JOURNAL OF COMPUTATIONAL PHYSICS **20**, 196–207 (1976)

Time-Differencing Schemes and Transform Methods

JENÖ GAZDAG

IBM Corporation, Palo Alto Scientific Center, 1530 Page Mill Road, Palo Alto, California 94304

Received June 17, 1975

In this paper, we study several time-differencing procedures for the numerical solution of partial differential equations. We find that "partially corrected" time-differencing schemes offer some advantages over single-step methods. Such differencing schemes consist of a predictor step and a corrector step, however, the time derivative is evaluated only *once* in the two steps. Partially corrected time-differencing schemes can be used with particular advantage in transform methods, where the numerical approximation of the derivative terms represents the major portion of computing. All differencing methods are tested on the nonlinear Vlasov–Poisson system of equations with two phase-space variables. In the case of the numerical example considered, the partially corrected schemes are only about 1 % slower than the corresponding single-step procedures without correction.

I. INTRODUCTION

Time-differencing procedures for solving partial differential equations numerically have been studied extensively [1–6]. The two most widely accepted single-step procedures appear to be the leapfrog scheme and the second-order Adams–Bashforth method [1, 4, 7]. It is interesting to note that both these schemes are unstable, which suggests that users place a great importance on the simplicity of the time-differencing procedures, even at the risk of numerical instabilities The numerical instabilities found in second-order single-step methods are absent in some of the commonly used predictor–corrector schemes [2, 8, p. 186]. In the conventional two-step procedures [2], the time derivative is calculated in both the predictor as well as the corrector steps. Although the accuracy of such two-step methods is higher, they require approximately twice as much computation as comparable single-step time-differencing schemes. As a result of this trade-off between higher accuracy and more computation, the advantages of such two-step methods are not always applicable to a given problem.

We found that it is possible to devise two-step time-differencing procedures, in which the time derivative is calculated only in one of the two steps. Such "partially corrected" procedures require only slightly more computation than

the single-step methods. Their error characteristics, however, are improved considerably by the corrector step. This is particularly true for small time steps, in which case the truncation errors become comparable to those in the conventional (fully corrected) schemes.

Partially corrected time-differencing procedures can be used with considerable advantage in transform methods. The term "transform method" refers collectively to those numerical procedures in which the space dependence of a function is expressed in terms of a set of orthogonal polynomials [9, 10], or in which some orthogonal transformation is used for the accurate and efficient computation of the space-derivative terms [11–13]. In such numerical approaches, the computation of the time derivative is usually the most costly operation in the numerical procedure. Consequently, the corrector step that does not involve the explicit recomputation of the time derivative represents a rather small fraction of the total computing.

In Section II, we review some of the single-step time-differencing procedures that have been used with success in transform methods. We discuss the corrected time-differencing schemes in Section III. We examine and compare the truncation errors associated with these methods in Section IV. To test these differencing schemes for the numerical solution of nonlinear partial differential equations, they were applied to the solving of the Vlasov–Poisson system of equations. Section V presents these results and discusses the accuracy obtained. Section VI concludes the paper.

II. Single-Step Time-Differencing Schemes

Consider the equation

$$\partial u/\partial t = G(u, x, t), \tag{1}$$

where x and t are distance and time, respectively. Perhaps the most basic approach to the numerical integration of (1) results from expressing $u[x, (m + 1)\,\Delta t]$ in a truncated Taylor series

$$u^{m+1} = \sum_{l=0}^{p} \frac{\partial^l u^m}{\partial t^l} \frac{(\Delta t)^l}{l!}, \tag{2}$$

where u^m stands for $u(x, m\,\Delta t)$. It can be shown [11] that this method is unstable for $p = 1$ and $p = 2$; however, it is stable for $p = 3$ and $p = 4$. The third-order scheme ($p = 3$) has been applied with success in several nonlinear partial differential equations including the Vlasov–Poisson system of equations in three phase-space variables [11–13]. The only disadvantage of this scheme has to do with the

computation of the second and third time derivatives. When Eq. (1) has a number of nonlinear terms in several space variables, the computation of the higher-order partial derivative terms becomes rather involved.

