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NUMERICAL SOLUTION OF THE PARTIAL DIFFERENTIAL EQUATIONS OF GAS DYNAMICS

By

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November 5, 1971
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This work was supported in part by the Advanced Research Projects Agency of the Department of Defense and was monitored by the U.S. Army Research Office-Durham under Contract No. DAHC04 72-C-0001.
ABSTRACT

In this report the relevant, practical criteria required for the numerical calculation of different types of gas dynamic flow fields are discussed. A classification for finite difference schemes is given. Numerical experiments are conducted on the non-linear Burger's equation using the Brailovskaya, Cheng-Allen, Dufort-Frankel, Crank-Nicolson and Lax-Wendnoff finite difference schemes as typical examples of different classes of finite differences schemes. The effect of time and space increments, types of boundary conditions, perturbations at the boundaries, truncation errors, convergence criteria and convergence rates are studied. It is shown that both the Cheng-Allen and Dufort-Frankel schemes have individual merits in different types of application.
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I. INTRODUCTION

Multidimensional flow problems are governed by physical laws which are mathematically represented by a set of partial differential equations. In attempting the solution of a multidimensional flow problem, one has recourse to (a) experimental methods, (b) pure analytical methods, and (c) computational methods using high speed electronic computers. Experimental techniques are usually confined to particular problems and yield a limited amount of information, while pure analytical methods can be applied to the most elementary cases, with many simplifying assumptions. While each of these two methods have their own individual and peculiar merits, computational methods with high speed electronic digital computers of the present and future generations, like the ILLIAC IV parallel processing machine, offer a number of advantages, among which are the following:

1. A numerical solution of the original partial differential equations governing the problem furnishes insight and valuable information about the inherent nature of the problem without any simplifying assumptions, or with a minimum of simplification.

2. Once a computational program has been developed, a wide spectrum of results and any required parametric studies are obtained with the least amount of effort and expenditure.

3. A single class of numerical methods can often be applied to a number of physical problems with different boundary conditions, whereas a physical experiment would necessitate expensive changes in equipment.

4. Computational procedures yield cross correlations between physical variables that are not readily available from experimental techniques.

5. Optimization of the related variables under given constraints and under physically realistic conditions is best accomplished computationally.

6. Numerical techniques are the only experimental tools available in certain problems because the nature of the physical phenomenon and its gigantic scale precludes any form of physical experimentation.
7. Coupled with experimental investigations and asymptotic analysis, computational techniques are a very powerful tool in obtaining a complete understanding of the physical problem.

Physical phenomena, in general, and multidimensional flow problems, in particular, can be described mathematically by a set of conservation laws in integral form. The equations are appropriately called conservation laws because they express the principle of conservation of mass, momentum and energy. These integral relations are readily reducible to a system of partial differential equations governing the flow. Together with prescribed initial and/or boundary conditions, the multidimensional flow problem reduces to a boundary value problem in the steady case or a coupled initial-boundary value problem in the non-steady case. Computationally it is oftentimes easier to solve even a steady state problem as the long time limit of the corresponding non-steady problem, since implicit difference schemes employing iterative techniques are generally required for the steady state formulation [1]. Moreover, in multidimensional flow problems, a time dependent formulation has decided advantages, even if for no other reason than that it is computationally simple. Such a method of computing the steady state solution as the long time limit of a sequence of temporal states, is often referred to as the "asymptotic method."

In the numerical solution of the partial differential equations of multidimensional fluid dynamics, the computational space is divided into smaller meshes or cells. The partial derivatives in the governing equations are approximated by finite differences of values at the mesh points. The problem is thus discretized and the dependent variables are calculated at a discrete set of mesh points comprising the computational grid in the flow field. The usual assumption made is that as the computational grid becomes smaller and smaller, the computed solution at a point converges to the actual true solution.

Numerical methods may be divided into three categories, depending on the construction of the computational grid and the calculation of the dependent variables. A brief description of the three methods serves to illustrate the advantages and disadvantages of each.
1.1 The Method of Finite Differences

This widely used method is applicable to both linear and non-linear partial differential equations of the hyperbolic, parabolic and elliptic type. It stems from the original work of Courant, Friedrichs and Levy [2]. The computational region is subdivided into smaller meshes which can have rectangular, cylindrical, spherical or other frames of reference, depending on the nature of the problem and its boundary (Figure 1). The grid lines are arbitrary.

The required dependent variables at any grid point, fixed in time and space, are obtained as a function of the variables at neighboring grid points. Computational ease and programming simplicity are greatly facilitated if no moving or stationary discontinuities exist in the flow. Whenever discontinuities do exist in the flow, special procedures are required to handle them depending on whether they are moving discontinuities or stationary discontinuities.

(a) Stationary Discontinuities

When the number of singularities is small and the discontinuities are fixed in time and space, the computational space can be treated as being composed of a number of separate regions. These regions have continuous solutions bounded by the singular discontinuous surfaces which satisfy boundary conditions appropriate to the problem. Finite difference methods are used in the regions with continuous solutions.

(b) Moving Discontinuities

(1) The initial formation and subsequent motion of the discontinuity may be followed by keeping track of the characteristics of the flow, which are the lines of propagation of discontinuities. Once the discontinuity has been thus located in space and time, it may be treated as a boundary point or surface, and the method of finite differences used for calculating the values at the remaining points.
FIGURE 1(a) ARBITRARY GRID IN THE METHOD OF FINITE DIFFERENCES

FIGURE 1(b) GRID FORMED BY CHARACTERISTIC LINES IN METHOD OF CHARACTERISTICS

FIGURE 1(c) CURVILINEAR GRID CONFORMING TO BODY SHAPE USED IN METHOD OF INTEGRAL RELATIONS
(2) In order to avoid the additional complication in programming logic as a result of finding the location of the moving discontinuity, certain devices may be employed which permit the use of finite differences alone throughout the flow, without the necessity of resorting to other methods like the method of characteristics. These devices are based on the physical nature of the discontinuous phenomenon, as for example, the use of artificial viscosity for smearing out shocks in hydrodynamic flow [3]. Such devices for computing across discontinuities should be used with caution as they introduce errors into the computation, resulting in loss of accuracy and resolution.

(3) Where feasible, problems with non-stationary singularities may be solved by using a movable grid attached to the singularity. This involves prior knowledge of the motion of the discontinuity. The transformation should, however, avoid the introduction of independent variables which map such grids into coordinate lines.

1.2 The Method of Characteristics

Numerical solutions of partial differential equations by the method of characteristics are possible only for equations of the hyperbolic type. In the method of finite differences, the computational grid may be constructed for any reference system of coordinates and may be superposed on the computational space at the very outset. However, in the method of characteristics, the computational grid must be bounded only by characteristic lines or surfaces which are drawn as the calculation proceeds in space and time. (See Figure 1b.) This is necessary since it is only along these characteristic lines or surfaces that the original non-linear partial differential equations can be reduced to simpler ordinary differential equations, called the compatibility conditions. In the three dimensional case, complexity of computational algorithm and difficulties in programming arise because of the complex behavior of the characteristic surfaces.

The method of characteristics is eminently suitable for flows containing a limited number of discontinuities, as it permits the accurate determination of the origin and subsequent propagation of shocks. Also, the method admits of considerable mathematical vigor, and uniqueness and convergence have been proved.
1.3 The Method of Integral Relations

This method, like the finite difference method, is applicable to hyperbolic, parabolic and elliptic partial differential equations. The computational space is divided into a series of curvilinear strips conforming to the shape of the boundary of the region of interest. (See Figure 1c.) The governing partial differential equations are written in divergence or conservation form and are integrated across these strips, with the functions occurring in the integrands being replaced by some interpolation expressions. Thus, in effect, it is the integrals that are being approximated, instead of the partial derivatives, as in the finite difference method. Since the governing equations are integrated in divergence or conservation form, the results obtained therefrom remain valid even when crossing a discontinuity.

Each of the above methods may be applied individually or in conjunction with any of the others depending on the nature and complexity of the problem. To name two examples, the supersonic flow over a satellite nose cone containing an ablative shield may be calculated by a combination of the method of characteristics and the method of integral relations. Flow of a viscous fluid in a boundary layer, may be calculated by the method of finite differences, the method of integral relations, or both.

Another very important factor to be considered in the selection of any one of the above three numerical methods is the type of computer employed and the programming language used. For computers like the parallel processing ILLIAC IV, maximum advantage must be taken of its capability to compute simultaneously in parallel. If the method of characteristics were used, the computational grid cannot be initially superposed on the flow field, and hence, until the flow has developed sufficiently, all the parallel processors cannot be put into operation simultaneously.

