Some Comments on the Numerical Integration of the Vorticity Equation and Related Equations

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Abstract

It is shown that if the streamfunction is specified over an Eulerian region R (x, y) at $t=0$, and on the boundaries of R (x, y) at $t > 0$, a solution of the vorticity equation which satisfies certain conditions of continuity will be unique. If vorticity is also specified at the inflow boundary, such a solution is excluded. In the latter case, an internal discontinuity propagates into the region along a material surface, and in principle solutions should be obtained separately for each sub-region and "matched" kinematically and dynamically at the interface. The associated analytical or numerical problems are prohibitive.

The problem of obtaining stable methods of numerical integration, specifying only the stream function on the boundary, is considered. Numerical integrations of a non-linear first order differential equation indicate that such stable methods may exist, in contradiction to linear theory.

The integration of the vorticity and associated equations for the first time-step is also considered. A method is presented which is not only simple to apply, but also maintains the same accuracy as succeeding time-steps for which centered difference techniques are used.

1. Introduction

In recent years, the numerical integration of non-linear partial differential equations has played an increasingly important role in scientific research. This is, perhaps, particularly true of meteorology. Since the early studies of CHARNEY, FJÖRTOFT, and VON NEUMANN (1950) numerical methods have been extensively used not only in meteorological research but also in operational forecasting.

The equations to be integrated have taken various forms, depending on the physical "model" to be studied and the degree to which simplifying assumptions are introduced. Nevertheless, many of the equations – and in particular the barotropic models – can be placed in the form:

$$\Delta\psi_t = g\left(\psi, \partial^n\psi/\partial x^m \partial y^{n-m}\right) \quad \begin{matrix} 0 \leq m \leq n \\ n = 1, 2, \ldots, k \end{matrix} \qquad (1)$$

where Δ is Laplace's operator, and the dependent variable ψ is a streamfunction or a quasi-streamfunction which determines or is closely related to the field of fluid motion. It is to be noted that (1) includes as a special case the unsteady state, two dimensional vorticy equation for a homogeneous fluid:

$$\Delta\psi_t = -J\left(\psi, \Delta\psi\right) + \nu\Delta^2\psi \qquad (2)$$

where ν is the kinematic viscosity and J represents the Jacobian with respect to an orthogonal cartesian coordinate system in the plane.

The numerical integration of equations of this class involve many mathematical problems which are at present only imperfectly understood. For example, the accumulation of truncation errors, and the associated problem of numerical stability, have not been adequately treated for these non-linear systems. A host

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of additional unsolved problems could be mentioned.

In the present paper three problems in particular will be discussed. First, a statement of sufficient boundary conditions will be developed for the uniqueness of solutions to differential equations of class (1). In order to simplify the notation, the derivation will be presented in terms of the vorticity equation for a perfect fluid (i.e., (2) without the viscous terms). This equation is, of course, of fundamental importance in many fields of fluid dynamics. However, it must be emphasized that the method of proof developed for the vorticity equation can be applied with only trivial modification to most equations of class (1) as well as to certain systems of such equations.

A second problem considered involves a definition and discussion of overspecification in numerical integration. It will be shown that in recent meteorological research, boundary conditions have been overspecified. Some of the consequences are considered; the relation between overspecification and numerical stability is discussed; and two possible means of avoiding overspecification are proposed, one in terms of an Eulerian and one in terms of a Lagrangian analysis.

The third problem investigated is the error in the first time step of a numerical integration, given the value of the dependent variable ψ in a region R (x, y) at time $t=0$. It is pointed out that the conventional method of using an uncentered difference for the first time step involves an error one order of magnitude larger than for all subsequent time steps. An alternative procedure is advanced which is simple to apply and which eliminates this increased error.

Throughout the text, numerical examples are included. For this purpose it is desirable to use a simplified non-linear partial differential equation for which the analytical solution is known. One convenient equation is:

$$u_t + uu_x = 0 \tag{3}$$

This equation, which has the solution:

$$u = \phi\,(x - ut) \tag{4}$$

provided $J\,(x - ut,\ t)$ is not zero, is of a type thoroughly discussed by LIGHTHILL (1955). Numerical integrations of (3) have been used to illustrate the effects of certain types of overspecification and of uncentered differences in the numerical procedure.

2. A Definition of "Overspecification" and of "Admissible Solution"

The concept of "overspecification" is so fundamental to the discussion which follows that it seems desirable to clarify its meaning at the outset. This concept is essentially related to the solution of differential equations, for which the dependent variables are to be determined everywhere within a specified region. Although it is possible to extend the meaning to difference equations, this will be deferred to a later section. In the discussion which immediately follows, the mathematics of continuous rather than of discrete systems is at issue.

It is interesting to note that even with regard to differential equations, there is much confusion in the literature concerning what constitutes "overspecification". Of course, "overspecification" occurs when the system of the differential equation and boundary conditions has no admissible solution. However, the fact has frequently been overlooked that to determine when a system is "overspecified", it is necessary to define "admissible solution". Usually, an "admissible solution" must satisfy not only the differential equation and the boundary conditions, but also additional restrictions as well.

This can be illustrated by a simple example. Consider the ordinary differential equation: $dy/dx = 1$. Most of us would agree, almost without thinking, that it would be an overspecification to demand that the solution pass through the two points: $x=0$, $y=0$; and $x=1$, $y=3$. Yet such a solution – in fact, an infinite number of such solutions – can be found provided we are willing to allow the dependent variable y to be multi-valued in x. Figure 1 a shows such a solution: namely, $(y-x-1)^2=1$. Furthermore, an additional infinite set of solutions can be found provided we are willing to allow the dependent variable to be discontinuous (i.e. provided we are willing to let $dy/dx=1$ except at one or more points where the derivative is not defined). An example of a single-valued solution of this type is shown in Figure 1 b. Even in this

