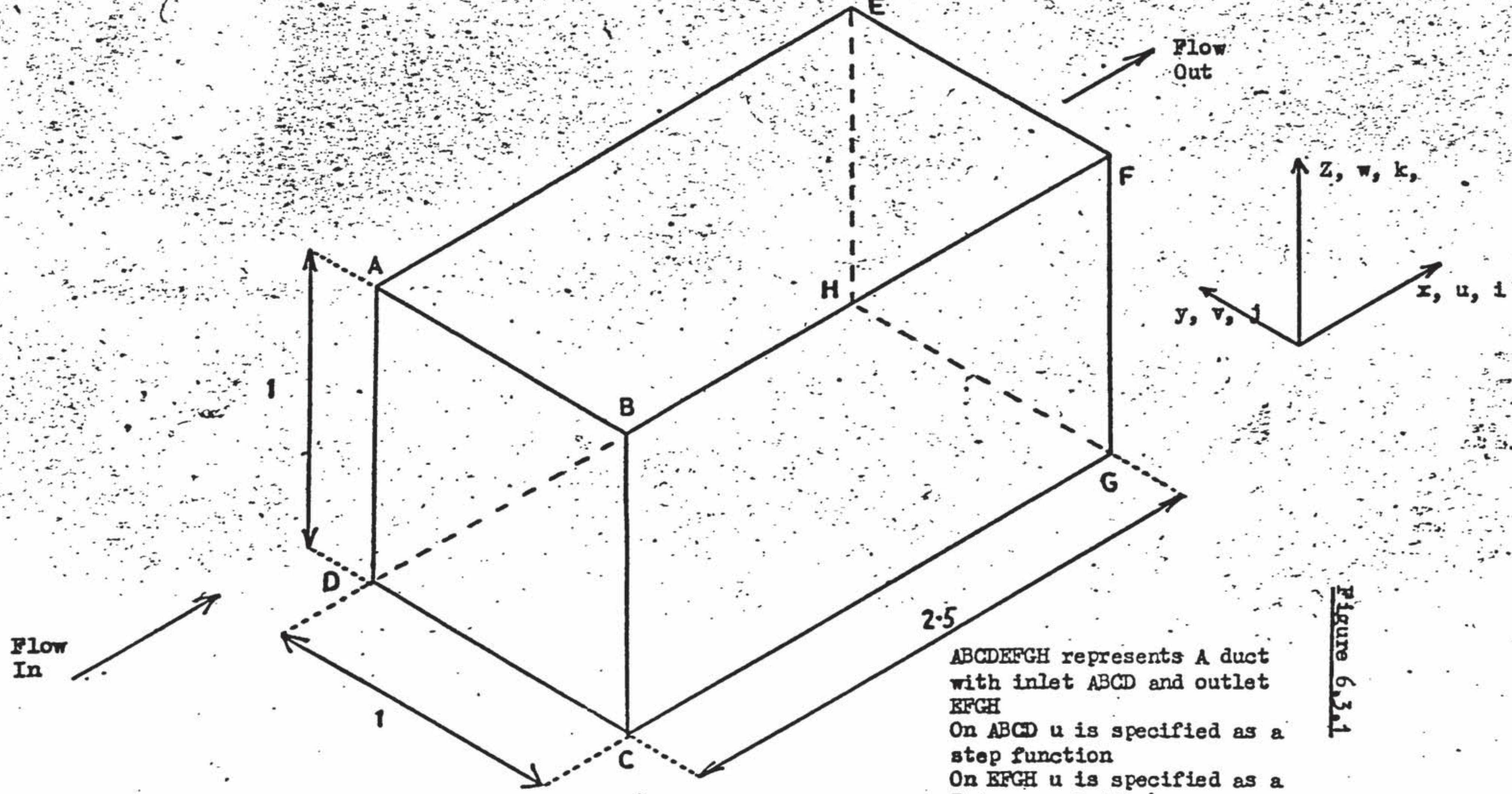
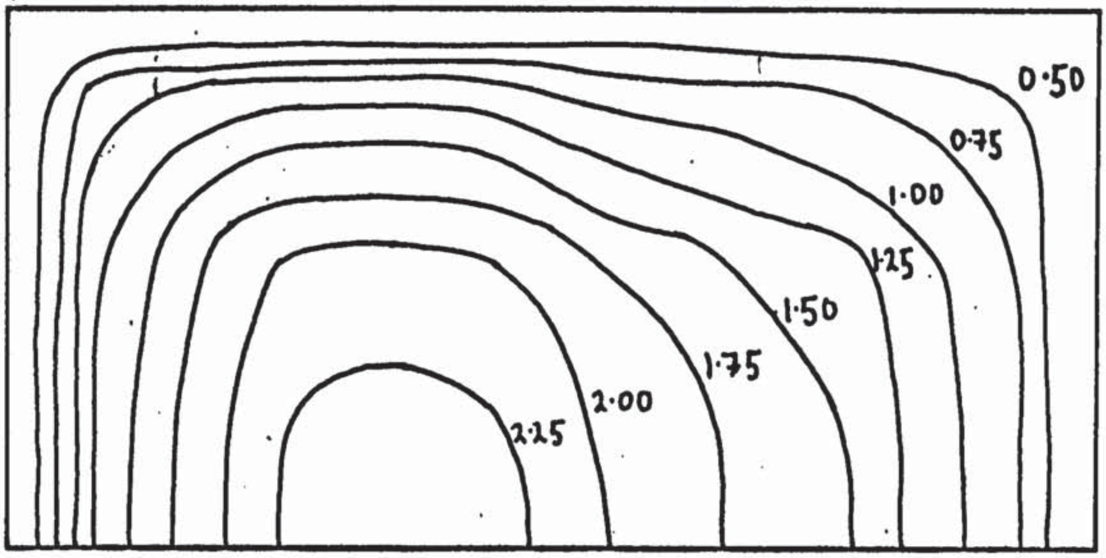


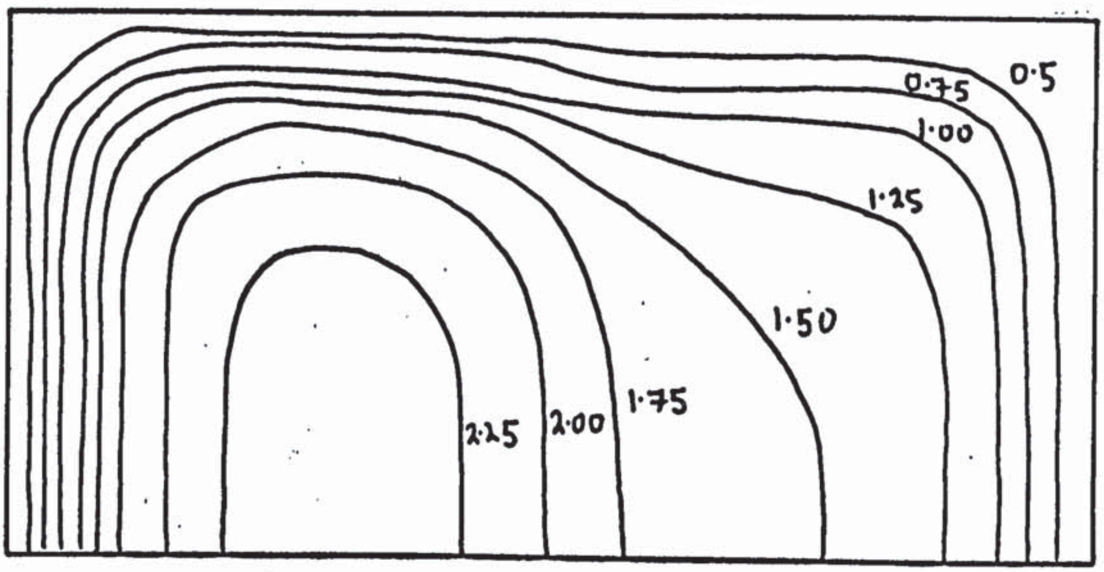
Figure 6.3.1

ABCDEFGH represents A duct with inlet ABCD and outlet EFGH
On ABCD u is specified as a step function
On EFGH u is specified as a Poisson solution
All other boundary velocities are zero

Figure 6.3.2

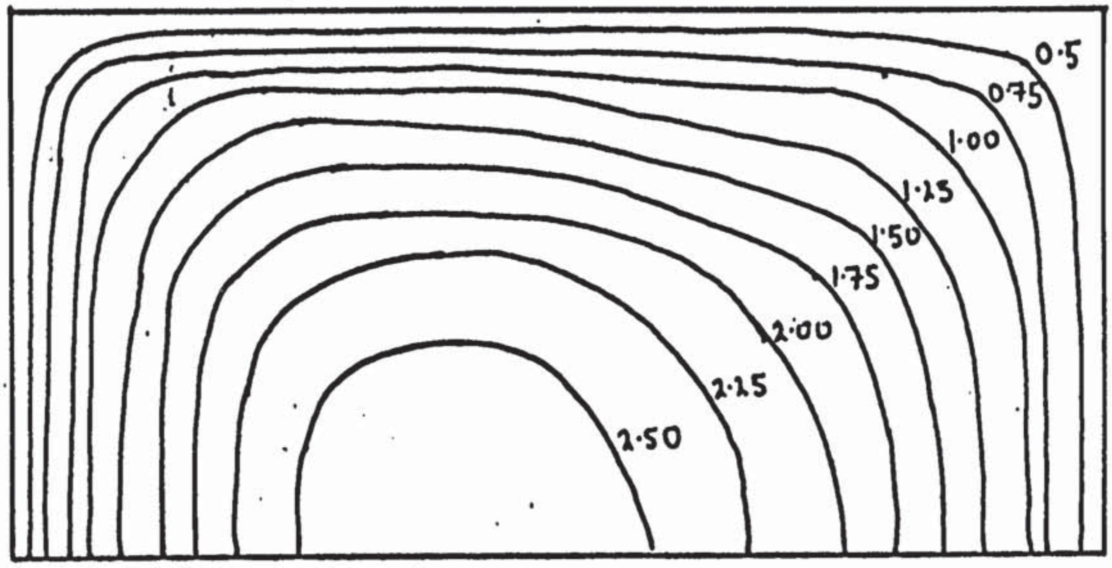


Roscoe contour plots of normal velocities at Plane 2.

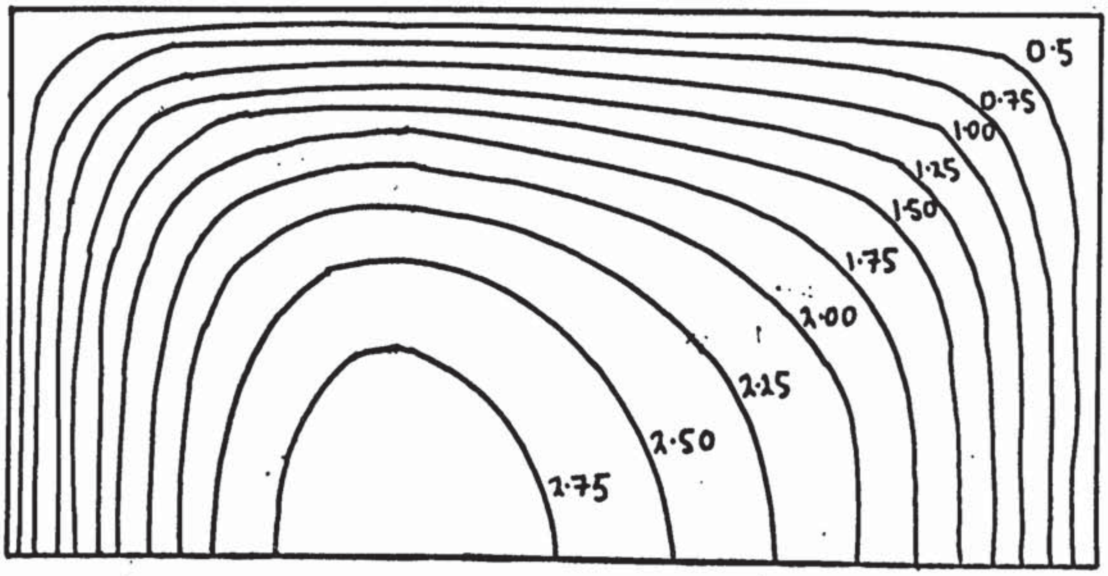


Aregbesola contour plots of normal velocities at Plane 2.

Figure 6.3.3

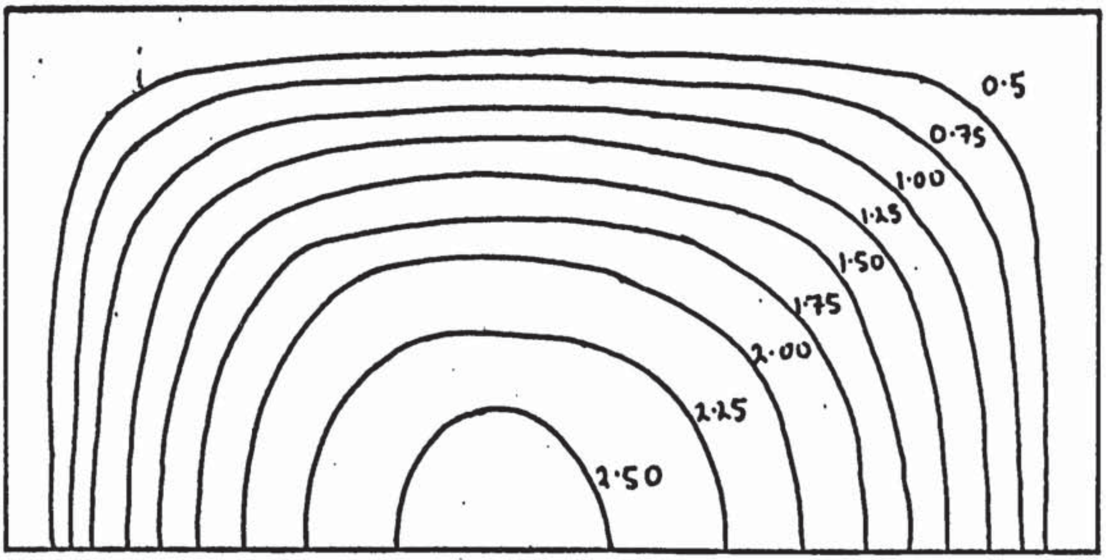


Roscoe contour plots of normal velocities at Plane 3.

