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Multidimensional Difference Schemes with Fourth-Order Accuracy

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An explicit finite-difference algorithm is presented for the solution of quasilinear divergence free multidimensional hyperbolic systems. The method consists of four steps per time level. The resulting scheme is fourth-order accurate in both space and time, though the intermediate steps are only first-order accurate. The family of schemes introduced is dissipative, and hence, suitable for both smooth flows and flows containing shocks. This method is compared, in several numerical examples, with both second-order schemes and others that are fourth order in space, but second order in time.

1. INTRODUCTION

With the advent of faster computers, it was realized that more complicated problems could be solved and with a higher degree of precision than previously obtainable. This advance in hardware has lead to a renewed study of algorithms that are more efficient at smaller error levels. Roberts and Weiss [22] first introduced schemes that are second-order accurate in time but fourth order in space.

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This concept was continued by Crowley [8], Kreiss and Oliger [16], and Gerrity, McPherson, and Polyer [12], among others. These schemes are nondissipative, and hence, their main application has been in meteorological problems where shocks do not arise. One could add an artificial dissipative term to these schemes, but it is difficult to choose the coefficients so that they prevent nonlinear instabilities while not smoothing out important data (compare, Kashara and Rao [15]). Other approaches to improving the accuracy in the spatial directions have been via spectral methods (e.g., Orszag [19]) and finite element techniques (e.g., Swartz and Wendroff [24]). These methods also seem to be most appropriate for problems where shocks do not occur and the solutions are sufficiently smooth.

Should one be interested in a general code that is accurate in smooth regions but gives the correct shock speeds, the most appropriate techniques are generalizations of the Lax–Wendroff method. A start in this direction was begun by Burstein and Mirin [7] and Rusanov [23] who introduced a three step third-order generalization of the Richtmyer scheme. For second-order methods in two space dimensions, one needs a minimum lattice of seven points at the previous time level (Livne [17]) while most schemes have a nine-point stencil for their domain of dependence. For third-order methods, one requires a domain of dependence of the order of 25 net points; this of course creates difficulties near boundaries. It was felt that once one uses this enlarged lattice, one might as well look for schemes that are fourth order in both space and time. For scalar equations, Abarbanel and Zwas [4] introduced a one-step method for conservation equations that in fact uses only a 21-point lattice. Later, Abarbanel and Gottlieb [2] suggested a family of multistep methods that are fourth order or higher for any quasi-linear divergence-free hyperbolic system.

Another approach is that known as the method of lines. In this technique, one first discretizes in space obtaining a system of differential–difference equations. This is then integrated in time using a standard O.D.E. routine. Gary [10] suggests using fourth-order accurate differencing in space followed by a fourth-order Runge–Kutta in time. This approach suffers from the serious handicap that at each time level, a net point needs information from an unacceptably large number of points at the previous time level. In the one space dimension case, the domain of dependence is 17 points, and in the two-dimensional case, it would be roughly a square of 17×17 mesh points. This causes difficulties near boundaries and also requires, for most problems, too fine a mesh. In view of all of this, we shall not make any numerical comparisons with such Runge–Kutta-like fourth-order accurate methods. Instead, we propose to investigate schemes that employ minimal domains of dependence. These will modify and extend the algorithm proposed by Abarbanel and Gottlieb [2].

The schemes introduced by Abarbanel and Gottlieb suffer from two disadvantages. First, the method requires seven steps for fourth-order accuracy. This

is considerably more than required for ordinary differential equations. Second, the multidimensional schemes use a diamond shaped domain of dependence that creates some difficulties near boundaries. Furthermore, there now exists two separate sets of nodes that can lead to weak instabilities (see Houghton, Kasahara, and Washington [14]). Later, Abarbanel, Gottlieb, and Turkel [3] (AGT) showed that one can construct a four step fourth-order method in a single dimension. This was done by either using a three-level method, or alternatively a two-level method, where the intermediate steps are only first-order accurate. In this paper, we shall extend these latter results to several dimensions. In addition, the domain of dependence is rectangular, which minimizes boundary problems. As a final bonus, the stability requirement seems to allow larger time steps than either the one-step Lax–Wendroff or two-step Richtmyer methods.

In many problems of physical significance, the major obstacle to obtaining high precision is the limited computer storage rather than time factors. For example, use of a fine grid over the surface of the globe, especially with multilayer models, quickly exhausts the high speed computer storage of present day machines. Use of auxiliary storage involves large time delays or else sophisticated software that is beyond the capability of most computer centers. In other applications, as in plasma physics, one integrates equation in physical-phase space. Hence, one-dimensional problems involve two computational dimensions, while two space dimensional problems imply the need of four computational dimensions in addition to the time variable. Thus, for the Vlasov equation, computer storage requirements are of extreme importance. Finally, the trend in computers is towards faster machines, for example, parallel mode operation. However, the high speed memory of these machines will not be much larger than present computers. For these reasons, we shall emphasize the core storage requirements of differing schemes in addition to comparing their efficiency in terms of running time.

2. Finite-Difference Scheme

We shall confine the derivation of the algorithm to the two-dimensional divergence equation

$$u_t + f_x + g_y = 0, \tag{1}$$

where f and g are vector functions of u. Identical results are true when f and g are functions of the space variables in addition to u. However, in order to minimize the algebra, we shall consider the case where they depend only on u. In one of the numerical examples presented in Section 4, f and g are functions of x and y.

The system (1) also can be written as a quasi-linear system

$$u_t + Au_x + Bu_y = 0. \tag{2}$$

We shall assume that this system is hyperbolic, i.e., A and B have a complete set of real eigenvalues and eigenvectors. To simplify the notation, we introduce the averaging and differencing operators.

$$\begin{aligned} \mu_x W_{i,j} &= \tfrac{1}{2}(W_{i+1/2,j} + W_{i-1/2,j}), \\ \delta_x W_{i,j} &= W_{i+1/2,j} - W_{i-1/2,j}, \end{aligned} \tag{3}$$

with corresponding notation for the y direction. Without loss of generality, one can always assume that $\Delta x = \Delta y$. We then define λ

$$\lambda = \frac{\Delta t}{\Delta x} = \frac{\Delta t}{\Delta y}, \tag{4}$$

where, as usual, Δt, Δx, Δy are the mesh spacings in the t, x, y directions, respectively.

In this paper, we consider Burstein-type centering, where the intermediate steps are defined at mesh points (i, j) or $(i + 1/2, j + 1/2)$. One could also consider Thommen-type centering, where the intermediate steps are centered at (i, j) or $(i + 1/2, j)$ or $(i, j + 1/2)$. The extension of MacCormack type schemes to fourth-order accuracy is difficult because of the lack of centering.

We now describe a general four-step scheme in two dimensions. In Appendix A, we extend this to three space dimensions. We denote the numerical approximation to $u(x, y, t)$ by $w_{i,j}^n$. By $f^{(k)}$, we mean $f(w_{i,j}^{(k)})$, where the superscript is the number of the intermediate level. When k is equal to zero, the superscript is omitted, and we are referring to the start of a time level.

$$w^{(1)} = \mu_x\mu_y w - \lambda a[\mu_y\delta_x f + \mu_x\delta_y g], \tag{5a}$$

$$\begin{aligned} w^{(2)} = {} & \epsilon_1 w + \epsilon_2\mu_x{}^2 w + \epsilon_3\mu_y{}^2 w + \epsilon_4\mu_x{}^2\mu_y{}^2 w \\ & - \lambda[\alpha_1(\mu_y\delta_x f^{(1)} + \mu_x\delta_y g^{(1)})] + \alpha_2(\mu_x\delta_x f + \mu_y\delta_y g)], \end{aligned} \tag{5b}$$

$$\begin{aligned} w^{(3)} = {} & \theta_1\mu_x\mu_y w + \theta_2\mu_x{}^3\mu_y w + \theta_3\mu_x\mu_y{}^3 w + \theta_4\mu_x{}^3\mu_y{}^3 w \\ & - \lambda[\beta_1(\mu_y\delta_x f^{(2)} + \mu_x\delta_y g^{(2)}) \\ & + \beta_2(\mu_x\delta_x f^{(1)} + \mu_y\delta_y g^{(1)}) + \beta_3(\mu_x\delta_x\mu_y{}^2 f^{(1)} + \mu_x{}^2\mu_y{}^2\delta_y g^{(1)}) \\ & + \beta_4(\delta_x\mu_y f + \mu_x\delta_y g) + \beta_5(\delta_x\mu_y{}^3 f + \mu_x{}^3\delta_y g) \\ & + \beta_6(\mu_x{}^2\delta_x\mu_y f + \mu_x\mu_y{}^2\delta_y g) + \beta_7(\mu_x{}^2\delta_x\mu_y{}^3 f + \mu_x{}^3\mu_y{}^2\delta_y g], \end{aligned} \tag{5c}$$

$$
\begin{aligned}
w^{(4)} = w - \lambda[&\gamma_1(\delta_x\mu_y f^{(3)} + \mu_x\delta_y g^{(3)}) \\
&+ \gamma_2(\mu_x\delta_x f^{(2)} + \mu_y\delta_y g^{(2)}) + \gamma_3(\mu_x\delta_x\mu_y{}^2 f^{(2)} + \mu_x{}^2\mu_y\delta_y g^{(2)}) \\
&+ \gamma_4(\delta_x\mu_y f^{(1)} + \mu_x\delta_y g^{(1)}) + \gamma_5(\delta_x\mu_y{}^3 f^{(1)} + \mu_x{}^3\delta_y g^{(1)}) \\
&+ \gamma_6(\mu_x{}^2\delta_x\mu_y f^{(1)} + \mu_x\mu_y{}^2\delta_y g^{(1)}) + \gamma_7(\mu_x{}^2\delta_x\mu_y{}^3 f^{(1)} + \mu_x{}^3\mu_y{}^2\delta_y g^{(1)}) \\
&+ \nu_1(\mu_x\delta_x f + \mu_y\delta_y g) + \nu_2(\mu_x\delta_x\mu_y{}^2 f + \mu_x{}^2\mu_y\delta_y g) \\
&+ \nu_3(\mu_x\delta_x\mu_y{}^4 f + \mu_x{}^4\mu_y\delta_y g) + \nu_4(\mu_x{}^3\delta_x f + \mu_y{}^3\delta_y g) \\
&+ \nu_5(\mu_x{}^3\delta_x\mu_y{}^2 f + \mu_x{}^2\mu_y{}^3\delta_y g) + \nu_6(\mu_x{}^3\delta_x\mu_y{}^4 f + \mu_x{}^4\mu_y{}^3\delta_y g)] \qquad (5d)
\end{aligned}
$$

(When the right-hand side of Eq. (1) is nonzero, Eq. (5) has additional terms multiplied by Δt. This inhomogenous case will be treated in a future paper on the shallow water equations.)