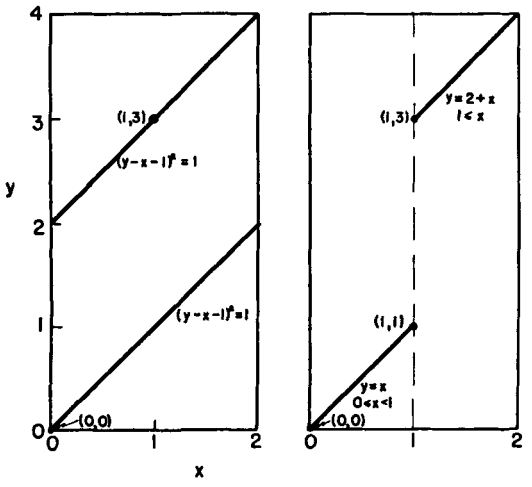

Fig. 1. Multivalued and discontinuous solutions of $dy/dx = 1$ passing through the points (0,0) and (1,3)

simple example, then, we can say the boundary conditions overspecify the differential equation *only* if we set up the arbitrary restriction that admissible solutions must be single-valued, continuous functions of x. Whether this limitation is a useful one or not depends upon the objectives of the investigator. Perhaps this is why the term "overspecification" appears so infrequently in mathematics, but is found so often in the literature of applied science.

In most physical problems, solutions are required in which the dependent variables are single-valued, continuous functions of the independent variables. This is not invariably the case, however. Obvious exceptions occur when the dependent variables are defined in a multiply connected region: e.g. the potential of the electromagnetic force field set up by current flowing in a wire of finite diameter. In other cases, dependent variables are deliberately allowed to be discontinuous on a given surface: e.g. the discontinuity in density and tangential velocity component at the interface between two homogeneous fluids, as in Helmholz waves. In the latter example, however, other requirements must be satisfied – namely, the kinematic and dynamic boundary conditions for the surface of internal discontinuity. In general, when discontinuity surfaces (in the dependent variables or their pertinent derivatives) occur within the region under consideration, solutions must be obtained independently for the regions on either side of the surface, and the solutions must then be "matched" in some suitable manner. We will have occasion to refer to this procedure in more detail below.

With these preliminary remarks in mind, let us return to differential equations of class (1). In meteorology, equations of this type are of primary interest in initial value problems. Values of the dependent variable ψ are specified over a region $R\ (x, y)$ at a time $t=0$. The task is to determine what additional boundary conditions (if any) are necessary and sufficient to determine a unique admissible solution for the dependent variable $\psi\ (x, y, t)$ within $R\ (x, y)$ over a certain time interval $0 \leq t < \tau$.

Before this question can possibly be answered, it will be necessary to decide what additional restrictions are to be imposed in the definition of "admissible solution". In this, we must be guided by the nature of the physical problem and by the objectives of the investigation. In the following paper it will be assumed that an admissible solution $\psi\ (x, y, t)$ satisfies the differential equation over the region $R\ (x, y)$ within the time interval $0 \leq t < \tau$, and also meets the following requirements:

(1) The function $\psi\ (x, y, t)$ must be a single-valued, continuous, real function of the independent variables. This assumption is justified since we shall generally be interested in regions $R\ (x, y)$ which are simply connected. In addition, if a "shock" develops (i.e. if ψ becomes multiple-valued within the region at $t=\tau$) the solution ceases to have physical validity. In such cases, no admissable solution of the differential equation may exist for $t \geq \tau$.

(2) The derivatives of ψ that appear in the differential equation are defined everywhere an admissible solution exists. This restriction is justified since we shall not generally be interested in the propagation of surfaces of discontinuity within the region $R\ (x, y)$. We shall, therefore, be permitted to solve the differential equation over the entire region, without matching solutions at some moving internal boundary.

(3) An admissible solution $\psi\ (x, y, t)$ can be expanded in a convergent power series in time. For every point with $R\ (x, y)$ and for $-\varepsilon \leq t < \tau;\ \varepsilon > 0$:

$$\psi\ (x, y, t) = \sum_{n=0}^{\infty} t^n \phi_n\ (x, y) \qquad (5)$$

The desirability of this restriction is by no means as obvious as the first two. However, it will be useful to investigate solutions which are very well behaved. The effect of relaxing the requirement that (5) be valid will be considered in a later section.

With the above definition of "admissible solution" we are now in a position to attack equations of class (1). Unfortunately, it has not been possible to determine the boundary conditions which are necessary and sufficient for a unique solution to exist. Nevertheless, if we assume an admissible solution exists over some range, sufficient boundary conditions for uniqueness can be established.[1]

3. Sufficient Conditions for the Uniqueness of Solutions to the Vorticity Equation

The following proof will be developed for the two-dimensional vorticity equation for a perfect fluid:

$$\triangle\psi_t = -J(\psi, \triangle\psi). \tag{6}$$

The proof can, however, by a trivial modification be extended to most equations of class (1). *It will be assumed* that the following boundary conditions are specified: (a) the value of ψ over $R(x, y)$ at $t = 0$; and (b) the value of ψ at the boundaries of $R(x, y)$ for $0 \leq t < \tau$. *It will be shown* that there exists no more than one admissible solution which satisfies these boundary conditions. In other words, the boundary conditions are sufficient to establish uniqueness.

The proof is straightforward. Assume two solutions ψ' and ψ'' which are admissible. Define a function $\Theta \equiv \psi' - \psi''$. Then Θ is zero over $R(x, y)$ at $t = 0$, and also is zero at the boundaries of $R(x, y)$ for $0 \leq t < \tau$. Substituting ψ' and ψ'' in (6):

$$\begin{aligned} \triangle\psi'_t &= -J(\psi', \triangle\psi') \\ \triangle\psi''_t &= -J(\psi'', \triangle\psi'') \end{aligned} \tag{7}$$

Or, subtracting:

$$\triangle\Theta_t = -J(\psi', \triangle\psi') + J(\psi'', \triangle\psi'') \tag{8}$$

