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Note

Difference Schemes with Uniform Second and Third Order Accuracy and Reduced Smoothing

1. Introduction

Difference schemes of space-time order three were first introduced in [1, 2] and generalized to the fourth order in [3]. In [5], the uniform third order accuracy was achieved in another way. A third order finite element representation was combined with an explicit evaluation of the space-time Taylor coefficients up to order three.

The third order schemes given in [1, 2, 5] contained enough inherent smoothing to be suitable for shock computation. In fact the computation of a one dimensional shock was used in [6, 7] as a nonlinear assessment of these difference schemes. It appeared that the third order schemes given in [1, 2, 5] produce similar shock diameters.

This result and the comparison with the behaviour of other difference methods [7] indicates that the inherent smoothing of schemes given in [1, 2, 5] is quite reasonable for situations with great change of the fields in one time step.

However, this will generally be too much smoothing for meteorological applications using the primitive equations and an explicit difference scheme. In such models gravitational shock waves are absent, but nevertheless determine the maximum allowable time step.

All relevant structures change relatively little in one time step. For this reason meteorological computations require schemes with very little inherent smoothing. Some dissipation is then introduced by explicit terms or smoothing [8]. Non-dissipative schemes are available which have a high order with respect to the space variable [9]. The purpose of the present paper is to develop reduced smoothing versions of the schemes with uniform second and third order accuracy introduced in [4, 5].

A characteristic feature of the ρ-th degree method is the varying treatment of neighbouring gridpoints, which arises naturally from the use of third and second order finite elements [11]. Therefore we are allowed more flexibility in designing schemes than would be the case if all gridpoints were treated the same, as in [1, 2].

As in [5], we will design the third order scheme by combining third order operations with the explicitly computed Taylor coefficients up to order three.

These operations are rather time consuming on computers, and certainly there is room for simplifications and improvements. For ordinary differential equations we have the example of the Runge–Kutta method, which achieves fourth order accuracy by a combination of first order operations. However, the scheme presented here is already rather effective from the economic point of view [5], because one set of Taylor

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coefficients is used to compute several degrees of freedom at a time. For example in one space dimension a coarse grid X_ν with gridlength ΔX is introduced. The third order finite element representation of fields is achieved by defining the field as third order polynomials for every grid interval $[X_\nu, X_{\nu+1}]$.

The polynomials fit together continuously at X_ν. The specification of the polynomials requires three amplitudes per grid interval. As amplitudes one may choose the gridpoint values of the field at X_ν and it's second and third derivatives at $X_{\nu+(1/2)}$ [4, 5] or alternatively the gridpoint values at X_ν, $X_{\nu+(1/3)}$ and $X_{\nu+(2/3)}$ [6]. All amplitudes can be chosen independently to describe initial values and are predicted at later times. A set of Taylor coefficients is computed for every interval $[X_\nu, X_{\nu-1}]$ and serves to compute the three amplitudes. The reduced smoothing version of the scheme uses the same amount of computation time per degree of freedom as the original one [5] which for a meteorological application [6] needed computation times comparable to those of the Eliassen scheme. The new version of the scheme will need to store the fields at two time levels. In comparison, the original version [5] needed storage for only one time level.

The scheme will be defined in Section 2. Section 3 gives a linear evaluation and in Section 4 a rotationally symmetric gravity wave is computed to exemplify the application.

2. The Finite Difference Scheme

The method is explained referencing definitions given in [5]. It is applicable to initial value problems of the form

$$(\partial/\partial t)\phi = F(\phi, D\phi), \tag{1}$$

with D being a differential operator of order smaller than 4.

As in [5], a field $\phi(X, Y)$ will at even time levels be defined by the constants

$$\begin{gathered} \phi_{\nu,\mu}, \qquad \phi_{\nu,\mu+(1/2),y2}, \qquad \phi_{\nu,\mu+(1/2),y3} \\ \phi_{\nu+(1/2),\mu,x2}, \qquad \phi_{\nu+(1/2),\mu,x3} \end{gathered} \tag{2}$$

with $\phi_{\nu,\mu+(1/2),x2}$, etc. being the respective spatial derivatives of ϕ.