In the method of finite differences, the division of the computational space into arbitrary grids can be accomplished at the very beginning. In many problems, calculations at several grid points proceed simultaneously and independently, so that each processor or arithmetic unit of a parallel processing machine can be assigned to a given grid point. In this way great saving in computational time is realized, making possible the calculation of solutions to problems that would otherwise be prohibitively time consuming.
consuming. In the parallel processing machine, the computation of points adjacent to shock discontinuities and of boundary points presents certain challenges. In the computation of shock boundaries, one simple expedient would be to incorporate a system of checks which would be processed by all the arithmetic units, but would be effective only if shocks were present.

Since the method of finite differences offers definite advantages, especially from the viewpoint of application to advanced parallel processing machines, we shall confine our attention to this numerical technique. For computation of three dimensional flow problems, finite difference techniques offer the maximum assistance in the natural extension from the two dimensional case.
2. CONSERVATION LAWS

The laws that govern the motion of a fluid or gas state that given a control volume $V$ bounded by a surface $S$, the sum total of all the phenomena occurring within the volume $V$ must be such that the overall mass, momentum and energy contained within the control volume are conserved. Expressed mathematically, the conservation laws may be written as follows:

Conservation of mass

$$\frac{\partial}{\partial t} \int_V \rho \, dv = \oint_S - \rho \vec{u} \cdot d\vec{s}$$  \hspace{1cm} (1)

Conservation of momentum

$$\frac{\partial}{\partial t} \int_V \rho \vec{u} \, dv = \oint_S \left[ - (\rho \vec{u}) \cdot \vec{u} - \rho \vec{p} + \vec{t} \right] \cdot d\vec{s} + \int_V \rho \vec{g} \, dv$$  \hspace{1cm} (2)

Conservation of energy

$$\frac{\partial}{\partial t} \int_V \rho (e + \frac{\vec{u}^2}{2}) \, dv = \oint_S \left[ - \rho \vec{u} \cdot (e + \frac{\vec{u}^2}{2}) + \vec{u} \cdot \vec{r} - \vec{u} \cdot \vec{\tau} \right] \cdot d\vec{s} + \int_V \rho \vec{H} \, dv + \int_V \rho \vec{g} \cdot \vec{u} \, dv$$  \hspace{1cm} (3)

where

- $\vec{u}$ = velocity vector
- $\rho$ = density
- $p$ = pressure
- $\vec{\tau}$ = shear stress tensor
\[ \vec{I} = \text{unit tensor} \]
\[ H = \text{heat conduction from external sources} \]
\[ \vec{g} = \text{body force vector} \]

While a number of solutions will satisfy the above conservation laws, the particular solution for any given problem is determined uniquely by its initial and boundary conditions. The choice of a reference coordinate system in a computational procedure employing finite differences is governed by the ease of obtaining a finite difference formulation as well as suitability for programming in various languages.

In particular, in Cartesian tensor notation, the conservation equations may be written as follows:

### Conservation of mass:

\[
\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 \tag{4}
\]

### Conservation of momentum

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) + \frac{\partial \rho}{\partial x_j} \delta_{ij} - \frac{\partial}{\partial x_j} \tau_{ij} - \rho g_i = 0 \tag{5}
\]

### Conservation of energy

\[
\frac{\partial \rho}{\partial t} \left( e + \frac{u^2}{2} \right) + \frac{\partial}{\partial x_j} \left[ \rho u_j \left( e + \frac{u^2}{2} \right) + \rho u_j - u_i \tau_{ij} \right] - \rho g_i u_i + \rho H = 0 \tag{6}
\]

where \( \delta_{ij} \) is the Kronecker delta.
The equations (4) through (6) can readily be obtained from the integral equations (1) through (3) by applying Gauss theorem

\[ \int_S \vec{b} \cdot \vec{n} \, ds = \int_V \nabla \cdot \vec{b} \, dV \]  

(7)

2.1 The Navier-Stokes Equations

If we assume that Stokes law of fluid friction applies, i.e., the shear stress is proportional to the rate of shear deformation, and if we assume that the constant of proportionality or viscosity coefficient \( \mu \) is a constant, and that the bulk viscosity coefficient is zero, we may write the shear stresses as follows for the two-dimensional case:

\[ \tau_{xx} = \frac{4}{3} \mu \frac{\partial^2 u}{\partial x^2} - \frac{2}{3} \mu \frac{\partial v}{\partial y} \]  

(8)

\[ \tau_{yy} = \frac{4}{3} \mu \frac{\partial^2 v}{\partial y^2} - \frac{2}{3} \mu \frac{\partial u}{\partial x} \]  

(9)

\[ \tau_{xy} = \tau_{yx} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \]  

(10)

When these values for the shear stress \( \tau_{ij} \) are incorporated into the conservation equations, they are called the Navier-Stokes equations.

It will now be shown that the conservation laws embodying the Navier-Stokes shear stress has the same vector form as the Burgers' equation [4]:

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{1}{Re} \frac{\partial^2 u}{\partial x^2} \]  

(11)
In the absence of the external body force \( g \) and heat addition from external sources, (which does not include heat generated or absorbed within the body from such causes as non-equilibrium chemical processes, etc.) we may write the conservation laws in one dimension, thus:

**Conservation of mass**

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0 \tag{12}
\]

**Conservation of momentum**

\[
\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2 + p - \frac{4}{3} \mu \frac{\partial u}{\partial x}) = 0 \tag{13}
\]

**Conservation of energy**

\[
\frac{\partial}{\partial t} \left( e + \frac{u^2}{2} \right) + \frac{\partial}{\partial x} \left[ \rho u \left( e + \frac{u^2}{2} \right) + pu - u \frac{4}{3} \mu \frac{\partial u}{\partial x} \right] = 0 \tag{14}
\]

If we now define the vectors

\[
U = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} \tag{15}
\]

\[
F = \begin{pmatrix} -\rho u \\ -(\rho u^2 + p) \\ -\rho u^2 (p+E) \end{pmatrix} \tag{16}
\]
\[ S = \begin{pmatrix} 0 \\ \frac{\partial}{\partial x} \left( \frac{4}{3} \mu \frac{u}{x} \right) \\ \frac{\partial}{\partial x} \left( u \frac{4}{3} \mu \frac{\partial u}{\partial x} \right) \end{pmatrix} \]  

(17)

where  
\[ E = \rho \left( e + \frac{u^2}{2} \right) \]  

(18)

we can write [5] one vector equation for the three conservation laws (12), (13), and (14) as

\[ U_t = A U_x + B U_{xx} \]  

(19)

where  
\[ A = \frac{\partial F}{\partial U} \quad \text{and} \quad B = \frac{\partial S}{\partial U_x} \]

Note that the conservation laws have the same vector form as the Burgers' equation (11)

\[ \frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} + \frac{1}{R_e} \frac{\partial^2 u}{\partial x^2} \]

The Burgers' equation (11), therefore, serves as a useful model for testing finite difference schemes, prior to actual use on the full Navier-Stokes equations. In this way, flexibility, ease of programming and a substantial saving in computational time are secured when testing a number of difference schemes, with the aim of studying the different characteristics of each scheme.
3. DIFFERENCE SCHEMES

The numerical solution of a given set of partial differential equations involves replacing the partial derivatives by finite differences which are functions of the discrete values at neighboring points. The finite difference representation is often involved and bears no resemblance to the original partial derivative. The choice of a difference scheme for a given problem involves careful consideration of a number of factors, including the following:

1. Consistency of the difference approximation.
2. Convergence and stability of computed results.
3. Truncation errors and accuracy.
4. Ease of programming.
5. Reasonable computation time.
6. Adaptability to different programming languages.
7. Applicability to present and future generation of computers.

A brief description of various types of difference schemes and various practical considerations pertaining to their use will be given in this section and in Section 4.

3.1 Types of Difference Schemes

The one-dimensional Burgers' equation

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{1}{Re} \frac{\partial^2 u}{\partial x^2}
\]

may also be represented as

\[
\frac{u_t}{u} = -f(u) \frac{u_x}{x} + \frac{1}{Re} \frac{u_{xx}}{x}
\]

where \( f(u) = u \).
Let $u_j^n$ be the value of the computed solution at point $(j,n)$ in computational space (Figure 2).