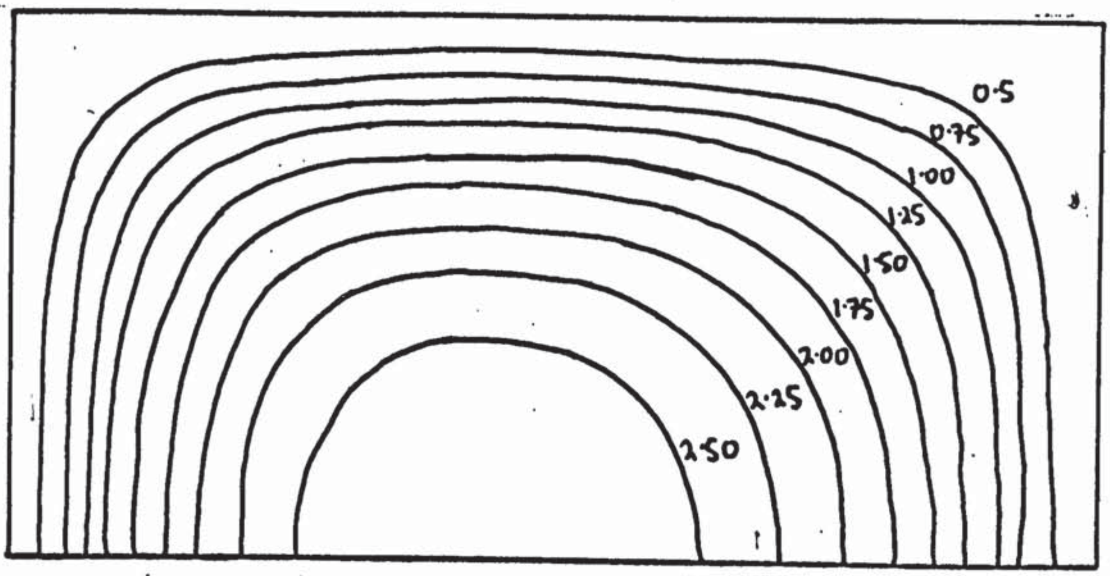


Aregbesola contour plots of normal velocities at Plane 3.

Figure 6.3.4



Roscoe contour plots of normal velocities at Plane 4.



Aregbesola contour plots of normal velocities at Plane 4.

obvious difficulty of there being no directly comparable points between the two discretisations, it was necessary for the two authors to define their mass flows in different fashions. The present author's results used the conditions on boundary pressure derived for Case (i) in Chapter 5.

Results

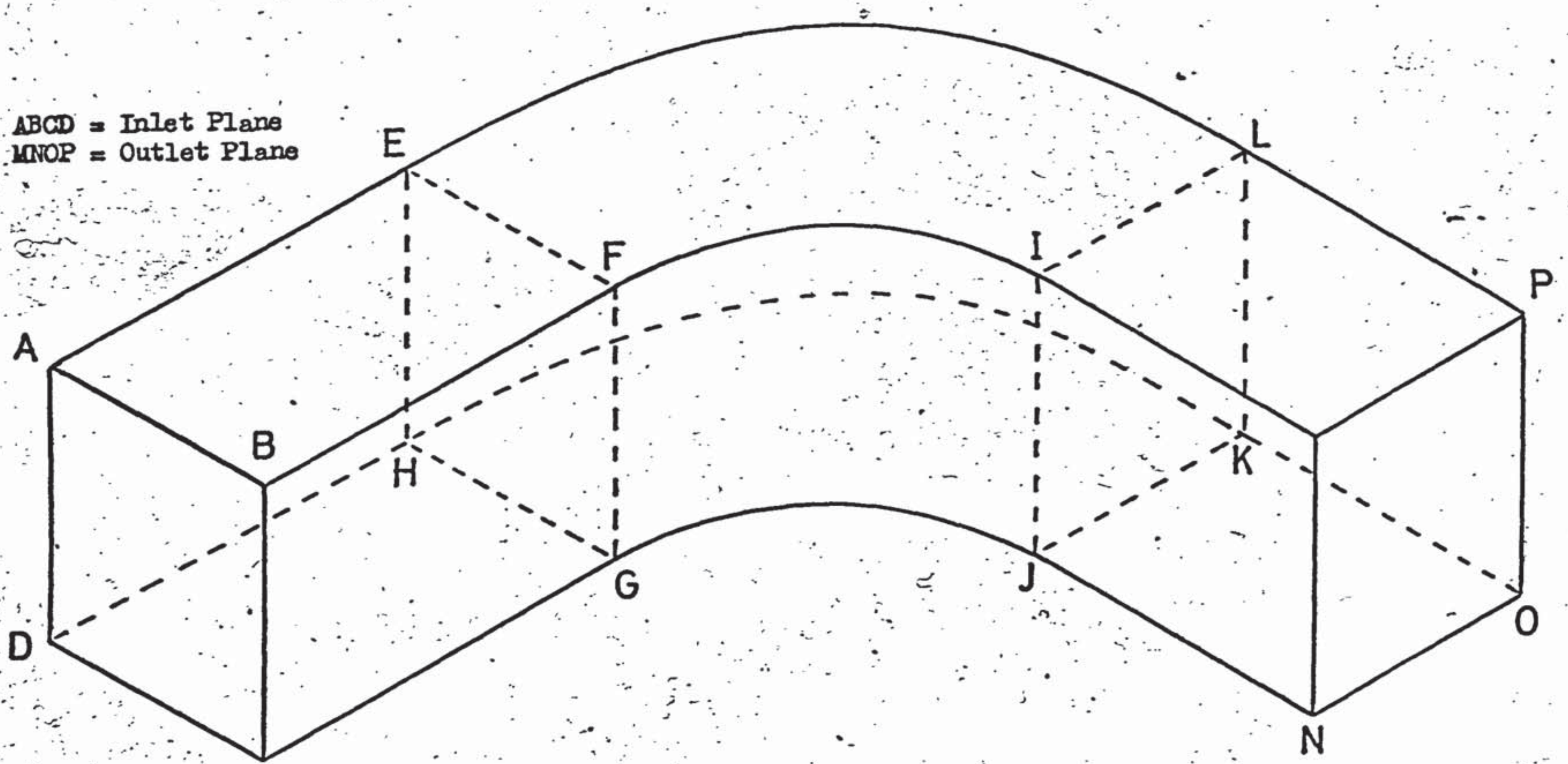
Figs 6.3.2. - 6.3.4. give normal velocity contour plots for the planes 2, 3 and 4 - most of the change in the flow occurs over these three planes. The present author's results are given at the top of each figure and Aregbesola's at the bottom of each figure.

There is excellent agreement in the prediction of the rate at which profile develops over the three planes with the two profiles of each figure being qualitatively similar. In each figure there is good quantative agreement for low value velocities, with only a moderate agreement for the high value velocities.

6.4 Comparisons of the Present Method with a Physical Experiment

The present method has been used in an attempt to reproduce the results of a wind tunnel experiment performed by Joy [51]. The geometry and dimensions of the wind tunnel are given in Fig 6.4.1. Stuart [37] applied his 3-D inviscid streamline curvature method to the same experiment and has predicted the main features of the flow. Fig 6.4.2 shows the total pressure contours on the inlet plane of

Figure 6.4.1



ABCDEFGH and IJKLMNOP are rectangular parallelepipeds. EFGHIJKL has a rectangular cross section, and the boundary lines FI, EL, GJ and HK all lie on circular arcs.

RADIUS ARC GJ = 12·5"

DC = 5"

BC = 10"

the duct. It can be seen that the flow is approximately symmetrical about the line XX'. Figs 6.4.3 - 6.4.5 give comparisons between Joy's measured total pressure contours and Stuart's predicted total pressure contours in the top half of each plane at 30°, 60° and 90° respectively. (Because of the 'symmetry' of the inlet data, the total pressure plots for the bottom half of each plane are similar).

For the initial development, the present author chose to neglect the straight inlet and outlet sections of the duct in order to simplify the programming details. Whilst this will clearly alter the quantative nature of any results, the qualatative effects of the duct geometry on the flow should still be visible. These effects are illustrated in Figs 6.4.3 - 6.4.5, and the main effect after 90°, in Fig 6.4.5, is a twisting of the total pressure contours.

This twisting gives rise to increasing total pressures towards the outside of the bend, along OX_1, and towards the top of the plane, along OX_2.

<u>General Difference form of $\tilde{T}$, the Momentum Operator</u>

Initially, finite difference equations of the form (4.3.12) were derived with $\tilde{T}$ having the original UDR form, in which the coefficients of an equation at (i, j, k) were all evaluated at (i, j, k). Following the solution procedures given in Chapter 5, converged solutions were obtained for a variety of boundary conditions, but all such solutions were very poor in comparison with experiment.

The numerical experiments were repeated with the modified $\tilde{T}$ whose general form is given at (4.2.16) (ie the form for which stability of the complete difference representation was proved). The results were, again, very poor. Finally it was decided to define $\tilde{T}$ in a conservative form based on the original UDR form. Thus, expressing the original UDR form as

$$\tilde{T}\,\psi_{ijk} = f_i\,\psi_{i+1jk} - (f_i + f_i\,g_i)\,\psi_{ijk} + f_i\,g_i\,\psi_{i-1jk}$$

$$+ \text{ (similar terms for j, k differences)} \qquad (6.4.1)$$

then the conservative $\tilde{T}$ is defined as

$$\tilde{T}\,\psi_{ijk} = f_{i+1}\,\psi_{i+1jk} - (f_i + f_i\,g_i)\,\psi_{ijk} + f_{i-1}\,\psi_{i-1jk}$$

$$+ \text{ (similar terms for j, k differences)} \qquad (6.4.2)$$

The coefficients f_i and g_i are the coefficients in (4.1.3). With the boundary conditions outlined below, this conservative form of $\tilde{T}$ proved to be partially successful.

Boundary Conditions

(i) For the Momentum Equations

On the inlet plane, and the solid boundaries, velocities were specified. On the exit plane, since the straight exit section was discarded, it was felt that specifying parallel flow would be too restrictive. Thus, the conditions assumed were that swirl was constant (ie the 'in-plane' velocities remain constant over the last two planes) and that the second normal derivative of the normal velocity was zero on exit ($\partial^2 u/\partial x^2 = 0$). These exit conditions include the parallel flow conditions, but allow more freedom in the final solution.

(ii) For the Pressure Equation

On the inlet plane, zero static pressure was assumed. On the solid boundaries, pressure was obtained by integrating the wall-tangential momentum equations along the solid boundaries from inlet to exit planes. At the walls, the second normal derivatives of the wall-tangential velocities were approximated by forward and backward differences into the flow, thus avoiding the arbitrary estimation of velocity components at fictitious points. To complete the pressure information on the inlet plane, and the solid boundaries, pressure differences across these boundaries were prescribed using the method of Case (i)(A) conditions explained on p. 62. Thus, on the inlet plane and the solid boundaries, Case (ii) conditions have been employed.

On the exit plane, Case (i) conditions are employed. To use Case (i) conditions we need to make a statement about the normal velocity near the exit planes, in addition to that already made. We say that $\partial^2 u/\partial x^2 = 0$ on the plane prior to the exit plane.

These conditions close the equations, and allow a solution to be obtained.

Results

These are given in Figs 6.4.6 - 6.4.8 for 30°, 60° and 90° respectively.

The 30° results appear quite good, although the total pressure seems to decrease more than should towards the outer boundary. The 'dip' in the contours at about the mid-plane agrees with observation, and the inner boundary results seem very good.

The 60° results bear only a slight resemblance to the experimental results at 60°, but they are similar to the 30° results.

The 90° results bear only a slight resemblance to the experimental results, except that there is agreement on the rise in total pressure towards the outside of the bend, and in a sense, the 90° results are quite similar to the 60° experimental results insofar as the 'high' total pressure contours tend to pass from the line of symmetry to the outer wall of the pipe.

In the author's view, these results represent a limited success, and are sufficiently good to indicate that further work could well be worthwhile.

Parameters of the Flow

Gas Medium:- Air

Density = 0.07 lbs/ft^3

Kinematic viscosity = 0.000143 ft^2/sec

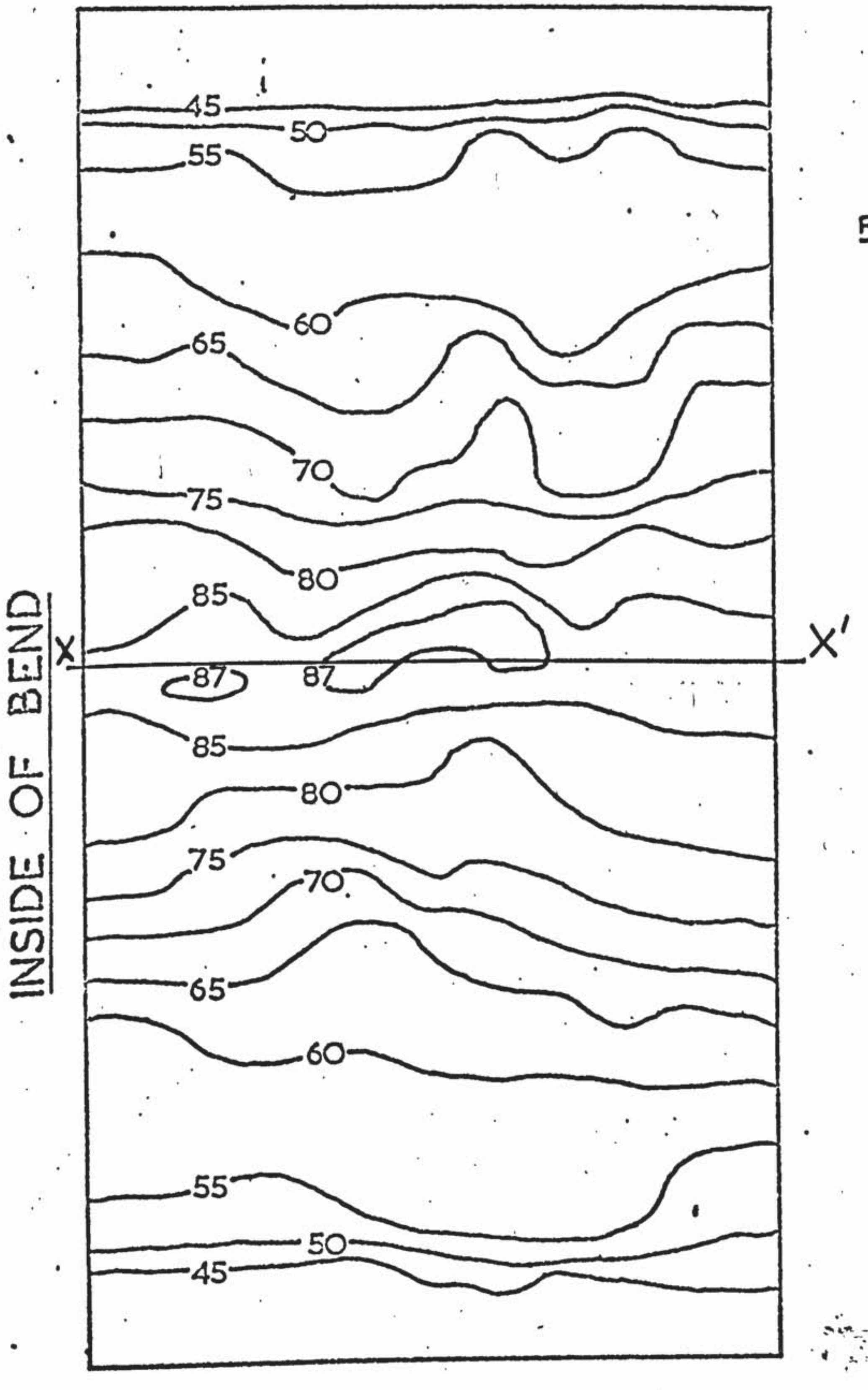
6.5 Possible Defects of the Model and a Suggested Remedy

From the point of view of calculating high Reynolds number flows, the present author feels that the main defect in his model is in the