Inside the grid square (X_ν, Y_μ), $(X_\nu, Y_{\mu+1})$, $(X_{\nu+1}, Y_{\mu+1})$, $(X_{\nu+1}, Y_\mu)$ the field is interpolated as a polynomial (see [5]). The polynomials corresponding to the different grid squares fit together continuously. At the odd levels the fields will be represented in a grid which is shifted by the amount $\Delta X/2$. A field in the shifted grid is represented by a set of parameters

$$\begin{gathered} \phi_{\nu+(1/2),\mu+(1/2)}, \qquad \phi_{\nu+(1/2),\mu,y2}, \qquad \phi_{\nu+(1/2),\mu,y3} \\ \phi_{\nu,\mu+(1/2),x2}, \qquad \phi_{\nu,\mu+(1/2),x3}. \end{gathered} \tag{3}$$

Equation (1), the equation of motion, allows the explicit computation of the Taylor coefficients

$$\phi_t(X, Y), \qquad \phi_{tt}(X, Y), \qquad \phi_{ttt}(X, Y). \tag{4}$$

As functions of X and Y, these coefficients are again developed into truncated Taylor series [5] up to order 3. In the shifted grid the development is around the point (X_ν, Y_μ):

$$\begin{aligned} \phi_{ttt}(X, Y) &= \phi_{ttt}(X_\nu, Y_\mu) \\ \phi_{tt}(X, Y &= \phi_{tt}(X_\nu, Y_\mu) \\ &+ \phi_{ttx}(X_\nu, Y_\mu) \cdot (X - X_\nu) \\ &+ \phi_{tty}(X_\nu, Y_\mu) \cdot (Y - Y_\mu) \end{aligned} \tag{5}$$

and analogously for $\phi_t(X, Y)$. In Eq. (5) X and Y must be inside the shifted grid square which is defined by its edges $(X_{\nu+(1/2)}, Y_{\mu+(1/2)})$, $(X_{\nu+(1/2)}, Y_{\mu+(3/2)})$, $(X_{\nu+(3/2)}, Y_{\mu+(3/2)})$, $(X_{\nu+(3/2)}, Y_{\mu+(1/2)})$.

These Taylor coefficients can be used to compute the fields at a later time level by using a third order version of the Leapfrog formula

$$\phi(X, Y, t + 2\,\Delta t) = \phi(X, Y, t) + 2\,\Delta t\left(\phi_t(X, Y, t + \Delta t) + \frac{\Delta t^2}{6}\,\phi_{ttt}(X, Y, t + \Delta t)\right) \tag{6}$$

However, it is not possible to interpret Eq. (6) as a finite difference equation for ϕ. According to Eq. (5) the coefficient of $2\,\Delta t$ is a piecewise polynomial function with possible discontinuities at the boundaries of the shifted grid square. Therefore the right hand side of Eq. (6) does not define a continuous piecewise polynomial function in the original grid.

In the terminology of [5], $\phi(X, Y, t)$ is an element of the space S_3 and $\phi_t(X, Y, t + \Delta t) + (\Delta t^2/6) \cdot \phi_{ttt}(X, Y, t + \Delta t)$ is an element of P_3'. S_3 contains continuous functions which are polynomials on every original grid square. P_3' contains functions which are polynomials on every shifted gridsquare. The functions of P_3 are not required to be continuous.

To obtain a difference equation, we must define $\phi(X, Y, t + 2\,\Delta t)$ as a function of S_3, when $\phi(X, Y, t)$ is given as a function of S_3. In [5] a mapping $Q'\colon P_3' \to S_3$ was defined. We now modify Eq. (6) to

$$\phi^{n+2}(X, Y) = \phi^n(X, Y) + 2\,\Delta t\, Q'\left(\phi_t^{n+1}(X, Y) + \frac{\Delta t^2}{6}\,\phi_{ttt}^{n+1}(X, Y)\right), \tag{7}$$

with n indicating the time level.

$$Q'\left(\phi_t^{n+1}(X, Y) + \frac{\Delta t^2}{6}\,\phi_{tt}^{n+1}(X, Y)\right)$$

is an element of the space S_3 and therefore can be represented by a set of parameters.

$$\phi^{RS^{n+1}}_{\nu,\mu} \qquad {}^{RS^{n+1}}_{\nu,\mu+(1/2),y2} \qquad \phi^{RS^{n+1}}_{\nu,\mu+(1/2),y3}$$
$$\phi^{RS^{n+1}}_{\nu+(1/2),\mu,x2} \qquad \phi^{RS^{n+1}}_{\nu+(1/2),\mu,x3} \tag{8}$$

According to Eq. 5 $\phi_t^{n+1}(X, Y) + (\Delta t^2/6)\, \phi_{ttt}^{n+1}(X, Y)$ is given by its Taylor coefficients up to order 3 at the points (X_ν, Y_μ). In [5] the parameters of Eq. (8) are given as linear functions of these coefficients.