The right hand side of (8) is identically zero over $R(x, y)$ at $t = 0$. In addition, $\Theta_t = 0$ at the boundary of $R(x, y)$ at $t = 0$. Therefore, from a well known theorem concerning Laplace's Equation, it follows that $\Theta_t = 0$ over the entire region $R(x, y)$ at $t = 0$. In addition differentiation of Θ_t with respect to x and y leads to the requirement:

$$\frac{\partial(\psi')^{n+1}}{\partial x^{n-m}\partial y^m \partial t} = \frac{\partial(\psi'')^{n+1}}{\partial x^{n-m}\partial y^m \partial t} \quad \begin{matrix} \text{over } R(x, y) \text{ at } t = 0 \\ 0 \leq m \leq n \\ 0 \leq n \leq 3 \end{matrix} \tag{9}$$

Equations (7) can now be differentiated with respect to time, and the difference again taken. This leads to the relationship:

$$\begin{aligned} \triangle\Theta_{tt} = &-J(\psi'_t, \triangle\psi') - J(\psi', \triangle\psi'_t) + \\ &+ J(\psi''_t, \triangle\psi'') + J(\psi'', \triangle\psi''_t) \end{aligned} \tag{10}$$

However, from (9) the right hand side of this equation is again identically zero over $R(x, y)$ at $t = 0$, and in addition $\Theta_{tt} = 0$ at the boundary of $R(x, y)$. Therefore, $\Theta_{tt} = 0$ over the region $R(x, y)$ at $t = 0$.

Repeating the above process, it can be shown that $\partial^p\Theta/\partial t^p = 0$ over $R(x, y)$ at $t = 0$, for all integral values of p. However, from (5) ψ' and ψ'' can be expanded in a Maclaurin Series in time. Thus, for any point X, Y, T within $R(x, y)$ where $0 \leq T < \tau$:

$$\begin{aligned} \Theta(X, Y, T) = &\Theta(X, Y, 0) + T\Theta_t(X, Y, 0) + \\ &+ \frac{T^2}{2!}\Theta_{tt}(X, Y, 0) + \ldots . \end{aligned} \tag{11}$$

All terms on the right hand side of (11) have been shown to be zero. Hence $\Theta(X, Y, T) = 0$ and ψ' is identically equal to ψ'' within the region and time limits considered. If a solution exists which meets the specified conditions, this solution must be unique.

4. Meteorological Implications of the Uniqueness Theorem

The implications of this uniqueness proof are of particular meteorological interest. In considering the problem of numerical integration of the equations for large scale atmospheric motions, CHARNEY ET AL. (1950) discussed

[1] Note that (5) is not equivalent to requiring that $\psi(x, y, t)$ be analytic, since the functions $\phi_n(x, y)$ are not necessarily analytic. A simple example of a non-analytic solution which satisfies the above conditions follows. Consider the linear equation $\psi_t + \psi_x + \psi_y = 0$, where ψ is to be determined in the region $0 \leq x \leq 1$, $0 \leq y \leq 1$. One solution is given by equation (5) where: $\phi_n = (-1)^n (n!)^{-1} (x - y)^{3/2} \exp[(x + y)/2]$. Note that the second and all higher space-derivatives of ψ are not defined along the line $x = y$, which bisects the region $R(x, y)$. The solution is clearly not analytic throughout the region, yet it is "admissible" according to the above definition.

the vorticity equation and on the basis of a heuristic argument concluded that the vorticity $\triangle\psi$ must be specified on those portions of the boundary along which the fluid was moving into the region under consideration (the socalled "inflow" boundaries). This argument has generally been accepted in subsequent literature dealing with problems or large scale atmospheric motions. In fact, some authors refer to this heuristic argument as a "proof" – presumably of the sufficiency and necessity of specifying the vorticity along the inflow boundaries. Yet it is clear from the discussion in the previous section that if a well-behaved solution exists, which is admissible according to the definition of Section 2, this solution will in general be excluded by specifying the vorticity on the inflow boundaries. In other words, the system will be overspecified.

This dilemma can be avoided in one of two ways. First, the boundary conditions can be reduced by assuming only the value of the stream function ψ on the boundaries of the region $R\ (x, y)$ at $t > 0$. If a solution exists over a region $0 \leq t < \tau$ which is admissible according to the definition of Section 2, this solution will then be unique. Alternatively, the definition of admissible solution can be relaxed in some specified manner – for example, the first two limitations of Section 2 could be retained, but (5) could be relaxed and the solution could be required to satisfy some less restrictive continuity requirement. A solution of the differential equation may then exist which satisfies not only the assumed values of ψ at the boundaries of $R\ (x, y)$, but also the assumed values of $\triangle\psi$ at inflow boundaries.

These alternatives can be illustrated by considering the simple non-linear differential equation:

$$u_t + uu_x = 0 \qquad (12)$$

This equation can be written in the form $du/dt = 0$, and in this sense is analogous to the vorticity equation $d\ (\triangle\psi)/dt = 0$. In this one dimensional problem, we will assume that u is specified along a segment of the x-axis, $R\ (x)$, at $t = 0$. The value of u is to be determined within $R\ (x)$ for $0 \leq t < \tau$.

Let us first consider a solution which is well-behaved, according to the definition of Section 2. It is not difficult to show by an obvious extension of the method of the previous section that if solutions are sought for which u, u_x, and u_t are single-valued and continuous, and for which u can be expanded as a power series in time, no additional boundary conditions should be specified. In particular, neither u nor its time variation should be specified along the inflow extremity of $R\ (x)$. Let us present a specific example. Let $u = 1.0 + 0.5 \cos x$ at $t = 0$ for $-\pi/2 \leq u \leq +\pi/2$. The unique admissible solution, applying the definition of Section 2, is: $u = 1.0 + 0.5 \cos (x - ut)$, and u and its derivatives are finite, single-valued, and continuous within the segment $R\ (x)$ for $0 \leq t < .9\pi$. At $t = .9\pi$ a "shock" enters the region. Beyond the shock line the solution is not admissible, since in such regions the dependent variable u becomes multi-valued. This inadmissibility corresponds to a lack of physical reality, since fluid velocity cannot have two or more values at a single point. This solution is shown in Figure 2 a. The straight lines are characteristics, of slope $1/u$, along which the velocity u is conserved.