15" x 90° BEND

STATION 1 - LOOKING UPSTREAM

FIG 6.4.2



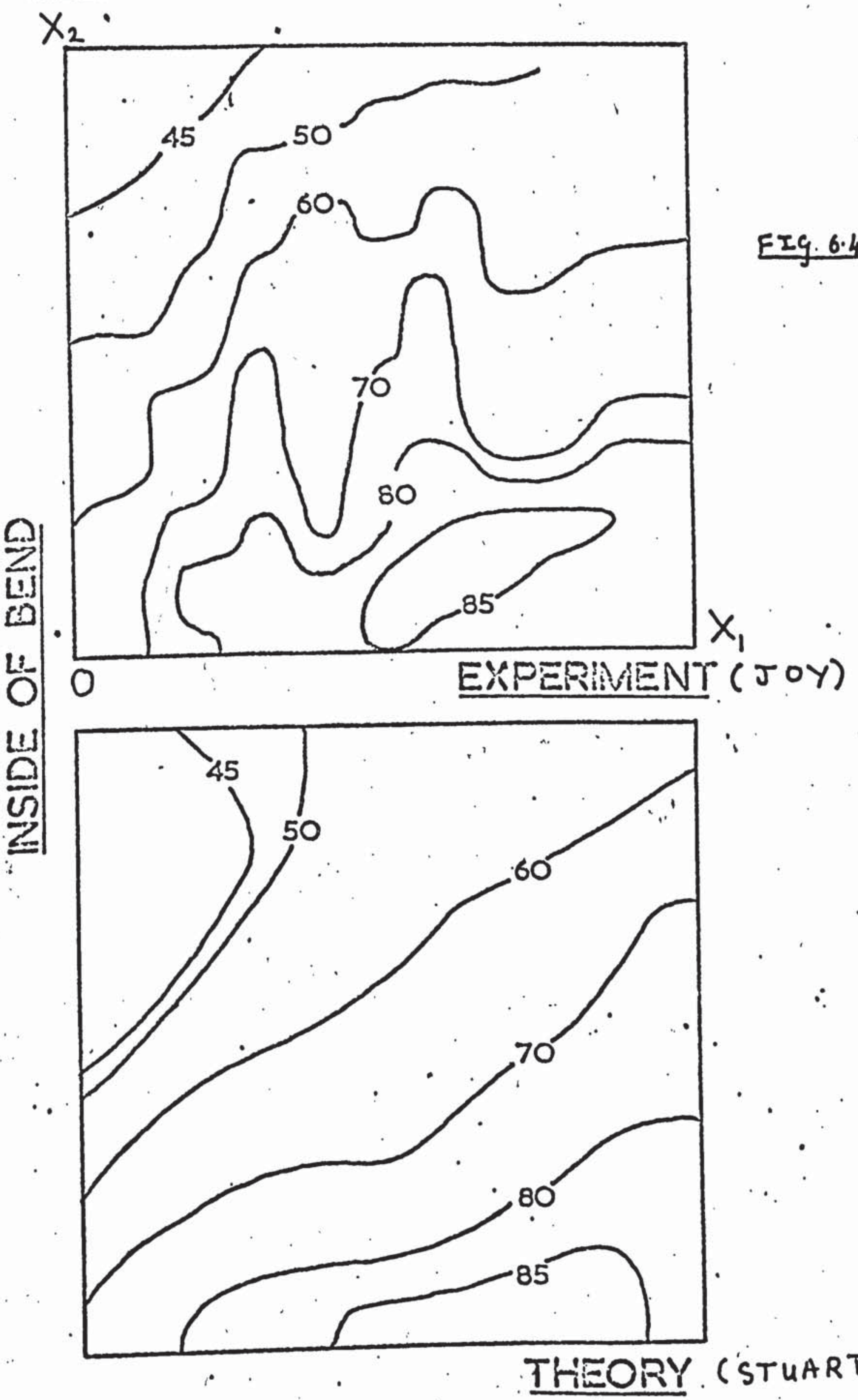
TOTAL PRESSURE CONTOURS

Stuart/Hetherington

15" x 90° BEND

STATION 2 - LOOKING UPSTREAM

FIG. 6.4.3.



Stuart + Hetherington

15" x 90° BEND

STATION 3 - LOOKING UPSTREAM

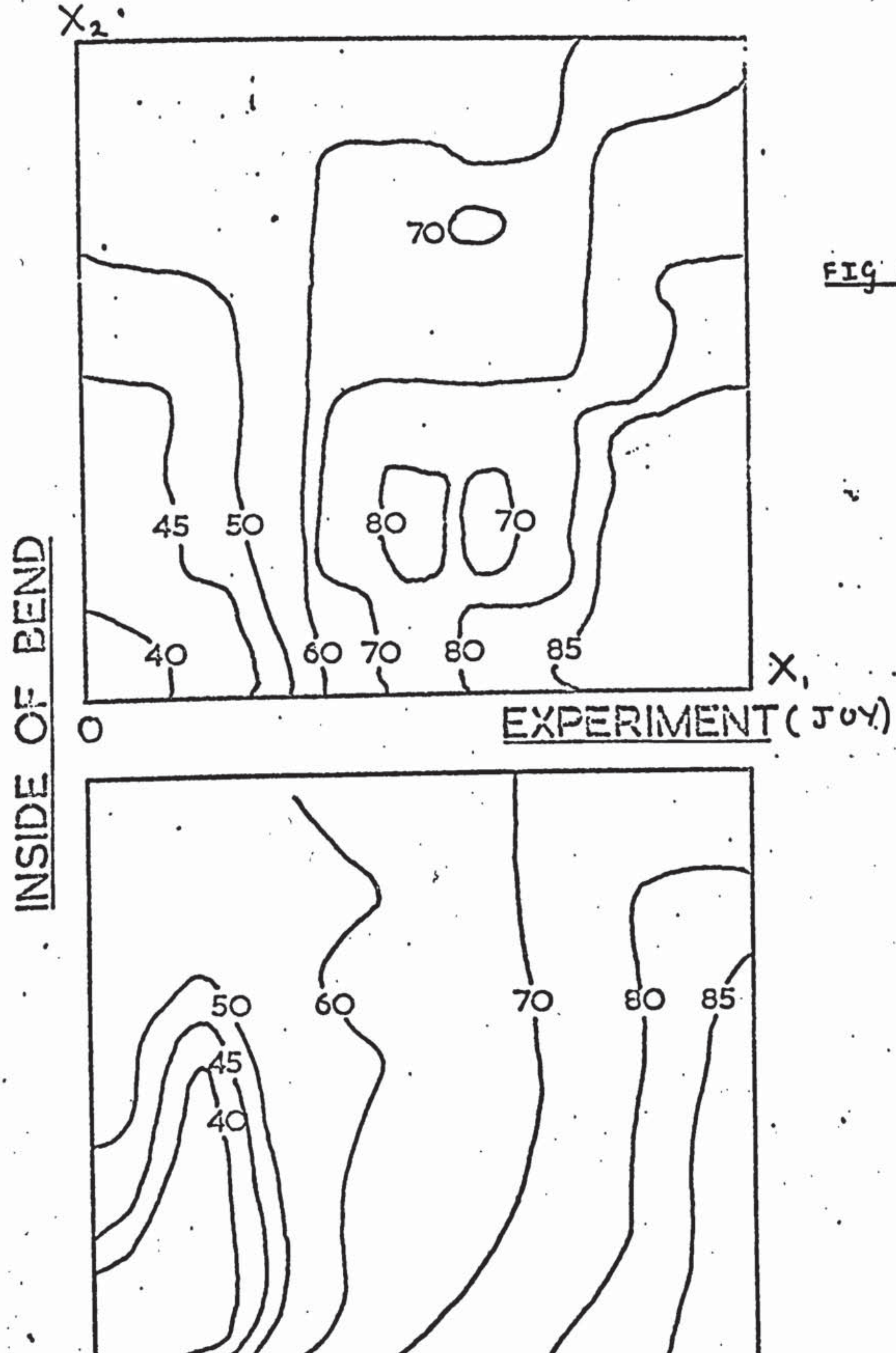


FIG 6·4·4·

15" x 90° BEND

STATION 4 - LOOKING UPSTREAM

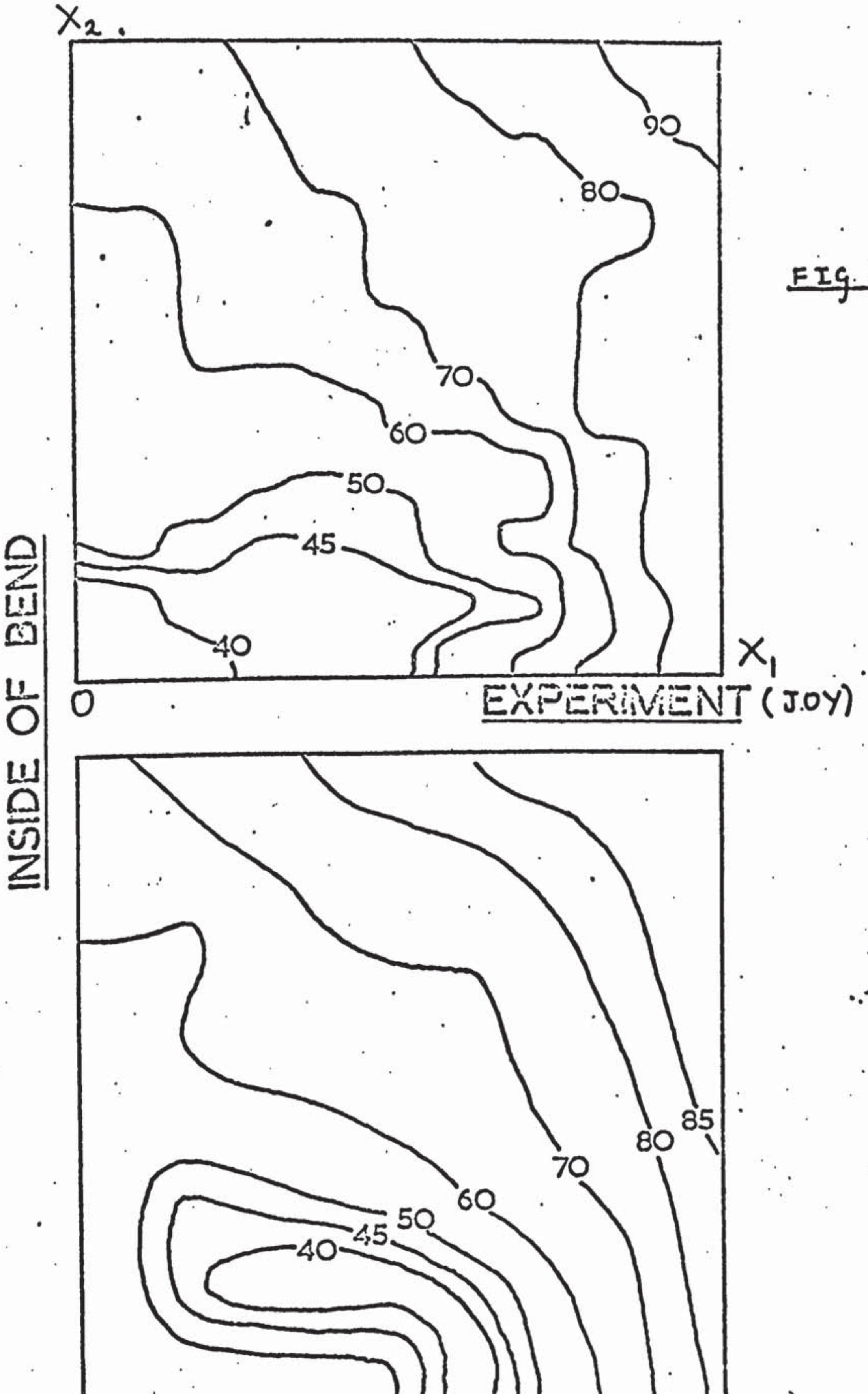
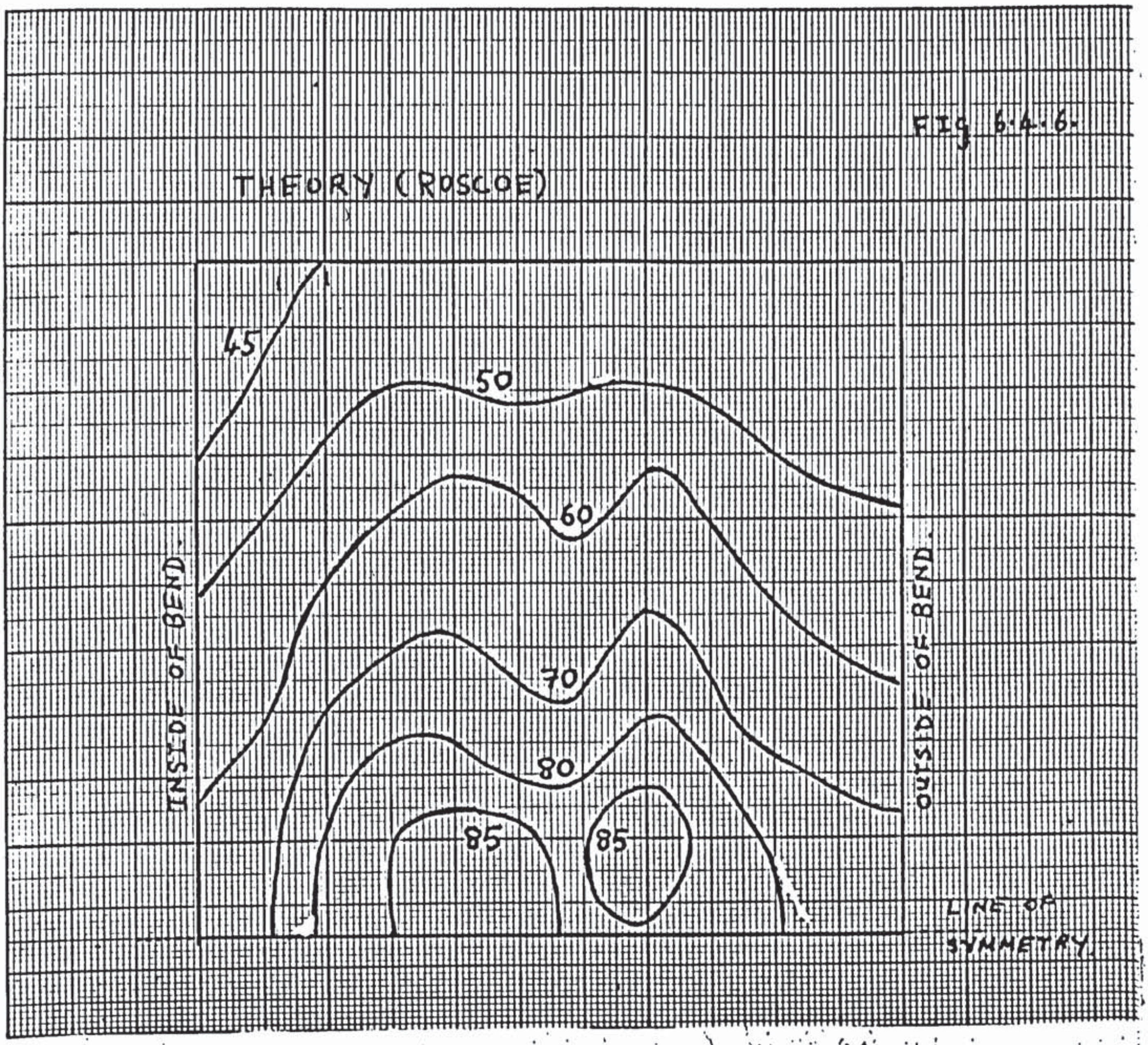