Having given this general algorithm, it remains to determine under which conditions is a scheme of fourth-order accuracy. We demand that the scheme be fourth-order in both space and time and for nonlinear as well as linear problems. Therefore, it is not sufficient to analyze the amplification matrix of the scheme. Instead, one must carry out the Taylor series and compare terms through fourth order in Δt and Δx. It was demonstrated in [3] that one cannot build such a scheme where the kth step is kth-order accurate. Hence, one must include all lower-order terms in the expansions and do comparisons only after calculating $w^{(4)}$. Then, $w^{(4)}$ is fourth-order accurate, but, in general, $w^{(1)}$, $w^{(2)}$, $w^{(3)}$ will only be first-order accurate. The complete expansion of $w^{(4)}$ is given in Appendix B. Here, we demonstrate the procedure for $w^{(1)}$ and $w^{(2)}$. Thus,

$$
\begin{aligned}
w^{(1)} &= \mu_x\mu_y w - \lambda a[\mu_y\,\delta_x f + \mu_y\,\delta_x g] \\
&= w + \frac{(\Delta x)^2}{8}(w_{xx} + w_{yy}) \\
&\quad - a\,\Delta t\left[f_x + g_y + \frac{(\Delta x)^2}{24}(f_{xxx} + 3f_{xyy} + g_{yyy} + 3g_{xxy})\right] \\
&= w + Dw.
\end{aligned}
$$

Then,

$$
\begin{aligned}
f^{(1)} &= f(w + Dw) \\
&= f + f_w Dw + \tfrac{1}{2}f_{ww}(Dw)^2 + \tfrac{1}{6}f_{www}(Dw)^3 + O((\Delta x)^4),
\end{aligned}
$$

where

$$
Dw = \frac{(\Delta x)^2}{8}\nabla^2 w + a\,\Delta t\left[w_t - \frac{(\Delta x)^2}{24}(f_{xxx} + g_{yyy} + 3(f_y + g_x)_{xy})\right].
$$

Differentiating, one finds that

$$f_x^{(1)} = f_x - a\,\Delta t\, w_{xt} + \tfrac{1}{2}(a\,\Delta t)^2\,(A_t w_t)_x - \tfrac{1}{6}(a\,\Delta t)^3\,(A_{tt}w_t - A_t w_{tt})_x + \frac{(\Delta x)^2}{8}\,(A(w_{xx} + w_{yy}))_x - \frac{a(\Delta t)(\Delta x)^2}{24}\,[A(f_x + 3g_y)_{xx} + 3A_t w_{xx} + A(3f_x + g_y)_{yy} + 3A_t w_{yy}]_x,$$

with a similar formula for $g_y^{(1)}$. Use is being made of the formulas

$$f_w = A, \qquad f_{ww} = \frac{A_t}{w_t},$$

$$f_t = A w_t, \qquad f_{www} = \frac{A_{tt}w_t - A_t w_{tt}}{w_t^3}.$$

One then substitutes these values of $f_x^{(1)}$ and $g_y^{(1)}$ into Eq. (5b). Then,

$$w^{(2)} = (\epsilon_1 + \epsilon_2 + \epsilon_3 + \epsilon_4)\,w + \frac{(\Delta x)^2}{4}\,[(\epsilon_2 + \epsilon_4)\,w_{xx} + (\epsilon_3 + \epsilon_4)\,w_{yy}] + (\alpha_1 + \alpha_2)\,\Delta t\, w_t + a\alpha_1(\Delta t)^2\, w_{tt} + \frac{1}{2}\,\alpha_1 a^2(\Delta t)^3\,[(A_t w_t)_x + (B_t w_t)_y] + \frac{\alpha_1(\Delta x)^2\,\Delta t}{8}\,[(A(w_{xx} + w_{yy}))_x + (B(w_{xx} + w_{yy}))_y + f_{xyy} + g_{xxy}] + \frac{\alpha_1 + 4\alpha_2}{24}\,(\Delta x)^2\,\Delta t(f_{xxx} + g_{yyy}).$$

One continues in this manner to evaluate $w^{(4)}$ (see Appendix B). This is then compared with $w(t + \Delta t)$ expanded in a Taylor Series, i.e., coefficients of $(\Delta t)^r$ in both, expansions are forced to be equal while coefficients of $(\Delta x)^k(\Delta t)^l$ in the expansion of $w^{(4)}$ are set equal to zero. When this is done for all the terms through $(\Delta t)^4$ (assuming $\Delta t/\Delta x$ is a constant), the following conditions are derived for the parameters appearing in formula (5).

(1) $\gamma_1 + \gamma_2 + \gamma_3 + \gamma_4 + \gamma_5 + \gamma_6 + \gamma_7 + \nu_1 + \nu_2 + \nu_3 + \nu_4 + \nu_5 + \nu_6 = 1,$

(2) $\gamma_1 t_3 + (\gamma_2 + \gamma_3)\,t_2 + (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\,t_1 = \tfrac{1}{2},$

(3) $\gamma_1 t_3^2 + (\gamma_2 + \gamma_3)\,t_2^2 + (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\,t_1^2 = \tfrac{1}{3},$

(4) $\gamma_1\beta_1 t_2 + \gamma_1(\beta_2 + \beta_3)\,t_1 + (\gamma_2 + \gamma_3)\,\alpha_1 t_1 = \tfrac{1}{6},$

(5) $\gamma_1 t_3^2 + (\gamma_2 + \gamma_3)\,t_2^3 + (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\,t_1^3 = \tfrac{1}{4},$

$$\gamma_1\beta_1 t_2 t_3 + \gamma_1(\beta_2+\beta_3)\, t_1 t_3 + (\gamma_2+\gamma_3)\,\alpha_1 t_1 t_2 = \tfrac{1}{8}, \tag{6}$$

$$\gamma_1\beta_1 t_2^2 + \gamma_1(\beta_2+\beta_3)\, t_1^2 + (\gamma_2+\gamma_3)\,\alpha_1 t_1^2 = \tfrac{1}{12}, \tag{7}$$

$$\gamma_1\beta_1\alpha_1 t_1 = \tfrac{1}{24}, \tag{8}$$

$$\gamma_1(\theta_1+4\theta_2+3\theta_4) + 2(\gamma_2+\gamma_3)(\epsilon_2+\epsilon_4) + \gamma_4+\gamma_5+\gamma_6+\gamma_7 = 0, \tag{9}$$

$$\gamma_1(\theta_1+4\theta_2+3\theta_4)\, t_3 + 2(\gamma_2+\gamma_3)(\epsilon_2+\epsilon_4)\, t_2 + (\gamma_4+\gamma_5+\gamma_6+\gamma_7)\, t_1 = 0, \tag{10}$$

$$2\beta_1\gamma_1(\epsilon_2+\epsilon_4) + \gamma_1(\beta_2+\beta_3) + (\gamma_2+\gamma_3)\,\alpha_1 = 0, \tag{11}$$

$$\gamma_1(\beta_1+4\beta_2+4\beta_3+\beta_4+\beta_5+7\beta_6+7\beta_7) + (\gamma_2+\gamma_3)(\alpha_1+4\alpha_2) + (\gamma_4+\gamma_5+\gamma_6+\gamma_7)\, t_1 = 0, \tag{12}$$

$$\gamma_1(\beta_1+2\beta_3+\beta_4+3\beta_5+\beta_6+3\beta_7) + (\gamma_2+\gamma_3)\,\alpha_1 + (\gamma_4+\gamma_5+\gamma_6+\gamma_7)\, t_1 = 0, \tag{13}$$

$$\gamma_1 + 4(\gamma_2+\gamma_3) + \gamma_4+\gamma_5 + 7(\gamma_6+\gamma_7) + 4(\nu_1+\nu_2+\nu_3) + 10(\nu_4+\nu_5+\nu_6) = 0, \tag{14}$$

$$\gamma_1 + 2\gamma_3 + \gamma_4 + 3\gamma_5 + \gamma_6 + 3\gamma_7 + 2\nu_2 + 4\nu_3 + 2\nu_5 + 4\nu_6 = 0, \tag{15}$$

$$\gamma_1 t_3 + 4(\gamma_2+\gamma_3)\, t_2 + (\gamma_4+\gamma_5+\gamma_6+\gamma_7)\, t_1 = 0, \tag{16}$$

$$\gamma_1 t_3 + 2\gamma_3 t_2 + (\gamma_4+3\gamma_5+\gamma_6+3\gamma_7)\, t_1 = 0, \tag{17}$$

where

$$t_1 = a, \tag{18}$$

$$t_2 = \alpha_1 + \alpha_2\,, \tag{19}$$

$$t_3 = \beta_1+\beta_2+\beta_3+\beta_4+\beta_5+\beta_6+\beta_7\,, \tag{20}$$

are the times at which the intermediate levels are located.

