# Numerical Integration of Navier-Stokes Equations

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## I. Introduction

THERE is extensive literature on the numerical integration of some difference forms of the Navier-Stokes equations. The references quoted herein are those relevant to later discussions and not intended to be complete. There is also extensive literature on the mathematics of difference methods for the solution of partial differential equations for which Ref. 1 is a comprehensive review and contains an extensive bibliography. The present paper is an attempt to develop the implications of a mathematical theorem, which, when put into proper perspective, offers a unified and coherent treatment of various practical aspects of computation.

Like approximate differential analyses and physical tests, numerical methods are fallible. Larger and faster computers offer no easy answer to computational difficulties like stability and convergence. Smooth and physically reasonable results of computation are often less accurate than those not so smooth. Since the true asymptotic nature is difficult to establish, both the difference and the differential approximations are nonrigorous; but they are useful, especially with the help of physical experimentation and rigorous mathematical results. We are sympathetic to such heuristic and nonrigorous analysis in favor of obtaining results useful in practice.

We shall consider only the difference form of the Navier-Stokes equations in Eulerian coordinates. Lagrangian coordinates are convenient for flows involving free-surface boundary or active processes associated with fluid elements. It suffers, however, from the serious distortions of the Lagrangian net and from the cummulative errors of the particle paths at large times. Thus various mixed or coupled Eulerian-Lagrangian schemes have been developed even for free boundary problems. Eulerian formulation, even for a single fluid in the absence of a free boundary, has its share of problems, which we shall discuss. We write, for the Navier-Stokes equations,

$$\begin{aligned} \partial\rho/\partial t + (\partial/\partial x_j)(\rho u_j) &= 0 \\ \partial(\rho u_i)/\partial t + (\partial/\partial x_j)(\rho u_i u_j + p\delta_{ij} - \tau_{ij}) &= 0 \\ \partial(\rho e)/\partial t + (\partial/\partial x_j)[\rho u_j(e + u_i u_i/2) + p u_j - u_i\tau_{ij}] &= 0 \end{aligned} \qquad (1)$$

They express the conservation of mass, momentum, and energy through the divergence of the fluxes of the respective quantities. Here $p$, $\rho$ and $e$ are the pressure, density and internal energy of the fluid with some algebraic equations of state $p = f(\rho,e)$. $\tau_{ij}$ is the Navier-Stokes stress tensor, linearly expressed in terms of the rate of strain of the fluid. It is posed as an initial value problem for $0 \leq t \leq T$ in a bounded domain of $x$ with appropriate boundary conditions.

If all $\partial/\partial t$ terms vanish in the limit of large times, the solution reaches a steady limit. Such a procedure of obtaining steady-state solution from time-dependent calculation[2-4] is sometimes referred to as "asymptotic method."[5] In the temporal approach a steady-state limit is not presumed and will not necessarily follow. Except for the errors and the limitations introduced by the solution and the formulation of the difference problem, this long time limit represents the physical situation more naturally than the solution of the steady state equation obtained formally from Eq. (1) by dropping all terms involving $\partial/\partial t$. If the physical flow is truly "steady," the long time limit of the temporal solution must be insensitive to reasonable variance of initial conditions and to reasonable disturbances of various forms and magnitudes in the transient stage, and should agree with the solution of the steady state equation.

Computationally, the solution of the temporal system is more convenient especially for flows in multispace dimensions.[5] The steady-state formulation generally requires the use of implicit difference schemes to be solved by various iterative methods.[5,6,etc.] The successive iterations may be looked upon as the evolution of the solution in some temporal sense. For certain simple difference schemes applied to simple equations, the correspondence can be precisely established. The fictitious temporal terms so introduced need not be in the same form as those given by Eq. (1). They may be introduced as artificial devices[4] in the form of transient forces or mass and energy sources and dipoles, etc., to improve computational stability or rate of convergence or to facilitate the computation in general without affecting the long time limit and the true steady-state solution.

To study the temporal development of a flowfield one must represent the temporal terms by a consistent difference formulation using a reasonable temporal and spatial resolution. The high wave number components of turbulent fluctuations cannot be represented with sufficient resolution.

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Presented as Paper 70-2 at the AIAA 8th Aerospace Sciences Meeting, New York, January 19–21, 1970; submitted March 6, 1970; revision received August 31, 1970. This research was sponsored by the U.S. Air Force Office of Aerospace Research under contract number AF-33-615-67-C-1065. The author wishes to thank the reviewers and other friends who offered their helpful criticisms and suggestions in the preparation of this revised manuscript.

It is doubtful that turbulence can be studied fruitfully with the difference methods discussed herein. For other difficult problems of fluid dynamics, numerical methods hold great promise especially when used along with asymptotic differential analysis and physical experimentation.

The mathematical theory of linear partial difference equations is rigorous and fairly complete. For quasi-linear equations which we encounter in fluid dynamics, the treatment is largely heuristic.[1] The local linearized stability analysis of v. Neumann is the only practical guide.[1] The convergence proofs of some difference forms for certain incompressible flows with periodic boundaries[7,8] for example, may be extended to other boundary value problems of practical interest.* We are more interested here in practical guidance.

It is not certain whether the "equivalence" between a given difference formulation and some differential formulation could be established mathematically for quasi-linear equations under conditions more restrictive than those required to establish such an equivalence between linear equations. However, if it should, the set of more restrictive conditions is expected to contain those required to establish the equivalence between the linear systems. Hence, we shall examine the conditions of stability, consistency, well-posedness and convergence in the sense of Lax's Equivalent Theorem as applied to the quasi-linear equations with the hope that some of the necessary consequences will provide us with some practical guidance.

To mathematicians, the investigation of the necessary consequences of an unproven extension of a theorem is indeed "awkward." The applied scientists, however, will not hesitate to derive benefit from such an approach with due care in interpreting the results, since our primary interest is to obtain approximate descriptions of a physical problem, not the solution of a specific mathematical equation.