Les us now consider solutions of (12) which can be obtained by specifying additional boundary conditions, and by relaxing in an appropriate manner the definition of an admissible solution. First, let us require a solution for which u, u_x, and u_t are defined and single valued in the region $R(x)$. Note that the restriction corresponding to (5) has been eliminated; however, the differential equation is valid everywhere in the region and an internal "matching" of dynamic or kinematic boundary conditions can be avoided. With this less restrictive definition of admissible solution, additional boundary conditions must be specified for uniqueness to exist. One possibility is to define u at inflow boundaries for $t > 0$. However, this must be done in a very particular manner: such that u_x and u_t are always defined at the characteristic passing through the lefthand extremity of $R(x)$. In the particular example considered previously, this would require that:

$$u_t = \frac{0.5\ u \sin (x - ut)}{1 - 0.5\ t \sin (x - ut)}$$
$$u_x = \frac{-0.5 \sin (x - ut)}{1 - 0.5\ t \sin (x - ut)} \qquad (13)$$

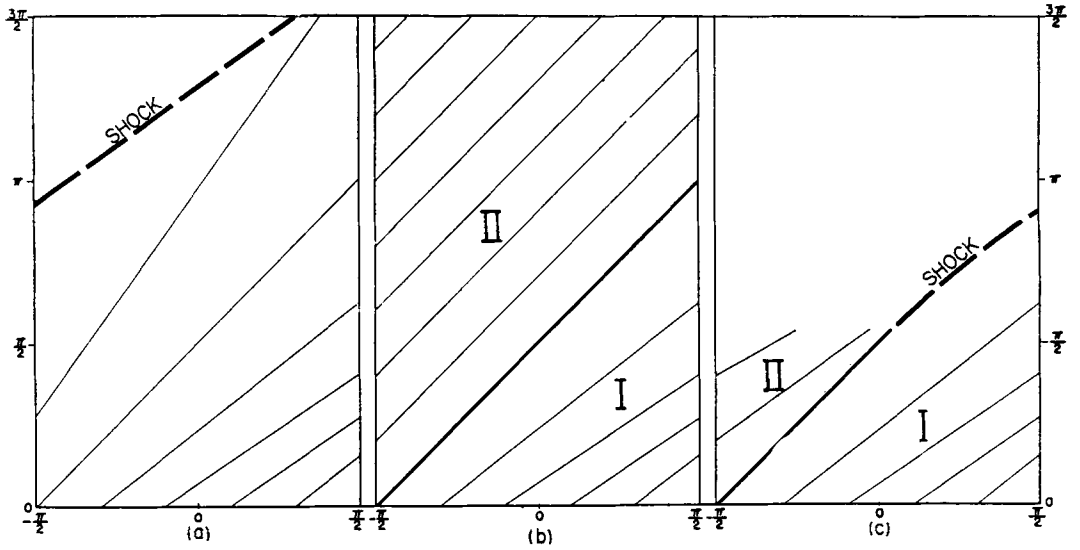

Fig. 2. Characteristic lines for three solutions of $u_t + uu_x = 0$, when $u(0, t) = 1.0 + 0.5 \cos x$ for $-\pi/2 \leq x \leq +\pi/2$. Value of u at inflow boundary obtained: (a) from analytical extension; (b) by setting $u_t = 0$; (c) by setting $u_t = 1$.

along the characteristic $x = x_0 + u_0 t$, where x_0 and u_0 are the values of x and u at the left-hand extremity of $R(x)$. Finding a distribution of u at the inflow boundary which satisfies (13) – and which differs from the result of Figure 2 a – is not difficult. One simple example is obtained by adding a function $(x - x_0 - u_0 t)^n$, $n > 1$, to the previous analytical solution, and by evaluating the result at $x = 0$ to obtain $u(0, t)$. However, the particular function selected for an additional boundary condition is not at issue. The major points to be made are: (1) if the differential equation is to be valid everywhere in the region over an appreciable time interval, the choice of the dependent variable at the inflow boundary is limited in a rigid manner, and (2) it is virtually impossible to meet these limitations *a priori* if the analytical solution is unknown.

The choice of u at the inflow boundary becomes simple *a priori* only when the definition of "admissible solution" is further relaxed so that u_x and u_t may be undefined at some internal boundary. In this case one has considerable freedom in specifying u at the inflow extremity. An obvious choice is to let u_t be zero at the inflow boundary for all $t > 0$. Such a solution to the previous example has been presented in Figure 2 b. Note that u_x and u_t are discontinuous along the characteristic passing through $x = -\pi/2$, $t = 0$, which has been entered as a heavy line. The differential equation is, of course, not satisfied along this characteristic. The solution in Sub-Region I (restricted to the fluid within the segment $R(x)$ at $t = 0$) is, as before, $u = 1.0 + 0.5 \cos(x - ut)$; the solution in Sub-Region II (fluid which entered the segment at $t > 0$) is $u = 1$. These two solutions are matched kinematically at the characteristic line passing through the inflow extremity. Note that in this case no shock phenomenon occurs.

The importance of the choice of u_t on the boundary is indicated in Figure 2 c. In this case it was assumed that u_t was a non-zero constant at $x = -\pi/2$: namely, $u_t = 1$. A shock forms rather quickly, as indicated. Before the shock forms (as t less than about $\pi/2$) the solution may again be divided into two sub-regions separated by the characteristic passing through the inflow extremity. At $t > \pi/2$, the kinematic boundary condition can no longer be satisfied at the surface of discontinuity and the dependent variable u becomes multi-valued at that point.

The implications of the above discussion with regard to the vorticity equation are evident. The alternatives are: (1) to specify only the streamfunction on the boundary of $R(x, y)$ at $t > 0$, to assume a solution exists according

to the definition of admissibility of Section 2, and to attempt to obtain this unique solution by some acceptable procedure; or (2) to specify in addition the value of the vorticity at the inflow boundary, and to relax the definition of admissibility. The latter alternative will in general mean that derivatives of the vorticity will not exist along an internal surface: namely, the boundary between the fluid originally within the region at $t=0$, and the fluid which moves into the region at a subsequent time. This discontinuity will propagate into the region, and at a later instant will define the boundary of two sub-regions. To solve the system analytically, solutions of the vorticity equation should be obtained separately for each sub-region, and the solutions should be matched along the material boundary so that the kinematic and dynamic boundary conditions are satisfied. In this process, the equation $f(x, y, t) = 0$ of the material boundary on which the discontinuities occur must be determined. The associated analytical problem – or its numerical analogue – is formidable.