We also demand that $w^{(2)}$, $w^{(3)}$ be at least first order, and hence,

$$\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4 = 1, \tag{21}$$

$$\theta_1+\theta_2+\theta_3+\theta_4 = 1. \tag{22}$$

Finally, from symmetry of x and y we have

$$\epsilon_2 = \epsilon_3\,, \tag{23}$$

$$\theta_2 = \theta_3\,. \tag{24}$$

(6)

We note that the first eight equations are identical with those of the fourth-order Runge–Kutta ordinary differential equations (see Ralston [21]). In sum, we have 24 nonlinear equations for 34 variables, and so expect that system (6) will represent a multiparameter fourth-order family of schemes. In fact, we shall assume that the parameters

$$t_1 , t_2 , \epsilon_2 , \theta_2 , \beta_2 , \beta_7 , \gamma_3 , \gamma_7 , \nu_3 , \nu_5 , \nu_6$$

can be chosen arbitrarily. We can then express the general solution to Eqs. (6) in terms of these 11 free parameters. For a solution to exist, we must assume that $t_1 \neq 1$ and $t_2 \neq 1$. Under these circumstances, we have two sets of solutions.

If $t_1 = t_2$, a solution exists only if $t_1 = 1/2$. However, in this case, the amplification matrix turns out to be unstable, and so we shall not describe this case. If $t_1 \neq t_2$ we must have $t_1 \neq 1/2$. In summary, the following conditions are assumed to hold

$$t_1 \neq 0, \quad t_1 \neq \tfrac{1}{2}, \quad t_1 \neq 1, \quad t_2 \neq 0, \quad t_2 \neq 1, \quad t_2 \neq t_1 .$$

The general solution to system (6) in terms of the above free parameters is

$$t_3 = 1, \qquad \text{(this is also true for O.D.E.)}$$

$$\gamma_1 = \frac{(1/4) - ((t_1 + t_2)/3) + (t_1 t_2/2)}{(1 - t_1)(1 - t_2)},$$

$$\gamma_2 = \frac{1 - 2t_1}{12t_2(1 - t_2)(t_2 - t_1)} - \gamma_3 ,$$

$$\bar{\gamma} = -\frac{1 - 2t_1}{12t_1(1 - t_1)(t_2 - t_1)},$$

$$\gamma_6 = -\frac{(1/2) + t_2 - 2t_1 + t_2 t_1 - t_2^2}{12t_1(1 - t_2)(t_2 - t_1)} - \gamma_7 ,$$

$$\gamma_5 = -\frac{\gamma_1}{2t_1} - \frac{\gamma_3 t_2}{t_1} - \frac{\bar{\gamma}}{2},$$

$$\gamma_4 = \bar{\gamma} - \gamma_5 - \gamma_6 - \gamma_7 ,$$

$$\nu_2 = -\frac{\gamma_1}{2}\left(1 - \frac{1}{t_1}\right) - \gamma_3\left(1 - \frac{t_2}{t_1}\right) - 2\nu_3 - \nu_5 - 2\nu_6 ,$$

$$\nu_1 = \frac{5}{3} - \frac{3\gamma_1 + 2(\gamma_2 + \gamma_3) + 3(\gamma_4 + \gamma_5) + \gamma_6 + \gamma_7}{2} - \nu_2 - \nu_3 ,$$

$$\nu_4 = \frac{1}{2}(\gamma_1 + \gamma_4 + \gamma_5 - \gamma_6 - \gamma_7) - \frac{2}{3} - \nu_5 - \nu_6 ,$$

$$
\begin{aligned}
\epsilon_3 &= \epsilon_2 , \\
\epsilon_4 &= \frac{t_2(1-2t_2)}{2t_1(1-2t_1)} - \epsilon_2 , \\
\epsilon_1 &= \frac{1}{2} - 2\epsilon_2 - \epsilon_4 , \\
\theta_3 &= \theta_2 , \\
\theta_1 &= \frac{3}{2} - \frac{1}{12t_1}\frac{(1/2)-t_2}{(1/4)-((t_1+t_2)/3)+(t_1t_2/2)} - \theta_2 , \\
\theta_4 &= 1 - 2\theta_2 - \theta_1 , \\
\alpha_1 &= \frac{t_2(t_2-t_1)}{2t_1(1-2t_1)} , \\
\alpha_2 &= t_2 - \alpha_1 , \\
\beta_1 &= \frac{1-2t_1}{12\gamma_1 t_2(t_2-t_1)} , \\
\beta_3 &= \frac{-\alpha_1(\gamma_2+\gamma_3)}{\gamma_1} + 2\beta_1(\epsilon_2+\epsilon_4) - \beta_2 , \\
\beta_6 &= -\frac{1}{6}\left[1 + 3(\beta_2+\beta_3) + \frac{1}{(1/4)-((t_1+t_2)/3)+(t_1t_2/2)}\right. \\
&\qquad \left. \times \left(\frac{(\alpha_1+4\alpha_2)(1-2t_1)}{12t_2} + \frac{1-2t_2}{12}\right)\right] - \beta_7 , \\
\beta_5 &= \frac{-\alpha_1(\gamma_2+\gamma_3) - \bar{\gamma}t_1}{2\gamma_1} - \frac{1}{2}(1-\beta_2-\beta_3+2\beta_7), \\
\beta_4 &= 1 - \beta_1 - \beta_2 - \beta_3 - \beta_5 - \beta_6 - \beta_7 , \\
a &= t_1 .
\end{aligned} \tag{7}
$$

We thus have a multiparameter family of schemes that is fourth order in both space and time. We would like to choose these parameters to optimize the properties of the scheme. For example, we would like to achieve a stability condition that allows a large Δt; we would also like to minimize the phase error. Furthermore, depending on the problem, we would like to either maximize or minimize the inherent dissipation of the scheme for long wave numbers. Thus, for smooth problems, we would like a small amount of dissipation, though it is obvious that we cannot eliminate it entirely. For problems with strong shocks, we would wish to maximize the dissipation to eliminate nonlinear instabilities. Since the dissipation

is inherent within the scheme, rather than imposed artificially, it is hoped that this inherent dissipation will yield physically meaningful results and not just smooth out all information, as can happen when adding a large amount of artificial dissipation to a nondissipative scheme.

In this paper, we shall not attempt to analyze the effects of choosing various sets of parameters. Instead, we shall find the amplification matrix, and arbitrarily choose one set of parameters that seems to allow large time steps consistent with stability. In a future paper, we shall analyze ways of improving the results of Section 4 by a more judicious choice of free parameters.

3. Amplification Matrix

Denoting the finite-difference scheme (5) by

$$w^{n+1} = C(t)\, w^{(n)},$$

we calculate the amplification matrix $G(\alpha, \beta)$ by the standard method

$$G(\alpha, \beta) = e^{-i(k_x \Delta x + k_y \Delta y)} C(t)\, e^{i(k_x \Delta x + k_y \Delta y)},$$

where

$$\alpha = k_x \Delta x, \quad \beta = k_y \Delta y; \quad -\pi \leqslant \alpha \leqslant \pi, \quad -\pi \leqslant \beta \leqslant \pi.$$

To simplify notation, we introduce new variables ξ, η defined by

$$\xi = \sin \frac{\alpha}{2}, \qquad \eta = \sin \frac{\beta}{2} \tag{8}$$

and consider G as a function of ξ and η. We note that the Fourier transform of μ_x is simply $(1 - \xi^2)^{1/2}$ while the Fourier transform of δ_x is just $2i\xi$, and similarly for the other space dimensions. We also introduce the matrices

$$\begin{aligned} M &= A\xi(1 - \eta^2)^{1/2} + B\eta(1 - \xi^2)^{1/2}, \\ R &= \xi\eta[A\eta(1 - \xi^2)^{1/2} + B\xi(1 - \eta^2)^{1/2}]. \end{aligned} \tag{9}$$