Another differencing method that has received a great deal of attention is the "midpoint leapfrog method" [1–8] in which u^{m+1} is approximated as

$$u^{m+1} = u^{m-1} + G^m 2\,\Delta t. \tag{3}$$

This method is second-order accurate in time, with attractive error characteristics. Morton [4] has studied seven different algorithms in detail and reached the conclusion that the leapfrog algorithm, Eq. (3), is the best of the generally applicable basic methods. However, the leapfrog method for hyperbolic problems is only marginally stable [6, p. 55]. Kreiss and Oliger [5] have given examples of numerical schemes that are unstable when leapfrog time differencing is used. This instability arises from a computational mode, leading to the separation of the solution at subsequent time steps. Such time-splitting instability has been also observed in the numerical solution of the Vlasov equation [14, p. 174]. As a result, the leapfrog scheme must be reinitialized after, say, 20 time steps [6, 14, 15]. Because of this major weakness, some do not consider the leapfrog scheme as a practical method [15].

After careful study of several methods, Lilly [1] found that the Adams–Bashforth method was preferable to the leapfrog scheme. The second-order Adams–Bashforth method advances Eq. (1) by the folllowing rule:

$$u^{m+1} = u^m + [3G^m - G^{m-1}]\,\Delta t/2. \tag{4}$$

This method is unconditionally unstable, with a weak divergence caused by an amplification factor $1 + O(\Delta t^2)$ [1, 6, p. 74]. Because the instability is weak, the method can be used for inviscid flow calculations for short time.

As we shall see, the third-order Adams–Bashforth scheme [16, p. 137, 17, p. 194]

$$u^{m+1} = u^m + [23G^m - 16G^{m-1} + 5G^{m-2}]\,\Delta t/12 \tag{5}$$

is stable. However, it requires an additional level of G values.

III. Corrected Time-Differencing Schemes

Here, we consider time-differencing schemes that are composed of two steps: (1) A predictor step, followed by (2) a corrector step. Results obtained from the predictor step will be denoted by a tilde mark, e.g., $\tilde{u}$. The corrected values from step (2) bear no tilde sign. The first method is a conventional (fully corrected)

two-step time-differencing procedure. Methods 2 and 3 are partially corrected schemes.

Method 1. *The corrected leapfrog scheme.* The predictor step is the leapfrog scheme,

$$\tilde{u}^{m+1} = u^{m-1} + G^m 2\,\Delta t, \tag{6}$$

followed by a trapezoidal corrector step,

$$u^{m+1} = u^m + (G^m + \tilde{G}^{m+1})\,\Delta t/2. \tag{7}$$

Method 2. *The partially corrected second-order Adams–Bashforth Scheme.* The predictor step is the same as Eq. (4),

$$\tilde{u}^{m+1} = u^m + (3\tilde{G}^m - \tilde{G}^{m-1})\,\Delta t/2 \tag{8}$$

and the corrector step is

$$u^{m+1} = u^m + (\tilde{G}^m + \tilde{G}^{m+1})\,\Delta t/2. \tag{9}$$

We note that in (6) and (7), G^m appears, which is computed from the corrected value u^m. In the partially corrected procedures, this step is omitted, and the uncorrected derivative, $\tilde{G}^m$, is used as in (8) and (9).

We have also considered the partially corrected leapfrog scheme, i.e., using

$$\tilde{u}^{m+1} = u^{m-1} + \tilde{G}^m 2\,\Delta t \tag{10}$$

in place of (8). For constant Δt, Method 2 is equivalent to (9) and (10). The advantage in using (8) instead of (10) is that (8) is easily generalized to variable time steps, whereas (10) is not, since it is based on the idea of time centering.

Method 3. *The partially corrected Adams–Bashforth scheme of order* 3. In this case, the predictor step is the same as (5),

$$\tilde{u}^{m+1} = u^m + [23\tilde{G}^m - 16\tilde{G}^{m-1} + 5\tilde{G}^{m-2}](\Delta t/12), \tag{11}$$

followed by the corrector step [16, p. 144]

$$u^{m+1} = u^m + [5\tilde{G}^{m+1} + 8\tilde{G}^m - \tilde{G}^{m-1}](\Delta t/12). \tag{12}$$

The expressions for the corrector step given by Eqs. (9) and (12) are the same as in the Adams–Moulton method [17, p. 143]. However, the present methods differ from the Adams–Moulton method in that the time derivative is computed after the first step only.