The values at neighboring points $u_{j+1}^n$, $u_{j-1}^n$, and $u_j^{n+1}$ can be obtained as functions of the value $u_j^n$ at point $(j,n)$ thus,

$$u_{j+1}^n = u_j^n + \Delta t \frac{\partial u}{\partial x} | _j^n + O(\Delta t)^2 \quad (21)$$

In this representation, we have made the following assumptions:

(a) The Taylor expansion about the grid point $(j,n)$ converges monotonically.

(b) This convergence is rapid enough to permit truncation of the series after the second term.

Therefore,

$$\frac{\partial u}{\partial t} | _j^n = \frac{u_{j+1}^n - u_j^n}{\Delta t} + O(\Delta t)$$

Thus forward (and backward) differencing involves an error of first order in $(\Delta t)$. 

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The second term in the Burgers equation (11) can be represented as

\[ f(u) \frac{u}{x} = \sum_{j}^{k} \frac{u_{j+1} - u_{j-1}}{2\Delta x} \]

and the third term as

\[ \frac{1}{Re} \frac{u}{xx} = \frac{1}{\Delta x^2 Re} \left[ u_{j+1}^m - 2u_j^p + u_{j-1}^q \right] \]

where \( k, \ell, m, p \) and \( q \) are either \( n+1 \) or \( n \). Thus the Burgers equation may be represented in general form as:

\[ u_{j}^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} \sum_{j}^{k} \left( u_{j+1}^k - u_{j-1}^\ell \right) + \frac{\Delta t}{\Delta x^2 Re} \left[ u_{j+1}^m - 2u_j^p + u_{j-1}^q \right] \]

\[ (22) \]

(a) **Explicit Schemes** - One step schemes

If \( k = \ell = m = p = q = n \), we have the Euler's scheme

\[ u_{j}^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} \sum_{j}^{k} \left( u_{j+1}^n - u_{j-1}^n \right) + \frac{\Delta t}{\Delta x^2 Re} \left( u_{j+1}^n - 2u_j^n + u_{j-1}^n \right) \]

\[ (23) \]

This is an explicit scheme where values at the \( (n+1) \)th time step are calculated directly from known values at the \( n \)th time step. No intermediate or provisional values of \( u_{j}^{n+1} \) are calculated.

(b) **Explicit Schemes** - Two step schemes

Quite often two-step explicit schemes are encountered of which the Richtmyer variation of the Lax-Wendroff scheme is a familiar example [6]. In the inviscid case \( (Re \rightarrow \infty) \), the scheme may be written as
\[ u_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{u_j^{n+1} + u_j^n}{2} + \frac{\Delta t}{2\Delta x} f_{j+\frac{1}{2}}^n \left[ u_{j+\frac{1}{2}}^n - u_{j-\frac{1}{2}}^n \right] \]

\[ u_j^{n+1} = u_j^n + \Delta t \frac{1}{\Delta x} f_j^{n+\frac{1}{2}} \left[ u_{j+\frac{1}{2}}^{n+1} - u_{j-\frac{1}{2}}^{n+1} \right] \]  \hspace{1cm} (24)

In this scheme, intermediate values centered at time \((n+\frac{1}{2})\) are first obtained before the final values at time \((n+1)\) are calculated. The intermediate values may also be calculated at time \((n+1)\) instead of \((n+\frac{1}{2})\) as is done in the Brailovskaya and Cheng-Allen schemes to be discussed later.

(c) Fully Implicit Schemes

If \(k = \lambda = m = p = q = n+1\), the calculation of \(u_j^{n+1}\) is more involved and iteration techniques are necessary. The fully implicit schemes can be shown to be unconditionally stable.

(d) Partially Implicit Schemes

If either the convective term or the viscous term alone is formulated implicitly and the other term is formulated explicitly, we have a partially implicit scheme. Thus, the convective term is formulated implicitly if

\[ k = \lambda = n+1 \text{ and } m = p = q = n, \]

and if

\[ k = \lambda = n \text{ and } m = p = q = n+1 \]

the viscous term is formulated implicitly. Calculation of \(u_j^{n+1}\) again involves iteration techniques.
(e) Quasi Implicit Schemes

If k = m = n and ℓ = p = q = n+1,

\[ u_{j}^{n+1} = u_{j}^{n} - \frac{\Delta t}{2\Delta x} f_{j}^{n}(u_{j+1}^{n} - u_{j-1}^{n}) + \frac{\Delta t}{\Delta x} e^{n} [u_{j+1}^{n} - 2u_{j}^{n+1} + u_{j-1}^{n+1}] \]

(25)

Values \( u_{j}^{n+1} \) can be calculated explicitly without any iteration techniques provided \( u_{j-1}^{n+1} \) is known at the left boundary. The scheme is then called a quasi-implicit scheme.

(f) Differencing in Integral Form

Finite difference schemes may be obtained directly from the integral conservation laws expressed in Equations (1) - (3). This method has been used by Roberts and Weiss [7] for unsteady convective problems and possesses certain advantages, especially in flows containing discontinuities, since the form of differencing embodies the conservation laws.

In a two-dimensional problem, a computational net may be defined as in Figure 3. An elemental volume \( \Delta V \) is then given by

\[ \Delta V = \Delta x \cdot \Delta y = (x_{+} - x_{-}) (y_{+} - y_{-}) \]

![Figure 3](image-url)

Using this difference formulation, Equation (1) may be written as:
\[
\frac{2}{\Delta t} \int_{\Delta V} \rho dx \, dy = \int_{y_-}^{y_+} \left\{ \frac{\partial}{\partial x} \left( \int_{x_-}^{x_+} (\rho u) \, dx \right) \right\} \bigg|_{y_-}^{y_+}
\] (26)

and similarly for Equations (2) and (3).

Another classification used in addition to the above is based on the number of time levels used in the difference formulation. Thus, the Dufort-Frankel and leap frog scheme can be calculated like an explicit scheme, but uses data points from two time levels \( n \) and \( (n-1) \) to calculate points on the time level \( (n+1) \). It is, therefore, called a "two level" scheme. Multi-level schemes vary from the fully explicit to the fully implicit category.
4. CONSISTENCY, ERRORS, STABILITY AND CONVERGENCE OF DIFFERENCE SCHEMES

4.1 Consistency

In finite difference methods, the continuous partial derivatives are approximated by functions or operators involving known values at a selected number of discrete points. The solution marches on from a given sequence of known initial and/or boundary values to another sequence of computed values, and so on, until the final solution is realized, also at a set of discrete points.

The difference formulation is said to be a consistent approximation if the final computed solution represents the true solution to the problem at the selected discrete points.

To insure consistency, a number of important practical guidelines must be observed.

(1) Since the finite difference computation is a step-by-step marching procedure, the difference scheme must be consistent at each step of the calculation.

Consider the calculation of $u_j^{n+1}$ from the known value $u_j^n$ for $-k \leq j \leq k$, where $k$ is a positive integer. Further assume that $U_j^n$ are exact values. If $O(\Delta t)$ is a finite difference operator such that it transforms points $u_j^n$ to $u_j^{n+1}$, i.e.,

$$O(\Delta t) u_j^n = u_j^{n+1}$$

then the difference operator $O(\Delta t)$ provides a consistent approximation if

$$|| u_j^{n+1} - u_j^{n+1} || \to 0 \text{ as } \Delta t \to 0, \ 0 \leq t \leq T$$ \hspace{1cm} (27)

Consistency of the overall calculation is secured by insuring consistency at each step of the calculation.
(2) The quantity under the norm in (27) can be written as

\[ U(t + \Delta t) - O(\Delta t) u(t). \]

This, in effect, is equivalent to saying that the truncation error of the difference operator \( O(\Delta t) \) must tend to zero as \( \Delta t \rightarrow 0 \).

(3) Since the solution marches from known values to a set of computed values, it would initially begin with a known sequence of exact boundary values. To ensure that the final computed solution is consistent with the true final solution, it is important that the finite difference formulation of the boundary conditions be consistent with the true physical conditions at the boundary.

(4) The final computed solution should depend continuously on the given initial and/or boundary conditions, once these boundary conditions are consistently represented. Since disturbances, in the form of changes in the flow field, propagate along characteristic lines, the final solution will depend continuously on the initial data if all points in the computational space are calculated from known data within the domain of dependence of the point being calculated. This principle is embodied in the Courant-Friedrichs-Lewy rule which states that the time increment \( \Delta t \) should satisfy the relation

\[ \Delta t < \frac{\Delta x}{|u| + a} \]  \hspace{1cm} (28)

where \( u \) is the flow velocity and \( a \) the speed of sound in the gas.