In terms of these variables we have, after a considerable amount of manipulation,

$$\begin{aligned} G(\xi, \eta) = I &+ 2i(1 - \xi^2)^{1/2}(1 - \eta^2)^{1/2}\, M[1 + (2/3)(\xi^2 + \eta^2) + \sigma_1 \xi^2 \eta^2] \\ &+ (2/3)\, iR[1 - 3\sigma_2(\xi^2 + \eta^2) + 3\sigma_3 \xi^2 \eta^2] \\ &- 2M^2[1 + (1/3)(\xi^2 + \eta^2) + 2\sigma_4 \xi^2 \eta^2] \\ &- 2/3(1 - \xi^2)^{1/2}(1 - \eta^2)^{1/2}(MR + RM) - 4\alpha_2 \gamma_2 R^2 \\ &- (4i/3)(1 - \xi^2)^{1/2}(1 - \eta^2)^{1/2}\, M^3 \\ &- 8i[\gamma_1 \beta_1 \alpha_2 M^2 R + \gamma_1 \beta_2 t_1 MRM + \gamma_2 \alpha_1 t_1 RM^2] + (2/3)\, M^4, \end{aligned} \tag{10}$$

where

$$\begin{aligned}
\sigma_1 &= \gamma_1\theta_4 + (\gamma_2 + \gamma_3)\,\epsilon_4 + \gamma_6 + \gamma_7 - \gamma_5 + \nu_5 + \nu_6 - \nu_3\,,\\
\sigma_2 &= \gamma_2(\epsilon_2 + \epsilon_4) + \gamma_6 - \gamma_5 - \nu_3 + \nu_4 + \nu_5\,,\\
\sigma_3 &= \sigma_2 - \gamma_2\epsilon_2 - \nu_4\,,\\
\sigma_4 &= \gamma_1(\beta_1\epsilon_4 + \beta_2 + \beta_3 - \beta_5 + \beta_6 + \beta_7) + (\gamma_2 + \gamma_3)\,t_2 + (\gamma_6 + \gamma_7 - \gamma_5)\,t_1\,,
\end{aligned} \tag{11}$$

the σ_i can be chosen arbitrarily without affecting fourth-order accuracy. We first consider the case where $\alpha_2\gamma_2 = 0$, i.e., the R^2 term vanishes. If A and B are scalar, we can choose ξ_0, η_0 so that $M = 0$. Then,

$$G(\xi_0, \eta_0) = I + \tfrac{2}{3}iR[1 - 3\sigma_2(\xi_0^2 + \eta_0^2) + 3\sigma_3\xi_0^2\eta_0^2],$$

and obviously,

$$|\,G(\xi_0, \eta_0)| > 1, \qquad \text{if } \xi_0, \eta_0 \text{ are small.}$$

Hence, if we wish stability for all scalar A and B, we must choose $\alpha_2\gamma_2 \neq 0$, in fact, $\alpha_2\gamma_2 > \frac{1}{18}$. Even in the case of scalar A and B, the stability criterion is far from trivial, and so the choice of the parameters is largely a question of intelligent guessing.

To select a set of parameters, we first set $\beta_7 = \gamma_7 = \nu_6 = 0$, to reduce the number of arithmetic operations in calculating the finite difference formula (5). We next note that in the amplification matrix the coefficients of M^2R, MRM, RM^2 are all free. We wish $G = S + iJ$ to have symmetric S and J when A and B are symmetric. We thus require

$$\gamma_1\beta_1\alpha_2 = (\gamma_1\beta_2 t_1/2) = \gamma_2\alpha_1 t_1\,.$$

If we also wish t_1 and t_2 to be rational, this implies $t_1 = \frac{1}{6}$, $t_2 = \frac{1}{3}$, and hence, determines β_1, β_2, γ_1, γ_2, α_1, α_2. The only free parameters remaining are ϵ_4, θ_4, ν_3, ν_5. We determine these by choosing values for the parameters σ_1, σ_2, σ_3, σ_4, which appear in the amplification matrix (Eqs. (10) and (11)).

A preliminary guess at appropriate values are $\sigma_1 = \sigma_2 = \sigma_3 = 0$ and $\sigma_4 = -\frac{1}{2}$. With this choice, the parameters in Eq. (5) take on the following values

$$\begin{array}{llllllll}
t_1{=}1/6, & t_2{=}1/3, & t_3{=}1, & & & & & \\
a{=}1/6, & & & & & & & \\
\alpha_1{=}1/4, & \alpha_2{=}1/12, & & & & & & \\
\epsilon_1{=}11/6, & \epsilon_2{=}{-}(4/3), & \epsilon_3{=}{-}(4/3), & \epsilon_4{=}11/6, & & & & \\
\beta_1{=}5, & \beta_2{=}5, & \beta_3{=}{-}(95/8), & \beta_4{=}{-}(22/3), & \beta_5{=}15/2, & \beta_6{=}65/24, & \beta_7{=}0, & \\
\theta_1{=}17/12, & \theta_2{=}5/6, & \theta_3{=}5/6, & \theta_4{=}{-}(25/12), & & & & \\
\gamma_1{=}1/5, & \gamma_2{=}2 & \gamma_3{=}{-}(1/2), & \gamma_4{=}{-}(1/5), & \gamma_5{=}1, & \gamma_6{=}{-}2, & \gamma_7{=}0, & \\
\nu_1{=}{-}(10/3), & \nu_2{=}25/6, & \nu_3{=}{-}(7/6), & \nu_4{=}8/3, & \nu_5{=}{-}(11/6), & \nu_6{=}0, & &
\end{array} \tag{12}$$

and the amplification matrix becomes

$$\begin{aligned} G(\xi, \eta) = I &+ 2i(1 - \xi^2)^{1/2}(1 - \eta^2)^{1/2} M[1 + (2/3)(\xi^2 + \eta^2)] + (2/3)\, iR \\ &- 2M^2[1 + (1/3)(\xi^2 + \eta^2) - \xi^2\eta^2] - (2/3)(1 - \xi^2)^{1/2} \\ &\times (1 - \eta^2)^{1/2}(MR + RM) - (2/3)\, R^2 \\ &- (4i/3)(1 - \xi^2)^{1/2}(1 - \eta^2)^{1/2}\, M^3 \\ &- (2i/3)(M^2R + 2MRM + RM^2) + (2/3)\, M^4, \end{aligned} \tag{13}$$

where ξ, η, M, R are given by Eqs. (8) and (9).

Thus far, we have been unable to derive analytically a sufficient stability criterion for this amplification matrix. Our experience has been that, if one restricts oneself to symmetric matrices A and B, then the worst case happens when A and B commute. Thus, for example, the Lax–Wendroff scheme has its most stringent stability conditions when $A = B$ (similarly, see Eilon, Gottlieb, and Zwas [9]). When A and B commute, one can use the spectral mapping theorem to replace the matrices A and B by their respective eigenvalues, and so reduce the problem to a scalar one. Even in this case, it is difficult to determine analytically the stability condition. However, in this case we can solve the problem computationally, i.e., we consider a range of scalars a, b, $-2 \leqslant a \leqslant 2$, $-2 \leqslant b \leqslant 2$ and evaluate G for a discrete set of ξ and η. We then find that a sufficient condition for $|\, G(\xi, \eta)| \leqslant 1$ is that

$$(\Delta t/\Delta x)\, \rho(A) \leqslant 1 \qquad \text{and} \qquad (\Delta t/\Delta y)\, \rho(B) \leqslant 1,$$

where $\rho(A) = a$ is the spectral radius of A. We note that this allows larger time steps than most second-order two-dimensional methods. Numerical experiments, with the two-dimensional wave equation, fluid dynamic system and the linear elastic system indicates that in these cases, we can exceed even these time steps and maintain stability. (The C.F.L. number for the fluid dynamic system exceeds 1.3).

4. Results

Swartz and Wendroff [24] have indicated that there are basically three ways of comparing schemes. The first is simply to run the schemes on several problems of interest and to compare them with respect to core storage requirements and efficiency in running time. Thus, we assume an error tolerance and decrease the space mesh width and/or time steps until this error level is reached. Of course, this assumes a knowledge of the analytic solution. This can be achieved either by choosing simple problems for which the analytic solution is known, or alternatively solving the problem computationally with a fine enough grid to ensure errors considerably below that which is being used in the test problems. This approach

seems to be the most practical from a users viewpoint, especially if he is interested in one particular system of equations. The main difficulties of the method are the programming problems. Thus, it is difficult to ascertain that the several programs have all been optimized to the same degree. For example, the comparisons may be very different if the programming is done in assembly language, at least in part, or completely in some higher compiler language. Also, results will vary, depending on whether the coding has attempted to minimize core storage or to minimize running time.

An alternative method of comparing schemes is to compare their truncation errors under the assumption that only the leading term is of importance. This method is, of course, limited to linear problems, as it is difficult to compare the effects of unknown nonlinear terms in the algorithm. On using this method for higher-order methods in space and time, one finds that the truncation error consists of sums of many higher-order derivatives with varying coefficients. This makes direct comparisons exceedingly complicated. A further difficulty is encountered in schemes that are more accurate in the space variables than the time dimension. One must decide in advance whether one considers a sequence for which $\Delta t/\Delta x =$ constant or $\Delta t/\Delta x \to 0$ as Δx approaches zero. The different assumptions will greatly affect the treatment of truncation errors or boundary treatment. However, in practice, one does not work with a sequence of meshes tending to zero, and so this should not affect practical considerations.

A third possibility is to compare the schemes with respect to very simple problems and assume that these results have general validity. This method is usually very disadvantageous to schemes that are of higher-order of accuracy in both space and time. First, one frequently only discretizes the space variables in such an analysis (see, for example, Kreiss and Oliger [16]). Thus, the whole advantage of higher temporal accuracy is lost. Furthermore, the obviously complicated formulas needed for higher time accuracy are obviously inefficient when the equations are simple. However, the additional work is of less importance if the calculation of the fluxes and forcing terms is of sufficient complexity. For these reasons, we have chosen to revert to the first idea and will compare schemes on the basis of actual computer runs on sample problems.