IV. Error Analysis

We shall examine the numerical error resulting in the three methods described in the previous section. To show the merits of these schemes, their error characteristics will be contrasted with those of some of the popular numerical methods. These errors are determined from the numerical solution of the simple convective equation

$$\partial u/\partial t = -v(\partial u/\partial x) \tag{13}$$

where v is constant. If we let

$$U(k, t) = \sum u(x, t) \exp(-ikx), \tag{14}$$

the trivial solution of (10) can be written as

$$U(k, t) = U(k, 0) \exp(i\omega t), \tag{15}$$

where $\omega = -kv$.

The differencing error ϵ is defined as the deviation of the numerical solution U_* from the true solution U in one time step Δt, i.e.,

$$\epsilon = (U_*^m - U^m)/U^m \tag{16}$$

under the assumption that

$$U_*^{m-1} = U^{m-1}. \tag{17}$$

In these equations, U^m stands for $U(k, m\,\Delta t)$.

Although ϵ depends on k, v, and Δt, its dependence can be expressed in terms of one variable [11]

$$\phi = -kv\,\Delta t = \omega\,\Delta t, \tag{18}$$

which represents the change in the phase angle of the wave in one time step.

The geometrical representation of ϵ is shown in Fig. 1, which also illustrates the definition of the amplitude error

$$\delta_a = (|\,U_*^m\,| - |\,U^m\,|)/|\,U^m\,| \tag{19}$$

and the phase error

$$\delta_p = (\phi_* - \phi)/\phi, \tag{20}$$

which are used often as a measure of goodness of differencing schemes.

In some cases, one may be interested in employing a method having more favorable dispersion characteristics at the expense of more amplitude error and vice versa. If, however, there are no special reasons for preferring one type of

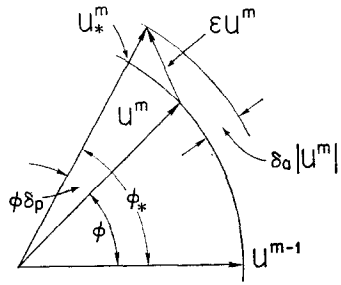

FIG. 1. Graphical representation of the differencing error ϵ, the amplitude error δ_a, and the relative phase error δ_p.

error to another, the magnitude of ϵ appears to be a good overall measure of accuracy. As can be seen in Fig. 1, ϵ accounts for the amplitude error as well as the phase error, and therefore, it provides an easy means of comparison between differencing schemes.

The magnitude of the differencing error ϵ versus $\omega\,\Delta t$ is shown in Fig. 2 for the time-differencing procedures discussed in Sections II and III. The partially corrected methods 2 and 3 have smaller differencing errors for $\omega\,\Delta t \leqslant 23°$ than the corresponding single-step differencing schemes. Unfortunately, Method 3 becomes unstable shortly after $\omega\,\Delta t = 24°$ and, therefore, its use is limited to cases in which one is willing to restrict oneself to small $\omega\,\Delta t$ values in order to maintain differencing errors at very small levels.

A rather attractive property of Method 2 is that its accuracy approaches that of Method 1, which is a fully corrected scheme, as $\Delta t \to 0$.

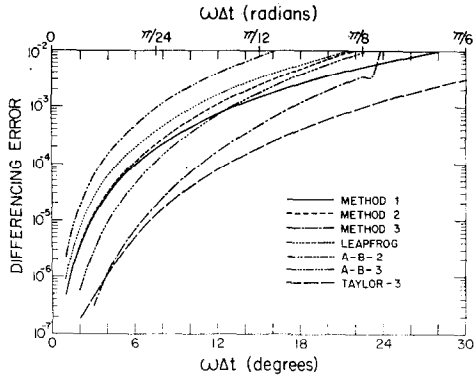

FIG. 2. Absolute value of differencing error vs $\omega\Delta t$ as defined by Eq. (16) and Fig. 1 for various numerical schemes. The second- and third-order Adams–Bashforth methods are indicated by A-B-2 and A-B-3, respectively.

As we see in Fig. 3, the small correction (9) applied after the otherwise unstable Adams–Bashforth scheme (Eqs. (4) and (8)), results in a stable time-differencing procedure, Method 2. A disadvantage of Method 3 is that it has positive amplitude error for $\omega \Delta t < 15°$ and, therefore, it is not a stable scheme. This very weak numerical instability, which is weaker than that of the second-order Adams–Bashforth scheme, is by no means a serious fault of the method.