For a given physical problem, a difference formulation is often derived from some well known differential formulation following some process of discretization, which, for boundary value problems, goes beyond the formal replacement of a derivative by the corresponding difference quotient. Since computational stability is usually obtained with much hard work, it is natural to postpone the question whether and to what extent an apparently smooth and physically reasonable solution from a stable computation does represent the solution of the physical problem. This question is crucial nevertheless. It is not just the question of convergence and the question of how well the computed results approximate the limit. There is also the question of how well the limit approximates the solution of the physical problem.

A direct mathematical approach to these problems, by analyzing the grid functions in the difference formulation is difficult because they are defined only at discrete points and cannot be differentiated in the usual sense. The postulate of equivalence between a difference formulation and certain differential formulation is particularly convenient because then we will not be forced to consider the grid functions and transform the problem into ground familiar to fluid dynamicists.

The "equivalence" between a difference and a differential formulation in the sense of Lax's theorem[1,9] for linear equations is more than a simple statement of convergence and needs much clarification even without attempting mathematical rigor. The result of computation based on a difference formulation will "converge" to the solution of the differential formulation if and only if a) the differential problem is "well-posed" and therefore posseses a genuine solution; b) the difference and the differential formulations are "consistent"; and c) the computation is "stable."

Now if the differential problem is ill-posed, its "solution" is either unbounded or indefinite. If a difference approximation should provide solutions converging to such a "solution," the computation must diverge or oscillate wildly. There is no hope of achieving stable computation in the strict sense. Even if the stability criterion is extended to include exponentially diverging solutions, the computed diverging results would not be meaningful since we cannot distinguish physical instability from numerical instability. Where the nature of physical instability is clear, we may introduce the proper physical factors to make the problem well-posed. For example, by adding surface tension in determining the growth of interfacial waves in Taylor Instability (see Ref. 1, p. 138). For most multidimensional flow problems, it is often not clear whether a problem is properly posed and we just try to achieve a stable computation.

The "convergence" is in some mean square sense where large or even unbounded local deviations are tolerated if the sum or integral of some kind of mean square or absolute deviation vanishes in the limit. This notion of convergence is similar to that of global asymptotic approximation, like inviscid approximation at small viscosities, familiar to fluid dynamicists. We should expect substantial local deviations and can only attempt to limit such large deviations from interfering with the main result rather than to suppress or avoid them completely.

The "consistency" between the difference and the differential formulation is required only in the limit of $\Delta t$ and $\Delta x \to 0$ in some manner subject to the stability restrictions in the form of inequality. For a given difference equation, the limiting form of the consistent differential equation can and will depend on the manner how the limit is taken. A well-known example (see Ref. 1, p. 176) is the DuFort-Frankel approximation to the simple diffusion equation. It is consistent with a wave equation with wavespeed depending on the ratio $\Delta t/\Delta x$ but is consistent with the diffusion equation if $\Delta t/\Delta x = 0(\Delta x)$ is maintained in the limit. This is not a singular example. What then is the limit of the "solution" which we obtain from a stable computation at some finite $\Delta t$ and $\Delta x$, not to mention how good is the computed result as an approximation to the physical problem? Moreover, it is debatable although initially suggested[9] to drop formally all the terms involving $\Delta t$ or $\Delta x$ and to claim the consistency between the difference and the differential operators so obtained, since higher-order derivatives can become large in the limit. On the other hand, if some of the higher-order terms should be kept, what is the rationale of such a stratagem?

The "consistency" requirements include also the location of the boundary and the specification of the boundary values or operators. Most of the physical problems of interest are boundary value problems. We often tolerate approximations in differential equations but maintain accurate boundary conditions to obtain physical approximations. It is doubtfully appropriate in the difference formulation of a physical problem to elaborate on the difference algorithm without paying due attention to the formulation on the boundaries. We are especially susceptible to such artifices of modifying the boundary operators when it appears to be a cause of computational instability and offer a possible quick remedy.

These questions will be pursued further with simple model equations through the investigation of the various restrictive conditions of "convergence" in the sense of the Lax Equivalence Theorem. The significance of the various inferences from this study, as applied to the Navier-Stokes equations of fluid dynamics, will then be illustrated.

## II. Pseudo-Diffusivity of Difference Approximation

### Linear Local Stability Criterion

For linear problems with constant coefficients, computational stability for the interior points (i.e., neglect the effect of boundary) can be analyzed with the stability analysis of v.

* Note added in Proof: A. Chorin informed the author that such an extension was completed very recently.

Neumann (see Ref. 1, p. 70), which considers the growth factor $g$ of a single Fourier component $e^{ikx}$ of small disturbances of wave number $k$. If there is only a scalar dependent variable, the condition of $|g| \leq 1$ is both sufficient and necessary for stability. The extended definition of computational stability which allows $|g| \leq 1 + 0(\Delta t)$ will not be adopted because of the previously mentioned difficulty in distinguishing physical and computational instability and because of our intention to take the large time limit so as to obtain steady state solutions. For the solution of a vector unknown governed by a system of linear partial differential equations with constant coefficients, the growth factor $g$ becomes an amplification matrix $G$. The stability condition $\|GG^*\| \leq 1$ based on some mean square norm is only necessary where $G^*$ is the Hermitian conjugate of $G$. It is sufficient only when $G$ is a normal matrix.

For the simple wave equation,

$$\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)u = 0 \tag{2}$$

the v. Neumann limit leads to $r = |c(\Delta t/\Delta x)| \leq 1$, where $c$ is the wave speed. This condition means that the zone of dependence of the difference formulation must include the zone of dependence of the differential problem. This is the Courant-Friedrichs-Lewy Condition (CFL)[10] to be observed for all hyperbolic systems. For the simple diffusion equation

$$(\partial/\partial t - \nu\partial^2/\partial x^2)u = 0 \tag{3}$$

with diffusivity $\nu$ the v. Neumann limit often takes the form $s = \nu(\Delta t/\Delta x^2) \leq \alpha$ where $\alpha$ is some constant like $\frac{1}{2}$. Most implicit schemes are always stable. A difference scheme that is stable for the diffusion equation is often unstable for the wave equation and vice versa. For the linearized Burgers' equation obtained by superposing Eqs. (2) and (3),

$$(\partial/\partial t + c\partial/\partial x - \nu\partial^2/\partial x^2)u = 0 \tag{4}$$

it was suggested (Ref. 1, p. 195) that the effect of lower-order term $c\partial/\partial x$ is not important, a statement justifiable only for certain difference schemes in view of the conflicting stability requirements of the simple wave and the simple diffusion equations.