Equations (3) are then implemented by

$$\phi^{n+2}_{\nu,\mu} = \phi^{n}_{\nu,\mu} + 2\,\Delta t\, \phi^{RS^{n+1}}_{\nu,\mu}$$
$$\phi^{n+2}_{\nu,\mu+(1/2),y2} = \phi^{n}_{\nu,\mu+(1/2),y2} + 2\,\Delta t \phi^{RS^{n+1}}_{\nu,\mu+(1/2),y2} \tag{9}$$

and analogously for the other parameters. This step is then combined with the dissipative time step of [5] as in the two step Lax–Wendroff scheme. The dissipative step is used for the transition $\phi^n \to \phi^{n+1}$, and according to Eqs. (9) we compute $(\phi^n, \phi^{n+1}) \to \phi^{n+2}$. As in [5], the second order version of the scheme is obtained by neglecting the third order terms.

3. Linear Evaluation

The linear evaluation of the scheme will be done for the linear advection equation in one space dimension

$$\frac{\partial \phi}{\partial t} = \frac{\partial \phi}{\partial X}. \tag{9}$$

We assume an initial field of the form

$$\begin{pmatrix} \phi_\nu{}^0 \\ \phi^0_{\nu+(1/2),x2} \\ \phi^0_{\nu+(1/2),x3} \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} i(2\pi\nu/L)$$

after n double time steps the field will be given by

$$\begin{pmatrix} \phi^{2n}_\nu \\ \phi^{2n}_{\nu+(1/2),x2} \end{pmatrix} = V^{2n} \begin{pmatrix} \phi_\nu{}^0 \\ \phi^0_{\nu+(1/2),x2} \end{pmatrix} \tag{10}$$

for the second degree method or

$$\begin{pmatrix} \phi^{2n}_\nu \\ \phi^{2n}_{\nu+(1/2),x2} \\ \phi_{\nu+(1/2),x3} \end{pmatrix} = V^{2n} \begin{pmatrix} \phi_\nu{}^0 \\ \phi^0_{\nu+(1/2),x2} \\ \phi_{\nu+(1/2),x3} \end{pmatrix} \tag{11}$$

for the third degree method. V is the amplification matrix. The stability of the scheme is investigated by numerically computing the eigenvalues of V for a range of parameters and testing whether the absolute values are smaller than one. As pointed out in [3], this procedure is not as reliable as the analytic derivation of stability conditions. However, it is applied here and in [3, 5] because the analytic derivation of stability conditions is a difficult problem for complex schemes. We obtain as Çourant Levy condition $\Delta t < 0.\ 3\,\Delta X = 0.9\,\Delta X'$ for the third degree method. The maximum allowable time steps are slightly greater than those of the smoothing versions of the schemes [4, 5]. The eigenvalues of V can be used to compare the computed phase velocity with the exact value $C_0 = -1$. Tables I and II give the relative phase velocities corresponding to the first eigenvalue, for the second and third degree methods, respectively.

The phase velocity errors of the schemes are slightly greater than those of the dissipative versions of the schemes [4, 5]. For the range of wavelengths considered, the accuracy shown in Table II is essentially that of the spectral method. For example the phase velocity error is smaller than 0.001 for $L > 8\,\Delta X$ with the spectral method [14] and for $L > 4\,\Delta X$ with the third degree method. To compare the efficiency with other methods, it should be observed that the third degree method uses three independent amplitudes to describe the field on an interval of length ΔX, and thus has the effective grid length $\Delta X' = \Delta X/3$. In a meteorological application [6] the third