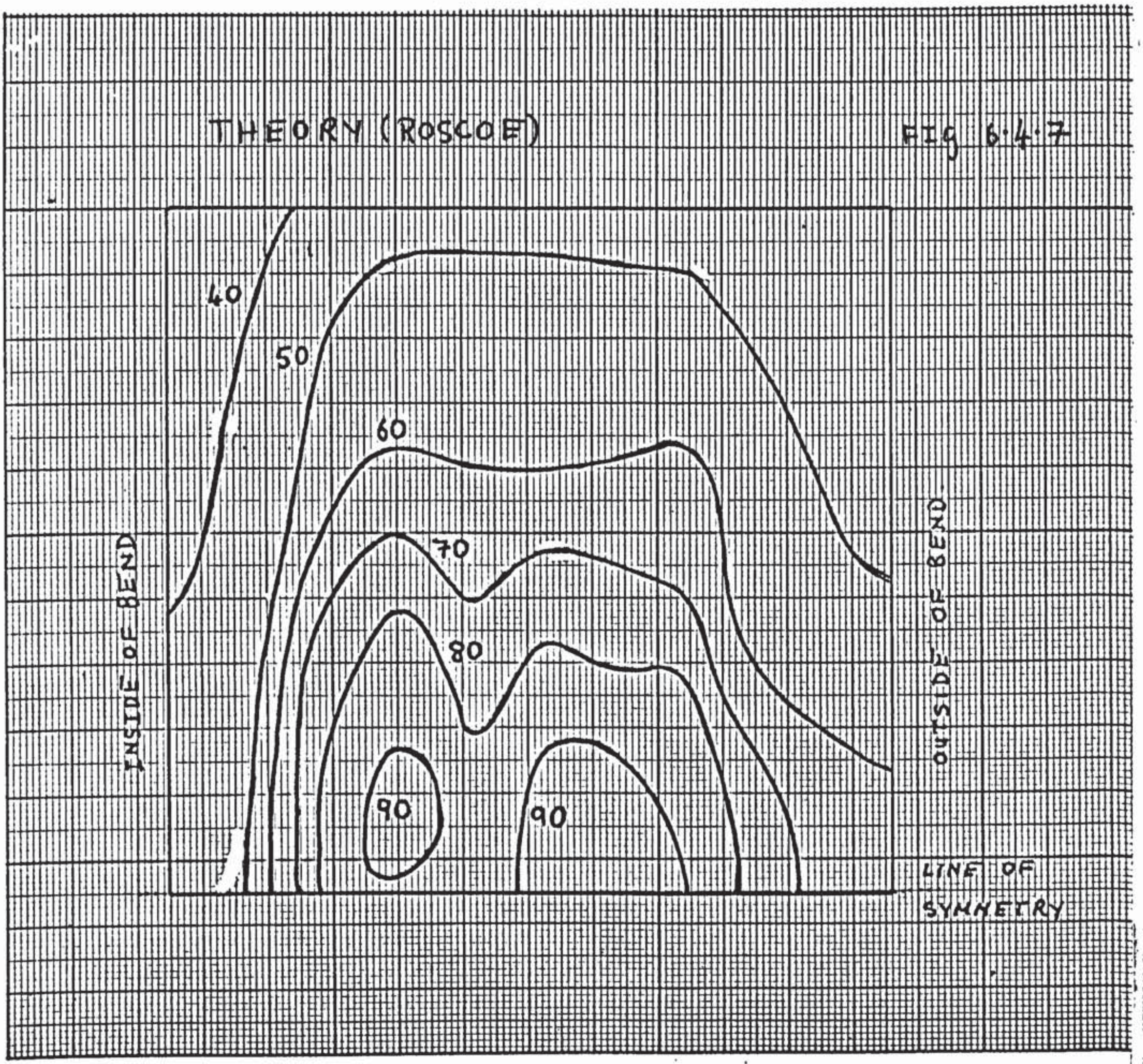
FIG. 6·4·5.

Stuart + Hatherington



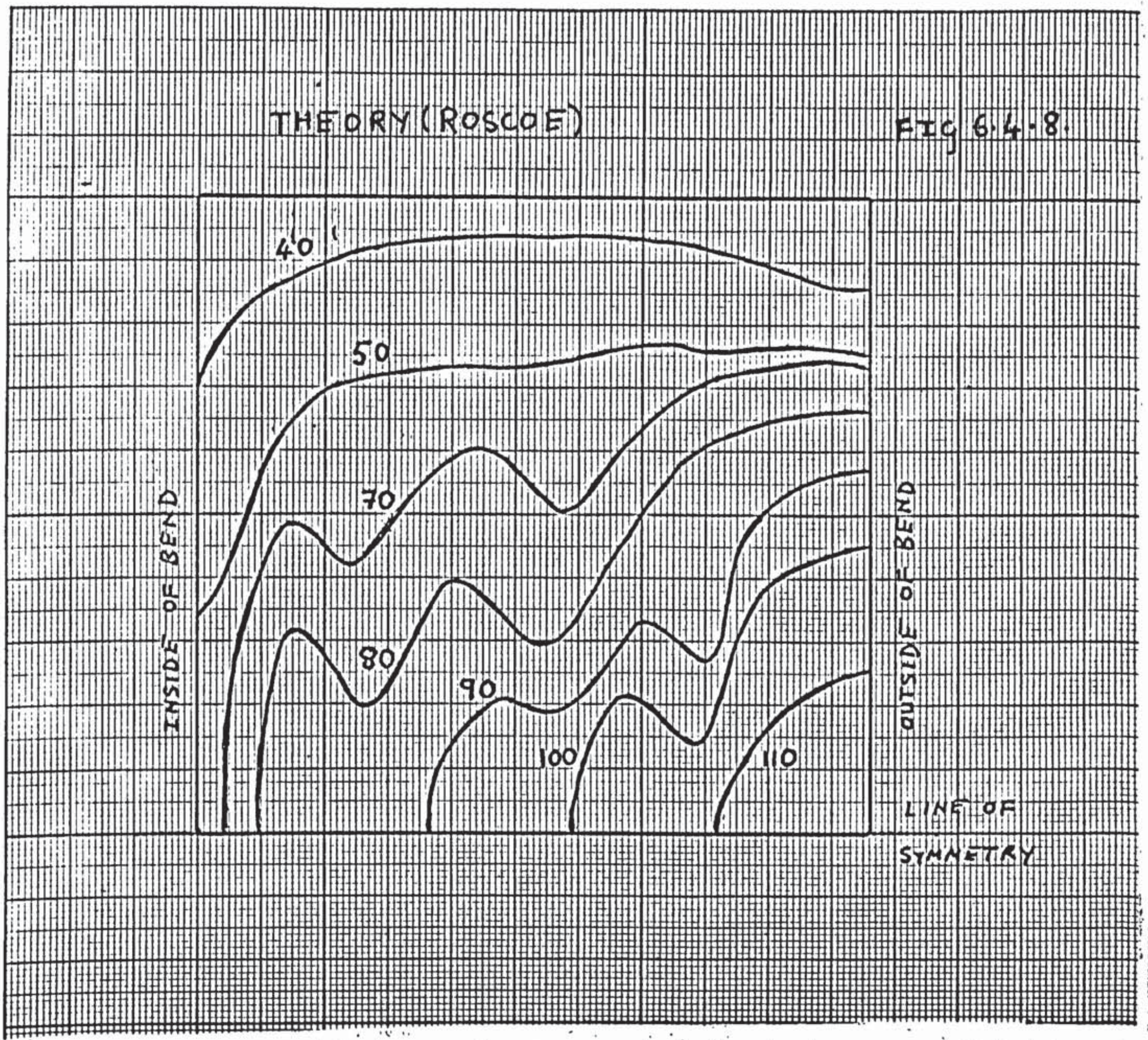
Total pressure contours at 30° of bend.

There is good agreement with the experiment results, Fig 6.4.3 (top)



Total pressure contours at 60^{o} of bend.

There is poor agreement with the experimental results, Fig 6.4.4 (top). The contours here appear to be a more developed version of the 30^{o} contours in Fig 6.4.6.

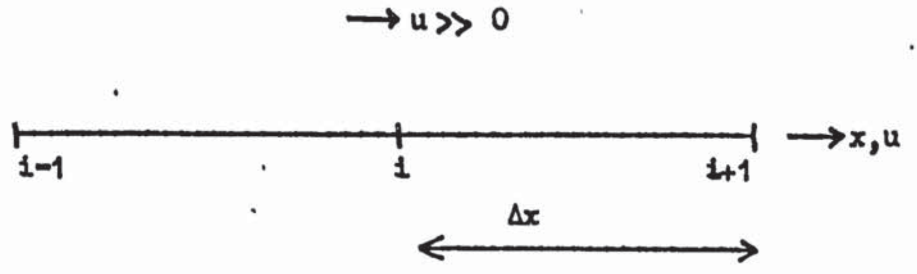


Total pressure contours at 90° of bend.

There is poor agreement with the experimental results, Fig 6.4.5 (top). However, these curves bear some resemblance to the 60° experimental curves, Fig 6.4.4 (top).

manner of representing the pressure/continuity terms, ie by using central difference formulae.

Figure 6.5.1



Consider the one dimensional diagram Fig 6.5.1, then in the limit of infinite Reynolds numbers (ie Kinematic viscosity tending to zero), at the point i, the UDR for $\left(u \frac{\delta u}{\delta x} - \nu \frac{\delta^2 u}{\delta x^2}\right)$ tends to $\frac{u_i}{\Delta x}$ $(u_i - u_{i-1})$ and the corresponding pressure gradient in our model is $\left(\frac{p_{i+1} - p_{i-1}}{2\Delta x}\right)$. Thus the momentum and pressure terms are centred at different points. Intuitively, we can see that the 'correct' form of the pressure gradient is $\left(\frac{p_i - p_{i-1}}{\Delta x}\right)$. In physical terms, we can equate this with the statement that for an inviscid fluid, the 'pressure force' accelerating a fluid particle from (i-1) to i arises from the pressure difference between i and (i-1).

Extrapolating this intuitive view to a high Reynolds number 3-D flow, we see that at a point (x, y, z) = (iΔx, jΔy, kΔz) then $\delta p/\delta x$, $\delta p/\delta y$ and $\delta p/\delta z$ are best approximated by 'upwind' differences, ie are best backward differenced relative to the respective directions of the velocity components u, v and w

$$\left.\begin{array}{ll} \text{Thus if } u_i > 0, \text{ then } \frac{\delta p}{\delta x} \simeq \frac{p_i - p_{i-1}}{\Delta x} \\ \text{if } u_i < 0, \text{ then } \frac{\delta p}{\delta x} \simeq \frac{p_{i+1} - p_i}{\Delta x} \end{array}\right\} \qquad (6.5.1)$$

etc.

This naturally begs the question of how to approximate the continuity equation. Theorem 4.2.2 supplies the answer to this question. Suppose that

$$\left.\begin{array}{l} D_i \, \underline{p} \simeq \frac{\delta p}{\delta x} \\ D_j \, \underline{p} \simeq \frac{\delta p}{\delta y} \\ D_k \, \underline{p} \simeq \frac{\delta p}{\delta z} \\ \tilde{D}_i \, \underline{u} + \tilde{D}_j \, \underline{v} + \tilde{D}_k \, \underline{w} \simeq \frac{\delta u}{\delta x} + \frac{\delta v}{\delta y} + \frac{\delta w}{\delta z} \end{array}\right\} \qquad (6.5.2)$$

Then, if T represents the UDR of the momentum operator, the equations of motion become

$$\begin{pmatrix} T & 0 & 0 & D_i \\ 0 & T & 0 & D_j \\ 0 & 0 & T & D_k \\ \tilde{D}_i & \tilde{D}_j & \tilde{D}_k & 0 \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{v} \\ \underline{w} \\ \underline{p} \end{pmatrix} = \underline{b} \qquad (6.5.3)$$

where $\underline{b}$ is the vector of boundary information. For stability, Theorem 4.2.2 implies that S defined by

$$S = \begin{pmatrix} 0 & 0 & 0 & D_i \\ 0 & 0 & 0 & D_j \\ 0 & 0 & 0 & D_k \\ \tilde{D}_i & \tilde{D}_j & \tilde{D}_k & 0 \end{pmatrix} \tag{6.5.4}$$

should be skew-symmetric. Thus, since we have deduced from physical considerations, forms for D_i, D_j and D_k, the requirement of skew-symmetry of S defines $\tilde{D}_i$, $\tilde{D}_j$ and $\tilde{D}_k$. We find the interesting result, that broadly speaking 'upwind' differences for the pressure derivatives implies 'downwind' differences for the continuity terms. More precisely, defining†

$$N_i = \text{Sign}(u_i) = \left.\begin{matrix} +1 & \text{if } u_i > 0 \\ -1 & \text{if } u_i < 0 \end{matrix}\right\} \tag{6.5.5}$$

then the approximations for $\partial p/\partial x$ and $\partial u/\partial x$ of the continuity equation are given by

$$\frac{\partial p}{\partial x} \simeq \frac{1}{\Delta x} \left[\left(\frac{1 - N_i}{2}\right) p_{i+1} + N_i \, p_i - \left(\frac{1 + N_i}{2}\right) p_{i-1}\right]$$

and

$$\frac{\partial u}{\partial x} \simeq \frac{1}{\Delta x} \left[\left(\frac{1 + N_{i+1}}{2}\right) u_{i+1} - N_i \, u_i - \left(\frac{1 - N_{i-1}}{2}\right) u_{i-1}\right] \tag{6.5.6}$$

---

† The treatment of N_i when $u_i = 0$ is complicated, and since the above ideas are not fully developed, no attempt will be made to explain this procedure.

The pressure equation arising out of these schemes turns out to be of second order only, and thus requires only one piece of pressure information at each point of the boundary. From this point of view, the schemes are more satisfactory than those already discussed.

The author is currently attempting to apply these schemes to the wind tunnel experiment discussed in 6.4.

APPENDIX I

A1.1 Derivation of UDR for Partial Differential Operators

Consider

$$TZ \;=\; a\frac{\partial^2 Z}{\partial x^2} + b\frac{\partial Z}{\partial x} + c\frac{\partial^2 Z}{\partial y^2} + d\frac{\partial Z}{\partial y} + fZ \;=\; 0 \qquad (A1.1.1)$$

The UDR will be derived on a uniform mesh. The extension to a non-uniform mesh will be obvious.