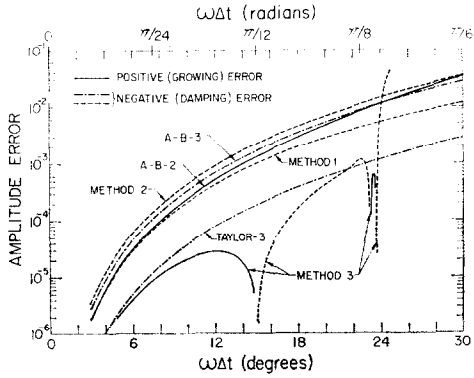

FIG. 3. Amplitude error vs $\omega \Delta t$ as defined by Eq. (19) and Fig. 1 for various numerical schemes.

The phase error curves (20) are shown in Fig. 4. We notice that the correction given by (9) applied in Method 2 results in improved phase-error characteristics over the second-order Adams–Bashforth scheme. The correction (12) applied in Method 3 to the third-order Adams–Bashforth scheme, however, does not reduce the phase error. On the contrary, after $\omega \Delta t = 23°$, the phase error of Method 3 grows very fast due to the instability mentioned earlier.

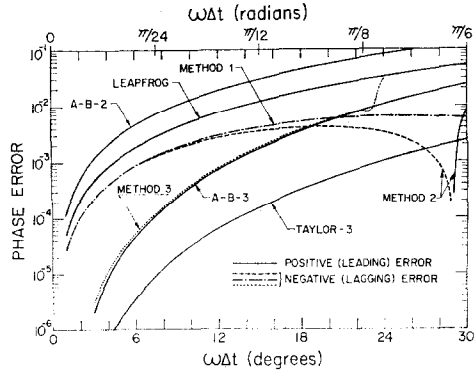

FIG. 4. Phase error vs $\omega \Delta t$ as defined by Eq. (20) and Fig. 1 for various numerical schemes.

V. Numerical Integration of the Vlasov Equation

The time-integration schemes described in Section III were tested by applying them to the Vlasov equation [12–14, 18]

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - E\frac{\partial f}{\partial v} = 0, \tag{21}$$

for the electron distribution $f(x, v, t)$, where the electric field $E(x, t)$ is given by the Poisson equation,

$$\partial E/\partial x = 1 - \int f\, dv. \tag{22}$$

These equations are written in dimensionless units [9]. The basic unit of time t and velocity v are the reciprocal of the plasma frequency $(\omega_p)^{-1}$ and the mean thermal velocity v_t. Length x is measured in units of the Debye length. The equilibrium electron distribution in all our computations is Maxwellian, i.e.,

$$f_0(v) = (2\pi)^{-1/2} \exp(-\tfrac{1}{2}v^2) \tag{23}$$

and the initial condition for the electron distribution is

$$f(x, v, 0) = f_0(v)(1 + \alpha \cos kx), \tag{24}$$

where k is the wavenumber and α is the initial perturbation amplitude. The initial electric field amplitude is

$$E_0 = \alpha/k. \tag{25}$$

The ASD method for the numerical solution of Eqs. (21) and (22), using a third-order Taylor series (2) time-integration scheme is described elsewhere [12, 13]. In this approach, all derivatives with respect to x and v are evaluated by means of finite-Fourier-transform methods. In order to test the present methods on a nonlinear partial differential equation, we developed programs for the solution of Eqs. (21) and (22) based on the ASD method using the various time-integration schemes discussed previously. We shall describe only the application of Method 2 to the Vlasov–Poisson system of equations. The other methods differ only in the time-integration scheme employed.