When the wave speed $c$ is replaced by $u$ and/or the diffusivity becomes a function of $u$, Eq. (4) becomes quasi-linear. Heuristically, if the instantaneous and the local values of $u$ are taken in evaluating the v. Neumann limit and if the most restrictive of these limits over the entire field of computation are taken at any instant in determining $\Delta t$, we would expect the computation to be stable. Tests with equations

$$\partial u/\partial t + u\partial u/\partial x = 0,\ \partial u/\partial t - (\partial^2/\partial x^2)(u^5) = 0 \tag{5}$$

have demonstrated that computational stability is indeed achieved. Since the limit depends on the solution $u$ as time evolves, the check of the stability condition and the choice of $\Delta t$ are repeated every few time steps.

The procedure just described is generally adopted, only that the Navier-Stokes equations are too complicated to yield a simple linearized local stability criterion to be tested over every point in the field of computation every few time steps. Accordingly the hyperbolic stability limit of the form $\Delta t < \Delta x/(|q| + |c|)$ is determined with diffusive terms neglected; and the diffusive stability limit of the form $\Delta t < \alpha(\Delta x)^2/\nu$ is obtained with convective terms neglected. The more restrictive of the two is taken as the stability limit of the system. It often fails even with an added factor of safety. Then, the boundary conditions or the difference scheme or both will be modified. The difficulties arise from various sources. One of them is that the superposition of the diffusion and the convective terms often yields more restrictive stability limit. If Eq. (4) is discretized with forward time, backward space difference for the convective term, and the centered space difference for the diffusion term, the v. Neumann stability limit is

$$\Delta t \leq (c/\Delta x + 2\nu/\Delta x^2)^{-1} \leq \text{Inf}\ [\Delta x/c, \tfrac{1}{2}\Delta x^2/\nu] \tag{6}$$

which is almost half the hyperbolic limit or the diffusion limit if they are nearly equal. When Eq. (4) is extended to two space dimensions as

$$\partial u/\partial t + c(\partial u/\partial x + \partial u/\partial y) = \nu(\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2) \tag{7a}$$

or

$$\partial u/\partial t + c\partial u/\partial x = \nu(\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2) \tag{7b}$$

we would have

$$\Delta t \leq \tfrac{1}{2}(c/\Delta x + 2\nu/\Delta x^2)^{-1} \tag{8a}$$

or

$$\Delta t \leq (c/\Delta x + 4\nu/\Delta x^2)^{-1} \tag{8b}$$

Here $c$ may be replaced by $|q| + |c|$ when applied to compressible flow problems. Some experiments demonstrated their usefulness with the nonlinear Burgers' and the Navier-Stokes equations.

The v. Neumann limit and most of the other stability criteria[1] are applicable only for interior points. Stable difference schemes in the sense of v. Neumann limit often leads to unstable computations under the "boundary effects." Sufficient stability criteria including the boundary effects can sometimes be obtained through the "energy analysis,"[1] but it is generally difficult even for simple difference equations. The v. Neumann analysis remains the most important practical guide (Ref. 1, p. 90). In fact, even the v. Neumann analysis is too complicated for the Navier-Stokes system; and there are other practical reasons that call for modifications of difference algorithms to suit particular problems. Simpler guidance, although less general, will be helpful especially if it appeals to physical intuition.

### Pseudo-Diffusivity

In the calculation of an inviscid shock at an unknown location, v. Neumann and Richtmeyer[11] added a viscous dynamic term $1^2(\partial u/\partial x)^2$ with $1 = a\Delta x$ into the inviscid equations before discretization to avoid tedious shock fitting. It also helps in achieving a stable computation and a smooth solution. The artificial viscous term so introduced is often of $0(\Delta x)$ to be effective. Alternatively, the formal expansion of the difference quotients into Taylor series often gives terms involving $\partial^2 u/\partial x^2$ and the like. The coefficients generally of $0(\Delta x)$ were referred[12,13] to as numerical viscosity. The former is a deliberate modification of the differential equation. The latter is implied in the difference approximation according to the formal interpretation. Although of different origin, they appear to play the same role in affecting computational stability. We shall examine first the notion of pseudo-diffusivity as to its ad hoc or heuristic content before demonstrating its usefulness in matters of practical computation.

Let $U_j^n$ be the grid function $U(n\Delta t, j\Delta x)$ obtained from a stable computation following a given difference formulation. Let $u(t,x)$ be the limit of $U_j^n$ when $\Delta t$ and $\Delta x$ approach zero in appropriate manners assuming convergence in the mean. Let $u_j^n$ represent $u(n\Delta t, j\Delta x)$ at the grid point $(n,j)$. The function $u(t,x)$ is the solution of a partial differential equation subject to the initial and the boundary conditions "consistent" with the difference formulation over the domain of computation in the appropriate limit. This function $u(t,x)$ is differentiable and expandable about any point $(n,j)$ in the domain. In what follows we shall illustrate the principle with the simple wave Eq. (2) rather than the Navier-Stokes Eqs. (1).