(A1.1.1) is partitioned into three bits. The procedure will be to develop a representation for each bit, and to take the UDR of (A1.1.1) as being a certain linear combination of these three representations. To this end consider

$$a\frac{d^2Z}{dx^2} + b\frac{dZ}{dx} \;=\; 0$$

$$c\frac{d^2Z}{dy^2} + d\frac{dZ}{dy} \;=\; 0 \qquad (A1.1.2)$$

The homogenous solutions are respectively

$$Z \;=\; 1 \text{ and } e^{-bx/a}$$

$$Z \;=\; 1 \text{ and } e^{-dy/c} \qquad (A1.1.3)$$

The corresponding finite difference solutions are

$$Z_i = 1 \text{ and } (e^{-b\Delta x/a})^i$$

$$Z_j = 1 \text{ and } (e^{-d\Delta y/c})^j \qquad \text{(A1.1.4)}$$

It follows that the auxiliary equations of the difference equations having (A1.1.4) as solutions are, respectively

$$(m - 1)(m - e^{-b\Delta x/a}) = 0$$

$$(n - 1)(n - e^{-d\Delta y/c}) = 0 \qquad \text{(A1.1.5)}$$

giving immediately, the difference equations

$$Z_{i+1} - (1 + e^{-b\Delta x/a}) Z_i + e^{-b\Delta x/a} Z_{i-1} = 0$$

$$Z_{j+1} - (1 + e^{-d\Delta y/c}) Z_j + e^{-d\Delta y/c} Z_{j-1} = 0 \qquad \text{(A1.1.6)}$$

Accordingly, there is chosen, for the UDR of (A1.1.1)

$$\hat{T}Z_{ij} = k_o [Z_{i+1j} - (1 + e^{-b\Delta x/a}) Z_{ij} + e^{-b\Delta x/a} Z_{i-1j}]$$

$$+ k_1 [Z_{ij+1} - (1 + e^{-d\Delta y/c}) Z_{ij} + e^{-d\Delta y/c} Z_{ij-1}]$$

$$+ fZ_{ij} = 0 \qquad \text{(A1.1.7)}$$

for some k_o and k_1. It remains to choose k_o and k_1. The procedure of section 2.3 cannot be followed, since as proven in Appendix IV, no elliptic difference equation with a finite number of terms, like (A1.1.7) can be an exact representation of an elliptic differential equation. Thus, k_o and k_1 are required such that (A1.1.7) is a 'good' representation of (A1.1.1) in some limited sense.

It will be shown, that the k_0 and k_1 turn out exactly as would k_0 and k_1 for the corresponding ordinary differential equations following the procedure of Section 2.3. Define

$$\psi(x,y) = l_0xy + l_1x + l_2y + l_3 \qquad (A1.1.8)$$

hence, the difference form of (A1.1.8) with obvious notation is

$$\psi_{ij} = (l_0\Delta x\,\Delta y)\,ij + (l_1\Delta x)\,i + (l_2\Delta y)\,j + l_3 \qquad (A1.1.9)$$

The criteria chosen for k_0 and k_1 of $\hat{T}Z_{ij}$ is that $\hat{T}$ and T (the operators of (A1.1.7) and (A1.1.1) are to be identical in their actions on ψ_{ij} and $\psi(x,y)$ respectively. Thus

$$T\psi(x,y) = b\,l_0y + d\,l_0x + b\,l_1 + d\,l_2 + f\psi(x,y)$$

$$= (b\,l_0\Delta y)\,j + (d\,l_0\Delta x)\,i + b\,l_1 + d\,l_2 + f\psi_{ij} \qquad (A1.1.10)$$

Substitution of (A1.1.9) into (A1.1.7) yields

$$\hat{T}\psi_{ij} = k_0\,[(l_0\Delta x\,\Delta y)\,j + l_1\Delta x]\,[(i+1) - (1 + e^{-b\Delta x/a})\,i + e^{-b\Delta x/a}\,(i-1)] + k_1\,[(l_0\Delta x\,\Delta y)\,i + l_2\Delta y]\,[(j+1) - (1 + e^{-d\Delta y/c})\,j + e^{-d\Delta y/c}\,(j-1)] + f\psi_{ij} = k_0\,[(l_0\Delta x\,\Delta y)\,j + l_1\Delta x]\,[1 - e^{-b\Delta x/a}] + k_1\,[(l_0\Delta x\,\Delta y)\,i + l_2\Delta y]\,[1 - e^{-d\Delta y/c}] + f\psi_{ij} \qquad (A1.1.11)$$

Comparing coefficients of i and j between (A1.1.10) and (A1.1.11) yields

$$k_o = \frac{b}{\Delta x\ (1 - e^{-b\Delta x/a})}$$

$$k_1 = \frac{d}{\Delta y\ (1 - e^{-d\Delta y/c})} \qquad (A1.1.12)$$

Comparison of (A1.1.12) with (2.3.5) shows that k_o and k_1 are essentially identical.

APPENDIX II

A DISCUSSION ON THE STABILITY OF SOME TAYLOR SERIES REPRESENTATIONS

A2.1 An Example

To illustrate one aspect of the stability problem, consider the simple system

$$\frac{d^2Z}{dx^2} + a\frac{dZ}{dx} = 0 \qquad (A2.1.1)$$

Three Taylor series representations of A21.1. are

$$\frac{1}{\Delta x^2}(Z_{i+1} - 2Z_i + Z_{i-1}) + \frac{a}{2\Delta x}(Zi+1 - Z_{i-1}) = 0 \qquad (A2.1.2)$$

$$\frac{1}{\Delta x^2}(Z_{i+1} - 2Z_i + Z_{i-1}) + \frac{a}{\Delta x}(Z_i - Z_{i-1}) = 0 \qquad (A2.1.3)$$

$$\frac{1}{\Delta x^2}(Z_{i+1} - 2Z_i + Z_{i-1}) + \frac{a}{\Delta x}(Z_{i+1} - Z_i) = 0 \qquad (A2.1.4)$$

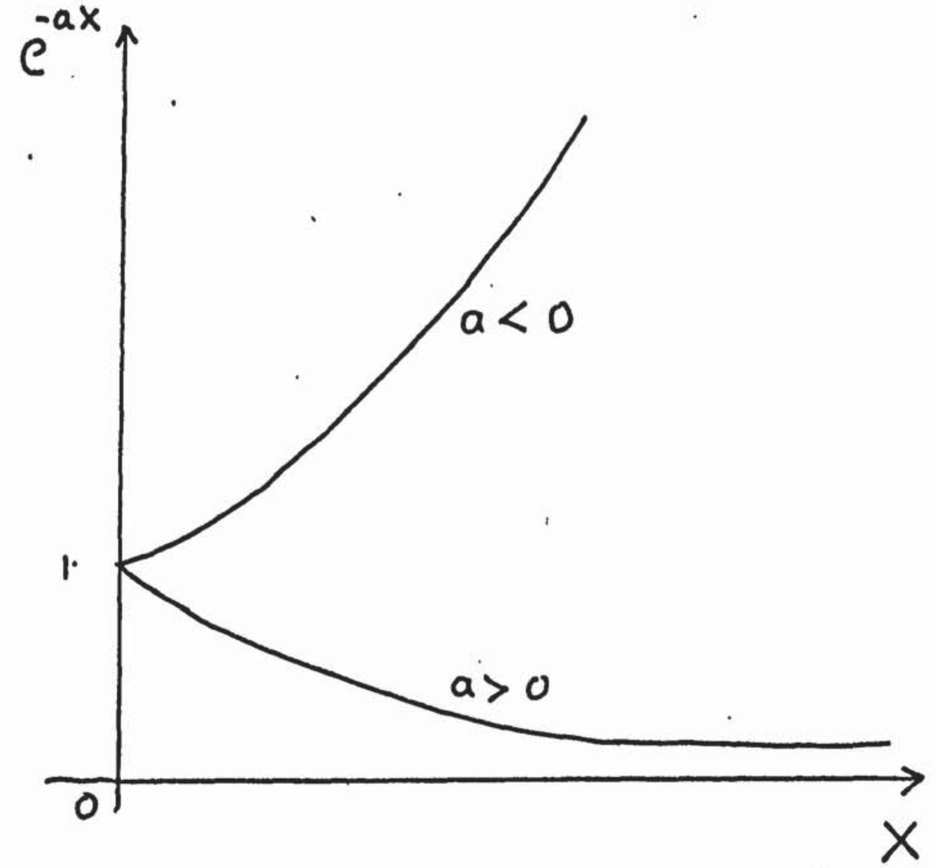
Now the true solution of (A2.1.1) is given by

$$Z(x) = A_0 + A_1 e^{-ax} \qquad (A2.1.5)$$

Each of the three representations (A2.1.2)-(A2.1.4) has A_0 as a solution, so the question is, how close are the non-constant components of their solutions to e^{-ax}?

The behaviour of the exponential term of (A2.1. 5) is illustrated in Fig. A2.1.1.

Figure A2.1.1



For positive a the function decays, and for negative a, the function increases.

The very least that should be expected of the finite difference solutions is that they behave monotonically as e^{-ax} for $a > 0$ and $a < 0$.

Each solution is considered in turn.

(i) (A2.1.2) yields the solution

$$Z_i = A_o + A_1 \left(\frac{2 - a.\Delta x}{2 + a.\Delta x} \right)^i \qquad (A2.1.6)$$

If the behaviour of the exponential term of (A2.1.6) is analysed, it is seen that it only displays the correct monotonic behaviour for $a > 0$ and $a < 0$ if the condition

$$\Delta x < \left| \frac{2}{a} \right| \qquad (A2.1.7)$$

is satisfied. If condition (A2.1.7) is contravened by equality, then the only solution of the difference equation is a constant, and thus two independent boundary conditions could not be fitted. The system is overdetermined. If (A2.1.7) is contravened by the opposite inequality, then the solution becomes oscillatory, and then although a solution can be found it is useless. Hence (A2.1.7) is the condition for stability of the difference equation.

(ii) (A2.1.3) yields the solution

$$Z_i = A_o + A_1 \, (1 - a.\Delta x)^i \qquad (A2.1.8)$$

Analysis of the exponential term yields that if

$$a > 0$$

then

$$\Delta x < \frac{1}{a} \tag{A2.1.9}$$

for the stability, and that if $a < 0$ there is no condition on Δx and proper behaviour is guaranteed for all Δx.

Again if $\Delta x = 1/a$, $a > 0$, then the system has only a constant as a solution.

(iii) (A2.1.4) yields the solution

$$Z_i = A_o + A_1 \left(\frac{1}{1 + a\Delta x}\right)^i \tag{A2.1.10}$$

Analysis of the exponential term yields that if

$$a < 0$$

then

$$\Delta x < -\frac{1}{a} \tag{A2.1.11}$$

for stability, and that if $a > 0$, there is no condition on Δx and proper behaviour is guaranteed for all Δx. $\Delta x = 1/a$ is the degenerate case.

To summarise these results there is

(i) A condition for stability always exists on the central difference scheme, and if 'a' becomes very large, then the condition (A2.1.7) would make a central difference scheme computationally infeasible.

(ii) The backward difference scheme is unconditionally stable if $a < 0$, but a restrictive condition holds if $a > 0$. Again if 'a' becomes very large and positive, then a backward difference scheme becomes infeasible.

(iii) The forward difference scheme is unconditionally stable if $a > 0$, but a restrictive conditions holds if $a < 0$. If 'a' becomes very large and negative, then a forward difference scheme becomes infeasible.

From these conclusions, it is reasonable to infer that if an equation like

$$\frac{d^2Z}{dx^2} + f(x)\frac{dZ}{dx} = 0 \qquad (A2.1.12)$$

where $f(x)$ takes both large positive and large negative values, is to be solved using one of the above schemes, then a stability condition

$$\Delta x < \frac{1}{|f(x)|_{max}} \qquad (A2.1.13)$$

must be applied. In the Navier-Stokes equations this precise situation holds where

$$f(x) = \frac{q}{\nu} \qquad (A2.1.14)$$

q being a flow velocity and ν being the kinematic viscosity. Thus, the condition (A2.1.13) gives the approximate requirement for a 3-D flow

$$\text{Max}\ (\Delta x,\ \Delta y,\ \Delta z) < \frac{\nu}{|q|_{max}} \qquad (A2.1.15)$$

In many situations (gas flows), $\nu \simeq 10^{-6}$, thus the condition (A2.1.15) makes the application of ordinary difference representations to many fluid flows problems completely infeasible.

A2.2 High Order Approximations to Derivatives

It often seems desirable to employ high order approximations in derivatives in order to reduce local truncation error. Such second order differences approximations to first order derivatives have been employed in this thesis at boundary points (See Chapter 5). However, care must be taken in their use. The reason is that an n-th order linear homogenous differential equation has n independent functions in its solution space, and any solution to the differential equation is made up as a linear combination of these n functions. Ideally, an n-th order difference representation is used because this also has n independent functions in its solution space, and if each of these n functions approximates one of the n functions of the differential equation and vice versa, then the difference solution will be a good approximation to the true solution.

However, suppose than an (n + 1)th order difference representation is used, then this will have (n + 1) functions in its solution space, and clearly, a 1:1 correspondence cannot be made between these functions, and those of the differential equation. If a correspondence between n of the functions can be made, and if the extra function decreases to zero as the solution proceeds, then the higher order scheme will be stable. In any other circumstance, eg the extra function increases as the solution proceeds, then the higher order scheme will be unstable.

<u>Example</u>

Consider the simple equation

$$\frac{dZ}{dx} = a \tag{A2.2.1}$$

then

$$Z(x) = ax + A_0 \tag{A2.2.2}$$

A_0 is the solution space of the homogenous form of (A2.2.1). The simplest approximation to (A2.2.1) is

$$Z_i - Z_{i-1} = a\Delta x \tag{A2.2.3}$$

therefore

$$Z_i = ai\Delta x + A_0 \tag{A2.2.4}$$

Thus, (A2.2.3) is in fact exact. However, a naive viewpoint might lead to a high order representation of (A2.2.1) being used, eg

$$\frac{Z_{i+2} - 4Z_{i+1} + 3Z_i}{-2\Delta x} = a \qquad (A2.2.5)$$

therefore

$$Z_{i+2} - 4Z_{i+1} + 3Z_i = -2a\Delta x \qquad (A2.2.6)$$

The homogenous solution of (A2.2.6) is

$$Z_i = A_o + A_1 3^i \qquad (A2.2.7)$$

The component A_o corresponds to the homogenous solution of (A2.2.1), but $A_1 3^i$ has no counterpart and renders the representation (A2.2.5) unstable.

The above is an exaggerated example, but it does illustrate a general principle:- it is good practice to only use schemes of order equal to that of the problem, and where this rule is not adhered to, extreme care must be taken.

APPENDIX III

THE CLASSIFICATION OF CERTAIN DIFFERENCE EQUATIONS INTO HYPERBOLIC, ELLIPTIC OR PARABOLIC TYPE

A3.1 Classification of a Prototype Equation †

A second order difference equation based on the central difference operators δ_i and δ_j defined by

$$\delta_i \psi_{ij} = \frac{\psi_{i+\frac{1}{2}j} - \psi_{i-\frac{1}{2}j}}{h}$$
$$\delta_j \psi_{ij} = \frac{\psi_{ij+\frac{1}{2}} - \psi_{ij-\frac{1}{2}}}{k} \qquad (A3.1.1)$$

is considered. h and k represent the distances between grid points of the mesh in the i and j directions respectively. The arguments to follow in no way exclude the treatment of equations based on other difference operators.