In Method 2, Eqs. (8) and (9), the electron distribution function is advanced by approximating $f(x, v, t + \Delta t)$ in two steps. In the first step, we obtain $\tilde{f}(x, v, t + \Delta t)$, an intermediate result, by implementing

$$\tilde{f}(x, v, t + \Delta t) = f(x, v, t) + \left[3\frac{\partial \tilde{f}(x, v, t)}{\partial t} - \frac{\partial \tilde{f}(x, v, t - \Delta t)}{\partial t}\right]\frac{\Delta t}{2}. \tag{26}$$

The final approximation is obtained from the corrector step

$$f(x, v, t + \Delta t) = f(x, v, t) + \left[\frac{\partial \tilde{f}(x, v, t)}{\partial t} + \frac{\partial \tilde{f}(x, v, t + \Delta t)}{\partial t}\right] \frac{\Delta t}{2}. \quad (27)$$

The time derivative of $\tilde{f}$ is obtained from the expression

$$\frac{\partial \tilde{f}}{\partial t} = -v \frac{\partial \tilde{f}}{\partial x} + \tilde{E} \frac{\partial \tilde{f}}{\partial v}, \quad (28)$$

where the partial derivatives of $\tilde{f}$ with respect to x and v are computed by the finite-Fourier-transform method as described elsewhere [11–13].

For the test problem, we chose the initial conditions given by (23) and (24), with $k = 0.5$ and $\alpha = 0.1$. All time-integration schemes gave the same well-known [9, 12, 13, 18] qualitative result for the electric field shown in Fig. 5. To make a

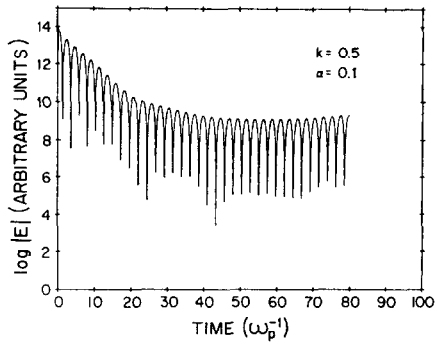

FIG. 5. Electric field vs time for a nonlinear wave.

quantitative comparison of the numerical inaccuracies in this nonlinear problem, we recorded the magnitude and the position (in time) of the thirteenth peak (see Fig. 5) in the vicinity of $t = 30$. The time of occurrence and the magnitude of $E_{\max}$ were calculated from three neighboring samples by means of second-order interpolation. These results are shown in Table I for two different time steps. In terms of the units employed in Table I, the initial amplitude of the wave at $t = 0$ is $E_0 = 100$. These results demonstrate conclusively that all methods considered are suitable for the numerical integration of the nonlinear Vlasov equation. The instability in the two unstable cases in Table I are due primarily to the $v(\partial f/\partial x)$ term in (21). By neglecting the $E(\partial f/\partial v)$ term in (21), we can write it as

$$\omega F + vkF = 0, \quad (29)$$

where

$$F = \int \int f(x, v, t) \exp[-i(kx + \omega t)]\, dx\, dt, \tag{30}$$

and obtain for $\phi = \omega\, \Delta t$, Eq. (18), the expression

$$\phi = -vk\, \Delta t \tag{31}$$

In the nonlinear example considered above, $v_{\max} = 5$ and $k_{\max} = 1.5$. Therefore, with $\Delta t = 0.075$, $| \phi_{\max} | > 0.56$ or 32°. According to Fig. 3, for $\phi > 30°$, numerical instability can be expected for both of the cases indicated by Table I.

TABLE I

The Magnitude and Position of $E_{\max}$[a]

	$\Delta t = 0.05$		$\Delta t = 0.075$	
	$\lvert E_{\max} \rvert$	t	$\lvert E_{\max} \rvert$	t
Taylor-3	1.3381	30.378	1.3354	30.378
Leapfrog	1.3348	30.349	1.3301	30.312
Adams–Bashforth-2	1.3338	30.304	Unstable	—
Adams–Bashforth-3	1.3315	30.379	1.3127	30.381
Method 1	1.3344	30.392	1.3119	30.410
Method 2	1.3311	30.393	1.3087	30.414
Method 3	1.3404	30.378	Unstable	—

[a] In the neighborhood of $t = 30.378$ in the numerical solution of Eqs. (21) and (22) for initial conditions (23) and (24) with $\alpha = 0.1$.

The t values in Table I are scattered about the value 30.378. Greater values correspond to methods with negative phase error, whereas smaller t values indicate leading (positive) phase error. In this respect, there is a good agreement between these t values and the phase error curves shown in Fig. 4. The only exception is the third-order Adams–Bashforth scheme, in which, in spite of its positive phase error, the peak appears slightly later than 30.378. The most probable cause for this is the relatively strong numerical damping in this scheme.