The first problem that we shall consider is the wave equation in two space dimension, with periodic boundary conditions, i.e.,

$$u_t = v_x + w_y, \qquad v_t = u_x, \qquad w_t = u_y, \tag{14}$$

with $0 \leqslant x \leqslant 2^{1/2}$, $0 \leqslant y \leqslant 2^{1/2}$, $0 \leqslant t \leqslant 2$, and initial conditions

$$\begin{aligned} u(x, y, 0) &= \sin(n\pi((x + y)/2^{1/2})], \\ v(x, y, 0) &= -(1/2^{1/2}) \sin[n\pi((x + y)/2^{1/2}], \\ w(x, y, 0) &= -(1/2^{1/2}) \sin[n\pi((x + y)/2^{1/2})], \end{aligned}$$

n an integer. The solution is then

$$\begin{aligned} u(x, y, t) &= \sin[n\pi((x + y)/2^{1/2} - t)], \\ v(x, y, t) &= -(1/2^{1/2}) \sin[n\pi((x + y)/2^{1/2} - t)], \\ w(x, y, t) &= -(1/2^{1/2}) \sin[n\pi((x + y)/2^{1/2} - t)]. \end{aligned} \tag{15}$$

As typical second-order methods, we choose the rotated Richtmyer scheme (see, for example, Wilson [28]) and the leapfrog method. For reasons of programming simplicity, the Kreiss–Oliger algorithm [16] was chosen to represent methods that are second order in time, but fourth order in space. This is by no means an exhaustive list, and there is need of additional tests.

As a measure of the accuracy of the numerical solution, we shall use a normalized L_2 norm. Thus, the error is defined as

$$E = \left(\frac{\sum [u(x, y, t) - u_{i,j}^n]^2}{\sum (u_{i,j}^0)^2} \right)^{1/2},$$

where the sum is over all net points within the period rectangle, and also, over all components of the vector.

In Table I, we give the mesh spacings and running times required for different

TABLE I

Wave Equation ($n = 1$)

Method	Mesh	$\Delta t/\Delta x$	Error	Time (sec)
Rotated Richtmyer	40 × 40	0.75	0.0712	93.5
Rotated Richtmyer	60 × 60	0.75	0.0318	306.0
Leapfrog	40 × 40	0.50	0.0261	5.2
Leapfrog	60 × 60	0.50	0.0115	16.3
Leapfrog	65 × 65	0.50	0.0098	21.0
Four step	19 × 19	1.30	0.0099	14.8

error levels, with the longest wave $n = 1$ (see Eq. (15)). This table compares the four-step method given by Eq. (5) and Eq. (12) with the second-order methods. Thus, it is estimated that, to achieve a one-percent error, the rotated Richtmyer method will take about 60 times as long as the four-step method and require much more storage.

The leapfrog scheme requires almost double the time of the fourth-order method. This comparative competitiveness of the leapfrog method will disapper with the

use of more complicated equations. Even in this simple case, the leapfrog method requires about 25 times as many net points as does the fourth-order method. Hence, for realistic problems, the core requirements of the second-order methods will greatly exceed the central storage capacities of any of the present day computing machines.

Before continuing, we shall briefly discuss the problem of programming. The Lax–Wendroff type schemes were programmed allowing general fluxes $f(u)$, $g(u)$ and minimizing computer storage. The coding for the leap frog and Kreiss–Oliger methods followed the general outline of the Williamson and Browning [27] program. As in all multilevel schemes, the storage requirements exceed those of

[redacted]

the core required by the fourth-order one-level method. As for running times, the ones obtained for the wave equation by the four-step scheme are much longer than could have been achieved by a different programming approach. The fourth-order method is at a disadvantage in timing analysis for a simple linear wave equation. For more realistic problems, where the fluxes are more complicated, the fourth-order method will improve relative to the other methods.

For methods that are of equal order, in both space and time, the error decreases as we increase the time step, for a fixed space mesh. That is, the error is smallest, for both shock and smooth problems, when the time step is chosen as close to the Courant number as possible. In Table II, we show the error that results from

TABLE II

Four-step Method with a Mesh of 18×18 ($n = 1$)

$\Delta t/\Delta x$	Error	Time
0.50	0.0178	32.4
0.75	0.0147	21.4
1.00	0.0121	16.5
1.10	0.0117	15.3
1.20	0.0116	14.0
1.25	0.0118	13.4
1.30	0.0122	12.8

using the four-step method with varying time steps, but a constant mesh width of 18×18. We see that the error is only mildly dependent on the time step, and the larger Δt yields a more efficient scheme.

When one considers methods that are second order in time, but fourth order

in space, this conclusion is no longer true. The choice of the most efficient time step now depends on the permitted error levels, the mesh width, and the wave lengths. In Table IIIa are listed the mesh spacings and running times required to give a one percent error ($E = 0.01$). This table is for the Kreiss–Oliger scheme, with varying time steps for the lowest frequency, $n = 1$. In Table IIIb, the results are given for $E = 0.005$. We see that for the low wave number and the proper

TABLE IIIa

Kreiss–Oliger Method ($n = 1$)

$\Delta t/\Delta x$	Mesh	Error	Time
0.50	65×65	0.0097	31.70
0.25	32×32	0.0095	7.80
0.15	12×12	0.0047	0.77
0.10	14×14	0.0081	1.75
0.05	16×16	0.0081	5.06

TABLE IIIb

$\Delta t/\Delta x$	Mesh	Error	Time
0.25	45×45	0.0049	21.45
0.15	22×22	0.0049	4.28
0.10	16×16	0.0033	2.56
0.05	18×18	0.0048	7.09

choice of Δt, the Kreiss–Oliger scheme is more efficient than the four-step method. However, the choice of $\Delta t = 0.5$ would have lead to a different conclusion. We also see that the error does not decrease monotonically as one decreases the step size in either the space or time directions. In Table IV, we show the error for fixed $\Delta t/\Delta x = 0.15$, while Δx, Δy vary. We see that the error does not decrease monotonically, even for small error levels, when, hopefully, the scheme is within its asymptotic range. The reason is that there is a fortuitous cancellation of errors at certain mesh lengths (see also Swartz and Wendroff [25]). Halving the mesh size reduces the error by a factor less than four. Hence, it may be more appropriate to consider sequences where $(\Delta t)^2/\Delta x$ is constant, rather than $\Delta t/\Delta x$. This, however, will affect the treatment of boundary conditions. In Tables Va and Vb, we fix the mesh at 15×15 and 30×30, respectively, and vary $\Delta t/\Delta x$. The error reaches

TABLE IV

Kreiss–Oliger Method ($\Delta t/\Delta x = 0.15$, $n = 1$)

Mesh	Error	Time
10×10	0.0252	0.46
11×11	0.0122	0.58
12×12	0.0047	0.77
13×13	0.0002	0.96
14×14	0.0024	1.18
15×15	0.0039	1.44
20×20	0.0052	3.27
25×25	0.0043	6.21
30×30	0.0033	10.78
40×40	0.0021	25.40

TABLE Va

Kreiss–Oliger Method (Mesh 15×15, $n = 1$)

$\Delta t/\Delta x$	Error	Time
0.50	0.1762	0.50
0.25	0.0332	0.88
0.15	0.0039	1.44
0.10	0.0052	2.13
0.05	0.0107	4.21

TABLE Vb

Kreiss–Oliger Method (Mesh 30×30, $n = 1$)

$\Delta t/\Delta x$	Error	Time
0.50	0.0451	3.38
0.25	0.0107	6.39
0.15	0.0033	10.79
0.10	0.0010	16.22
0.05	0.0003	32.36

a minimum at some $\Delta t/\Delta x$, which decreases with finer mesh spacings. As $\Delta t/\Delta x$ goes to zero, for fixed Δx, Δy, the error does not continually decrease (compare with Gary [10]). It is not clear what affect this will have on techniques utilizing Richardson extrapolation.

The Kreiss–Oliger method was then used to solve the wave equation with an initial wave number of two. In Table VI, we see that the mesh widths required for a 0.01 error are not half of those required for $n = 1$ and the same error level (Table IIIa). For example, for $\Delta t/\Delta x = 0.25$, $n = 1$ and $E = 0.01$, we require a mesh of 32×32 (Table IIIa). When we increase to $n = 2$ the Kreiss–Oliger scheme now requires a mesh of 90×90 (Table VIa). This is half the mesh width that was used when $n = 1$, but $E = 0.005$ (Table IIIb). Thus, it is not enough to specify the number of mesh points per wavelength, but one must state with respect to which wave number. Even if one chooses $\alpha = (\Delta t)/(\Delta x)^2$ constant the optimal α is wave number dependent.

TABLE VIa

Kreiss–Oliger Method ($n = 2$)

$\Delta t/\Delta x$	Mesh	Error	Time
0.25	90×90	0.0099	168.5
0.15	44×44	0.0098	33.5
0.10	31×31	0.0084	17.8
0.05	36×36	0.0097	55.2

TABLE VIb

Four-Step Method

$\Delta t/\Delta x$	Mesh	Error	Time
1.30	41×41	0.0147	148.5
1.30	46×46	0.0095	211.5

The four-step fourth-order method is more efficient than the Kreiss–Oliger method for sufficiently small error levels. The exact level of this error tolerance will depend on the complexity of the equations. The above argument shows that the fourth-order method will also be more effcient when we fix the error level, but allow higher frequencies to enter the solution. Thus, even in the simple wave equation, the four-step method is faster if n is chosen sufficiently large. For realistic

problems it is not clear what wavelengths will appear, and hence, what is the optimal choice of $\Delta t/\Delta x$ for the second-order time but fourth-order space schemes. Thus, much of its speed advantages at low frequencies may not be realizable. At higher frequencies, the unequal treatment of space and time is a disadvantage.

It is obvious that, as the computational time needed for an evaluation of the flux terms increases, that the four-step method becomes more competitive. Thus, for sufficiently complex f and g, the four-step method requires four flux evaluations for f and g at each mesh point. The optimal time step for the Kreiss–Oliger scheme is about one tenth that of the fourth-order method. Hence, in this case, the Kreiss–Oliger method will take about two and one-half times as long to compute the solution on the same mesh.