The prototype equation to be studied is

$$\hat{a}\,\delta_i^{\,2}\,\psi_{ij} + \hat{b}\,\delta_i\,\delta_j\,\psi_{ij} + \hat{c}\,\delta_j^{\,2}\,\psi_{ij} = 0 \qquad (A3.1.2)$$

For simplicity $\hat{a}$, $\hat{b}$ and $\hat{c}$ are treated as constants. Consider the linear combination of differences

$$m\,\delta_i\,\psi_{ij} + n\,\delta_j\,\psi_{ij} = e_{1ij} \qquad (A3.1.3)$$

where m and n are to be determined (and assumed constants). From this last equation operating through by δ_i and δ_j in turn, there are obtained the relations

† So far as the present author is aware the ideas of this section are new.

$$\left.\begin{aligned} m\,\delta_i^{\,2}\,\psi_{ij} + n\,\delta_i\,\delta_j\,\psi_{ij} &= e_{2ij} \\ m\,\delta_i\,\delta_j\,\psi_{ij} + n\,\delta_j^{\,2}\,\psi_{ij} &= e_{3ij} \end{aligned}\right\} \qquad (A3.1.4)$$

where the commutivity of δ_i and δ_j has been used in the last of (A3.1.4), and where $e_{2ij} = \delta_i\,e_{1ij}$, $e_{3ij} = \delta_j\,e_{1ij}$.

Equations (A3.1.2) and (A3.1.4) together give

$$\begin{pmatrix} \hat{a} & \hat{b} & \hat{c} \\ m & n & o \\ o & m & n \end{pmatrix} \begin{pmatrix} \delta_i^{\,2}\cdot\psi_{ij} \\ \delta_i\cdot\delta_j\cdot\psi_{ij} \\ \delta_j^{\,2}\cdot\psi_{ij} \end{pmatrix} = \begin{pmatrix} 0 \\ e_{2ij} \\ e_{3ij} \end{pmatrix} \qquad (A3.1.5)$$

Thus if m and n satisfy

$$\begin{vmatrix} \hat{a} & \hat{b} & \hat{c} \\ m & n & o \\ o & m & n \end{vmatrix} = 0 \qquad (A3.1.6)$$

ie, if

$$\frac{n}{m} = \frac{\hat{b} \pm \sqrt{(\hat{b}^2 - 4\hat{a}\hat{c})}}{2\hat{a}} \qquad (A3.1.7)$$

then equation (A3.1.2) can be expressed as a linear combination of the equations of (A3.1.4). If $\hat{b}^2 - 4\hat{a}\hat{c} \geq 0$, then this linear combination is real. Before interpreting this result, notice that (A3.1.3) may be rearranged as

$$e_{1ij} = \left(\frac{m}{h}\;\psi_{i+\frac{1}{2}j} + \frac{n}{k}\,\psi_{ij+\frac{1}{2}}\right) - \left(\frac{m}{h}\;\psi_{i-\frac{1}{2}j} + \frac{n}{k}\,\psi_{ij-\frac{1}{2}}\right) \qquad (A3.1.8)$$

or as

$$e_{1ij} = \left(\frac{m}{h}\ \psi_{i+\frac{1}{2}j} - \frac{n}{k}\ \psi_{ij-\frac{1}{2}}\right) - \left(\frac{m}{h}\ \psi_{i-\frac{1}{2}j} - \frac{n}{k}\ \psi_{ij+\frac{1}{2}}\right) \qquad \text{(A3.1.9)}$$

In either case, e_{1ij} is expressed as a sum of two linear functionals along mesh diagonals, as indicated in Fig A3.1.1.

Hence, since (A3.1.4) is derived from linear operations on (A3.1.8) or (A3.1.9), then if (A3.1.7) holds, then (A3.1.2) can be considered as linear combinations of e_{1ij} evaluated at various points of the difference mesh.

In equation (A3.1.7), three cases arise, each of which will now be interpreted in turn.

<u>Case (i)</u> $\hat{b}^2 - 4\hat{a}\hat{c} > 0$

In this case, there are two real values of n/m which allow (A3.1.2) to be written as linear combinations of e_{1ij} defined at various mesh points. Suppose that the $\frac{1}{2}$ interval points like $(i + \frac{1}{2}, j - \frac{1}{2})$, $(i, j + \frac{1}{2})$, etc, occur explicitly as mesh points, and that therefore by implication the corresponding function values occur explicitly in the difference equation, (the procedure in the opposite case will be explained shortly) then e_{1ij} can be considered as a dependant variable transformation for ψ_{ij}. It follows that (A3.1.2) can

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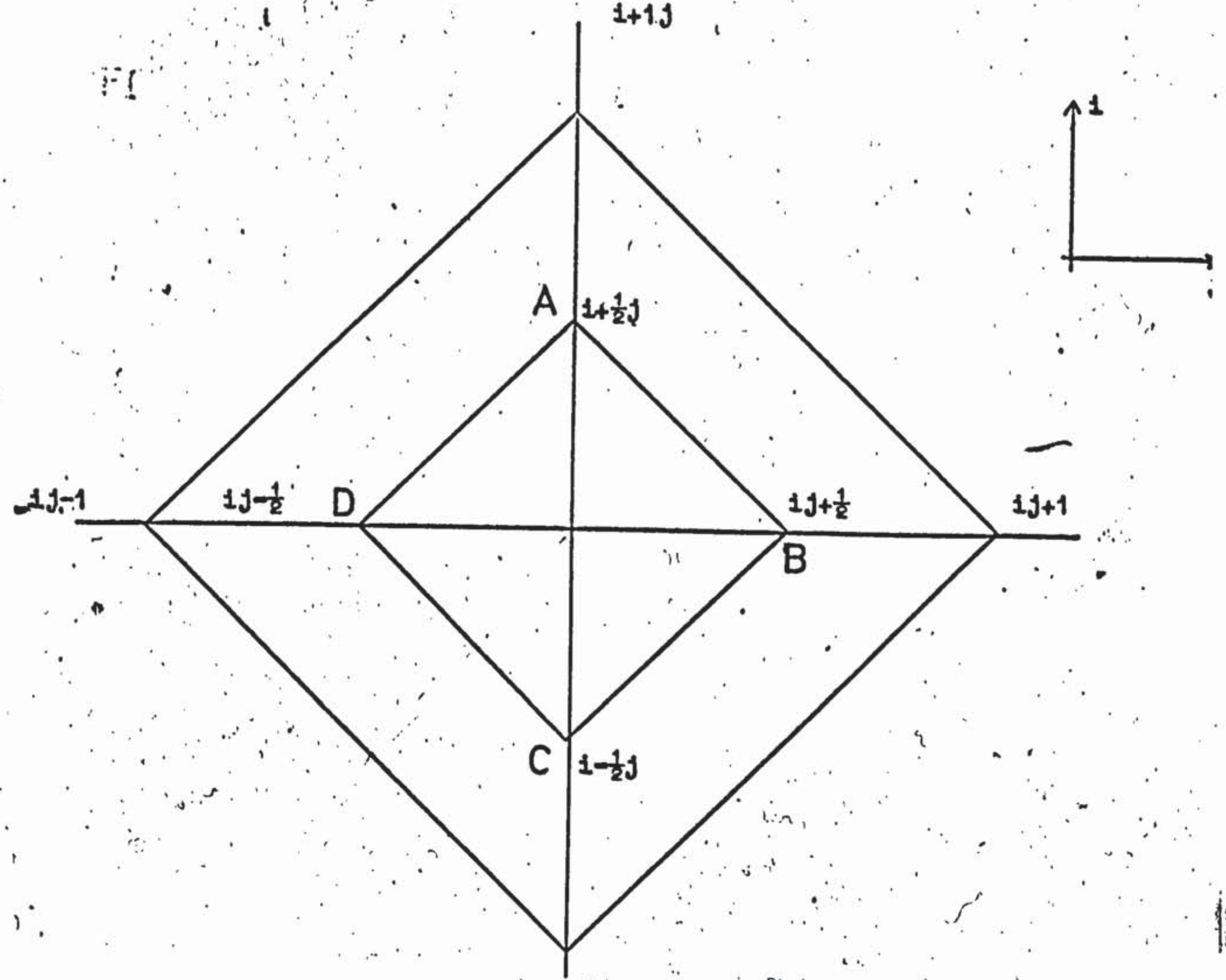
To ensure consistency with the hyperbolic differential equation analysis, notice that depending on the sign of n/m, an appropriate choice of either (A3.1.8) or (A3.1.9) will ensure that e_{1ij} is defined in terms of weighted differences along mesh diagonals, rather than weighted sums. These two values of n/m will be seen to correspond to the two characteristic directions obtained in the analysis of the second order hyperbolic differential equation.

Figure A3.1.1



The RHS of equation (A3.1.8) is the sum of two linear functions, one on AB and the other on CD. Likewise, the RHS of (A3.1.9) is the sum of linear functions on BC and DA.

then be solved for e_{1ij} everywhere. Thus, suppose that e_{1ij} is known over the whole difference domain, and that $n/m > 0$ so that e_{1ij} is arranged in the form (A3.1.9), ie in terms differences along mesh diagonals rising from left to right, as in Fig A3.1.2). Let the sense of Fig A3.1.2 be in the sense of Fig A3.1.1, then along XX' of Fig A3.1.2, e_{1ij} has the form

$$\left.\begin{aligned} e_{1ij} &= \left(\frac{m}{h}\psi_{A1} - \frac{n}{k}\psi_{Ao}\right) - \left(\frac{m}{h}\psi_{Bo} - \frac{n}{k}\psi_{B1}\right) \\ e_{1i+\frac{1}{2}j+\frac{1}{2}} &= \left(\frac{m}{h}\psi_{A2} - \frac{n}{k}\psi_{A1}\right) - \left(\frac{m}{h}\psi_{B1} - \frac{n}{k}\psi_{B2}\right) \\ e_{1i+1j+1} &= \left(\frac{m}{h}\psi_{A3} - \frac{n}{k}\psi_{A2}\right) - \left(\frac{m}{h}\psi_{B2} - \frac{n}{k}\psi_{B3}\right) \end{aligned}\right\} \qquad (A3.1.10)$$

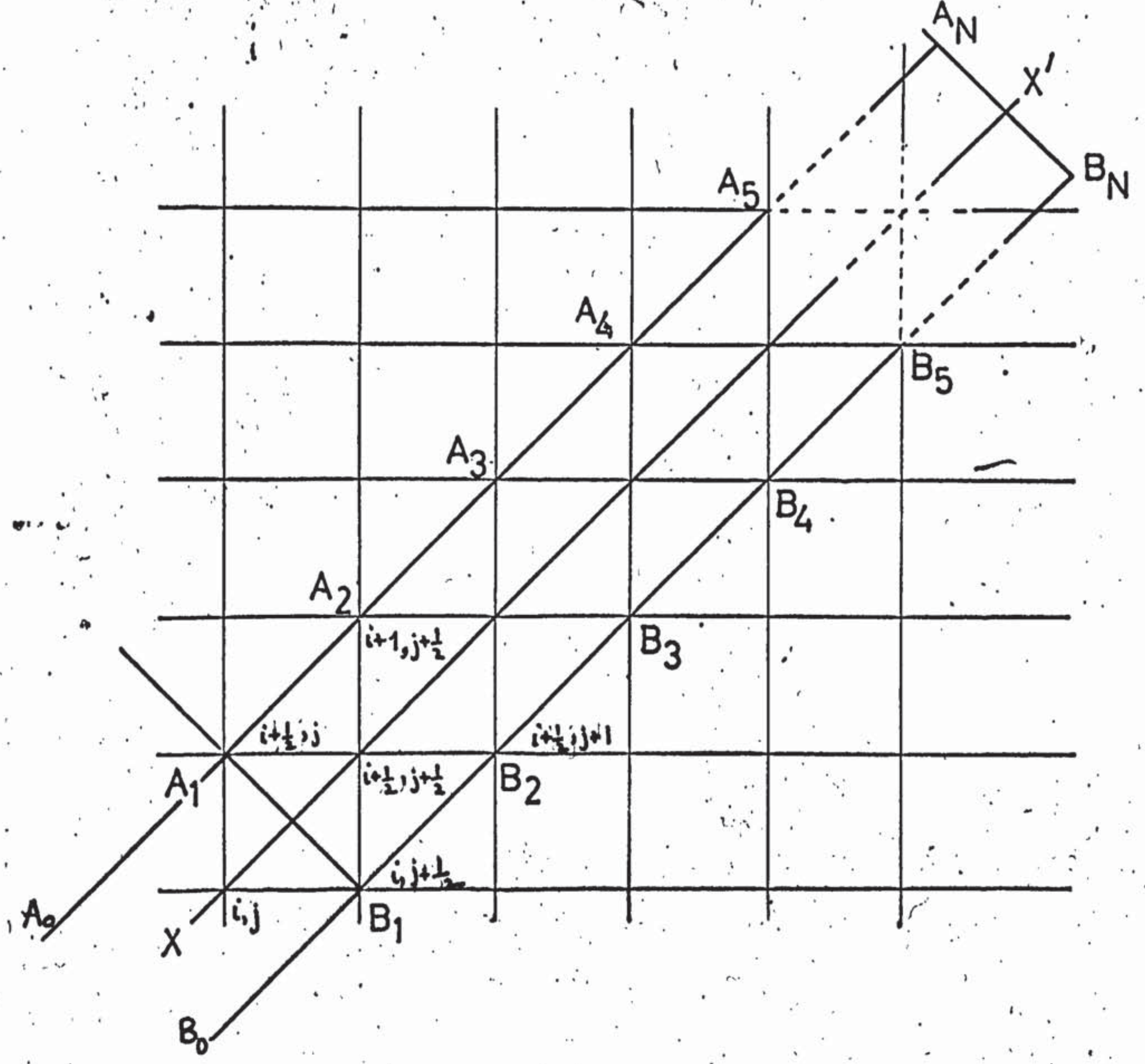
. . .