These questions can be avoided by accepting the definition of an "admissible solution" presented in Section 2. Fortunately, this poses no difficulties in meteorological problems, for the dependent variable and its derivatives are not subject to control at $t > 0$, and can only be estimated for use as boundary conditions by subjective means at best. Certainly if the techniques of solving large scale meteorological equations were analytical rather than numerical, there would be nothing to gain and much to lose by arbitrarily introducing internal discontinuities. Unique solutions could be obtained by specifying the streamfunction at all boundaries; the vorticity would not be specified either at inflow or outflow boundaries for $t > 0$. Whether these conclusions need be modified when numerical methods are applied will be considered in the following sections.

5. Boundary Conditions for Numerical Integration

When differential equations are translated into difference equations, and solutions are attempted by numerical means, it is found that a variety of methods of integration can be devised – each of which will yield a specific numerical result. Furthermore, these methods can be adapted to all sorts of different boundary conditions. Thus, in the case of the vorticity equation, methods of integration can readily be developed for which the vorticity is specified at all boundaries at $t > 0$, at only the inflow boundary, or at no boundary at all. In the sense that each of these procedures leads to a particular answer, the methods can easily be made unique.

For this reason, the concept of necessary and sufficient boundary conditions for the existence and/or uniqueness of an admissible solution has meaning in the numerical problem only in terms of the differential equation we are attempting to solve by approximate methods. We can therefore arbitrarily define "overspecification" of a system of difference equations as a statement of boundary conditions which would constitute overspecification in the continuum, as the grid spacing approaches zero. Similarly, "necessary" or "sufficient" conditions can also be defined in terms of the associated differential equation. This terminology will be followed below.

One additional fact must be pointed out. Since numerical methods are an attempt to obtain approximate solutions to a differential equation, the integration procedures devised must not be in conflict with theory applicable to the continuum. This is of importance in the present discussion in connection with the occurrence of discontinuity surfaces propagating into the region $R(x, y)$. We have already seen that in solving the differential equation under such circumstances, solutions must be obtained separately in each sub-region and matched at the moving surface of discontinuity. If numerical methods are applied under similar conditions, an equivalent procedure should in principle be followed. This would, of course, be extremely difficult to do – especially since the discontinuity is a Lagrangian surface moving in a finite Eulerian grid.

In practice, the discontinuity introduced by specifying vorticity on the inflow boundary has been ignored. The discontinuity cannot be detected with a finite grid, and application of a differencing procedure across the discontinuity results in an arbitrary "smearing". Although such a process can possibly be rationalized on purely pragmatic grounds, little theoretical justification exists. When we integrate numerically across discontinuities

along which the differential equation (and hence the difference equation) is not valid, we have no way of knowing what errors are introduced. If numerical methods are to achieve an adequate scientific basis, such arbitrary procedures must be carefully avoided.

In the numerical integration of the vorticity equation, therefore, it is extremely desirable to develop a method which will not require the specification of vorticity on either the inflow or the outflow boundaries at $t > 0$. Another problem must be faced, however. To be useful, such a method must be simple to apply; must not accumulate errors too rapidly; and must remain numerically stable.

The latter two requirements have so far proved to be a substantial stumbling block. According to PLATZMAN (1954) two methods of estimating vorticity at the outflow boundary were used by the research group at the Institute for Advanced Study at Princeton. The first method involved setting the vorticity at an outflow point equal to the vorticity at the first interior grid point; the second involved a linear extrapolation from two interior grid points. These methods were used only at the outflow boundaries, the vorticity on the inflow boundaries being specified in accordance with the conclusions of CHARNEY ET AL. (1950). Nevertheless, a rapid accumulation of errors occurred near the outflow boundary, and (in some cases at least) numerical instability resulted.

An analysis of this behavior must involve an investigation of truncation error and stability criteria in non-linear systems. This is beyond the scope of the present paper. However, it is certainly not proper on the basis of these experiences to take the negative point of view that overspecification is necessary if instability is to be avoided. Certainly, some numerical methods may exist which do not overspecify and which are not unstable. One (a Lagrangian approach) is discussed in Section 7; a second possible procedure (in Eulerian form) is presented in Section 8. Neither of these procedures may at present be feasible for operational forecasting. Each will have value as a research procedure.

6. A Numerical Example

In order to provide a partial check on the effect of non-linearity on stability and truncation error, a numerical solution of a first order equation ($u_t + uu_x = 0$) was undertaken. The investigation of PLATZMAN (1954) on the linear form of this equation ($u_t + ku_x = 0$ where k is constant) made the attempt particularly interesting. Platzman found that complete overspecification (i.e. assigning the value of u at both inflow and outflow extremities of the segment R (x)) assured numerical stability, while either of two methods of computing the value of u at the outflow extremity resulted in numerical instability. It is important to determine whether these surprising conclusions are applicable to the non-linear model.

The non-linear equation ($u_t + uu_x = 0$) assures the formation of shock phenomena somewhere in the $x-t$ plane if u_x is not everywhere positive. An example was therefore chosen for which the analytical solution showed all shocks occurred downstream from the segment R (x) considered. Numerical integrations are therefore unaffected by multiple-valued solutions of the differential equation.