TABLE I

Second Degree Method, First Eigenvalue

	Relative phase velocities			
$\Delta t/\Delta X$	$L = 2\Delta X$	$L = 4\Delta X$	$L = 8\Delta X$	$L = 16\Delta X$
0.02	0.8	0.98	0.997	0.9994
0.1	0.8	0.98	0.997	0.9994
0.2	0.9	0.98	0.998	0.9995

TABLE II

Third degree method, first eigenvalue

	Relative phase velocities			
$\Delta t/\Delta X$	$L = 2\Delta X$	$L = 4\Delta X$	$L = 8\Delta X$	$L = 16\Delta X$
0.02	1.05	1.001	1.0001	1.00002
0.1	1.05	1.001	1.0001	1.00002
0.2	1.02	1.001	1.0001	1.00001

degree method needed as much computation time as a model using the Eliassen grid with grid length $\Delta X/2$. In relation to its effective grid length $\Delta X' = \Delta X/3$, the third degree method appears to be inferior to the spectral method. However, when relating the accuracy achieved to the computation time needed in a nontrivial application, the third degree method achieves the accuracy of the spectral method for wavelengths near 4 ΔX and needs the same amount of computation time as the Eliassen scheme.

The damping factors A^{n+1}/A^n corresponding to the eigenvalues of the second and third degree schemes, respectively, are given in Tables III, IV.

TABLE IIIa

Second degree method, first eigenvalue

	Damping factor A^{n+1}/A^n			
$\Delta t/\Delta X$	$L = 2\Delta X$	$L = 4\Delta X$	$L = 8\Delta X$	$L = 16\Delta X$
0.02	0.999	0.99996	0.999996	$>1 - 10^{-6}$
0.1	0.99	0.9998	0.9999	0.99999
0.2	0.99	0.997	0.9996	0.99997

TABLE IIIb

Second degree method, second eigenvalue

	Damping factor A^{n+1}/A^n			
$\Delta t/\Delta X$	$L = 2\Delta X$	$L = 4\Delta X$	$L = 8\Delta X$	$L = 16\Delta X$
0.02	0.99996	0.999994	$>1 - 10^{-6}$	$>1 - 10^{-6}$
0.1	0.999	0.99995	0.99999	$>1 - 10^{-6}$
0.2	0.998	0.9998	0.99999	$>1 - 10^{-6}$

TABLE IVa

Third degree method, first eigenvalue

	Damping factor A^{n+1}/A^n			
$\Delta t/\Delta X$	$L = 2\Delta X$	$L = 4\Delta X$	$L = 8\Delta X$	$L = 16\Delta X$
0.02	0.99996	0.999994	$>1 - 10^{-6}$	$>1 - 10^{-6}$
0.1	0.999	0.99995	0.99999	$>1 - 10^{-6}$
0.2	0.998	0.9998	0.99999	$>1 - 10^{-6}$

In view of meteorological applications, the behaviour of the schemes for small Δt is most interesting. For $\Delta t/\Delta X = 0.02$, the modes corresponding to the first eigenvalue are nearly undamped. This is desirable with respect to meteorological applications.

The scales belonging to the second and third eigenvalue are predicted very inaccurately. Therefore it would be desirable to damp them, which is not achieved by the damping factors given in Tables IIIb and IVb, c. When solving linear equations, this leads to an accumulation of small scale features during the time development. For nonlinear equations, the use of these schemes without an additional smoothing operation will generally lead to nonlinear instability, because there is no damped mode.

TABLE IVb

Third degree method, second eigenvalue

	Damping factor A^{n+1}/A^n			
$\Delta t/\Delta X$	$L = 2\Delta X$	$L = 4\Delta X$	$L = 8\Delta X$	$L = 16\Delta X$
0.02	0.999995	0.9998	0.9995	0.999
0.1	0.99998	0.995	0.99	0.95
0.2	0.9995	0.99	0.95	0.9

TABLE IVc

Third Degree Method, Third Eigenvalue

	Damping factor A^{n+1}/A^n			
$\Delta t/\Delta X$	$L = 2\Delta X$	$L = 4\Delta X$	$L = 8\Delta X$	$L = 16\Delta X$
0.02	0.99998	0.998	0.998	0.998
0.1	0.98	0.95	0.95	0.95
0.2	0.95	0.9	0.85	0.85

The lack of damping for wavelengths smaller than $6\,\Delta X'$ is a rather undesirable feature. To achieve a damped mode one might use the scheme in combination with highly selective smoothing operations, like those defined in [8]. This will probably be the best solution in view of an optimal treatment of the wavelengths greater than $6\,\Delta X'$. A reasonable performance of the scheme is also obtained by combining the non-smoothing scheme and the version defined in [5] to achieve the desired degree of smoothing.