Rising along the diagonal XX', the equations of (A3.1.10) can be used to form an equation in which the explicit appearance of ψ_{A1}, ψ_{A2}, ... ψ_{AN-1} is eliminated to obtain a relationship of the form

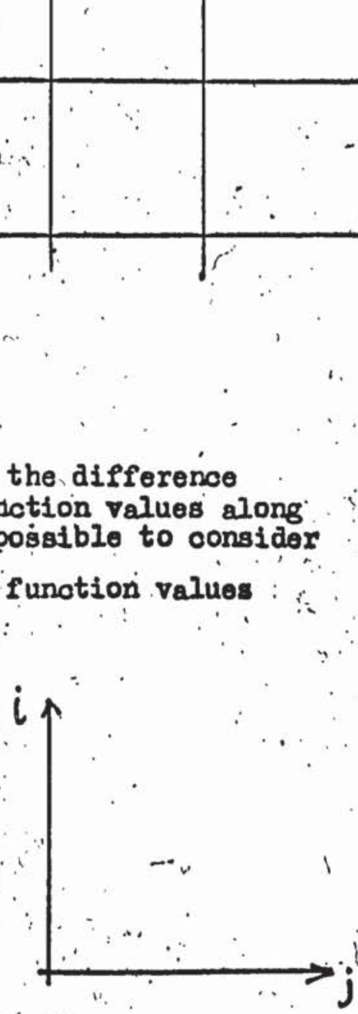
$$\varepsilon_o \psi_{Ao} + \varepsilon_N \psi_{AN} + \sum_{i=0}^{N} \lambda_i \psi_{Bi} = \Delta \qquad (A3.1.11)$$

where Δ is known, ie an explicit relationship between function values on a known line on the finite difference mesh is obtained. It follows that such a line cannot be considered as a physical boundary along which arbitrary function values may be specified. Such a condition typifies the hyperbolic differential equation, and consequently a difference equation of the form (A3.1.2) for which $\hat{b}^2 - 4\hat{a}\hat{c} > 0$ is classified as a HYPERBOLIC DIFFERENCE EQUATION. Notice that if

Figure A3.1.2



In the case of n/m real, it is shown that the difference equations yield a relationship between function values along the line $A_o\ B_o\ B_n\ A_n$, and thus it is not possible to consider the line as a boundary on which arbitrary function values can be prescribed.



$$\frac{k}{h} = \frac{n}{m} \quad , \frac{n}{m} > 0 \tag{A3.1.12}$$

then (A3.1.9) is a relationship of exact differences along mesh diagonals, so that (A3.1.11) reduces to a relationship of the form

$$\varepsilon_0 \psi_{AO} + \varepsilon_N \psi_{AN} + \lambda_0 \psi_{BO} + \lambda_N \psi_{BN} = \Delta \tag{A3.1.13}$$

ie a relationship between end-point values on the two lines $A_1 A_N$ and $B_0 B_N$. This is the result obtained along the characteristics of the differential equation analogous to the difference equation (A3.1.2). If $n/m < 0$, and if $k/h = -n/m$, then use of (A3.1.8) achieves the same result. Thus it is reasonable to associate the mesh diagonals on the two distinct meshes given by

$$\left.\begin{aligned} \frac{k}{h} &= \left|\frac{\hat{b} + \sqrt{(\hat{b}^2 - 4\hat{a}\hat{c})}}{2\hat{a}}\right| \\ &\text{and} \\ \frac{k}{h} &= \left|\frac{\hat{b} - \sqrt{(\hat{b}^2 - 4\hat{a}\hat{c})}}{2\hat{a}}\right| \end{aligned}\right\} \tag{A3.1.14}$$

along which e_{1ij} is a relationship between differences, with the distinct characteristics obtained from the hyperbolic differential equation that is analogous to the difference equation (A3.1.12). †

Suppose that no $\frac{1}{2}$-interval function values occur in the difference equation (A3.1.12), then the set of equations represented by this difference equation can be considered as an incomplete set, the set being completed by the addition of an arbitrary, but independent, set of equations in the function e_{1ij} at $\frac{1}{2}$-interval mesh points.

---

† Where if $n/m < 0$, the diagonal associated with the characteristic goes from left to right, and vice versa if $n/m > 0$.

The above remarks will then apply.

<u>Case (ii)</u> $\hat{b}^2 - 4\hat{a}\hat{c} = 0$

In this situation, one real value of n/m exists which allows (A3.1.2) to be written as a linear combination of (A3.1.4), and the difference equation is therefore classified as a PARABOLIC DIFFERENCE EQUATION. The interpretation is similar to that of the hyperbolic case, and again the main result is that it is impossible to choose an arbitrary closed line on which arbitrary function values can be obtained.

<u>Case (iii)</u> $\hat{b}^2 - 4\hat{a}\hat{c} < 0$

In this situation, no real values of n/m exist which enable (A3.1.2) to be written as linear combinations of (A3.1.4). The main consequence is that it is possible to define an arbitrary closed line containing the difference mesh on which arbitrary function values may be specified. In this situation, the difference equation is classified as an ELLIPTIC DIFFERENCE EQUATION.

A3.2 The Inclusion of Certain First Order Differences

Having analysed the situation for the prototype equation, (A3.1.2) a particular difference equation will be considered, whose form can be identified with the UDR of a differential equation of the form

$$a\frac{\partial^2\psi}{\partial x^2} + b\frac{\partial\psi}{\partial x} + c\frac{\partial^2\psi}{\partial y^2} + d\frac{\partial\psi}{\partial y} = 0 \qquad (A3.2.1)$$

where $ac \neq 0$. Consider the equation

$$a\,\delta_i^{\,2}\,\psi_{ij} + c\,\delta_j^{\,2}\,\psi_{ij} - d_{ij} \;=\; 0 \qquad \text{(A3.2.2)}$$

where d_{ij} is a function of $(\psi_{ij} - \psi_{i-1j})$, $(\psi_{ij} - \psi_{ij-1})$, $(\psi_{i+1j} - \psi_{ij})$ and $(\psi_{ij+1} - \psi_{ij})$. For the purposes of development, suppose that

$$d_{ij} \;=\; \lambda\,\frac{(\psi_{ij} - \psi_{i-1j})}{h} \;+\; \varepsilon\,\frac{(\psi_{ij} - \psi_{ij-1})}{k} \qquad \text{(A3.2.3)}$$

Now it is clear that d_{ij} cannot be represented as any linear combination of e_{1ij}, as defined at (A3.1.3), and so it follows that (A3.2.2) can never be written as any linear combination of elements e_{1ij} at points in the mesh and consequently, (A3.2.2) cannot be classified as hyperbolic for any a, c, h or k in the manner of the previous section. However, it will be shown how (A3.2.2) can, in a certain sense, be classified as hyperbolic or elliptic.

Write

$$\left.\begin{aligned}
\psi_{ij} - \psi_{1-ij} &= -\tfrac{1}{2}\,(\psi_{i+1j} - 2\,\psi_{ij} + \psi_{i-1j}) + \tfrac{1}{2}\,(\psi_{i+1j} - \psi_{i-1j}) \\
\psi_{ij} - \psi_{ij-1} &= -\tfrac{1}{2}\,(\psi_{ij+1} - 2\,\psi_{ij} + \psi_{ij-1}) + \tfrac{1}{2}\,(\psi_{ij+1} - \psi_{ij-1})
\end{aligned}\right\} \qquad \text{(A3.2.4)}$$

then using (A3.2.4) in (A3.2.3) and subsequently in (A3.2.2) then (A3.2.2) becomes

$$\frac{2a + \lambda h}{2}\;\delta_i^{\,2}\,\psi_{ij} + \frac{2c + \varepsilon k}{2}\;\delta_j^{\,2}\,\psi_{ij}$$

$$-\,\frac{\chi}{2h}\,(\psi_{i+1j} - \psi_{i-1j}) - \frac{\varepsilon}{2k}\,(\psi_{ij+1} - \psi_{ij-1}) \;=\; 0 \qquad \text{(A3.2.5)}$$

It follows immediately that if

$$\frac{2a + \lambda h}{2h^2} + \frac{2c + \varepsilon k}{2k^2} = 0 \qquad (A3.2.6)$$

then the explicit appearance of ψ_{ij} in (A3.2.5) is eliminated, and (A3.2.5) can then be expressed as a linear combination of function values along the mesh diagonals depicted in Fig A3.2.1, and thus, as in the case of the hyperbolic equation of the previous section, lines exist on the difference mesh along which arbitrary function values cannot be specified, ie the equation has a hyperbolic nature.

Certainly, if (A3.2.6) is true, then

$$\left(\frac{2a + \lambda h}{2}\right) \cdot \left(\frac{2c + \varepsilon k}{2}\right) \leqq 0 \qquad (A3.2.7)$$

and thus, a necessary condition for a difference equation of the type (A3.2.2) to be hyperbolic is that (A3.2.7) is true.† Conversely, a sufficient condition for equation (A3.2.2) to be elliptic in nature is that

$$\left(\frac{2a + \lambda h}{2}\right) \cdot \left(\frac{2c + \varepsilon k}{2}\right) > 0 \qquad (A3.2.8)$$

Referring to the UDR's of equations of the type (A3.2.1), it is shown in Chapter III that if

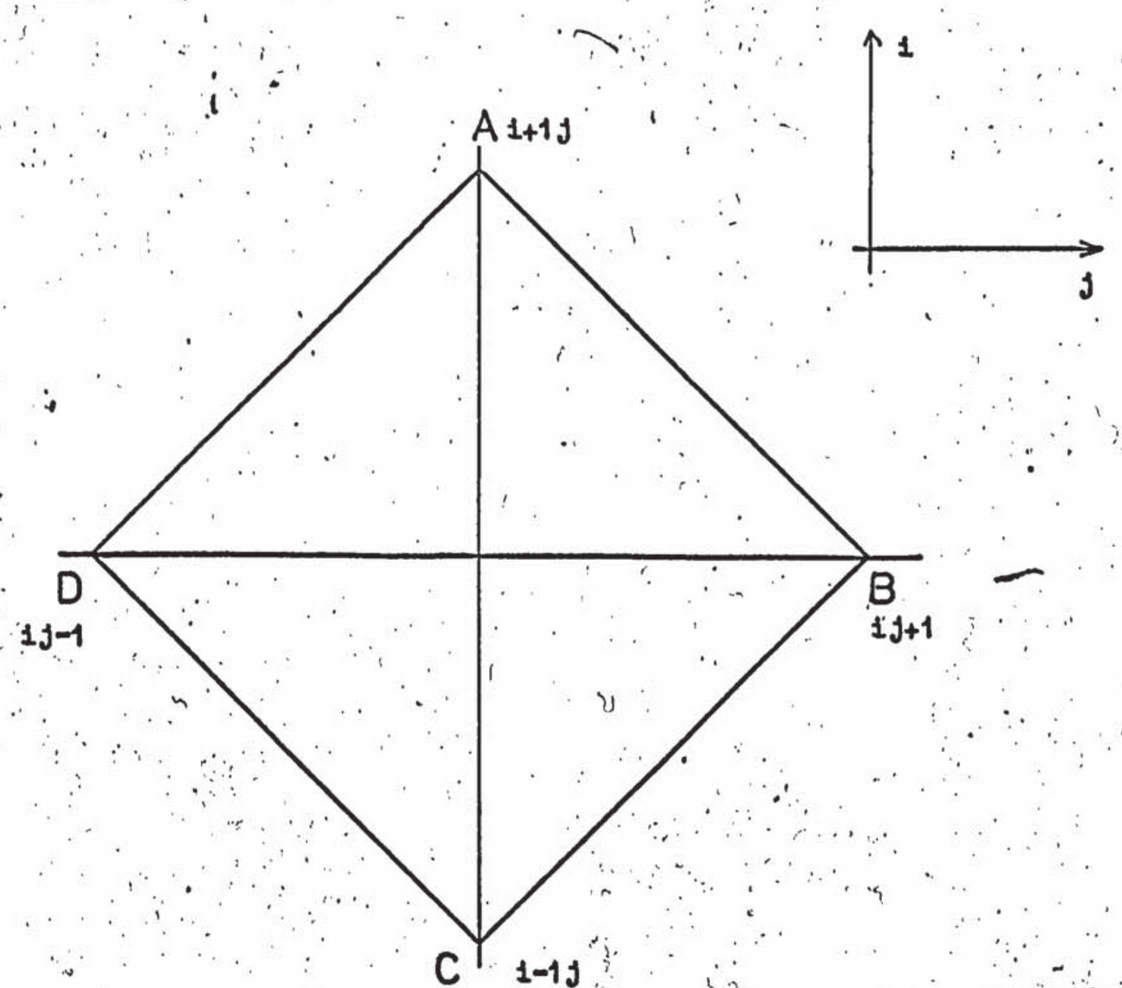
$$ac > 0, \text{ then } \left(\frac{2a + \lambda h}{2}\right) \cdot \left(\frac{2c + \varepsilon k}{2}\right) > 0$$

and if

$$ac < 0, \text{ then } \left(\frac{2a + \lambda h}{2}\right) \cdot \left(\frac{2c + \varepsilon k}{2}\right) < 0 \qquad (A3.2.9)$$

† The equation may be considered as hyperbolic to within a truncation error.

Figure A3.2.1



Equation (A3.2.5) can be considered as a sum of linear functions on DA and CB, or on AB and CD. In either case, the equation has a hyperbolic nature.

for all values of h and k, and thus if the original differential equation is elliptic in nature, then the UDR is guaranteed to be elliptic, and if the original differential equation is hyperbolic then a necessary condition for the UDR to be hyperbolic is satisfied, and in fact in this situation, an appropriate choice of h and k will make the UDR hyperbolic in the sense of Section A3.2.

An interesting result follows. Suppose that (A3.2.6) is true, then use of (A3.2.6) allows (A3.2.5) to be written in the form

$$\frac{\sqrt{-[(2a + \lambda h)\,(2c + \epsilon k)]}}{2} \cdot \frac{(\psi_{i+1j} + \psi_{i-1j} - \psi_{ij+1} - \psi_{ij-1})}{hk}$$

$$= G\,[(\psi_{i+1j} - \psi_{i-1j}),\,(\psi_{ij+1} - \psi_{ij-1})] \qquad \text{(A3.2.10)}$$

Now identify co-ordinates (ξ , η) with the diagonal directions, and express (h, k) in terms of ($\Delta\xi$, $\Delta\eta$), and write

$$\left.\begin{aligned} (\psi_{i+1j} - \psi_{i-1j}) &= (\psi_{i+1j} - \psi_{ij+1}) + (\psi_{ij+1} - \psi_{i-1j}) \\ (\psi_{ij+1} - \psi_{ij-1}) &= (\psi_{ij+1} - \psi_{i-1j}) + (\psi_{i-1j} - \psi_{ij-1}) \end{aligned}\right\} \qquad \text{(A3.2.11)}$$

then (A3.2.10) may be considered as a difference form of

$$\frac{\partial^2\psi}{\partial\xi\,\partial\eta} = F\left(\frac{\partial\psi}{\partial\xi}, \frac{\partial\psi}{\partial\eta}\right) \qquad \text{(A3.2.12)}$$

This is the standard form of the hyperbolic equation. We consequently would expect that if the orginating equation was elliptic, then a necessary condition for the stability of the difference equation is

(A3.2.8), and similarly, if the original equation was hyperbolic, then a necessary condition for the stability of the difference equation is (A3.2.7).

By (A3.2.8), the UDR's for hyperbolic and elliptic equations guarantee the satisfaction of these conditions. A quantative study of these outline ideas may be fruitful.

The Parabolic Equation

Consider

$$\frac{\partial^2 \psi}{\partial x^2} + d\,\frac{\partial \psi}{\partial y} = 0 \qquad \text{(A3.2.13)}$$

and a difference approximation to it

$$\delta_i^2 \psi_{ij} + d\left(\frac{\psi_{ij+1} - \psi_{ij}}{k}\right) = 0 \qquad \text{(A3.2.14)}$$

Writing

$$\frac{\psi_{ij+1} - \psi_{ij}}{k} = \frac{k}{2}\left(\frac{\psi_{ij+1} - 2\psi_{ij} + \psi_{ij-1}}{k^2}\right) + \left(\frac{\psi_{ij+1} - \psi_{ij-1}}{2k}\right) \qquad \text{(A3.2.15)}$$

then (A3.2.14) becomes

$$\delta_i^2 \psi_{ij} + d\,\frac{k}{2}\,\delta_j^2 \psi_{ij} + \frac{d}{2k}\left(\psi_{ij+1} - \psi_{ij-1}\right) = 0 \qquad \text{(A3.2.16)}$$

If $d < 0$, then by choosing

$$\frac{k}{h} = \frac{\sqrt{-dk}}{2} \qquad \text{(A3.2.17)}$$

the equation (A3.2.16) can be written in terms of linear combinations of ψ_{ij} along mesh diagonals, and the solution can be propagated along the diagonals, in the manner of a hyperbolic equation. If d > 0, then this cannot be done, and (A3.2.16) has no preferred direction. If in (A3.2.14), $\partial\psi/\partial y$ were approximated using backward differences, then the opposite results on 'd' are true. Now, on a given y = constant, the solution of (A3.2.13) behaves as the solution of a two point boundary value problem, in the sense that on y = constant, the solution at any point depends on the solution at every other point, and the solution does not propagate along preferred directions in the hyperbolic manner. Thus, the condition (A3.2.17) must never be true. It follows that if d > 0, then forward differences on $\partial\psi/\partial y$ should be used, and if d < 0, the backward differences on $\partial\psi/\partial y$ should be used. For example, in the equation

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2} \qquad \text{(A3.2.18)}$$

d < 0, and the above analysis implies the difference scheme

$$\frac{\psi_{ij} - \psi_{ij-1}}{\Delta t} = \frac{\psi_{i+1j} - 2\psi_{ij} + \psi_{i-1j}}{\Delta x^2} \qquad \text{(A3.2.19)}$$

ie, the implicit scheme whose stability is well-known.