This condition also states that discontinuities in the flow should be properly demarcated, so that the characteristic lines do not cross them. Otherwise, the final solution would not depend continuously on the initial data. This precludes the possibility that the operator \( O(\Delta t) \) would contain points on the opposite side of a discontinuity.
4.2 Errors and Accuracy

Consider the equation

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0 \]  \hspace{1cm} (29)

and a finite difference formulation to it

\[ L(u) = \frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} + u_{j}^{n} \frac{(u_{j+1}^{n} - u_{j}^{n})}{\Delta x} = 0 \]  \hspace{1cm} (30)

Expanding \( u_{j}^{n+1} \) and \( u_{j+1}^{n} \) about the point \( u_{j}^{n} \), using Taylor's series in powers of \( t \) and \( x \) respectively, it is shown that

\[ L(u) - (\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x}) = \Delta t \frac{\partial^{2} u}{\partial t^{2}} + \cdots + \Delta x \frac{\partial^{2} u}{\partial x^{2}} + \cdots \]  \hspace{1cm} (31)

The error of truncating the Taylor series is, therefore, of order \( \Delta t \) and \( \Delta x \).

Besides truncation errors, other types of errors introduced into a calculation are:

(a) Boundary errors introduced into the computational space at the boundary, by incorrect formulation of the boundary conditions.

(b) Inconsistency errors.

(c) Machine roundoff errors.

These errors propagate and accumulate in complex fashion to yield a gross error in the computed result.
4.3 Stability and Convergence

The finite difference solution to a given system of partial differential equations involves a marching procedure applied to a sequence of discrete points in computational space. The difference operator $O(\Delta t)$ applied once transforms initial values $u_j^0$ to values $u_j^1$ at the first level of computation. Let $N$ levels of computation be required to attain the final solution. Since the operator $O(\Delta t)$ contains an intrinsic error, there exists the possibility that the cumulative error over $N$ computational levels becomes unmanageable. Hence, the computation is said to be stable if given a value $\Delta t$ such that $0 \leq \Delta t \leq \tau$, $O(\Delta t)^N$ is uniformly bounded for $0 \leq N \Delta t \leq T$, where $T$ is the time at the final solution.

This final solution is said to converge to the true solution at any time level if the norm of the difference between the computed solution and the true solution tends to zero as $\Delta t$ tends to zero.

Let $U_j^n$ be the true solution at point $(j,n)$, and $u_o$ be initial values. The difference approximation is convergent if

$$|| O(\Delta t)^n u_o - U_j^n || \rightarrow 0 \text{ as } \Delta t \rightarrow 0$$

(32)

for all $j$.

Stability and convergence are synonymous as proved by P. Lax for linear partial differential equations. Lax's equivalence theorem [8] states that, given a properly posed initial value problem and a consistent finite difference approximation to it, stability is the necessary and sufficient condition for convergence. Although the theorem is proved only in the linear case, it is quite common to assume that it applies locally to the quasi-linear partial differential equations of fluid dynamics.

In practical computations, the non-linear partial differential equations do not readily admit to a simple stability analysis. At best, stability is investigated with a simplified linear form of the original equations. The Von-Neumann analysis, which is the most commonly used procedure
for testing stability, studies the behavior of a sinusoidal error superposed on the true solution. If the amplitude of the error increases as calculation proceeds, the difference operator is considered unstable. A more difficult means of studying the stability of a difference operator is the so-called energy method, which provides information at both interior and boundary points. The essential feature of this method is to show that the increase in a specific norm of the solution vector is no greater than $1 + 0 (\Delta t)$ between the two successive time steps. If this norm can then be shown equivalent to the $L_2$ norm, stability in this norm is assured. In fairly simple cases, the physical energy of the system provides such a norm, and hence the method is called the energy method. The mathematical analysis is quite complicated, and, unlike the Von-Neumann analysis, the energy method does not provide a physical insight into the manner of error propagation.

In practice the norm used in Equation (32) to test for convergence takes various forms. Let $u_j^n$ be the computed points and $U_j^n$ the values of the true solution at these points.

Let $N_o = a$ certain number of iterations

$\epsilon = a$ given positive quantity independent of $N$

If the condition

$$| U_j^n - u_j^n | \leq \epsilon$$

(33)

is satisfied for $N > N_o$, convergence has been attained in the maximum modulus norm. The computed solution converges uniformly to the true solution. Since a convergence criterion based on the maximum modulus norm implies uniform convergence, a necessary condition for such a criterion to be used is that the true solution $U_j^n$ must be continuous.

Another common norm employed to test for convergence in numerical applications is the mean square error norm, which can be stated as follows:
\[ \frac{1}{J} \sum_{j=1}^{J} (U^n_j - u^n_j)^2 \Delta t \leq \varepsilon \]  

for \( N > N_0, 0 \leq \Delta t \leq \tau. \)

This is a measure of the mean quadratic error and insures convergence in the mean. If the sequence of points \( U^n_j \) of the true solution is continuous and has continuous partial derivatives, then convergence in the mean and uniform convergence are equivalent.
5. NUMERICAL EXPERIMENTS WITH FINITE DIFFERENCE SCHEMES

In the foregoing the salient features of obtaining the numerical solution of a set of partial differential equations have been described, and among the three main methods of approach, the method of finite differences has been singled out for particular attention. The integral conservation laws which are the underlying physical basis for the governing partial differential equations are given, and methods of obtaining their finite difference formulation are discussed. Various considerations of practical relevance, in regard to consistency, error propagation, stability and convergence of difference schemes have been given.

The selection of a difference scheme for a particular problem constitutes a first step in the solution of a given system of partial differential equations. A number of workers have made comparative studies of different classes of difference schemes. Emery [9] has made an evaluation of five difference schemes for one- and two-dimensional, non-steady inviscid flow. They are:

(a) Lax's centered time, forward space difference scheme

(b) Rusanov's [10] scheme which is an improvement of Lax's scheme, possesses the minimum artificial viscosity at each nodal point, and also weights the importance of neighboring points

(c) Landshoff's scheme which introduces an artificial pressure on the lines of Richtmyer's and Von-Neumann's artificial viscosity

(d) The Lax-Wendroff scheme

(e) Richtmyer's variation of the Lax-Wendroff scheme.

Applied to a moving shock problem, most of the schemes show a visible overshoot at the shock front. It is found that Lax's scheme is easy to program and of good resolution. Rusanov's method is more versatile and also possesses good resolution. A modified version of the Lax-Wendroff scheme is shown to yield a resolution which is spatially three times as great as that obtained by
Lax's method for the same number of nodal points. Computational times are minimum in Lax's method and Richtmyer's variation of the Lax-Wendroff method, and maximum in the Lax-Wendroff method. A great deal of difficulty in programming is experienced with the Lax-Wendroff scheme, even in the inviscid case.

Fourth order accurate, conservative difference schemes derived directly from the integral formulation of the conservation laws were studied by Roberts and Weiss [7]. The schemes are shown to be free from numerical dispersion, and thereby to yield accurate results in the convective problems studied. The schemes are correctly centered in time and space so that the modulus of the amplification factor is exactly unity, and, hence, stability is assured. Extension of the scheme to three space dimensions is indicated.

A similar technique based on Godunov's [11] method was utilized by Taylor and Masson [12] to calculate flow over bodies with boundaries of large curvature. A curvilinear co-ordinate system was used. This method, like that of Roberts and Weiss involves the calculation of fluxes across cell boundaries. The difference equation for each cell is derived by integrating the governing equations over the volume of the cell.

Rubin and Burstein [5] investigated the use of the Richtmyer two-step variation of the Lax-Wendroff scheme for both inviscid and viscous flow in the case of a moving shock. The full Navier-Stokes equations in one dimension are used in the viscous flow calculation. The difference formulation in the viscous case is very susceptible to numerical instability. Once a stable formulation has been successfully established, the Courant-Friedrichs-Lewy stability criterion must be strictly enforced.

More recently Rubin and Preiser [13] generalized the Richtmyer method to three space dimensions and time. The resulting formulation is obtained directly from the integral conservation laws, with some approximation.