The equivalence between a difference and a differential formulation implies taking the limit of $\Delta t$ and $\Delta x$ approaching

zero in some manner under the restraint in the form of some inequality because of the consideration of computational stability. The limit must be taken along some specified path in the $t$-$x$ plane. Hence we shall not treat $t$ as an independent variable and for the simple wave Eq. (2), take $r = \Delta t/\Delta x =$ constant in taking the limit. A difference equation, $L_\Delta(U) = \Sigma a_{nj} U_j^n = 0$ as an approximation to the differential Eq. (2), $L(u) = (\partial/\partial t + c\partial/\partial x)u = 0$, can be expanded into Taylor series when $U_j^n$ is replaced by $u_j^n$ with leading terms identified as $(\partial/\partial t + c\partial/\partial x)u$ and the "higher-order small terms" involving $\partial^2/\partial t^2$, $\partial^3/\partial t^3$ . . . along with $\partial^2/\partial x^2$, $\partial^3/\partial x^3$ . . . etc. Those temporal derivatives will be eliminated in succession with *the successive differential approximations to the difference equation*. Thus we arrive at a differential equation of the form

$$(\partial u/\partial t + c\partial u/\partial x) - \nu_e \partial^2 u/\partial x^2 + \alpha_1 \partial^3 u/\partial x^3 + \beta_2 \partial^4 u/\partial x^4 + \alpha_3 \partial^5 u/\partial x^5 - \beta_4 \partial^6 u/\partial x^6 + \ldots = 0 \quad (9)$$

where

$$\nu_e = 0(\Delta x),\ \beta_{2j} = 0(\Delta x)^{2j+1},\ \alpha_{2j-1} = 0(\Delta x)^{2j}$$

Here $\nu_e$ is the pseudo- or numerical viscosity. If in the limit of $\Delta x \to 0$, none of the higher-order derivatives should become large, we would have the desired limit $L(u) = (\partial/\partial t + c\partial/\partial x)u$.

Now "convergence in the mean" does permit finite size deviations over mesh sizes of $0(\Delta x)$. As $\Delta x \to 0$, the derivatives of $\partial/\partial x$ will become large. Neither can we visualize how such mesh to mesh deviations in computed results would disappear in the limit. Short of dealing exclusively with the difference equation, can we benefit from conventional asymptotic approximations to Eq. (9) if there could be a rationale for the approach? Assuming small relative errors, we may resolve the error into its Fourier components and refer to them as error waves with long wave lengths comparable to the dimension of the field of computation and with the shortest wave length equal to $2\Delta x$. In the limit of $\Delta x \to 0$, the ratio of wave length $\lambda$ to mesh size $\Delta x$ may be anywhere from $0(\Delta x)^{-1}$ to $\geq 2$. It is therefore pertinent to investigate the behavior of such error waves in the various limiting processes with $\Delta x/\lambda$ vanishing in different manners, for example $\lambda \sim (\Delta x)^m$ with $m = \frac{1}{2}, \frac{2}{3}, \frac{3}{4}$, etc. By keeping $\lambda(\Delta x)^{-m}$ constant, and letting $\Delta\xi = \Delta x/\lambda \to 0$, we may drop terms in Eq. (9) of higher order in $\Delta\xi$ assuming that all derivatives of $\xi$ be of order of unity. The last assumption means the neglect of the error waves with wave numbers higher than those considered, an adequate approximation if we are interested primarily in the accuracy of our computed solution in the global sense when the fine scale mesh to mesh fluctuations are ignored.

For $m = \frac{1}{2}$, we have to keep only the term with $\nu_e \partial^2 u/\partial x^2$ in Eq. (9) and for $m = \frac{2}{3}$, we have to keep both $\nu_e$ and $\alpha_1$ terms. For $m = \frac{3}{4}$, we have to include $\beta_2$ term also. If we should consider the limit of $\lambda/\Delta x =$ const, i.e., $m = 1$, we find that all terms in Eq. (9) must be included and such information is then contained only in the difference equation itself. Thus, except for the very fine scale error-waves of the order of mesh to mesh fluctuations, the asymptotic global behavior of the "limit" of our computed solution can be studied without resort to the difference equation, albeit the true asymptotic nature is not mathematically established.

The elementary wave solutions for Eq. (9) can be given as

$$u \sim \exp[-D_e k^2 t] \cdot \exp[ik(x - c_e t)]$$

with

$$D_e = \nu_e + k^2\beta_2 + k^4\beta_4 + \ldots$$
$$C_e = c - k^2\alpha_1 + k^4\alpha_3 + \ldots \quad (10)$$

$D_e$ is the pseudo-diffusivity and $C_e$ is the effective wave-velocity, both depending on the wave number $k$ as power series in terms of $(\Delta x)^{2(1-m)}$ when $k = 2\pi/\lambda \sim 0(\Delta x)^{-m}$ with $0 < m < 1$. The series may be terminated for some fixed choice of $m$. The precise magnitudes of $\nu_e$, $\beta_s'$ and $\alpha_s'$ depend on the difference algorithm and the differential equation.

If $D_e < 0$ for some wave number $k$, the solution of Eq. (10) diverges and Eq. (9) is ill-posed. The computation will necessarily be unstable in the strict sense. Since instability is inferred from illposedness of the limiting form of the difference formulation, we can say little about the nature of computational instability[12] encountered at finite $\Delta t$ and $\Delta x$.

It may be simply verified that the condition of $\nu_e > 0$ applied to Eq. (2) with many difference algorithms leads to identical stability criteria as those from v. Neumann analysis. We must not, however, be misled by such agreement. V. Neumann analysis applies to all error waves. The analysis of any truncated expression of $D_e$ considers only part of the error waves with $m < 1$. If all $\beta_s' \geq 0$, the most critical stability limit will be $\nu_e \geq 0$. When some of the $\beta_s'$ become $<0$, the result of v. Neumann analysis will be more restrictive.

Although less general and heuristic, the concept of pseudo-diffusivity is meaingful and often useful where v. Neumann analysis fails, since the v. Neumann analysis for the complete equation of fluid dynamics is just too complicated to be carried out and to yield simple stability criterion. The difference algorithms often have to be modified in practice for various computational reasons. The change in the pseudo-diffusivity resulting from the modification of a difference quotient replacing a derivative is a useful indication of the change of the stability behavior of the computation of the complicated system of equations.