The solution chosen was:

$$u = {}^1/_2 \exp\,[(x-ut)^2 \ln 0.2/144]. \quad (14)$$

The distribution of u at $t=0$ was in the form of an error function. The initial values were computed on the x-axis at unit intervals for $-12 \leq x \leq 12$; the time increment was set equal to unity. At $t=0$, u was 0.1 at each

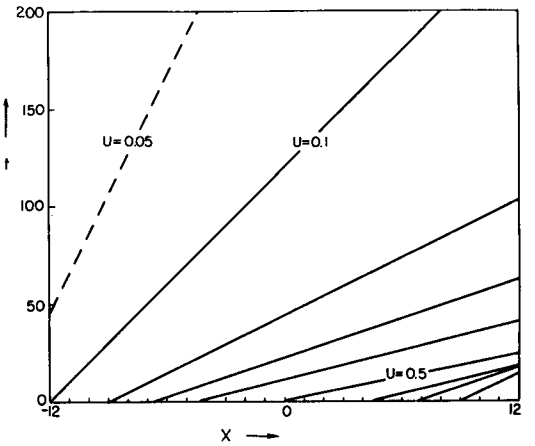

Fig. 3. Graphical solution of $u_t + uu_x = 0$. Straight lines are characteristics along which u is conserved. The distribution of u at $t=0$ is an error function with maximum at $x=0$.

extremity and 0.5 at the origin. The characteristic solution of (14) is shown in Figure 3.

Numerical integrations were performed using five different procedures:

(1) u was held constant at both inflow and outflow boundaries.
(2) u was held constant at the inflow boundary, and was computed at the outflow boundary using a quadratic extrapolation from two interior points. (This is a "first order" procedure as defined below.)
(3) u was computed at both inflow and outflow boundaries using a quadratic extrapolation from two interior points. (A "first order" procedure.)
(4) u was computed at both boundaries during the integration, using values of u_x on the boundaries obtained from interior values of u. (A "second order" approximation, discussed below.)
(5) u was computed at both boundaries using a somewhat different "second order" procedure, described below.

At the inflow boundary in Method 2, and at both boundaries in Method 3, the following equations were used:

$$\begin{aligned} u_{12} &= 2\,u_{11} - u_{10} + \Theta(\alpha^2) \\ u_{-12} &= 2\,u_{-11} - u_{-10} + \Theta(\alpha^2) \end{aligned} \qquad (15)$$

where α is the increment in x, and $\Theta(\alpha^2)$ indicates that terms involving α^2 and higher have been dropped from the appropriate Taylor Expansions. Note that although (15) is accurate to α^2, this is a first order procedure since u_x is the quantity actually used in the numerical integration, and the corresponding values of u_x at first interior points are:

$$\begin{aligned} (u_x)_{11} &= \frac{u_{11} - u_{10}}{\alpha} + \Theta(\alpha) \\ (u_x)_{-11} &= \frac{u_{-10} - u_{-11}}{\alpha} + \Theta(\alpha) \end{aligned} \qquad (16)$$

Methods 4 and 5 involve second order approximations for u_x. The respective relationships near the outflow boundary are:

$$\text{Method 4: } (u_x)_{12} = \frac{4u_{11} - 3u_{12} - u_{10}}{2\alpha} + \Theta(\alpha^2) \qquad (17)$$

$$\text{Method 5: } (u_x)_{11} = 2(u_x)_{10} - (u_x)_9 + \Theta(\alpha^2)$$

The first expression can be derived from Taylor Expansions about $x = 12$. Similar expressions are used near the inflow boundary.

Integrations were carried out for 20 time steps, and for $t = 1$, 5, 10 and 20 the root-mean-square difference between each numerical solution and the analytical solution was evaluated and expressed as a percentage of the average value of u. The results are presented in Table I. In general, there is not too much difference between Methods 2, 3 and 4. However, one second order procedure (Method 5) shows signs of accumulating errors near the boundaries. The strongly overspecified procedure (Method 1) is definitely inferior to all others, with an average error of 35 % at the end of 20 iterations. Strong corrugations appear near the outflow boundary, and the maximum value of u has increased from 0.50 to 0.85 (clearly an error, since the value of u should be conserved). At this stage it appeared that a moderate extension of the computation would result in the onset of numerical instability in Method 1, although if Platzman's conclusions were applicable to the non-linear system this should have been the only stable method of the group.

To see whether instability would develop, the numerical integrations were extended to 200 iterations for Methods 1, 2, 3 and 4. The second order procedure (Method 4) became unstable after about 110 iterations. Interestingly enough, the other three methods remained stable, although in Method 1 the maximum value of u exceeded unity for 21 consecutive iterations (from $t = 22$ through $t = 42$). The

Table 1. Root-Mean-Square Errors for five methods of numerical integration, expressed as percentage of mean value of dependent variable

	Method of Numerical Integration				
t	1.	2.	3.	4.	5.
1	0.3	0.4	0.5	0.2	0.2
5	1.3	0.8	0.5	0.3	0.3
10	3.3	1.5	0.9	0.6	1.3
20	34.9	3.7	3.0	3.5	11.7

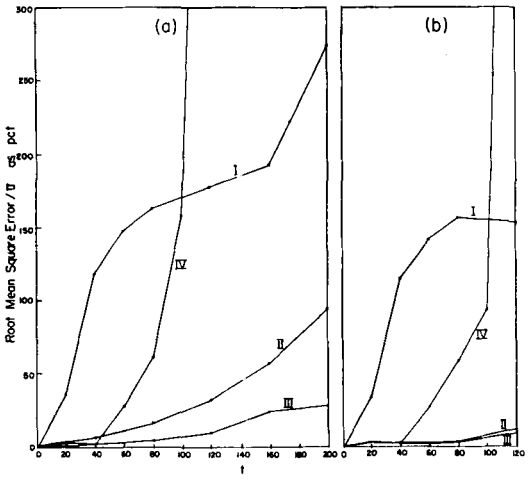

Fig. 4. Average root-mean-square errors of four methods of numerical integration of the equation $u_t + uu_x = 0$, expressed as percent of average value of dependent variable u. Time scale is normalized: t equals number of iterations.

root-mean-square errors for each method are shown in Figure 4: (a) for the entire set of 25 points; and (b) for those points occupied by fluid originally within the region R (x). The latter graph is terminated at $t = 120$, since beyond this most of the original fluid has left the Eulerian region. Method 3 remains amazingly accurate, while Method 2 has greater limitations. As a result of numerical "smoothing" across a surface that is an internal discontinuity in the continuum, Method 2 is slightly less accurate than Method 3 even for the portions of the $x-t$ plane where the analytical solutions are identical. This is shown in Figure 4 (b). On the other hand, Method 1 is so inaccurate as to be virtually useless after about 20 iterations. By $t=80$, corrugations of wave length two extend throughout the entire set of 25 points. Method 4 starts out well, but is unstable and becomes virtually useless after about 55 iterations.