The $| E_{\max} |$ values depend on both the amplitude error and the phase error. For example, the leapfrog scheme with "zero damping" results in a smaller $| E_{\max} |$ value than Taylor-3. The reason for this is that the numerical model has excessive phase mixing due to the leading phase error of the leapfrog scheme.

Similarly, in the second-order Adams–Bashforth scheme, the rather large positive phase error results in a smaller $|E_{\max}|$ value, in spite of the positive amplitude error that should lead to growth.

As we stated earlier, the additional amount of computation required in the corrector step of Methods 2 and 3 is relatively small. In the numerical example discussed above, Method 2 required about 1% more computation than the leapfrog or the second-order Adams–Bashforth method.

VI. Conclusions

We have described partially corrected time-differencing schemes and compared their error characteristics with several well-known differencing methods. An important feature of these numerical procedures is that the corrector step does not involve the recomputation of the time derivative of the function to be integrated. Therefore, when these schemes are applied in transform methods, the computation required in the corrector step is only a very small fraction of that in the predictor step. We found, however, that this simple corrector step improves the error characteristics of the predictor step. This is true particularly in the case of Method 2, which uses the second-order Adams–Bashforth schemes as predictor. While this predictor scheme is unstable, the corrected differencing scheme is stable. Thus, the instability of the predictor has very little effect on the stability of the result after the corrector is applied.

All the differencing methods considered in this paper were tested on the nonlinear Vlasov–Poisson system of equations with two phase–space variables x and v. The results of these tests were consistent with the truncation error properties of these differencing schemes as we discussed in Section V. In this test, Methods 2 and 3 required about 1% more computation than the single-step procedures without the corrector step. Method 1, however, in which the customary predictor–corrector concept is used, requires about twice as much computation as the leapfrog scheme. The Taylor-3 method, (2), which is the most accurate, is approximately three times slower (per time step) than the leapfrog scheme. This is because each time step requires three time-derivative computations. Among the time-differencing procedures studied in this paper, Method 2 appears to be the most attractive practical method. For very high accuracy, Method 3 should be considered.

Acknowledgment

The author wishes to thank Piero Sguazzero for numerous useful discussions.

REFERENCES

1. D. K. LILLY, *Mon. Weather Rev.* **93** (1965), 11.
2. J. A. BYERS, *J. Comput. Phys.* **1** (1967), 496.
3. A. GRAMMELTVEDT, *Mon. Weather Rev.* **97** (1969), 384.
4. K. W. MORTON, *Proc. Soc. London A.* **323** (1971), 237.
5. H. O. KREISS AND J. OLIGER, *Tellus* **24** (1972), 199.
6. P. J. ROACHE, "Computational Fluid Dynamics," Hermosa, Albuquerque, N. M. 1972.
7. S. A. ORSZAG AND M. ISRAELI, *Ann. Rev. Fluid Mech.* **6** (1974), 281.
8. R. W. HAMMING, "Numerical Methods for Scientists and Engineers," McGraw–Hill, New York, 1962.
9. T. P. ARMSTRONG, R. C. HARDING, G. KNORR, AND D. MONTGOMERY, *Methods Comput. Phys.* **9** (1970), 30.
10. S. A. ORSZAG, *J. Fluid Mech.* **49**, 75, Part 1 (1971).
11. J. GAZDAG, *J. Comput. Phys.* **13** (1973). 100.
12. J. GAZDAG, Proc. Int. Symp. on Computing Methods in Applied Sciences and Engineering, Versailles, France, December 17–21, 1973; "Lecture Notes in Computer Science," Vol. 11, Part 2, p. 37. (G. Goos and J. Hartmanis, Eds.) Springer–Verlag, New York/Berlin, 1974.
13. J. GAZDAG, *J. Comput. Phys.* **19** (1975), 77.
14. G. KNORR, *J. Comput. Phys.* **13** (1973), 165.
15. J. E. FROMM, Private communication.
16. R. W. HAMMING, "Introduction to Applied Numerical Analysis," McGraw–Hill, New York, 1971.
17. F. CESCHINO AND J. KUNTZMAN, "Numerical Solution of Initial Value Problems," Prentice–Hall, Englewood Cliffs, N.J. 1966.
18. J. CANOSA AND J. GAZDAG, *Phys. Fluids* **17** (1974), 2,030.