When a term $\partial\psi/\partial y$ occurs by itself in the differential equation, the UDR method will not assign a unique differencing to $\partial\psi/\partial y$, since it does not distinguish between $(\psi_{ij+1} - \psi_{ij})$ and $(\psi_{ij} - \psi_{ij-1})$.

Consequently, parabolic equations are not considered in the UDR analysis.

APPENDIX IV

THE POSSIBILITIES OF DERIVING EXACT DIFFERENCE SCHEMES FOR HYPERBOLIC AND ELLIPTIC OPERATORS

A4.1 Hyperbolic Operators

In this section it is proved (by example) for certain simple hyperbolic differential operators, it is possible to make the solution space of the difference operator coincide with the solution space of the differential operator. Two examples are considered

(1) $$\frac{\partial Z}{\partial x} + \frac{\partial Z}{\partial y} = 0 \qquad (A4.1.1)$$

The solution space of (A4.1.1) is given by all once differentiable functions of the type H(x-y). By stipulating that the difference equation has as its solution space the difference analogue of H(x-y), there will be derived the exact representation of (A4.1.1).

In general, the solution space of a difference equation can be written as

$$[S] = [A^i B^j] \qquad (A4.1.2)$$

where A and B are arbitrary constants. Let h,k be the step lengths such that $x_i = ih$ and $y_j = jk$.

Suppose that

$$B = A^t \qquad (A4.1.3)$$

where t is some number, then a typical solution of the difference equation is, from (A4.1.2) of the form

$$Z_{ij} = A^{i+tj} \tag{A4.1.4}$$

therefore

$$\begin{aligned} A^{i+tj} &= \hat{A}^{x-y} \\ &= \hat{A}^{h(i-kj/h)} \end{aligned} \tag{A4.1.5}$$

by constraint for some $\hat{A}$. Hence, if $A = \hat{A}^h$ then

$$i + t_j = i - \frac{k}{h} j \tag{A4.1.6}$$

and therefore

$$t = -\frac{k}{h} \tag{A4.1.7}$$

Thus, from (A4.1.3) there is

$$B\, A^{k/h} = 1 \tag{A4.1.8}$$

(A4.1.8) defines the auxiliary equation of the difference equation and gives immediately

$$(E_j\, E_i^{k/h} - 1)\, Z_{ij} = 0 \tag{A4.1.9}$$

where

$$\left.\begin{aligned} E_j\, Z_{ij} &= Z_{ij+1} \\ E_i\, Z_{ij} &= Z_{i+1j} \end{aligned}\right\} \tag{A4.1.10}$$

These give from (A4.1.9) the difference equation

$$Z_{i+k/h,j+1} - Z_{ij} = 0 \qquad (A4.1.11)$$

A precise interpretation to (A4.1.11) can only be given when k/h is integer. In this circumstance, for the appropriate boundary conditions, (A4.1.1) and (A4.1.11) have identical solutions.

That this is true is simple to see if k/h = 1 for then (A4.1.11) becomes

$$Z_{i+1,j+1} - Z_{ij} = 0 \qquad (A4.1.12)$$

where the mesh is square. Now the characteristics of (A4.1.1) are given by

$$\frac{dy}{dx} = 1 \qquad (A4.1.13)$$

and along these

$$dZ = 0 \qquad (A4.1.14)$$

ie moving on a straight line of gradient unity, Z is a constant. This is precisely the statement made at (A4.1.12).

(ii) $$\frac{\partial^2 Z}{\partial x^2} - \frac{\partial^2 Z}{\partial y^2} = 0 \qquad (A4.1.15)$$

The solution space of (A4.1.15) is the set of all twice differentiable functions of the form $h(x \pm y)$. Following the previous example, solutions of the required difference equation have the typical form

$$Z_{ij} = A^i B^j = A^{i+tj} \qquad (A4.1.16)$$

using $B = A^t$. Thus by constraint

$$A^{i+tj} = \hat{A}^{x\pm y} = \hat{A}^{h(i\pm kj/h)} \qquad (A4.1.17)$$

for some $\hat{A}$ such that $A = \hat{A}^h$. Hence, comparing powers of A and $\hat{A}^h$

$$t = \pm\frac{k}{h} \qquad (A4.1.18)$$

Hence, using $B = A^t$

$$\left.\begin{array}{l} B = A^{+k/h} \\ \text{or} \\ B = A^{-k/h} \end{array}\right\} \qquad (A4.1.19)$$

The equations (A4.1.19) give the auxiliary equation of the difference equation

$$(BA^{-k/h} - 1)\,(BA^{k/h} - 1) = 0 \qquad (A4.1.20)$$

Hence

$$(E_j E_i^{-k/h} - 1)\,(E_j E_i^{+k/h} - 1)\, Z_{ij} = 0 \qquad (A4.1.21)$$

therefore

$$(E_j - (E_i^{k/h} + E_i^{-k/h}) + E_j^{-1})\, Z_{ij} = 0 \qquad (A4.1.22)$$

In particular, if $k/h = 1$ (ie a square mesh) then (A4.1.22) yields

$$Z_{i+1j} - Z_{ij+1} - Z_{ij-1} + Z_{i-1j} = 0 \qquad (A4.1.23)$$

as the difference equation which exactly solves the differential equation (A4.1.15) on a square mesh. On the square mesh (A4.1.23) is identical to the standard Taylor series form of (A4.1.15).

Now suppose that $k/h = 2$, ie the aspect ratio of the mesh is two, then (A4.1.22) yields

$$Z_{ij+1} - Z_{i+2j} - Z_{i-2j} + Z_{ij-1} = 0 \qquad (A4.1.24)$$

as the difference equation which exactly solves the differential equation on a mesh with aspect ratio, $k/h = 2$. Equation (A4.1.24) will not naturally arise from a Taylor series approach.

Thus, in simple situations it is certainly possible to construct a difference equation having the desired property. It would possibly be a fruitful avenue of research to see if an approximation of this principle could be applied to produce good schemes for hyperbolic equations of a practical relevance.

A4.2 Elliptic Operators

It will be proved for the simplest elliptic differential operator, that it is impossible to write down a polynomial difference operator (ie one with a finite number of terms) whose solution coincides with the differential operator.

Consider

$$\frac{\partial^2 Z}{\partial x^2} + \frac{\partial^2 Z}{\partial y^2} = 0 \qquad (A4.2.1)$$

The solutions of (A4.2.1) are combinations of all functions of the type $H(x \pm \sqrt{-1}y)$ (ignoring the simple polynomial solutions). The corresponding solutions of the required difference operator are all functions of the type

$$Z_{ij} = A^i B^j$$

$$= A^{i+tj} \qquad (A4.2.2)$$

using $B = A^t$ for some t. Thus, by constraint, it is required that

$$A^{i+tj} = \hat{A}^{x \pm \sqrt{-1}y}$$

$$= \hat{A}^{h(i \pm \sqrt{-1}\, kj/h)} \qquad (A4.2.3)$$

for some $\hat{A}$ such that $A = \hat{A}^h$. Hence comparing powers of A and $\hat{A}^h$

$$t = \pm \sqrt{-1}\, \frac{k}{h} \qquad (A4.2.4)$$

Using $B = A^t$, there are the relationships

$$B = A^{\sqrt{-1}\, k/h}$$

$$B = A^{-\sqrt{-1}\, k/h} \qquad (A4.2.5)$$

These give the auxiliary equation of the difference equation

$$(BA^{-\sqrt{-1}\,k/h} - 1)\,(BA^{\sqrt{-1}\,k/h} - 1) \quad = \quad 0 \qquad (A4.2.6)$$

Hence

$$(E_j\,E_i^{-\sqrt{-1}\,k/h} - 1)\,(E_j\,E_i^{\sqrt{-1}\,k/h} - 1)\,Z_{ij} \quad = \quad 0 \qquad (A4.2.7)$$

After suitable manipulation, this yields

$$(E_j - (E_i^{\sqrt{-1}\,k/h} + E_i^{-\sqrt{-1}\,k/h}) + E_j^{-1})\,Z_{ij} \quad = \quad 0 \qquad (A4.2.8)$$

Using the relationship $E_i = e^{hD}$ where $D = d/dx$, (A4.2.8) yields

$$(E_j - 2\,\mathrm{Cos}\,(\frac{k}{h}\log(E_i)) + E_j^{-1})\,Z_{ij} \quad = \quad 0 \qquad (A4.2.9)$$

Thus the difference equation whose exact solution is that of (A4.2.1) is

$$Z_{ij+1} - 2\,\mathrm{Cos}\,(\frac{k}{h}\log(E_i))\,Z_{ij} + Z_{ij-1} \quad = \quad 0 \qquad (A4.2.10)$$

Since (A4.2.10) contains an infinite number of terms, the original statement is proven.

To show that (A4.2.10) yields the standard approximation, use $E_i = e^{hD}$ therefore

$$Z_{ij+1} - 2\,\mathrm{Cos}\,(K\frac{\partial}{\partial x})\,Z_{ij} + Z_{ij-1} \quad = \quad 0 \qquad (A4.2.11)$$

therefore

$$Z_{ij+1} - 2\,(1 - \frac{k^2}{2}\frac{\partial^2}{\partial x^2})\,Z_{ij} + Z_{ij-1} \quad \simeq \quad 0 \qquad (A4.2.12)$$

$$\frac{(Z_{ij+1} - 2\,Z_{ij} + Z_{ij-1})}{K^2} + \frac{\partial^2}{\partial x^2}\,Z_{ij} \simeq 0 \qquad (A4.2.13)$$

for the result.

Since the result is true for the simplest of elliptic differential operators, it is reasonable to suppose that it is true for all elliptic differential operators. Consequently, so far as elliptic equations are concerned, some form of partitioning in the differential operator has to be resorted to (eg Chapter 3).

APPENDIX V

CERTAIN PRECISE DETAILS OF THE SOLUTION PROCEDURE

A5.1 A Typical Cartesian Momentum Equation

In full, a typical 3-D (x,u) momentum equation is given by

$$h(r,t) = e^{-\frac{\rho r t}{\mu}}$$

$$\frac{+\rho U_{ijk}}{\Delta x\,(1 - h(U_{ijk}, \Delta x))}\left\{ U_{i+1jk} - U_{ijk}\,(1 + h(U_{ijk}, \Delta x)) + U_{i-1jk} \cdot h(U_{ijk}, \Delta x)\right\}$$

$$\frac{+\rho V_{ijk}}{\Delta y\,(1 - h(V_{ijk}, \Delta y))}\left\{ U_{ij+1k} - U_{ijk}\,(1 + h(V_{ijk}, \Delta y)) + U_{ij-1k} \cdot h(V_{ijk}, \Delta y)\right\}$$

$$\frac{+\rho W_{ijk}}{\Delta z\,(1 - h(W_{ijk}, \Delta z))}\left\{ U_{ijk+1} - U_{ijk}\,(1 + h(W_{ijk}, \Delta z)) + U_{ijk-1} \cdot h(W_{ijk}, \Delta z)\right\}$$

$$+\left(\frac{p_{i+1jk} - p_{i-1jk}}{2\,\Delta x}\right) = 0 \qquad \text{(A5.1.1)}$$

For simplicity, now define

$$\left.\begin{aligned} h_u &= h(U_{ijk}, \Delta x) \\ C_u &= \frac{+\rho U_{ijk}}{\Delta x\,(1 - h_u)} \end{aligned}\right\} \qquad \text{(A5.1.2)}$$

and similarly for h_v, h_w, C_v and C_w.

From (A5.1.1) a successive over-relaxation (SOR) scheme can be defined, viz

$$U^{n+1}_{ijk} = U^{n}_{ijk} + \lambda \Big\{ C_u \left(U_{i+1jk} - (1 + h_u) U_{ijk} + h_u U_{i-1jk}\right)$$

$$+ C_v \left(U_{ij+1k} - (1 + h_v) U_{ijk} + h_v U_{ij-1k}\right)$$

$$+ C_w \left(U_{ijk+1} - (1 + h_w) U_{ijk} + h_w U_{ijk-1}\right) - \left(\frac{P_{i+1jk} - P_{i-1jk}}{2 \Delta x}\right)\Big\} \Big/$$

$$\Big\{ C_u (1 + h_u) + C_v (1 + h_v) + C_w (1 + h_w) \Big\} \qquad \text{(A5.1.3)}$$

where the relaxation factor is given by

$$\varepsilon_{ijk} = \lambda / \left(C_u (1 + h_u) + C_v (1 + h_v) + C_w (1 + h_w)\right) \qquad \text{(A5.1.4)}$$

The denominator of ε_{ijk} is just the coefficient of the diagonal term U_{ijk}, and can therefore be viewed as a scaling factor for the equations to make the coefficient of all diagonal terms unity and of all off-diagonal terms less than unity.

From (A5.1.3) there is now defined

$$\hat{U}^{n+1}_{ijk} = U^{n}_{ijk} + \lambda \Big\{ C_u \left(U_{i+1jk} - (1 + h_u) U_{ijk} + h_u U_{i-1jk}\right)$$

$$+ C_v \left(U_{ij+1k} - (1 + h_v) U_{ijk} + h_v U_{ij-1k}\right)$$

$$+ C_w \left(U_{ijk+1} - (1 + h_w) U_{ijk} + h_w U_{ijk-1}\right)\Big\} \Big/$$

$$\Big\{ C_u (1 + h_u) + C_v (1 + h_v) + C_w (1 + h_w) \Big\} \qquad \text{(A5.1.5)}$$

and

$$U^{n+1}_{ijk} = \hat{U}^{n+1}_{ijk} + \lambda \left(\frac{P_{i+1jk} - P_{i-1jk}}{2 \Delta x}\right) \Big/$$

$$\Big\{ C_u (1 + h_u) + C_v (1 + h_v) + C_w (1 + h_w) \Big\} \qquad \text{(A5.1.6)}$$

Equations (A5.1.5) and (A5.1.6) are typical of those used in practice.

Typically $\lambda = -0.5$

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GLOSSARY OF TERMS

μ	= kinematic viscosity
ρ	= fluid density
ν	= μ/ρ
∇^2	= the Laplacian
(u, v, w)	= the velocity vector
p	= static pressure
$\Delta x, \Delta y, \Delta z$	= increments in x, y, z directions, respectively.
$\underline{y}^*$	= conjugate transpose of arbitrary matrix
Total pressure	= $p/\rho + \frac{1}{2}(u^2 + v^2 + w^2)$
g_{ij}	= covariant components of the metric tensor
g^{ij}	= contravariant components of the metric tensor
g	= determinant of the matrix (g_{ij})
v_i	= <u>contravariant</u> velocity components in curvilinear co-ordinates (standard notation is v^i)