For the boundary points the v. Neumann analysis does not apply while the energy analysis is difficult. The pseudo-diffusivity analysis will here yield some useful information. For example, the integration of Eq. (2) with the leap-frog scheme subject to the first-order accurate extrapolation boundary condition $u_J^n = U_{J-1}^n$ at $j = J$ is locally unstable, since the resulting difference equation $(U_{J-1}^{n+1} - U_{J-1}^{n-1}) + r(U_{J-1}^n - U_{J-2}^n) = 0$ gives negative pseudo-diffusivity:

$$D_e = \frac{r\Delta x}{2}\left[1 - r^2k^2\Delta x^2 - \frac{2k^2\Delta x^2}{4!}(1 + r^2k^2\Delta x^2) - \frac{2(k\Delta x)^4}{6!}(1 + \ldots) + \ldots\right] \quad (11)$$

when $k\Delta x = \pi$ or slightly less. The local exact solution of the difference equation is known (see Ref. 1, p. 142) to diverge. When the second and higher-order accurate extrapolation conditions are used, the exact solution of the difference equations are not so easy to find. The resulting pseudo-diffusivity can, however, be seen as approximately 2 and 6 times, respectively, that given in Eq. (11). Thus the extrapolation boundary condition cannot be usefully applied to the integration of simple wave equation with leap-frog difference algorithm.

When Friedrich's scheme is used with these extrapolation boundary conditions, the difference equation near the boundary gives $\nu_e$ and $\beta_2$, which are positive if $r \leq 1$. Thus we need not expect destabilizing influence from such extrapolation boundary conditions. However, only extrapolation schemes of second-order accuracy and higher should be used; otherwise, the local wave speed becomes $[(1 + r)/2r]\,c$ instead of the correct speed $c$.

### Error Dispersion and Formal Accuracy

The effective velocity $c_e$ given in Eq. (10) differs from the wave velocity $c$ of the genuine solution of Eq. (2). The error waves generated at some point will propagate away from its source with speeds depending on the wave number $k$. Large local errors in the computation not excluded by the "convergence in the mean" will be dispersed, causing severe errors elsewhere. Although such dispersed waves may be

damped through large positive pseudo-diffusivity, Eq. (9) becomes a poor approximation of the genuine solution of Eq. (2). In the results of calculation[4,11,14] of an inviscid shock wave, such dispersed error waves often appear downstream of the shock. They are generated by the large computational errors in the shock region. Substantial reduction of the amplitudes of such error waves could be achieved if the difference scheme were reduced to first-order accuracy by adding artificial viscous terms of $0(\Delta x)$ as was shown by Godunov.[15]

From Eq. (10) the logarithmic decrement of an error wave generated at the instant $t_0$ during the time of propagation $t - t_0$ is $D_e k^2(t - t_0)$. The distance $L$ of propagation of the error wave from its source for it to decay by a factor $\Delta x$ is obtained by replacing $t - t_0$ by $L/c_e$. Since both $\alpha_j$ and $\beta_j$ are of the order of $c(\Delta x)^{j+1}/(j+1)!$, we have

$$L \sim \Delta x\,|\ln \Delta x|(m^*!)/(k\Delta x)^{m^*} \tag{12}$$

where $m^*$ is $q+1$ or $q+2$ according as the formal order of accuracy of the difference algorithm $q$ is odd or even. That $L \sim \Delta x|\ln \Delta x|$ for all error waves in a given difference scheme is identical as the result of Kreiss and Lundquist,[16] but their condition requiring the difference scheme to be "contractive" is missed entirely. Relation (12) suggests further the importance of the wave number per mesh ($k\Delta x$) and of the formal order of accuracy $q$.

For first order accurate difference formulations, we have $\nu_e = 0(c\Delta x)$ With $k\Delta x = 2\pi\Delta x/\lambda$ the amplitude of such dispersed waves will be reduced over a wave length $\lambda$ by the ratio

$$g \sim \exp[-(2\pi)^2(\Delta/\lambda)(c/c_e)] \tag{13}$$

where $c/c_e$ is expected to be 0(1). Thus all waves with wave length $10\Delta x$ or less will be strongly damped so that such waves simply cannot propagate. On the other hand, those waves with wave lengths appreciably larger than $10\Delta x$ are comparable to the characteristic length and not perceptible unless the magnitudes are large. Therefore, the results of computation obtained with the first order accurate difference schemes will not display wavy disturbances in agreement with the result of Ref. 15.

For second order accurate difference formulations, we have $\nu_e = 0$ by definition. The leading dissipative term will be $\beta_2\partial^4 u/\partial x^4$ with $\beta_2/c(\Delta x)^3 = 0(1)$. Thus the error wave will be damped over a wave length by the ratio

$$g \sim \exp\left[-k^4\lambda(\Delta x)^3\frac{\beta_2}{c(\Delta x)^3}\frac{c}{c_e}\right] = \exp\left[-2(\pi)^4\left(\frac{\Delta x}{\lambda}\right)^3\frac{\beta_2}{c(\Delta x)^3}\frac{c}{c_e}\right] \tag{14}$$

For the Lax-Wendroff scheme applied to the simple wave equation $\beta_2/c(\Delta x)^3 = (1-r)/8r$. Thus waves with $\lambda = 4\Delta x$, for example, are damped mildly ($\lesssim 10^{-1}$) while those shortest waves with $\lambda = 2\Delta x$ will be damped by $10^{-2}$ over a wave length. Hence, in the inviscid shock wave calculations, waves with $\lambda = 4\Delta x$ decaying from the shock front are distinctly visible while those with $\lambda = 2\Delta x$ are not.

The third-order accurate schemes can apparently offer little improvement in decay rate over the second-order accurate schemes, since $\beta_2$ term remains the leading dissipative term. The fourth-order accurate schemes with leading dispersive term $\beta_5\partial^5 u/\partial x^5$ and leading dissipative term $\beta_6\partial^6 u/\partial x^6$ may increase the logarithmic decrement somewhat while considerably complicating the difference algorithm. Such higher-order accurate schemes may be necessary for suppressing "phase errors" that are particularly important in periodic problems.