Obviously, not too many conclusions should be drawn on the basis of a single example. Nevertheless, several points are evident. First, the stability criteria developed by PLATZMAN (1954) for a linear system cannot be applied to a non-linear system. The method of integration which showed earliest signs of instability was the one which (according to linear theory) should have been the only stable procedure. Furthermore, the best method was one which (according to linear theory) should have been unstable. Second, increased stability cannot be assured by higher order difference approximation near the boundaries. This is not too surprising, since after a large number of iterations the truncation error may be extremely large compared to the differencing error. Third, using a first order approximation the dependent variable was successfully computed at both inflow and outflow points, and this method was definitely superior to the one which involved overspecification at the inflow boundary.

These results may not, of course, be applicable to third order differential equations in two dimensions. Nevertheless, when considered in connection with the theoretical results of earlier sections, they indicate a careful re-evaluation of current practices is in order.

7. A Lagrangian Method of Integration

The discussion of sufficient boundary conditions would not be complete without mention of a Lagrangian solution. The difficulties in the Eulerian methods arise from the propagation into the region R (x, y) of a material surface, separating the fluid within the region at $t = 0$ from the fluid which enters at a later time. These difficulties can, of course, be avoided by conducting the numerical integration in terms of a Lagrangian grid. In the case of the vorticity equation, this approach completely removes one question of overspecification, since the vorticity is known throughout the Lagrangian region at all time.

In terms of three dependent variables (x, y, and ψ) the vorticity equation of a perfect fluid becomes:

$$x_t = J(\psi, x)$$

$$y_t = J(\psi, y)$$

$$\begin{aligned} f(a, b) &= J(x_t, x) + J(y_t, y) \qquad (18)\\ &= \psi_{aa}(x_b^2 + y_b^2) + 2\psi_{ab}(x_a x_b + y_a y_b)\\ &\quad + \psi_{bb}(x_a^2 + y_a^2) - \psi_a(x_a x_{bb} - x_b x_{ab}\\ &\quad + y_a y_{bb} - y_b y_{ab}) - \psi_b(x_b x_{aa} - x_a x_{ab}\\ &\quad + y_b y_{aa} - y_a y_{ab}) \end{aligned}$$

Here J is the Jacobian in terms of the independent variables (a, b) – where (a, b) are the values of (x, y) at $t=0$. Use has been made of the Lagrangian equation of continuity: $J(x, y)=1$. The function $f(a, b)$ is the known distribution of vorticity at the initial time. It is important to note that the third equation is always elliptic, with constant characteristic slopes $\pm 2i$. Thus, if the streamfunction is specified at the boundary points at all time, and if the coefficients remain finite, a unique single-valued solution exists in the interior.

Equations (18) can be re-written in difference form for numerical integration without difficulty. The procedure for integration is as follows:

(1) Values of x_t and y_t are computed everywhere in the interior at $t = t_0$.
(2) From this, values of x and y are computed at each interior grid point (a, b) at $t_1 = t_0 + \gamma$, where γ is the time increment. Values of x and y are computed at boundary points using an equation of the form (15).
(3) The coefficients of the third equation of (18) are evaluated at t_1 using centered differences in the (a, b) grid.
(4) The elliptic equation is solved for the streamfunction at all points.
(5) The above procedure is repeated.

In addition to theoretical advantages, such a numerical solution will yield particle trajectories, since the position (x, y) of a particle (a, b) is explicitly evaluated as a function of time. Difficulties include the increased storage to carry the values of three dependent variables, possible increase in truncation error, and problems in converting to an Eulerian system for purposes of plotting weather charts. However, with continued improvements in high speed computers, at least some of these difficulties are becoming less serious. Until Eulerian integrations can be conducted on a hemispheric scale, the Lagrangian system offers many unique advantages.

8. The First Time Step in Numerical Integration

One additional problem will now be considered: the errors introduced in integrating from $t=0$ to $t=\gamma$ (where γ is the time increment in the integration). The conventional method employs a forward (uncentered) difference for the first step. This introduces an error of the order of γ^2 in ψ, whereas all subsequent steps in centered time difference form introduce errors of the order γ^3. For:

$$\psi_{i,j}^{(1)} = \psi_{i,j}^{(0)} + \gamma\,(\psi_t)_{i,j}^{(0)} + \Theta(\gamma^2)$$
$$\psi_{i,j}^{(k+1)} = \psi_{i,j}^{(k-1)} + 2\gamma\,(\psi_t)_{i,j}^{(k)} + \Theta(\gamma^3) \qquad (19)$$

One immediate consequence of this increased error can be noted. In the vorticity equation in Eulerian form:

$$\Delta\psi_t = -J(\psi, \Delta\psi) \qquad (20)$$

the Jacobian is zero at maxima and minima of the streamfunction field (i.e. at centers of cyclones and anticyclones). If a forward time difference is employed, the vorticity at these important points cannot change in the first time step, although in actuality a significant variation may occur. This difficulty would be avoided by a higher order approximation, since even though $\Delta\psi_t$ were zero, the vorticity could pass smoothly through a maximum or minimum at $t=0$.

Various methods have been suggested for avoiding the increased error of a forward difference in the first time step, but none have been generally accepted because of their difficulty of application. The method suggested below, however, is very simple to apply and requires a minimum of additional programming.

Let us differentiate the vorticity equation with respect to time. Then:

$$\Delta\psi_{tt} = -J(\psi_t, \Delta\psi) - J(\psi, \Delta\psi_t). \qquad (21)$$

A program of computation can now be devised which only makes use of centered differences and higher order Taylor Expansions:

(1) From (20) compute $\Delta\psi_t$ at each interior grid point at $t=0$.
(2) Given (as boundary conditions) ψ_t on the boundary of $R(x, y)$, compute ψ_t at each grid point.
(3) From (21) compute $\Delta\psi_{tt}$ at each interior grid point at $t=0$. In this step it will be necessary to evaluate first space derivatives of $\Delta\psi_t$ at first interior grid points using a method analogous to (16).
(4) Given (as boundary conditions) ψ_{tt} on the boundary of $R(x, y)$, compute ψ_{tt} at each grid point.