The principle of the Lax-Wendroff scheme [14] was applied, in non-conservation form by Moretti and Salas [15] to the problem of shock formation caused by an accelerating piston. Consistency of formulation is maintained in a transformed co-ordinate system, which insures virtually no overshoot in the high pressure side of the shock. Since the equations are not maintained in conservation form, the Jacobian of the transformation, encountered while
evaluating the time derivatives in terms of space derivatives, is no longer present. The flow variables are evaluated only at the specified nodal points and no half incremental values are necessary as in the Richtmyer variation of the Lax-Wendroff scheme. Moretti [16] has also tested a number of difference schemes applied to the one-dimensional equations in divergence form and in non-divergence form.

A modification of a scheme originally proposed by Brailovskaya [17] was used by Cheng and Allen [18]. Stability of the modified scheme is shown to be independent of the Reynolds number for the linear case.

While many different schemes were used for specific problems, and in some instances, comparisons were made among different schemes of similar construction, a number of questions still need to be answered, among which are the following:

1. What is the effect of the space increment $\Delta x$ on accuracy, convergence rate and resolution?
2. What is the influence of the time step $\Delta t$ on accuracy and computational time in seeking a steady state solution?
3. What is the effect of different types of boundary conditions on the different schemes?
4. How do different formulations of the same boundary conditions affect the problem?
5. How do the different convergence criteria compare?
6. What is the effect of different classes of difference schemes on computational time?
7. What is the effect of Reynolds number on accuracy, stability and convergence in a viscous flow situation?
8. How do the schemes tested compare with regard to stability, accuracy and convergence rates?
9. How do various schemes compare for application to different categories of computers, like parallel processing machines, pipe line machines, etc.

In order to find answers to these questions, the following finite difference schemes were tested with the non-linear Burgers equation [11]:
(1) Erailovskaya Scheme

\[
\frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} = -\frac{1}{4\Delta t} \left[ (u_{j+1}^{n})^2 - (u_{j-1}^{n})^2 \right] + \frac{1}{Re \Delta x^2} \left[ u_{j+1}^{n} - 2u_{j}^{n} + u_{j-1}^{n} \right]
\]

(35)

\[
\frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} = -\frac{1}{4\Delta t} \left[ (u_{j+1}^{n+1})^2 - (u_{j-1}^{n+1})^2 \right] + \frac{1}{Re \Delta x^2} \left[ u_{j+1}^{n+1} - 2u_{j}^{n+1} + u_{j-1}^{n+1} \right]
\]

Truncation error is of order \(\Delta t, \Delta x^2\).

Stability condition: \(\Delta t \leq \min \left( \frac{\Delta x}{\max |u|}, \frac{\Delta x^2 Re}{4} \right) \)

(36)

(2) Dufort-Frankel Scheme

\[
\frac{u_{j}^{n+1} - u_{j}^{n-1}}{\Delta t} = -\frac{1}{4\Delta x} \left[ (u_{j+1}^{n})^2 - (u_{j-1}^{n})^2 \right] + \frac{1}{\Delta x^2 Re} \left[ u_{j+1}^{n} - u_{j}^{n+1} + u_{j-1}^{n} - u_{j}^{n-1} \right]
\]

(37)

Truncation error: \(O(\Delta x^2, \Delta t^2)\)

Stability condition: \(\Delta t \leq \frac{\Delta x}{\max |u|} \)

(38)

(3) Cheng-Allen Scheme

\[
\frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} = -\frac{1}{4\Delta x} \left[ (u_{j+1}^{n})^2 - (u_{j-1}^{n})^2 \right] + \frac{1}{Re \Delta x^2} \left[ u_{j+1}^{n+1} - 2u_{j}^{n+1} + u_{j-1}^{n+1} \right]
\]

\[
\frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} = -\frac{1}{4\Delta x} \left[ (u_{j+1}^{n})^2 - (u_{j-1}^{n})^2 \right] + \frac{1}{Re \Delta x^2} \left[ u_{j+1}^{n} - 2u_{j}^{n} + u_{j-1}^{n} \right]
\]
\[
\frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} = -\frac{1}{4\Delta x} \left[ (u_{j+1}^{n})^2 - (u_{j-1}^{n})^2 \right] + \frac{1}{\text{Re}\Delta x^2} \left[ u_{j+1}^{n+1} - 2u_{j}^{n+1} + u_{j-1}^{n+1} \right]
\]

Truncation error: \( O(\Delta t, \Delta x^2) \)

Stability condition: \( \Delta t \leq \frac{\Delta x}{\max |u|} \)

(4) **Crank-Nicolson Scheme**

\[
\frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} = -\frac{1}{4\Delta x} \left[ \frac{(u_{j+1}^{n})^2 - (u_{j-1}^{n})^2 + (u_{j+1}^{n+1})^2 - (u_{j-1}^{n+1})^2}{2} \right]
\]

\[
+ \frac{1}{\text{Re}\Delta x^2} \left[ \frac{u_{j+1}^{n+1} - 2u_{j}^{n+1} + u_{j-1}^{n+1}}{2} \right]
\]

Truncation error: \( O(\Delta t, \Delta x^2) \)

Unconditionally stable.

(5) **Lax-Wendroff Scheme**

Richtmyer's two step method was employed for this scheme. As in the above formulations, bars denote the intermediate steps.

\[
\frac{u_{j+1/2}^{n+1}}{2} = \frac{1}{2} (u_{j+1}^{n} + u_{j}^{n}) - \frac{1}{2\Delta x} \left[ \frac{(u_{j+1}^{n})^2 - (u_{j}^{n})^2}{2} \right] + \frac{1}{2} \frac{\Delta t}{\text{Re}\Delta x^2}
\]

\[
(u_{j+2}^{n} - u_{j+1}^{n} - u_{j}^{n} + u_{j-1}^{n})
\]
\[
\frac{u_j^{n+1/2}}{} = \left( \frac{u_{j+1}^n + u_{j-1}^n}{2} \right) - \frac{1}{4} \frac{\Delta t}{\Delta x} \left[ (u_{j+1}^n)^2 - (u_{j-1}^n)^2 \right] \\
+ \frac{\Delta t}{\Delta x^2 \text{Re}} \left[ u_{j+1}^n - 2u_j^n + u_{j-1}^n \right] 
\]

The final scheme for calculating values at the next time step is given by

\[
u_j^{n+1} = u_j^n - \frac{\Delta t}{4\Delta x} \left( u_{j+1}^n + u_{j-1}^n \right) \left( \frac{u_{j+1}^n - u_{j-1}^n}{2} + \frac{u_{j+1/2}^{n+1} - u_{j-1/2}^{n+1}}{2} \right) \\
+ \frac{\Delta t}{\Delta x^2 \text{Re}} \left[ u_{j+1}^n - 2u_j^n + u_{j-1}^n \right] 
\]

Truncation error: \( O(\Delta t, \Delta x^2) \)

Three other formulations for the Lax-Wendroff scheme were tested and found to be unstable.

According to the classification in Section 3, both the Brailovskaya and Cheng-Allen schemes are two-step explicit schemes. The Dufort-Frankel scheme is an explicit, two-level, one-step scheme. The Crank-Nicolson scheme is implicit, while the Lax-Wendroff scheme is a two-step explicit scheme. Attention has been focused mainly on explicit schemes because of the ease in programming in three dimensions. The Crank-Nicolson implicit scheme is commonly employed in the solution of the parabolic heat conduction equations. Since the Navier-Stokes equations are a mixed parabolic-hyperbolic system, we are interested in observing the behavior of the Crank-Nicolson scheme in comparison with the other four schemes.

Two sets of boundary conditions were chosen to test their effect on the final solution.

Set I

L. Boundary \( u(0) = 1 \)
R. Boundary \( u(1) = -1 \)
Set II

L. Boundary $u(0) = 1$

R. Boundary $u(1) = 0$

for $0 \leq x \leq 1$

The exact solution of the Burgers equation for the steady case is given by

$$u(x) = A \tanh \left( A(B-x) \frac{Re}{2} \right)$$

where $A$ and $B$ are determined from the boundary conditions. For boundary conditions I, there is a sharp discontinuity at $x = 0.5$, while for B.C.II, there is a sharp discontinuity at $x = 1$.

No special provision is made for these discontinuities in the numerical scheme, to observe how well they perform under extreme conditions where discontinuities may exist in the flow.

For a meaningful comparison of the various schemes, the arithmetic statements in the computer program were made as identical as possible, except for essential differences necessitated by the special characteristics of the individual difference schemes.