The apparently smooth computed results from first-order accurate schemes are not really preferable to those not so smooth results from second-order accurate schemes of comparable mesh size. The slowly decaying, long wave-length components (including fixed errors in boundary value) of computational disturbances emanating from various sources are not easily visible but adversely affect the results over the entire field of computation. It is difficult in practice to keep the main portion of the flowfield not substantially affected by such long error waves if not carefully controlled. Using smaller mesh sizes offers no simple solution, since the demand on the computational time and the memory capacity increase with $1/\Delta x$ at an exponent higher than 1, especially for flow problems in multispace dimensions.

In computing an inviscid flowfield, the magnitude of the Reynolds number based on the pseudo-diffusivity $D_e$ is a measure how inviscid the computed results are. Let $D$ be the reference dimension and divided into $D/\Delta x$ meshes. For a first-order accurate scheme, $D_e \cong \nu_e \cong u\Delta x$, the effective Reynolds number is $Re_{D_e} \cong uD/\nu_e \cong D/\Delta x$. If $D/\Delta x \sim 10$ to 30 then $Re_{D_e} \sim 10$ to 30, too small to represent an inviscid flow field. We should expect at least $Re_{D_e} \sim D/\Delta x \sim 10^2$ or $10^3$. Suppose now a second-order accurate scheme is adopted with $D_e \sim k^2c(\Delta x)^3$ then $Re_{D_e} \sim (D/\Delta x)^3/(kD)^2$. Since we are concerned here only with the disturbances with wave lengths comparable to the characteristic dimension, we have $Re_{D_e} \sim 10^2$ to $10^3$ even with $D/\Delta x$ 10 to 30. Thus, second-order accurate schemes will provide accurate inviscid solutions with $D/\Delta x \sim 10$ to 30.

For viscous problems, we wish to investigate the effect of fluid viscosity $\nu$. Thus we have to require $D_e \ll \nu$ or $Re_{D_e} \gg Re = UD/\nu$. If we take $D$ as the boundary-layer thickness, then $Re$ is generally $\gtrsim 10^2$. Other viscous characteristic dimensions would lead to much larger $Re$. Hence with less than 100 mesh points over the viscous dimension, the first-order accurate schemes can not even be considered to yield any quantitative results. With a second-order accurate scheme, the requirement becomes, after dropping $kD$ as 0(1), the inequality $D/\Delta x \gg Re^{1/3}$ or $Re_{\Delta x} \ll Re^{2/3}$. When $Re \sim 10^2$ to $10^3$, the minimum requirement of the resolution will be over 20 meshes over the characteristic viscous dimension, or $Re_{\Delta x} \sim 1$ to 10. Third-order accurate schemes offer little improvement in this respect. Fourth-order accurate schemes relax the requirement of resolution to $D/\Delta x \gg Re^{1/5}$ or $Re_{\Delta x} \ll Re_D^{4/5}$. Suppose some viscous calculation is performed with $D/\Delta x = 100$, then the first-, second-, third-, and fourth-order accurate difference schemes would promise to achieve engineering accuracies to viscous problems with $Re \sim 10$, $10^3$, $10^3$ and $10^5$, respectively.

## III. Consistency of Difference Formulation

### Extraneous Initial and Boundary Conditions

The proper formulation of the initial and the boundary condition for the difference form of the Navier-Stokes equations in multispace dimensions is quite uncertain. They are introduced as needed to initiate and perpetuate the computation. Instability often results with "stable" difference algorithm under certain boundary conditions, which are often modified intuitively to achieve stable computation. How well such results approximate the solution of our physical problem is uncertain. Moreover, judged by practical rules concerning the extent, the type, and the number of boundary conditions applicable to partial differential equations, the difference formulation often appears to be over specified. The apparent "over specification" is necessary for the following reasons:

For Eq. (2) the initial value $u(t = 0, x \geq 0)$ specified along the line segment $AB$ with $A$ at $x = 0$ will determine $u(t,x)$ in the segment between $AB$ and the characteristics through $A$, i.e., $x \geq ct$. Since the zone of dependence of any stable difference formulation includes that of the differential problem, the initial values along $AB$ determines $u(t,x)$ only in the region $x \geq (c/r)t$ where $r = c\Delta t/\partial x < 1$. To determine

$u(t,x)$ in the triangular region $(c/r)t > x \geq ct$ through difference calculation, extraneous conditions either as initial value at $t = 0$ extending beyond $BA$ or as boundary values on $x = 0$, are necessary.

The differential equation "equivalent" to an ordinary difference equation or any equation with a retarded variable is of infinite order. Its solution requires infinite numbers of boundary conditions, which may be specified by some continuous extension of the function outside the prescribed boundary. A truncated equation of order $n$ requires $n$ boundary conditions, with the truncation visualized as equivalent to assigning zero values to all the derivatives of order $n + 1$ and higher. If the original equation is of first order, we need $(n - 1)$ extraneous boundary conditions. In the $n$th order accurate difference algorithm, the $(n - 1)$ extraneous conditions may be the values of the function at $(n - 1)$ neighboring mesh points.

The two sources of extraneous boundary conditions are distinct. The former arises from the stability consideration pertaining to hyperbolic equations; the latter is due to the higher-order accuracy of difference approximations, applicable to ordinary equations as well. The resulting difficulty is the same regardless of its source. Unless specified according to the genuine but unknown solution, they will inevitably cause errors. We can only hope to minimize the errors and to have them sufficiently damped so as not to interfere with the results in the main portion of the field of computation.

### Conservative Difference Formulation

Conservative differencing commonly refers to writing the conservation laws as differential equations in the form of divergence of the flux quantities before discretization.[9,14] There is no apparent reason why such a procedure should yield more accurate results.[17,8,13] The differential equations of fluid dynamics express the conservation of mass, momentum, and energy of the fluid elements in any form and in whichever variables. Errors in the flux quantities are still introduced by the discretization of the differential equations in divergence form. To reduce the computational errors, conservation laws should be strictly enforced in the difference form.