4. A Nonlinear Computation

The application of the schemes is exemplified by a solution of the shallow water equations:

$$\begin{aligned} U_t &= -UU_x - VU_y - H_x \\ V_t &= -UV_x - VV_y - H_y \\ H_t &= -(HU)_y - (HV)_y \end{aligned} \tag{12}$$

The computation will be done on a 31×31 point grid using the second degree method with $\Delta X = 381$ km. The distance of the opposing boundaries is $29\,\Delta X$. The boundary conditions were chosen such that upper and lower boundaries are reflective and the right and left boundaries are open to gravity waves [13]. The

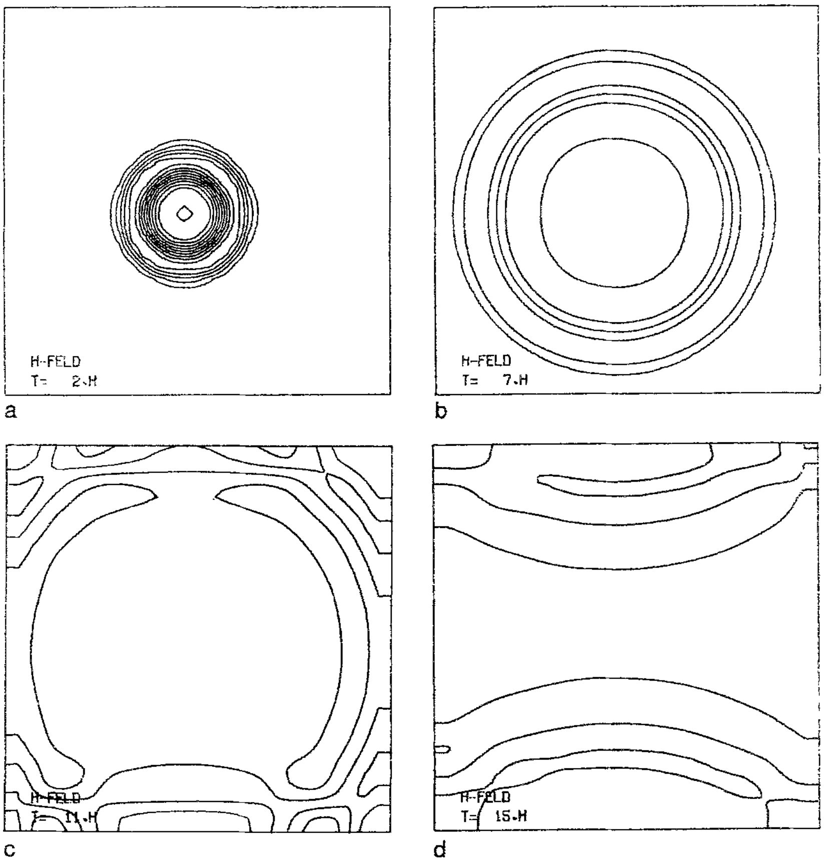

Fig. 1. The H field of the circular symmetric gravity wave at different time computed by the smoothing version of the second degree method. (a) $t = 2.2$ hr; (b) $t = 6.6$ hr; (c) $t = 11.1$ hr; (d) $t = 15.5$ hr.

initial condition is chosen to produce a circular symmetric gravity wave. In Eqs. (13) U, V, H replace the ϕ of Eq. (2).

$$
\begin{aligned}
U_{\nu+(1/2),\mu,x2} &= U_{\nu,\mu+(1/2),y2} = U_{\nu,\mu} = 0 \\
V_{\nu+(1/2),\mu,x2} &= V_{\nu,\mu+(1/2),y2} = V_{\nu,\mu} = 0 \\
H_{\nu+(1/2),\mu,x2} &= H_{\nu,\mu+(1/2),y2} = 0 \\
H_{\nu,\mu} &= 2(381\ \text{km/hr})^2 \qquad \text{for} \quad \nu, \mu \neq (15, 15) \\
H_{15,15} &= 8(381\ \text{km/hr})^2
\end{aligned}
\tag{13}
$$

This situation is appropirate to see the effect of numerical accuracy and to test the behaviour of the scheme near boundaries.