As a second problem, we consider wave motion down an infinite elastic plate. The equations are those of linear elasticity, i.e.,

$$\begin{aligned}
\rho u_t &= \tau_{11,x} + \tau_{12,y}\,, \\
\rho v_t &= \tau_{12,x} + \tau_{22,y}\,, \\
\tau_{11,t} &= (2\mu + \lambda) + \lambda v_y\,, \\
\tau_{12,t} &= \mu(u_y + v_x), \\
\tau_{22,t} &= \lambda u_x + (2\mu + \lambda)\, v_y\,,
\end{aligned}$$

where ρ, λ, μ are positive constants. The solution is periodic in the x direction, and so we integrate the equations in the domain $0 \leqslant x \leqslant 1$, $0 \leqslant y \leqslant 1$. We assume periodic boundary conditions in the x direction and symmetry about the y-axis, $y = 0$. At $y = 1$, we have free surface conditions, $\tau_{12} = \tau_{22} = 0$. For details of this problem and its solution, see Mindlin [18] and Turkel [26]. As a measure of accuracy of the solution, we shall now consider phase velocities rather than L_2 errors.

Let pos(u) denote the position of the zero of the u component of velocity. This is found for each y and then averaged in the y direction. We then define the phase error by

$$E_p = \frac{\text{pos}(u(x, y, t)) - \text{pos}(u^n_{i,j})}{\text{pos}(u(x, y, t))}\,.$$

We also define the energy loss by

$$\text{WCHG} = \frac{\text{initial energy} - \text{energy at time } t}{\text{initial energy}}\,,$$

the solution was calculated using a mesh of 16×16 and time steps

$$\Delta t = \frac{\text{CFL} \cdot (\Delta x)}{((\lambda + 2u)/\rho)^{1/2}}\,,$$

with CFL = 0.471, and CFL = 0.754. The numerical solution was found for four periods of the analytic solution. For the analytic solution, WCHG is identically zero, and hence, a negative numerical WCHG indicates instability.

The periodicity conditions in the x direction and the axis of symmetry, $y = 0$, pose no special problems for a fourth-order method. However, the boundary $y = 1$ requires special treatment. Any fourth-order method in the space direction requires a domain of dependence of at least two mesh widths in each direction. Hence, the standard difference equations cannot be used along the lines $y = 1$ and $y = 1 - \Delta y$. Once the solution is known along $y = 1 - \Delta y$, the solution on the upper boundary $y = 1$ can be found by space extrapolation. The four-step method is not dissipative in the sense of Kreiss, since $|G(\pi, \pi)| = 1$. Nevertheless, space extrapolation does not seem to cause serious difficulties.

Along the line interior to the boundary, two techniques were tried. The first was to use a second-order two step method. Several such methods were tried, but the resultant hybrid schemes were all unstable. Preliminary analysis indicates that the difference in phase speeds in the two sets of equations, second and fourth order, leads to incorrect coupling of the solutions (compare Browning, Kreiss, and Oliger [6]). Evidently, the boundary value problem still requires much analysis. As a substitute method, the analytic solution was prescribed along $y = 1 - \Delta y$ and space extrapolation used for $y = 1$. This time, no instabilities were detected. In Table VII, the results of the four-step method are compared with several second-order methods. As expected, the phase error and dissipation are both decreased when using higher-order methods. The dissipation in the fourth-order method decreases markedly as the time step is increased, consistent with stability requirements. In fact, for CFL = 1.047, the energy loss is about $\frac{1}{25}$ of that found for CFL = 0.471.

As a third problem, we consider a rotating cone, or the color problem (see Burstein and Mirin [7], Orszag [19]). The equation is given by

$$r_t - yr_x + xr_y = 0, \qquad -1 \leqslant x \leqslant 1, \quad -1 \leqslant y \leqslant 1, \tag{17}$$

where r denotes the height of the cone. Though the problem is linear, the coefficients are now functions of the space variables. The initial condition is

$$= 0, \qquad (x - x_0)^2 + y^2 > r^2.$$

The solution is simply the inverted cone rotating uniformly about the origin. In Table VIII is shown that the maximum and minimum of the solution at mesh points, after one complete revolution with $x = y = \frac{1}{32}$. The pseudospectral method includes wave numbers through 16. We see that the fourth-order method

TABLE VIIa

Elastic Waves (Mesh 16 × 16, CFL = 0.471)

Scheme	WCHG	E_p
Lax–Wendroff	0.130	0.027
Leapfrog	−0.009	0.029
Time splitting	0.176	0.026
Rotated Richtmyer	0.171	0.068
Burstein	0.035	0.047
Fourth order	0.116	0.001

TABLE VIIb

Elastic Waves (Mesh 16 × 16, CFL = 0.754)

Scheme	WCHG	E_p
Lax–Wendroff	−0.748	0.020
Leapfrog	Unstable	—
Time splitting	0.179	0.020
Rotated Richtmyer	0.209	0.060
Burstein	−0.028	0.042
Fourth order	0.025	0.001

TABLE VIII

Rotating Cone (Mesh 32 × 32, One Complete Revolution)

Method	Maximum at gridpoint	Minimum
Arakawa second order	0.51	−0.23
Arakawa fourth order	0.83	−0.10
Pseudospectral (k = 16)	0.98	−0.02
Four step fourth order	0.78	−0.09

decreases the amplitude of the cone. This is to be expected, since the scheme is dissipative. The dissipation is about the same as the second order in time and fourth order in space Arakawa scheme, but considerably less than second-order methods. The dissipation of the fourth-order method also decreases the negative overshoots. It still remains to be determined if the pseudospectral method requires prohibitive running times, especially for complicated boundary shapes.

As a final application, we consider a fluid dynamic problem with a strong shock. The equations are

$$\begin{aligned} \rho_t + (\rho u)_x + (\rho v)_y &= 0, \\ (\rho u)_t + (\rho u^2 + p)_x + (\rho uv)_y &= 0, \\ (\rho v)_t + (\rho uv)_x + (\rho v^2 + p)_y &= 0, \\ E_t + (u(E + p))_x + (v(E + p))_y &= 0, \end{aligned} \tag{18}$$

with $p = 0.4\rho e$, $E = \rho[e + \frac{1}{2}(u^2 + v^2)]$.

The initial conditions represent a circular diaphragm problem, i.e., two sets of constant states, separated by a diaphragm which is removed at $t = 0$. Thus, for $x^2 + y^2 \leqslant 1$,

$$\begin{aligned} \rho(x, y, 0) &= 1, \qquad u(x, y, 0) = 0, \\ v(x, y, 0) &= 0, \qquad p(x, y, 0) = 1, \end{aligned}$$

while for $x^2 + y^2 > 1$, the initial condition is

$$\begin{aligned} \rho(x, y, 0) &= 4, \qquad u(x, y, 0) = 0, \\ v(x, y, 0) &= 0, \qquad p(x, y, 0) = 4. \end{aligned}$$

The solution consists of a shock wave that implodes towards the origin. Upon reaching the origin, the shock reflects and expands outwards. The analytic solution to this problem is not known. However, by introducing polar coordinates, one can reduce this to a one-dimensional problem, which then can be solved with a fine mesh. It is obvious that the two-dimensional approach cannot be as efficient as the one-dimensional method. The purpose is not to gain new answers to the cylindrical shock problem, but to demonstrate that the fourth-order method automatically handles even strong shocks. The solution to the two-dimensional problem by the fourth-order method is compared with the solution obtained by Abarbanel and Goldberg [1] to the one-dimensional problem. For the $2D$ problem, a mesh was chosen so that there are 25 points per radius. Since the domain of integration is $-2 \leqslant x \leqslant 2$ and $-2 \leqslant y \leqslant 2$, the total mesh was 100×100,

not including reflection lines to handle the exterior boundaries. It was found that one could choose the time step so that

$$\Delta t \leqslant 1.2\Delta x/\max_{i,j}[|u| + c; |v| + c].$$

The one-dimensional problem used as the standard solution was solved using 100 points per radius. Figure 1 gives the pressure versus radius curves at various times using the fourth-order method. Figure 2 shows the curves obtained by Abarbanel and Goldberg ([1, Fig. 3]). The qualitative agreement between the two graphs is apparent. More specifically, the arrival time of the converging shock at

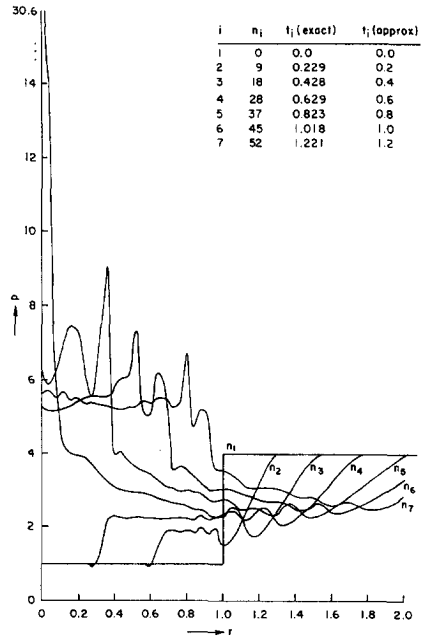

FIG. 1. Pressure versus radius for given times. Four-step two-dimensional method with $\Delta x = \Delta y = 1/25$ and CFL = 1.2.

the center is estimated from Fig. 1 to be $t \approx 0.60$ as compared to 0.57 in [1]. Even this relatively small error might be attributable to the inaccuracies in describing the initial circle of discontinuity by a coarse mesh. This indicates that indeed the four-step fourth-order accurate scheme can handle shocked-flows. Even for a relatively coarse mesh, the shock speed was fairly accurate. Note that no special treatment at the center is necessary (compare [1]). A change of the parameters in Eq. 5 could make the scheme more dissipative and eliminate the post shock oscillations.