For a second-order accurate difference scheme, an error of $0(\Delta x)^2$ would be neglected in those quantities to be conserved by the physical laws. Such errors are often systematic and will accumulate when summed over a large number of cells. The accumulated errors in one spatial dimension may reach $0(\Delta x)$, and those in two spatial dimensions may reach $0(1)$. Thus the numerical solution, even if satisfactory in every other respect, will not be an adequate approximation to the physical problem with the integrals of motion specified by the boundary values. Instead of attempting the tedious schemes accurate to $0(\Delta x)^4$ or $0(\Delta x)^5$, over-all second-order accuracy can be maintained by preventing the error accumulation. The conservative difference formulation to be described below is one that does not permit such errors to accumulate when summed over arbitrary combinations of neighboring mesh cells.[13] The integrated conservation relations for each computational cell derived from Eqs. (1) express the temporal changes of the conserved quantities $\int \rho dv$, $\int \rho u dv$, and $\int \rho e dv$ in each cell of volume $\Delta v$ in terms of the flux quantities crossing the cell boundary where $dv$ is to be interpreted as including the Jacobian of the transformation from the physical space to the parametric space adopted in the computation. The fluxes must be evaluated on the cell boundary while the conserved quantities are determined only as the averages over the cell. Difference approximations are here introduced a) by assigning the average values of $\rho$, $\rho u$ and $\rho e$ at some cell centers and b) by evaluating the fluxes on the boundary in terms of the average values in the neighboring cells through some difference approximation. If the fluxes crossing the boundary between two neighboring cells are invariant with respect to the order of the cell indices, they will cancel on the interior boundaries when summed over any group of neighboring cells. The integrals of motion of the conserved quantities over arbitrary combinations of neighboring cells will be no more in error than those of the boundary errors.

Asymmetric difference schemes likely lead to formulations that are not conservative in the sense described previously. Centered or symmetric difference schemes when applied to Cartesian coordinates in physical space will conserve the fluxes whether the convective terms are differenced in the divergence form or not.[13] However, centered or symmetric spatial difference schemes applied to differential equations expressed in curvilinear coordinates in physical space[2,18] or Cartesian coordinates in parametric spaces will not necessarily lead to conservative difference formulation because of the presence of the metric coefficients and the Jacobian for the volume element. By properly choosing the centroids where the average conserved quantities are assumed to be located and by taking an appropriate form of the average in evaluating the flux quantities on the boundary in such parametric spaces, we can achieve conservation over every cell. The resulting difference form, however, often becomes complicated. We prefer simpler difference formulations although they may promise conservation only when summed over a specified small group of, say, 4 neighboring cells.[19] In the limit of $\Delta x \to 0$, no excessive error accumulation results. In this sense, such schemes are also conservative.

A conservative difference formulation of the flow problem arrived at in the manner described previously can be visualized as based directly on the first principles without taking the limit of $dv \to 0$ to obtain differential equations and undoing it by discretization and possibly introducing some errors thereby. The conceptual limit and the postulated convergence, etc., are avoided. The solution of the difference formulation is a physical approximation within the resolution afforded by the Eulerian cell size, satisfying the integrated conservation laws over "quite arbitrary" volumes. It is the Eulerian counterpart of the PIC (particles in cell) method[20] of the Lagrangian formulation. Where a fluid particle represents a collection of differential elements or molecules of fluid in the PIC, a Eulerian cell of $0(\Delta x)^3$ represents a collection of differential volumes. Instead of requiring the dynamic laws to be satisfied by every differential fluid element or in every differential volume, we are satisfied with having the dynamic laws hold for each Lagrangian particle or Eulerian cell and for arbitrary groups of such particles or cells.

The concept of maintaining integrated conservation laws over each cell is often helpful in formulating boundary conditions, and in the following example,[21] it turned out to be critical. When a supersonic flow with a boundary layer turns over a sharp corner to form a closed recirculatory wake, an isolated stagnation point is present downstream of the base. The flow is partly subsonic, partly supersonic, with a boundary-layer-like region in between and with an emerging shock. There are two important sources of errors in treating the flow around the sharp corner: the local scale of the flow phenomena is too small to be properly resolved by the mesh size and the formulation of the boundary condition is difficult regardless of the mesh sizes. The errors around this sharp corner are very large. We have only been able to obtain stable and reasonable results using a conservative difference formulation.[21,22] Sizable disturbances emanating from the corner are discernible but the flow field a few cells away from the corner is insensitive to the details of the conserved treatment of the boundaries; Ref. 21 gives the details.

## IV. Error Estimate and Accuracy

### Steady Flow Problems

An error analysis, based on the same postulate as in this paper, was carried out for second order approximations for the Burgers' equation.[13] The qualitative and the quantitative

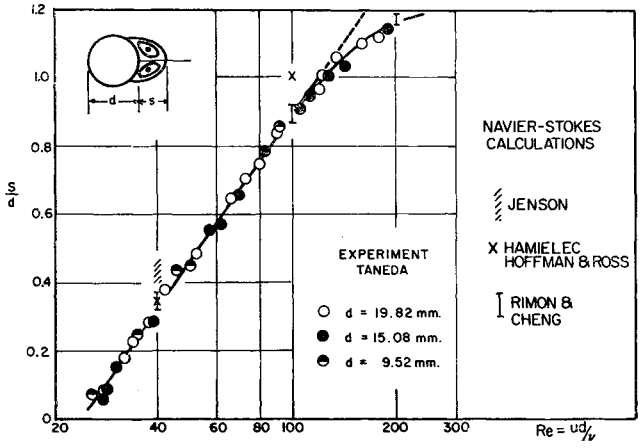


Fig. 1 Near wake length of sphere.