At first the computation is done with $\Delta t = 1/12$ hr, using the smoothing version of the second degree method [4]. The time development of the gravity wave is shown

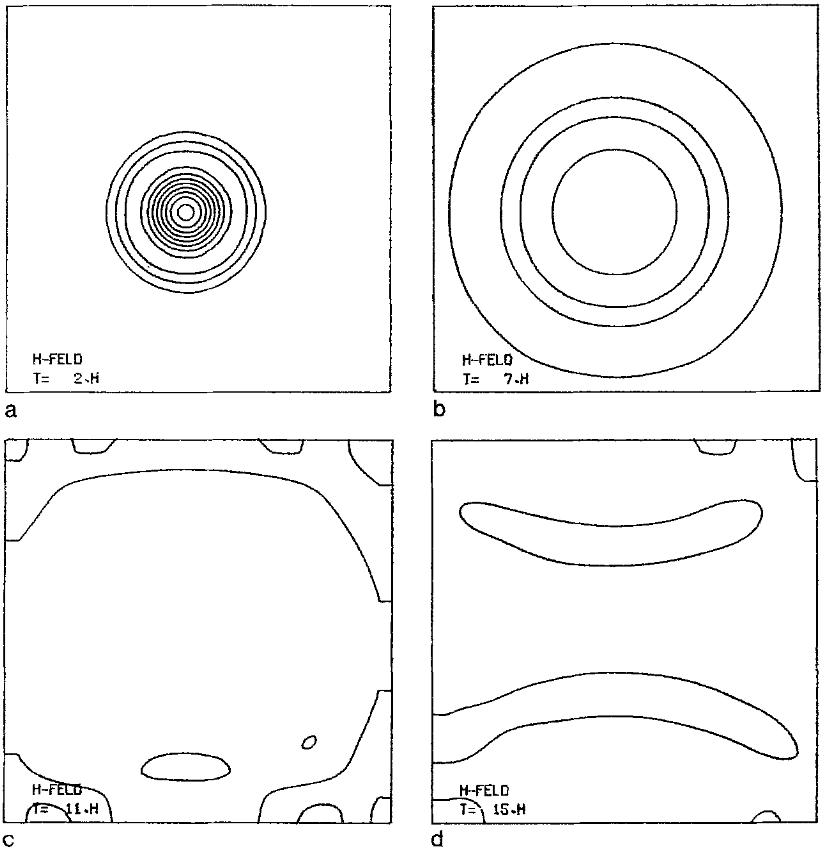

FIG. 2. As Fig. 1, but with the time step reduced by a factor 4. (a) $t = 2.2$ hr; (b) $t = 6.6$ hr; (c) $t = 11.1$ hr; (d) $t = 15.5$ hr.

in Fig. 1. The numerical solution is circular symmetric to good approximation, even after reflection at the boundary.

The test computations given in [5, 13] indicate that the smoothing version of the second degree method contains an appropriate degree of smoothing when there is a considerable change of the fields in one time step. This means that the phenomenon to be computed determines the Courant Levy time step. This situation occurs in the computation shown in Fig. 1. However, in meteorology we often have a situation where less smoothing is required. In models using explicit schemes for the primitive equations, the time step is determined by the gravity and sound waves. The relevant meteorological phenomena change very little during one time step. Therefore such models require difference schemes with reduced smoothing.

We simulate this situation by doing the computation of the gravity wave with a time step which is much smaller than required by the Courant Levy condition.