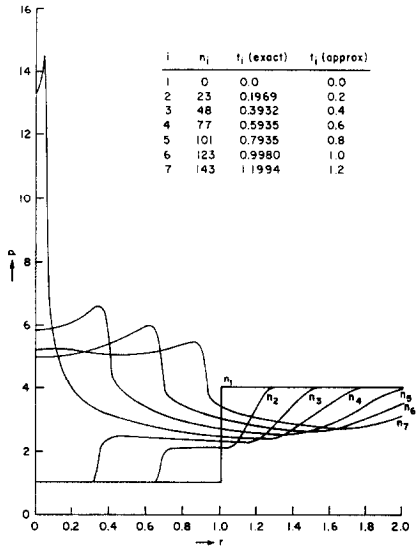

FIG. 2. Pressure versus radius for given times. From Abarbanel and Goldberg [1] using a one-dimensional code.

For problems where shocks are the only phenomenon of importance, fourth-order methods will not offer great efficiency. In the shock region itself, all schemes have basically first-order accuracy, though Apelkrans [5] and Orszag–Jayne [20] have shown that, even here, high-order methods offer slight advantages using a fixed mesh. Another advantage is in contact discontinuity problems. Finite-difference methods will diffuse the contact discontinuity at the rate of $(n)^{1/k}$, where k is the order of the method and n is the number of time step. In multidimensional problems, the meshes are, of necessity, coarse. Hence, the only practical method of following these discontinuities for any appreciable length of time (without special methods, see, e.g., Harten [13] is to use high-order methods, where k is large. Nevertheless, a major application of high-order methods will be to problems where shocks may occur, but the smooth portion of the flow is also of interest. Thus, one wishes to use a method that solves the smooth portion accurately, but still is not nonlinearly unstable and yields the correct shock speeds.

5. CONCLUSIONS

A method is presented for solving nonlinear hyperbolic systems with fourth-order accuracy, in both space and time. Since the equations are expressed in divergence free form, shocks are automatically handled correctly. The most general

scheme can be expressed in terms of 11 free parameters. One particular scheme was chosen on heuristic grounds. However, there is an obvious need to study this family in further detail, to try and optimize its properties. For the scheme chosen computational results indicate a stability criterion

$$\frac{\Delta t}{\Delta x}\rho(A) \leqslant 1, \qquad \frac{\Delta t}{\Delta x}\rho(B) \leqslant 1, \qquad \rho = \text{spectral radius},$$

at least for equations that are simultaneously symmetrizable.

A series of problems are studied numerically and comparisons made with other methods. In general, any of the methods that are fourth order in space are much more efficient than second-order methods. Within the class of fourth-order space methods, the choice is problem dependent. For problems that are sufficiently simple, e.g., the wave equation, the schemes of Kreiss–Oliger type scheme seem to be the most efficient. Here, it is difficult to justify the extra work required for fourth-order accuracy in time. Similarly, methods that require Fourier expansions or inversions of implicit methods will not be efficient for such problems. Yet, even in this simple case, the Kreiss–Oliger method has several disadvantages. The optimal time step is dependent on the error tolerance as well as the wave numbers included within the solution. In general, this optimal time step cannot be predicted in advance. It is not clear whether this applies to all methods that are second order in time but higher order in space. Second, the leapfrog (time) methods usually suffer from the generation of wakes behind places where the solution is not sufficiently smooth (see, for example, Abarbanel, Gottlieb, and Turkel [3]).

For problems of increased complexity, the advantages of the total fourth-order approach are more apparent. When the fluxes are sufficiently complex, one can compare methods strictly on the basis of counting flux evaluations. The four-step method thus requires four evaluations per time step. The Kreiss–Oliger scheme requires only one evaluation per time step. However, since its time steps are generally one-tenth of those required for the four-step methods, the Kreiss–Oliger method will require about 10 flux evaluations for the same time period. The pseudo-spectral method requires time steps that are $1/\pi$ times as small. Thus, about the same number of flux evaluations are required, though the spectral methods require Fourier expansions. The comparisons, with implicit methods as finite element or fourth-order space and time implicit schemes, are more difficult to evaluate. For example, integrating equations over the surface of the globe frequently requires Fourier cutoffs for stability reasons. Here, the larger allowable time steps of the four-step methods, are advantageous. Similar situations occur when the forcing terms in the differential equations are themselves solutions of an elliptic boundary value problem. Hence, there is still further need of comparisons of these various methods on specific problems of wide interest.

The four-step method is also able to handle problems where shocks, or severe gradients, may appear in the course of time. Most other high-order methods are [illegible] Gazdag [11]). It appears, however, that in dealing with problems containing discontinuities, higher-order methods will be limited to problems with contact discontinuities, or else problems that contain shocks, but the main interest is within the smooth regions of the solution.

There is still additional work being done to improve the characteristics of the scheme by choosing different choices of the free parameters. At present, the method is being adopted for the integration of the primitive equations over the surface of the globe. Also, the effect of imposing various boundary conditions is presently being studied.

Appendix A

We want to approximate numerically the quasi-linear hyperbolic system

$$u_t + f_x + g_y + h_z = 0, \tag{A.1}$$

where f, g, and h are vector functions of u. We denote the numerical approximation to $u(x, y, z, t)$ by $w^n_{i,j,k}$. The averaging and differencing operators that we use, μ and δ, respectively, are defined by an obvious extension of Eq. (3). Then, the extension of Eq. (5) to the three-dimensional case is given by,

$$w^{(1)} = \mu_x\mu_y\mu_z w - \lambda a[\mu_y\mu_z\delta_x f + \mu_z\mu_x\delta_y g + \mu_x\mu_y\delta_z h],$$

$$\begin{aligned} w^{(2)} = {} & \epsilon_1 w + \epsilon_2\mu_x{}^2 w + \epsilon_3\mu_y{}^2 w + \epsilon_4\mu_x{}^2\mu_y{}^2 w + \epsilon_5\mu_z{}^2 w + \epsilon_6\mu_y{}^2\mu_z{}^2 w + \epsilon_7\mu_z{}^2\mu_x{}^2 w \\ & + \epsilon_8\mu_x{}^2\mu_y{}^2\mu_z{}^2 w - \lambda[\alpha_1(\mu_y\mu_z\delta_x f^{(1)} + \mu_z\mu_x\delta_y g^{(1)} + \mu_x\mu_y\delta_z h^{(1)}) \\ & + \alpha_2(\mu_x\delta_x f + \mu_y\delta_y g + \mu_z\delta_z h)], \end{aligned}$$

$$\begin{aligned} w^{(3)} = {} & \theta_1\mu_x\mu_y\mu_z w + \theta_2\mu_x{}^3\mu_y\mu_z w + \theta_3\mu_x\mu_y{}^3\mu_z w + \theta_4\mu_x{}^3\mu_y{}^3\mu_z w \\ & + \theta_5\mu_x\mu_y\mu_z{}^3 w + \theta_6\mu_x\mu_y{}^3\mu_z{}^3 w + \theta_7\mu_x{}^3\mu_y\mu_z{}^3 w + \theta_8\mu_x{}^3\mu_y{}^3\mu_z{}^3 w \\ & - \lambda[\beta_1(\mu_y\mu_z\delta_x f^{(2)} + \mu_z\mu_x\delta_y g^{(2)} + \mu_x\mu_y\delta_z h^{(2)}) \\ & + \beta_2(\mu_x\delta_x f^{(1)} + \mu_y\delta_y g^{(1)} + \mu_z\delta_z h^{(1)}) + \beta_3(\mu_x\mu_y{}^2\mu_z{}^2\delta_x f^{(1)} \\ & + \mu_y\mu_z{}^2\mu_x{}^2\delta_y g^{(1)} + \mu_z\mu_x{}^2\mu_y{}^2\delta_z h^{(1)}) + \beta_4(\mu_y\mu_z\delta_x f + \mu_z\mu_x\delta_y g + \mu_x\mu_y\delta_z h) \\ & + \beta_5(\mu_y{}^3\mu_z{}^3\delta_x f + \mu_z{}^3\mu_x{}^3\delta_y g + \mu_x{}^3\mu_y{}^3\delta_z h) \\ & + \beta_6(\mu_x{}^2\mu_y\mu_z\delta_x f + \mu_x\mu_y{}^2\mu_z\delta_y g + \mu_x\mu_y\mu_z{}^2\delta_z h) \\ & + \beta_7(\mu_x{}^2\mu_y{}^3\mu_z{}^3\delta_x f + \mu_x{}^3\mu_y{}^2\mu_z{}^3\delta_y g + \mu_x{}^3\mu_y{}^3\mu_z{}^2\delta_z h), \end{aligned}$$