Tests were run at different Reynolds number $Re$, and at different space increment $\Delta x$. The Reynolds number was varied from 10 to 1000. The number of space intervals varied from 10 to 58 as 60 points was near the upper storage limit of the CDC 1604 computer used in the calculations. For a given space increment $\Delta x$ and Reynolds number $Re$, the time step was varied such that

$$\frac{\Delta x^2 Re}{4} \leq \Delta t \leq \Delta x$$

This range of $\Delta t$ was employed to subject the schemes to the most difficult conditions possible, both at the low Reynolds number limit and at the inviscid...
high Reynolds number limit. The criterion used to test for convergence to the steady state was

$$\max_j |u_{n+1}^j - u_n^j| \leq 10^{-5}$$

(46)

at any time step. This is analogous to the maximum modulus norm and implies uniform convergence. The quantity

$$\frac{1}{J} \sum_{j=1}^{J} |(u_{n+1}^j)^2 - (u_n^j)^2|$$

(47)

was also calculated for comparison. This is analogous to the mean square error norm, because $u_{n+1}^j$ tends to the true solution $u_n^j$ as $n$ increases. It implies convergence in the mean. It is thus possible to compare the two norms for convergence.

The computational program is coupled to a graph-plotting subroutine, which traces out the required curves on an oscilloscope from which photographs may be made directly. One feature of this plotting routine to be kept in mind while examining the results, is that it selects the most suitable scale for each specific plot within the sweep of the beam. Thus, if the final solution is calculated using different schemes, and if in any one solution so calculated, there is a peak or overshoot, the plotting subroutine automatically changes the scale for this particular curve. If now the different final solutions were photographed on a single film, the solution with the overshoot would be displaced from the other solutions, even though the curves represented the same numerical values, except for the overshoot.
6. RESULTS AND DISCUSSION

6.1 Comparison of the Different Schemes

Figures 4(a) and 4(b) show the computed solution with boundary conditions I and II, respectively. Figure 4(a) contains all the five schemes tested. The four explicit schemes are practically indistinguishable as they overlap over one another in the photograph. The smoother, less accurate curve is the solution from the Crank-Nicolson scheme. Figure 4(b) contains only the solution from the four explicit schemes. The mean square difference of the solution computed with the explicit schemes was only 0.008 compared to an ideal step function, while for the implicit scheme it was 0.04. As can be seen from the figure, the accuracy of all four explicit schemes compares favorably. The implicit scheme contains an additional iteration for each computed time step in the evolution of the steady state solution. The overall accuracy of the implicit scheme is dependent on the accuracy of the intermediate iterative step as well as the accuracy of the implicit scheme itself. The intermediate iterative step also consumes a good deal of computational time, making the implicit scheme slower than the explicit schemes.

The Brailovskaya scheme yields results comparable in accuracy to the other explicit schemes provided the time step is well within the stability limits dictated by the linear analysis. This limitation on the time step is even more stringent with the Lax-Wendroff scheme. The Cheng-Allen scheme, developed from the Brailovskaya scheme, possesses the best stability properties. Its theoretical stability limit is independent of the Reynolds number based on the linearized analysis. With this scheme a larger time step can be used at low Reynolds numbers than is permissible with the other explicit schemes. It was found by experiment that even at high Reynolds numbers, where the C.F.L. criterion is less than the viscous limit, a much larger time step could be used with the Cheng-Allen scheme.
FIGURE 4(a)

FIGURE 4(b)

FIGURE 4. ALL FIVE SCHEMES
RE = 60
DT = \( \frac{DX^2 \times RE}{4} \)
DX = 1/20
Tests with the Lax-Wendroff scheme show that, as the high Reynolds number inviscid limit is approached, this scheme yields the most accurate results. Figure 5 shows the computed solution at a Reynolds number of 1000. Two curves are distinguishable. The plot with the maximum waviness is the solution obtained from the Brailovskaya, Cheng-Allen and Dufort-Frankel schemes superimposed on one another. Within this curve is another curve, obtained from the Lax-Wendroff scheme which is smooth except for wiggles at either end of the discontinuity at $x = 0.5$. All other conditions being the same, the Lax-Wendroff scheme performs better at high Reynolds numbers. A stable formulation of the Lax-Wendroff scheme for viscous flows is however quite difficult. Before the stable scheme $^{(42)}$, $^{(43)}$ was arrived at, three other formulations were experimented with but without success. A similar difficulty has been experienced by Rubin and Burstein $[5]$. 

Table I shows the number of iterations and the computational time (sec) for a typical run with Reynolds number $Re = 60$, and the number of space intervals $= 40$.

$$\Delta t_{\frac{1}{4}} \text{ is equal to } \frac{Ax^2Re}{4} \text{ and } \Delta t_{\frac{3}{4}} = \Delta x,$$

with three intermediate steps in between. Schemes 1 through 5 correspond to the Brailovskaya, Dufort-Frankel, Cheng-Allen, Crank-Nicolson and Lax-Wendroff schemes. The number of iterations for the Crank-Nicolson scheme is not given, because the Crank-Nicolson scheme is implicit with an intermediate iteration step involved between two successive time steps. This, in effect, is tantamount to altering the scale of the time step, and hence a meaningful comparison cannot be made.

The table shows that the Dufort-Frankel scheme requires the least number of iterations for convergence, and also that the computational time is minimum in this case. This is because the Dufort-Frankel scheme is
FIGURE 5. INFLUENCE OF HIGH REYNOLDS NUMBER
RE = 1000  DT = 0.01  DX = 1/50
THE LAX–WENDROFF SCHEME IS THE BEST SCHEME

FIGURE 6. INFLUENCE OF SPACE STEP SIZE
CHENG–ALLEN SCHEME
RE = 60  DT = DX^2 RE/4
DX = 1/10, 1/20, 1/40 AND 1/50
<table>
<thead>
<tr>
<th>Scheme</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
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<tr>
<td>$\Delta t_1$</td>
<td>129</td>
<td>116</td>
<td>134</td>
<td></td>
<td>121</td>
</tr>
<tr>
<td>$\Delta t_2$</td>
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<td>81</td>
<td>103</td>
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<tr>
<td>$\Delta t_3$</td>
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<td>86</td>
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<tr>
<td>$\Delta t_4$</td>
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<td>75</td>
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<td>N.C.</td>
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<tr>
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<td>N.C.</td>
<td>37</td>
<td>68</td>
<td></td>
<td>N.C.</td>
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</tbody>
</table>

<table>
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<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t_1$</td>
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<td>13</td>
<td>20</td>
<td>59</td>
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<tr>
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<tr>
<td>$\Delta t_5$</td>
<td>N.C.</td>
<td>4</td>
<td>10</td>
<td>26</td>
<td>N.C.</td>
</tr>
</tbody>
</table>

$Re = 60$, $\Delta x = 1/40$

1 = BRLA
2 = DUFL
3 = CH-AL
4 = CR-NL
5 = LAX-WENDROFF
N.C. = DID NOT CONVERGE
<table>
<thead>
<tr>
<th>Space Increment - $\Delta x$</th>
<th>Computing time, sec.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/10</td>
<td>1.0</td>
</tr>
<tr>
<td>1/20</td>
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</tr>
<tr>
<td>1/50</td>
<td>29.0</td>
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</table>
a one step scheme and, therefore, requires a minimum number of arithmetic operations for the calculation of a mesh point. From the table it is also seen that the Crank-Nicolson scheme requires the longest computational time. At larger values of the time step, the Brailovskaya and Lax-Wendroff scheme do not converge. They therefore require strict enforcement of the stability criterion.

6.2 Effect of Space Increment on Accuracy and Resolution

Since truncation errors constitute the major source of inaccuracies, reducing the mesh size by reducing the space and time increments should result in an improvement in accuracy. Figure 6 shows the solution computed with the Cheng-Allen scheme with the space increment varying from 1/10 to 1/50.

With $\Delta x = 1/10$ the solution is found to be quite poor and the final solution inaccurate. With $\Delta x = 1/20$ (the curve above that for $\Delta x = 1/10$), there is a substantial improvement in accuracy. However, with a further reduction in $\Delta x$ to 1/30, 1/40 and 1/50, there is no discernable improvement. Thus there is an optimum $\Delta x$, beyond which, if the space increment is reduced, there is nothing to be gained either in accuracy or resolution.

A comparison of the computational times for satisfying the same convergence criterion is given in Table II. It shows that for $\Delta x = 1/10$ convergence is extremely rapid, but the figure shows the resolution is unsatisfactory. For $\Delta x = 1/30$, the accuracy is as good as for $\Delta x = 1/50$, but the computing time for reaching the steady state is only one-fifth of the computational time at $\Delta x = 1/50$.