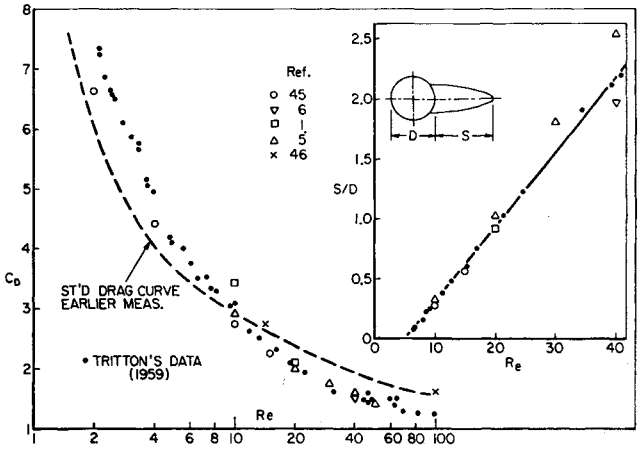


Fig. 2 Drag and near wake length of cylinder.

results were verified by actual computation when compared with the exact solution. Many practical conclusions of general interest are obtained and verified, all of which are in agreement with the qualitative inferences described in previous sections based on pseudo-diffusivity analysis. The usefulness of these results in multidimensional flow problems are demonstrated for the uniform flow of an incompressible fluid over a sphere. Reference 13 gives the details. The comparison of the near wake length is shown in Fig. 1 as an example.[19,23,25] The conservative formulation adopted in Ref. 19 did yield accurate results, adequate for most scientific and engineering purposes.

The uniform flow of an incompressible fluid over a cylinder has also been computed with various numerical procedures.[26–30] While generally satisfactory, there is some scatter among both the calculated and the experimental results[31] of $C_D$ and wake length (Fig. 2). It is uncertain how nearly the integrals of motion are conserved in these calculations. Neither is it clear which set of experimental data is more nearly correct. Nevertheless, it is fair to conclude that numerical integration of the Navier-Stokes equations when properly formulated and carefully executed can yield quantitatively meaningful results for steady flow problems with accuracy comparable to that of physical experimentation.

### Time Dependent Flows

For time dependent flows of slow and monotonic variation the decay of the error waves alone are important. For oscillatory flows the phase errors caused by dispersion become serious and difference schemes of higher than second-order accuracy are preferred.[32] Consider the damped oscillation, $u(t,x) =$

$$[\cos(x - 2t) + \sin(x - 2t)]/[e^x + \tfrac{1}{2}\cos(x - 2t)] \quad (15)$$

for $0 \leq t \leq T$ and $0 \leq x \leq L$ satisfying the Burgers' equation

$$\partial u/\partial t + (\partial/\partial x)(u^2/2) - \partial^2 u/\partial x^2 = 0 \quad (16)$$

The following sets of calculations were made for $T = 3.4$ and $L = 10$ with the two step Lax-Wendroff scheme (Ref. 1, p. 300).

1) All initial and boundary values are evaluated from the known exact solution, with $\Delta t = 0.01$ and $\Delta x = 0.2$.

2) Same as 1 for the first step. Use interpolation for the second step.

3) Same as 2 except that the downstream boundary values are approximated by $U_J^n = U_{J+1/2} = 0$.

4) Same as 2 except that the downstream boundary values $U_J^n$ and $U_{J+1/2}$ are evaluated from second order accurate extrapolation.

5) Repeat 3 and 4 with a) $\Delta t = 0.02$, $\Delta x = 0.30$ ($s = \frac{1}{2}$); b) $\Delta t = 0.04$, $\Delta x = 0.20$ ($s = 1$); c) $\Delta t = 0.04$, $\Delta x = 0.30$ ($s = \frac{4}{9}$).

Comparison of the results showed the following:

1. The influence of the extraneous initial and boundary conditions are inconsequential.

2. The dominant error in the computation is generated from the interior at about $\frac{1}{4}$ wave length where phase shift leads to large fractional error.

3. With the second order accurate (both in time and in space) two step Lax-Wendroff scheme, a spatial resolution of 30 meshes per wave length and 300 time steps per cycle can provide over-all engineering accuracy only for the first wave length (Fig. 3). Beyond this range the accuracy of the solution deteriorates rapidly. Schemes of first order temporal accuracy yields much less satisfactory results even with same space resolution.

For turbulent flow problems, sufficient resolution can be achieved only for those long waves with scales comparable to body dimension. We cannot expect the difference methods described previously to follow with quantitative details the temporal fluctuations of a turbulent field even with computers much larger and faster than currently available. The gross effect of the small scale eddies will still have to be represented phenomenologically, i.e., the closure problem will still be with us. The difference calculations described here will lead to some kind of "turbulent" fields, but they are domi-

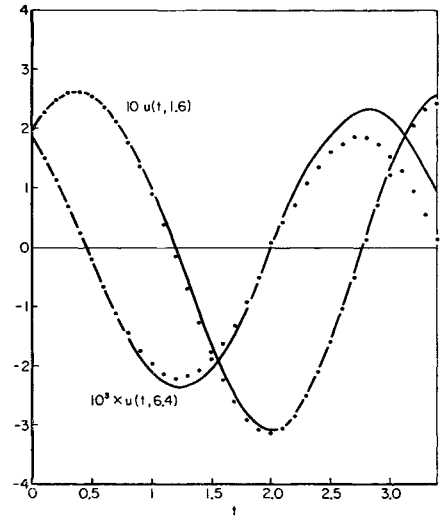


Fig. 3 Damped oscillation in first period at about ¼ and a full wave length (dots ~ computed value line ~ exact solution).

nated by "numerical turbulence" as a result of the more or less random nature of the errors introduced by difference methods with little resemblance to the "fluid turbulence."

## V. Conclusions

The heuristic content of the concept of pseudo-diffusivity is investigated. It is shown how its analysis can help to achieve computational stability for both the interior and the boundary points, and how the analysis of the decay of the dispersive waves describes the nature of error propagation.

The conservative difference formulation directly from first principles rather than the discretization of the differential equations is proposed as an Eulerian counterpart of the PIC method for the Lagrangian formulation. It is important to avoid the accumulation of errors in the physically conserved quantities over arbitrary volumes for quantitative accuracy. It is also beneficial in other aspects of computation.

With proper attention to the details, computed results for steady flows can be as accurate as the results of physical experimentation. However, for oscillatory flows, the phase error becomes important. Second-order accurate difference schemes do not appear suitable for the detailed study of turbulent flow fields and turbulence.

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