(5) Using the values of ψ_t and ψ_{tt} from steps (2) and (4) compute ψ at $t=\gamma$ using a Taylor Series expansion:

$$\psi_{i,j}^{(1)} = \psi_{i,j}^{(0)} + \gamma\,(\psi_t)_{i,j}^{(0)} + \frac{\gamma^2}{2!}(\psi_{tt})_{i,j}^{(0)} + \Theta(\gamma^3) \qquad (22)$$

Note that this method results in the same accuracy in the first time step as in each succeeding step. The procedure will be simple to program, since steps (1) and (2) are used throughout the entire computation, and the relaxation (or matrix inversion) in step (4) is identical in procedure to that in step (2). The method can be generalized easily to any equation in which only first time derivatives appear.

In order to check the improvement resulting from the application of this method, the simplified equation ($u_t + uu_x = 0$) was again considered. Six examples were considered, with u chosen as sine waves of various wave lengths and amplitudes at $t=0$. An interval of 2π on the x-axis was selected, in order that cyclic continuity would be preserved and no errors would be introduced at the boundaries of the segment. Numerical integrations were carried through ten time steps, using two methods. Method (a) used forward difference at $t=0$; Method (b) solved numerically the equations:

$$\begin{aligned} u_t &= -uu_x \\ u_{tt} &= -uu_{xt} - u_t u_x = 2uu_x^2 + u^2 u_{xx} \end{aligned} \qquad (23)$$

in centered difference form at $t=0$, and used a Taylor expansion similar to (22). At all later time steps, identical procedures were employed for both methods. Differences between the results could therefore be attributed entirely to the first step.

After 1, 2, 5 and 10 iterations, the root-mean-square error was computed for each method, using the analytical solution as a standard. The average results, normalized in terms of the error in the first time step for Method (b), are shown in Figure 5. The error in Method (b) increased regularly with time. The error in the first time step of Method (a) was about five times as great as in Method (b). Some recovery occurred at the second iteration, but beyond that the error curves became parallel, and the difference between the two curves remained essentially constant

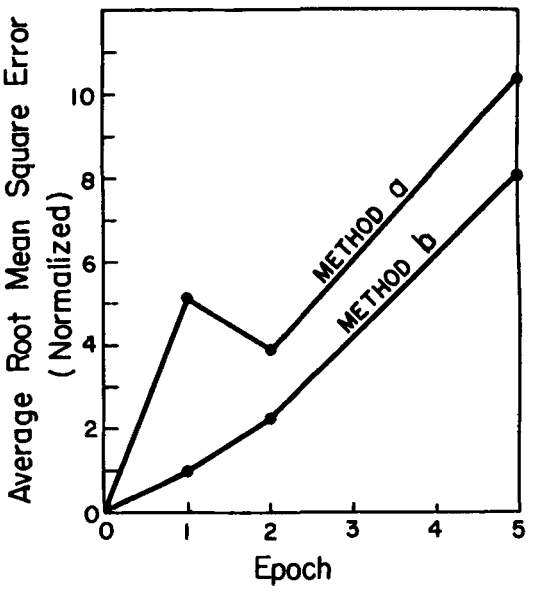

Fig. 5. Average root-mean-square errors of two methods of numerical integration of the equation $u_t + uu_x = 0$. Method b is identical to Method a, except that a higher order forward difference is used at $t=0$.

through the tenth iteration. At $t = 5\gamma$, the average error in Method (a) was about 30 % greater; at $t = 10\gamma$, it was about 15 % greater. In view of the small additional effort required to achieve this increase in accuracy, it is believed the method is worthy of routine application.

One final possibility suggests itself. Equations (20) and (21) can be used at any stage of the integration to the same order of accuracy as the centered difference form. This may not be operationally profitable, since two relaxations or matrix inversions are required at every time step. However, there are certain advantages which make this method of interest for research purposes. Thus, as (23) shows for the simplified equation, a certain "smoothing" is introduced by terms of the form u^2u_{xx} in the expression for the higher order time derivative. This should make the numerical integration more stable, while not causing the result to change appreciably from the analytical solution (which identically satisfies both equations in (23)).

This idea was tested using the numerical example of Section 6. Equations (23) were integrated through 200 iterations, using the

Table 2. Root-Mean-Square Errors for two methods of numerical integration, expressed as a percentage of mean value of dependent variable

	Entire Region		Original Fluid	
t	Method 3	Method b	Method 3	Method b
20	3.0	2.0	2.8	0.6
40	2.3	1.3	1.9	0.2
60	2.7	2.0	1.8	0.2
80	4.0	2.6	2.8	0.2
120	10.3	3.9	9.6	0.2
160	23.9	5.0	20.2	0.2
200	28.4	6.1	21.5	0.3

Method (b) discussed above at *each* time step. The root-mean-square errors are compared in Table II with Method 3 of Section 6, which was by far the best procedure previously tested over this extended period. It is interesting to note that Method (b) was definitely superior, both in the region occupied by the original fluid and over the entire set of 25 grid points.

In addition, absolutely no sign of instability appeared in Method (b), even after 200 iterations. Careful examination of the results show that centered difference estimates of u_x, u_t, u_{xx}, and u_{tt} remain consistent in sign from one grid point to the next (except at appropriate maxima and inflection points). On the other hand the results of Method 3 show oscillations in sign of u_{tt} after the second iteration; in u_{xx} after 16 iterations; in u_x after 17 iterations; and in u_t after 27 iterations. These oscillations persist, although they do not grow to substantial magnitude. The results seem to indicate clearly that the new method may have research value in numerical integrations for which stability is difficult to achieve.

It is important to emphasize that this method is equally applicable to the full vorticity equation. If the results of the non-linear first-order equation are any guide, it should be possible to use this method to integrate the vorticity equation for an Eulerian grid, without overspecification. Such an integration – and comparison of the results with the overspecified system – will throw more light on the effect of the current practice of assuming vorticity on the boundary of a fixed region.

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