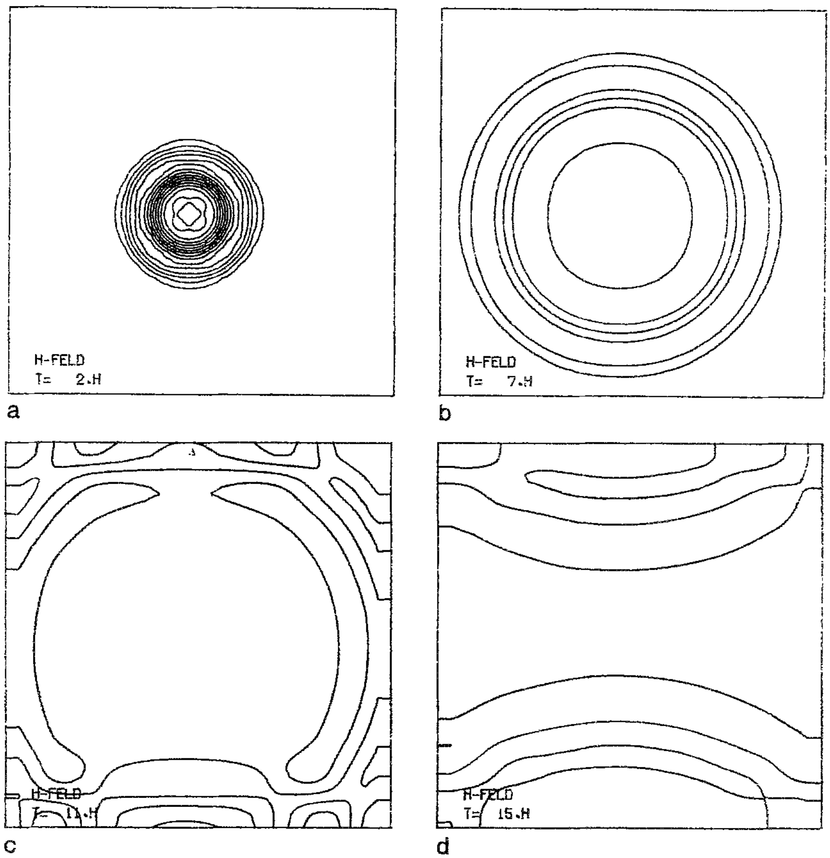

FIG. 3. As Fig. 2, but using the reduced smoothing version of the second degree method together with the smoothing version. One smoothing step was used on four non smoothing steps. A restoration of the amplitudes is achieved. (a) $t = 2.2$ hr; (b) $t = 6.6$ hr; (c) $t = 11.1$ hr; (d) $t = 15.5$ hr.

Figure 2 is the same as Figure 1, except that the computation was done with a time step reduced by a factor 4. With the dissipative version of the second degree method this means four times as much smoothing as before, since the scheme described in [4] involves a smoothing operation every time step. Figigure 2 shows the amplitudes to be considerably reduced, compared with Fig. 1. The main loss of amplitude occurs at the beginning of the forecast, in the presence of small scales. Figure 3 shows the same forecast, but using the smoothing and nonsmoothing versions of the second degree method in turn. One smoothing step to four non-smoothing steps is used. A comparison of Figs. 1 and 3 shows that the procedure leads to a restoration of the amplitudes.

Figures 1 to 3 show the gravity waves to be circular symmetric to good approximation. This can be considered as an effect of the numerical accuracy of the scheme. The reflection of the gravity wave at the boundary indicates that the reduced smoothing version of the second degree method may be as well behaved with respect to boundaries as the smoothing version [12]. In the present note it is not intended to use the circular symmetric gravity wave for a systematic comparison of difference schemes, as done in [7] for the one dimensional shock wave. Therefore we refrain from showing the results of other difference schemes. Schemes with ordinary accuracy, like the centered difference method, will more or less destroy the circular symmetry of the phenomenon. In particular the reflection at the boundary is often misrepresented.

5. Conclusions

The reduced smoothing versions of the second and third degree method have slightly greater phase velocity errors than the dissipative schemes. For the range of amplitudes considered, the linear analysis still showed phase velocities comparable to those of the spectral method. By using the smoothing and the reduced smoothing version together, one obtains an overall smoothing which is appropriate for synoptic scale meteorological calculations.

A nonliner example showed that the reduced smoothing scheme leads to greater amplitudes, when applied in a situation where the original version forced too much damping. The example also showed that the new version of the scheme is as well behaved with respect to boundaries as the original one. The good preservation of the circular symmetry of the solution is an indication of the accuracy of the schemes.

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J. Steppeler
Deutscher Wetterdienst
Offenbach, West Germany