$$
\begin{aligned}
w^{(4)} = w &- \lambda(\gamma_1(\mu_y\mu_z\delta_x f^{(3)} + \mu_z\mu_x\delta_y g^{(3)} + \mu_x\mu_y\delta_z h^{(3)}) \\
&+ \gamma_2(\mu_x\delta_x f^{(2)} + \mu_y\delta_y g^{(2)} + \mu_z\delta_z h^{(2)}) + \gamma_3(\mu_x\mu_y{}^2\mu_z{}^2\delta_x f^{(2)} + \mu_x{}^2\mu_y\mu_z{}^2\delta_y g^{(2)} \\
&+ \mu_x{}^2\mu_y{}^2\mu_z\delta_z h^{(2)}) + \gamma_4(\mu_y\mu_z\delta_x f^{(1)} + \mu_z\mu_x\delta_y g^{(1)} + \mu_x\mu_y\delta_z h^{(1)}) \\
&+ \gamma_5(\mu_y{}^3\mu_z{}^3\delta_x f^{(1)} + \mu_z{}^3\mu_x{}^3\delta_y g^{(1)} + \mu_x{}^3\mu_y{}^3\delta_z h^{(1)}) \\
&+ \gamma_6(\mu_x{}^2\mu_y\mu_z\delta_x f^{(1)} + \mu_x\mu_y{}^2\mu_z\delta_y g^{21)} + \mu_x\mu_y\mu_z{}^2\delta_z h^{(1)}) \\
&+ \gamma_7(\mu_x{}^2\mu_y{}^3\mu_z{}^3\delta_x f^{(1)} + \mu_x{}^3\mu_y{}^2\mu_z{}^3\delta_y g^{(1)} + \mu_x{}^3\mu_y{}^3\mu_z{}^2\delta_z h^{(1)}) \\
&+ \nu_1(\mu_x\delta_x f + \mu_y\delta_y g + \mu_z\delta_z h) + \nu_2(\mu_x\mu_y{}^2\mu_z{}^2\delta_x f + \mu_x{}^2\mu_y\mu_z{}^2\delta_y g \\
&+ \mu_x{}^2\mu_y{}^2\mu_z\delta_z h) + \nu_3(\mu_x\mu_y{}^4\mu_z{}^4\delta_x f + \mu_x{}^4\mu_y\mu_z{}^4\delta_y g + \mu_x{}^4\mu_y{}^4\mu_z\delta_z h) \\
&+ \nu_4(\mu_x{}^3\delta_x f + \mu_y{}^3\delta_y g + \mu_z{}^3\delta_z h) \\
&+ \nu_5(\mu_x{}^3\mu_y{}^2\mu_z{}^2\delta_x f + \mu_x{}^2\mu_y{}^3\mu_z{}^2\delta_y g + \mu_x{}^2\mu_y{}^2\mu_z{}^3\delta_z h) \\
&+ \nu_6(\mu_x{}^3\mu_y{}^4\mu_z{}^4\delta_x f + \mu_x{}^4\mu_y{}^3\mu_z{}^4\delta_y g + \mu_x{}^4\mu_y{}^4\mu_z{}^3\delta_z h).
\end{aligned}
$$

Note that the two-dimensional case is recovered by setting $\delta_z = 0$, $\mu_z = 1$, and $\epsilon_5 = \epsilon_6 = \epsilon_7 = \epsilon_8 = \theta_5 = \theta_6 = \theta_7 = \theta_8 = 0$. The consistency equations for the various parameters are still Eqs. (6) with the appropriate generalizations for the ϵ's and θ's.

Appendix B

The complete expansion of $w^{(4)}$ in terms of w at the start of time step is given below. The expansion is then compared with that for $w(t + \Delta t)$. Equating coefficients of $(\Delta x)^k(\Delta t)^l$ through fourth-order terms yields Eq. (6).

$$
\begin{aligned}
w^{(4)} = w &+ \Delta t(\gamma_1 + \gamma_2 + \gamma_3 + \gamma_4 + \gamma_5 + \gamma_6 + \gamma_7 \\
&+ \nu_1 + \nu_2 + \nu_3 + \nu_4 + \nu_5 + \nu_6)\, w_t \\
&+ (\Delta t)^2(\gamma_1 t_3 + (\gamma_2 + \gamma_3)\, t_2 + (\gamma_4 - \gamma_5 + \gamma_6 + \gamma_7)\, t_1)\, w_{tt} \\
&+ (\Delta t)^3\{(1/2)[\gamma_1 t_3{}^2 + (\gamma_2 + \gamma_3)\, t_2{}^2 + (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\, t_1{}^2] \\
&\times [(A_t w_t)_x + (B_t w_t)_y] \\
&+ [\gamma_1\beta_1 t_2 + \gamma_1(\beta_2 + \beta_3)\, t_1 + \alpha_1(\gamma_2 + \gamma_3)\, t_1][(A w_{tt})_x + (B w_{tt})_y]\} \\
&+ (\Delta t)^4\{(1/6)[\gamma_1 t_3{}^3 + (\gamma_2 + \gamma_3)\, t_2{}^3 + (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\, t_1{}^3]
\end{aligned}
$$

$$
\begin{aligned}
&\times [(A_{tt}w_t)_x + (B_{tt}w_t)_y] \\
&+ [\beta_1\gamma_1 t_2 t_3 + (\beta_2 + \beta_3)\,\gamma_1 t_1 t_3 + \alpha_1(\gamma_2 + \gamma_3)\,t_1 t_2 \\
&- (1/6)(\gamma_1 {t_3}^3 + (\gamma_2 + \gamma_3)\,{t_2}^3 + (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\,{t_1}^3)] \\
&\times [(A_t w_{tt})_x + (B_t w_{tt})_y] \\
&+ (1/2)[\beta_1\gamma_1 {t_2}^2 + (\beta_2 + \beta_3)\,\gamma_1 {t_1}^2 + \alpha_1(\gamma_2 + \gamma_3)\,{t_1}^2] \\
&\times [(A(A_t w_t)_x)_x + (B(A_t w_t)_x)_y + (A(B_t w_t)_y)_x + (B(B_t w_t)_y)_y] \\
&+ \alpha_1\beta_1\gamma_1 t_1[(A(Aw_{tt})_x)_x + (B(Aw_{tt})_x)_y + (A(Bw_{tt})_y)_x + (B(Bw_{tt})_y)_y]\} \\
&+ (\Delta x)^2\,\Delta t[\gamma_1 + 4(\gamma_2 + \gamma_3) + \gamma_4 + \gamma_5 + 7\gamma_6 + 7\gamma_7 + 4(\nu_1 + \nu_2 + \nu_3) \\
&+ 10(\nu_4 + \nu_5 + \nu_6)][f_{xxx} + g_{yyy}] \\
&+ (\Delta x)^2\,\Delta t[\gamma_1 + 2\gamma_3 + \gamma_4 + 3\gamma_5 + \gamma_6 + 3\gamma_7 + 2\nu_2 + 4\nu_3 + 2\nu_5 + 4\nu_6] \\
&\times [g_{xxy} + f_{xyy}] \\
&+ ((\Delta x)^2\,\Delta t/8)[\gamma_1(\eta_1 + 4\eta_2 + 3\eta_4) + 2(\gamma_2 + \gamma_3)(\epsilon_2 + \epsilon_4) \\
&+ (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)] \cdot [(Aw_{xx})_x + (Bw_{xx})_y + (Aw_{yy})_x + (Bw_{yy})_y] \\
&+ ((\Delta x)^2(\Delta t)^2/8)[\gamma_1 t_3(\eta_1 + 4\eta_2 + 3\eta_4) + 2(\gamma_2 + \gamma_3)(\epsilon_2 + \epsilon_4)\,t_2 \\
&+ (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\,t_1][(A_t w_{xx})_x + (B_t w_{xx})_y + (A_t w_{yy})_x + (B_t w_{yy})_y] \\
&+ ((\Delta x)^2(\Delta t)^2/8)[2\beta_1\gamma_1(\epsilon_2 + \epsilon_4) + \gamma_1(\beta_2 + \beta_3) + \alpha_1(\gamma_2 + \gamma_3)] \\
&\times [(A(Aw_{xx})_x)_x + (A(Bw_{xx})_y)_x + (B(Aw_{xx})_x)_y + (B(Bw_{xx})_y)_y \\
&+ A(Aw_{yy})_x)_x + (A(Bw_{yy})_y)_x + (B(Aw_{yy})_x)_y + (B(Bw_{yy})_y)_y] \\
&+ ((\Delta x)^2(\Delta t)^2/24)[\gamma_1(\beta_1 + 4\beta_2 + 4\beta_3 + \beta_4 + \beta_5 + 7\beta_6 + 7\beta_7) \\
&+ (\gamma_2 + \gamma_3)(\alpha_1 + 4\alpha_2) + (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\,t_1] \\
&\times [(Af_{xxx})_x + (Bf_{xxx})_y + (Ag_{yyy})_x + (Bg_{yyy})_y] \\
&+ ((\Delta x)^2(\Delta t)^2/8)[\gamma_1(\beta_1 + 2\beta_3 + \beta_4 + 3\beta_5 + \beta_6 + 3\beta_7) \\
&+ (\gamma_2 + \gamma_3)\,\alpha_1 + (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\,t_1] \\
&\times [(Ag_{xxy})_x + (Bg_{xxy})_y + (Af_{xyy})_x + (Bg_{xyy})_y] \\
&((\Delta x)^2(\Delta t)^2/24)[\gamma_1 t_3 + 4(\gamma_2 + \gamma_3)\,t_2 + (\gamma_4 + \gamma_5 + \gamma_6 + \gamma_7)\,t_1] \\
&\times [f_{xxxt} + g_{yyyt}] \\
&+ ((\Delta x)^2(\Delta t)^2/8)[\gamma_1 t_3 + 2\gamma_3 t_2 + (\gamma_4 + 3\gamma_5 + \gamma_6 + 3\gamma_7)\,t_1] \\
&\times [g_{xxyt} + f_{xyyt}].
\end{aligned}
$$

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