Therefore for any given problem an optimum mesh size should be selected which gives the best resolution at a maximum saving of computational time.

6.3 The Influence of the Time Step

Tests with the selected schemes show that the size of the time step is governed mainly by stability considerations. It is found that for a given increment, the use of a smaller time step does not increase the overall
accuracy of the steady state solution. See Figure 7. The important criterion is that the size of the time step in obtaining the asymptotic steady state solution should be such as to yield a convergent solution. Some schemes like the Cheng-Allen scheme permit the use of time steps in excess of the time increment demanded by stability criteria. For other schemes, like the Brailovskaya and Lax-Wendroff schemes, the time increment should be well below the theoretical stability limit for convergence.

In obtaining the asymptotic, steady state solution, the cumulative effect of errors must be considered. For example, if two different time increments \( \Delta t_1 \) and \( \Delta t_2 \) are used such that \( \Delta t_2 = 2\Delta t_1 \), it is found that the mean square difference of the computed solution from the true solution changes by about 0.0001. Since the total time \( T \) to attain the steady state solution is constant, the number of iterations in time \( N_2 \sim N_1/2 \). The cumulative Fourier components of the error function over \( N_2 \sim N_1/2 \) iterations is less than over \( N_1 \) iterations. But the amplitudes are larger over \( N_2 \) iterations than with \( N_1 \) iterations. These two factors tend to even out, producing the same overall error with \( N_2 \) iterations with large \( \Delta t \) as with \( N_1 \) iterations with small \( \Delta t \).

In actual practice it would therefore be advisable to select as large a time step as permissible to obtain good resolution while ensuring stability of computation.

6.4 Boundary Conditions

Figures 8 and 9 show solutions obtained with boundary conditions I and II respectively under identical run conditions, and Table III shows the number of iterations and computational times for reaching the steady state also under identical, but different run conditions. When the boundary conditions are such that a discontinuity exists at one boundary, the number of iterations and computational time are both higher. This is due to the fact that with B.C.1, the effects of the discontinuity at the center are compensated by positive and negative effects on either side, while with B.C.2, the effects of the one-sided differencing across the discontinuity take longer to be damped out.
FIGURE 7. INFLUENCE OF TIME STEP. CHENG–ALLEN SCHEME

$RE = 60 \quad DX = 1/30 \quad DT = DX$ AND $DT = DX^2 RE/4$
FIGURES 8 AND 9. INFLUENCE OF DIFFERENT BOUNDARY CONDITIONS ON EXPPLICIT SCHEMES

$RE = 60 \quad DX = 1/30 \quad DT = DX^2 \frac{RE}{4}$
### Table III

#### Number of Iterations

<table>
<thead>
<tr>
<th>Scheme</th>
<th>B.C.1</th>
<th>B.C.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>65</td>
<td>96</td>
</tr>
<tr>
<td>2</td>
<td>52</td>
<td>76</td>
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<td>3</td>
<td>63</td>
<td>90</td>
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<tr>
<td>5</td>
<td>58</td>
<td>86</td>
</tr>
</tbody>
</table>

#### Computing Time

<table>
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<th>Scheme</th>
<th>B.C.1</th>
<th>B.C.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>4</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>5</td>
</tr>
</tbody>
</table>

- \( \text{Re} = 40 \)
- \( \text{Dx} = 1/20 \)
- \( \Delta t = \Delta x^2 \text{Re}/4 \)

6.5 **Formulation of the Boundary Conditions**

The calculation of the first mesh point next to the prescribed boundary requires some additional information. In actual calculations the boundary points present the greatest difficulty. The results of the numerical experiments with the Burgers equation stress the importance of the correct formulation of the boundary conditions in a way that is as close to physical reality as possible.

Tests were conducted with different formulations for calculating the point immediately next to the boundary with schemes 1, 2 and 3, namely
the Brailovskaya, Dufort-Frankel and Cheng-Allen schemes. The Brailovskaya and Cheng-Allen schemes need one extra point beyond the boundary if the formulation for the other interior points and for the point next to the boundary is to be the same.

\[
\begin{array}{c}
F \quad E \quad D \quad G \\
A \quad B \quad C \\
x_1 \quad x_2
\end{array}
\]

FIGURE 10

The most common procedure in practice under these conditions is to assume reflection conditions at the boundary, i.e. to stipulate that the values of C and A in Figure 10 are the same. This arbitrary specification of values leads to inaccuracies and longer computational times.

Table IV compares the number of iterations and computational times for the Brailovskaya and Cheng-Allen schemes for two different formulations of the same boundary conditions given by Set I. In formulation 1 reflection conditions are assumed as shown in Figure 10. Formulation 2 is arrived at in a more physically realistic way.

Since the Burgers equation is analogous to the momentum conservation equation, the finite difference scheme for the cell adjacent to the boundary is derived from the integral formulation applied to this cell. Thus

\[
\frac{\partial}{\partial t} \int_{x_1}^{x_2} u \, dx + \frac{1}{2} \int_{x_1}^{x_2} \frac{\partial (u^2/2)}{\partial x} \, dx = \frac{1}{\text{Re}} \int_{x_1}^{x_2} \frac{\partial^2 u}{\partial x^2} \, dx
\]

Table IV

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Formulation 1</th>
<th>Formulation 2</th>
<th>Computing Time</th>
</tr>
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<tr>
<td>1</td>
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<td>37</td>
<td>13</td>
</tr>
<tr>
<td>3</td>
<td>44</td>
<td>38</td>
<td>4</td>
</tr>
</tbody>
</table>

\[\text{Re} = 40\]
\[\text{Dx} = 1/20\]
\[\text{Dt} = 0.01\]
The calculations show that convergence is more rapid and accurate with formulation 2 than with formulation 1. Hence in actual calculations the boundary conditions should be formulated in such a way as to represent the physical boundary conditions as closely as possible without introducing extraneous numerical errors from extrapolation formulae [19].

6.6 Perturbation of Boundary Conditions

To study the influence of arbitrary perturbations in boundary conditions, such as would be the case where unwanted and undetected errors crept into an actual computation at the boundary, tests were run where an error of +0.001 was introduced at the left boundary, and an error of -0.001 was introduced at the right boundary with boundary condition I, at every 10th point on the time axis. No convergence was obtained with any of the schemes when the perturbation was introduced at every 5th point. With the boundary values perturbed at every tenth point convergence was obtained at low values of the time increment with all the schemes, except the Dufort-Frankel scheme, Table V. As the time increment was increased, the Cheng-Allen and Crank-Nicolson schemes retained their stability while the Brailovskaya and Lax-Wendroff schemes became unstable.

6.7 The Convergence Criterion and Convergence Rates

Two convergence norms were monitored during the calculations namely

$$\max_j |u_j^n - u_j^m|$$

and

$$\sum_j [ (u_j^{n+1})^2 - (u_j^n)^2 ]$$

Figure 11 shows how the mean square difference between successive time iterations varies as a function of real time plotted on the x axis. It is seen that the curve consists of two sections— an initial segment where the
Table V

Boundary Values Perturbed at Every Tenth Point

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Number of Iterations</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Δt₁</td>
<td></td>
<td>129</td>
<td>unstable</td>
<td>136</td>
<td>127</td>
<td></td>
</tr>
<tr>
<td>Δt₂</td>
<td></td>
<td>97</td>
<td>&quot;</td>
<td>107</td>
<td>unstable</td>
<td></td>
</tr>
<tr>
<td>Δt₃</td>
<td></td>
<td>unstable</td>
<td>&quot;</td>
<td>88</td>
<td>&quot;</td>
<td></td>
</tr>
<tr>
<td>Δt₄</td>
<td></td>
<td>&quot;</td>
<td>&quot;</td>
<td>78</td>
<td>&quot;</td>
<td></td>
</tr>
<tr>
<td>Δt₅</td>
<td></td>
<td>&quot;</td>
<td>&quot;</td>
<td>69</td>
<td>&quot;</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Computing Time (sec)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Δt₁</td>
<td></td>
<td>29</td>
<td>unstable</td>
<td>20</td>
<td>59</td>
<td>16</td>
</tr>
<tr>
<td>Δt₂</td>
<td></td>
<td>22</td>
<td>&quot;</td>
<td>16</td>
<td>45</td>
<td>unstable</td>
</tr>
<tr>
<td>Δt₃</td>
<td></td>
<td>unstable</td>
<td>&quot;</td>
<td>13</td>
<td>38</td>
<td>&quot;</td>
</tr>
<tr>
<td>Δt₄</td>
<td></td>
<td>&quot;</td>
<td>&quot;</td>
<td>12</td>
<td>32</td>
<td>&quot;</td>
</tr>
<tr>
<td>Δt₅</td>
<td></td>
<td>&quot;</td>
<td>&quot;</td>
<td>10</td>
<td>26</td>
<td>&quot;</td>
</tr>
</tbody>
</table>
mean square difference remains almost steady and is of the order of 0.1 and a second segment where the curve dips downward until it finally attains a value of order $10^{-6}$. These two sections of the curve depict two different stages in the evolution of a convergent, asymptotic, steady-state solution from a given initial solution.

During the early part of the calculation, the time dependent solution is tending towards the steady state solution at a rapid rate. In fact, it is desirable to have this segment of the curve rise rapidly if one is interested in the final steady state solution alone. This would ensure a fast rate of convergence. If the study of the temporal development of the flow is the object of the calculation, it would then be preferable to have this part of the curve drop gradually all the way.

The second segment of the curve in Figure 11 shows a uniform drop to a low value. This portion of the curve is significant from a stability viewpoint. The solution becomes unstable unless the mean square difference tends to zero. Figure 12 shows the variation of the mean square difference in a divergent situation. It is seen that although the curve remains flat for a major part of the time, it finally yields increasing values of the mean square difference at the long time limit, thus leading to a non-converging solution.

Figure 13 shows the effect of the space increment on convergence rates. The space increment decreases from 1/10 through 1/20, 1/40 and 1/50 as the curves progress toward the right. With $\Delta x = 1/10$, the initial segment of the curve rises sharply and falls steeply to yield a high convergence rate. A similar trend is observed for $\Delta x = 1/20, 1/40$ and 1/50 although the convergence rate is less rapid. The fast convergence rates of the Cheng-Allen scheme render it suitable for computing the asymptotic steady state solution without great attention to temporal resolution, while the Dufort-Frankel scheme focuses on the temporal evolution of the final solution. Further the Dufort-Frankel scheme is second order accurate in time, while the Cheng-Allen scheme is only first order accurate.
FIGURE 11. DUFORT-FRANKEL SCHEME
RE=50  DX=1/20  DT=0.02

FIGURE 12. BRAILOVSKAYA SCHEME
RE=30  DX=30  DT=0.02

FIGURE 11 AND 12. R.M.S. DIFFERENCE BETWEEN SUCCESSIVE ITERATIONS PLOTTED AGAINST TIME TO SHOW THE CONVERGENCE CHARACTERISTICS OF DIFFERENT SCHEMES
FIGURE 13. INFLUENCE OF SPACE STEP INCREMENT ON CONVERGENCE CHARACTERISTICS. CHENG–ALLEN SCHEME
RE = 60  DT = DX^2 * RE / 4  DX = 1/10, 1/20, 1/40 AND 1/50
Figure 14 shows the value

$$(u_j^n - u_j^n)$$

i.e., the difference between the true and computed solutions plotted along the y axis for B.C.I. The solution is quite good, except at the discontinuity where large gradients exist. This leads to large values for the derivatives

$$\frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}, \frac{\partial^3 u}{\partial x^3}$$

at the discontinuity. The influence of this is discussed in the next section.

6.8. Influence of Reynolds Number

Figure 15 shows the steady state solutions for B.C.I for Reynolds numbers ranging from 20 to 200, calculated with the Dufort-Frankel scheme. Similar calculations for B.C.II obtained with the Brailovskaya scheme are shown in Figure 16. In either figure the curves with the discontinuity spread out over the largest number of meshes correspond to the lowest value of the Reynolds number. As the Reynolds number increases, the discontinuity thickness becomes smaller and smaller. However, as the discontinuity becomes sharper, wiggles form at the transition as shown in Figure 15 for Re = 200. This oscillation at the discontinuity is caused by the phenomenon mentioned at the end of the last section. With an increase in Reynolds number, the discontinuity becomes stronger, with the result that the gradients

$$\frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}, \frac{\partial^3 u}{\partial x^3}$$

increase in magnitude. Since we are differencing across the discontinuity without making any special provision for it, the truncation errors which are
FIGURE 14. DIFFERENCE BETWEEN TRUE AND COMPUTED STEADY STATE SOLUTION. BRAILOVSKAYA SCHEME. 
$DX = 1/20, \ DT = 0.02, \ RE = 50.$
FIGURE 15. DUFOURT–FRANKEL SCHEME
\[ \text{RE} = 20, 40, 60, 100, 200 \]
\[ \text{DX} = 1/30 \quad \text{DT} = \text{DX}^2 \text{RE}/4 \]

FIGURE 16. BRAIOVSKAYA SCHEME
\[ \text{RE} = 10, 20, 40, 60 \]
\[ \text{DX} = 1/20 \quad \text{DT} = \text{DX}^2 \text{RE}/4 \]

FIGURES 15 AND 16 SHOW THE INFLUENCE OF REYNOLDS NUMBER ON THE COMPUTED SOLUTION.
proportional to these derivatives become significant at the discontinuity, leading to the formation of wiggles. This is verified in Figure 17 which is the same case as Figure 16 but with $\Delta x = 1/50$ instead of $\Delta x = 1/30$. No waviness appears at the discontinuity at $Re = 200$ because of reduced truncation errors, even though we are differencing across a discontinuity.

Conclusions

Tests with the non-linear Burgers equation have illustrated a number of important aspects of the finite difference solution of partial differential equations. Comparison was made between explicit and implicit schemes, and also between one-step and two-step schemes. The tests show that the Dufort-Frankel one-step scheme and the Cheng-Allen two-step scheme both possess definite advantages compared to the other schemes, namely the Brailovskaya, Crank-Nicolson and Lax-Wendroff schemes. The Cheng-Allen scheme possesses the best stability properties when the boundary conditions are perturbed. This allows the use of a large time step. The Dufort-Frankel scheme possesses good temporal resolution, and, in addition, is only a one-step scheme. It requires the shortest computing time while providing results which compare with the Cheng-Allen scheme in accuracy.

The size of the space increment is governed mainly by how good the resolution should be. The use of as large a space increment as possible for the kind of resolution required is recommended. This results in a lower number of mesh points and also permits the use of a larger time step. Discontinuities in the flow must be properly treated and boundary conditions must be as close to physical reality as possible for meaningful results. The use of a large time step results in much saving in computational time. For any one problem an optimum balance among all these factors must be struck.
FIGURE 17. INTERACTION OF SPACE STEP SIZE AND REYNOLDS NUMBER EFFECTS.
RUN CONDITIONS SAME AS FIGURE 15, EXCEPT DX = 1/50 INSTEAD OF 1/30.
Application to Parallel Processing Machines

The Cheng-Allen scheme requires data from five points at time level n for the calculations of one point at time level (n+1) if the calculations are made at one pass. However, by calculating all the intermediate quantities at one pass, and then computing the required final values at time level (n+1) at the second pass through the arithmetic units, the calculation of a point at level (n+1) would always require only three values stored at different locations at time level n. The Dufort-Frankel scheme requires fewer arithmetic operations, resulting in a saving in computational time especially in three dimensional problems. Should storage space be at a premium, the values at time level (n+1) can be calculated at one pass from stored values. Thus both the Cheng-Allen and Dufort-Frankel schemes possess desirable characteristics.
REFERENCES


NUMERICAL SOLUTION OF THE PARTIAL DIFFERENTIAL EQUATIONS OF GAS DYNAMICS

S. Rajan

November 5, 1971

DAHC04 72-C-0001

ARPA Order No. 1899

CAC Document No. 20

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None

U. S. Army Research Office-Durham
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Durham, North Carolina

In this report the relevant, practical criteria required for the numerical calculation of different types of gas dynamic flow fields are discussed. A classification for finite difference schemes is given. Numerical experiments are conducted on the non-linear Burger's equation using the Brailovskaya, Cheng-Allen, Dufort-Frankel, Crank-Nicolson and Lax-Wendnoff finite difference schemes as typical examples of different classes of finite differences schemes. The effect of time and space increments, types of boundary conditions, pertubations at the boundaries, truncation errors, convergence criteria and convergence rates are studied. It is shown that both the cheng-Allen and Dufort-Frankel schemes have individual merits in different types of application.
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