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Time-difference schemes with spectral-like resolution

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Abstract—An efficient time-difference scheme is introduced for spectrum or finite-difference methods. The time step of the scheme can be determined by the required resolution relative to the frequencies associated with the physics of the problems. © 1998 Elsevier Science Ltd.

INTRODUCTION

Many physical phenomena involve traveling waves with a wide range of wave lengths and frequencies. Typical examples are turbulent flows and heat transfer, microscale heat transfer, Solar winds, and formations of planets. An acceptable numerical model must be able to resolve all relevant scales in order to accurately simulate physics. Spectral methods can be used to provide the required spectral resolution for space derivatives, but are impractical for time derivatives. Lele [1] has suggested compact finite-difference schemes with spectral-like space resolution. On the other hand, an efficient time-resolution scheme relative to the frequencies associated with the physics has never been proposed and discussed in the literature. Such a method is in demand for an accurate numerical simulation of unsteady physics. On this note, we will follow the principle used by Lele to develop efficient time-difference schemes for spectral methods and finite-difference methods.

A space discretization method usually results a nonlinear ordinary differential equation as

$$\frac{\mathrm{d}f}{\mathrm{d}t} = F(t,f). \qquad (1)$$

The function f is a real dependent variable for a space finite-difference method, or it can be a complex amplitude function for spectral methods [2], and a complex amplitude density function for spectral-eigenfunction method [3, 4]. In Section 2, a time-difference scheme suitable for spectral methods is presented, and its resolution characteristics are compared with commonly used time advancing schemes, such as Adams–Bashford and Adams–Moulton methods. The resolution characteristics, as defined by Lele, are the accuracy with which the difference approximation represents the exact result over the full range of frequencies that can be realized for a given time step. In Section 3, a time advancing scheme is suggested for finite-difference methods.

TIME ADVANCING SCHEME FOR SPECTRAL METHODS

Equation (1), after being discretized, can be in the form

$$\frac{f_n - f_{n-1}}{h} + b\frac{f_n - f_{n-2}}{2h} + c\frac{f_n - f_{n-3}}{3h} = \alpha f_n + \beta f'_{n-1} + \chi f'_{n-2} + \delta f'_{n-3} \qquad (2)$$

where h is the time step, the subscript indicates the time level, and $f'_n = F(t_n, f_n)$ denotes the approximation of the time derivative of the function f. The relations between the coefficients b, c and α, β, χ, δ are derived by matching the Taylor series coefficients at time step n of various orders. The first unmatched coefficient determines the formal truncation error of the approximation in equation (2). These constraints are:

$$1+b+c = \alpha+\beta+\chi+\delta \quad \text{(first order)} \qquad (3)$$

$$1+2b+3c = 2(\beta+2\chi+3\delta) \quad \text{(second order)} \qquad (4)$$

$$1+2^2b+3^2c = 3(\beta+2^2\chi+3^2\delta) \quad \text{(third order)} \qquad (5)$$

Since it is impractical to use a time difference scheme of too many multiple steps, we will not list constraints for higher orders. It is obvious that $\alpha = 0$ is for explicit schemes, such as Adams–Bashford methods. A few commonly used schemes are summarized below:

1. The first-order forward Euler (FE) method is, by selecting $b = c = \alpha = \chi = \delta = 0$, and $\beta = 1$,

$$\frac{f_n - f_{n+1}}{h} = f'_{n-1}.$$

2. The second-order Adams–Bashford (AB2) is by $b = c = \alpha = \delta = 0$, and $\beta = -1/2$, $\chi = 3/2$.
3. The third-order Adams–Bashford (AB3) is by $b = c = \alpha = 0$, and $\beta = 23/12$, $\chi = 4/3$, $\delta = 5/12$.
4. The first-order backward Euler (BE) is by $b = c = \beta = \chi = \delta = 0$, ad $\alpha = 1$.

5. The second-order Crank–Nicolson (CN) is by $b = c = \chi = \delta = 0$, and $\alpha = \beta = 1/2$.
6. The third-order Adams–Moulton is (AM3) by $b = c = \delta = 0$, and $\alpha = 5/12$, $\beta = 2/3$, $\chi = -1/12$.

The resolution characteristics of the above schemes can be studied by a Fourier analysis. If $i = \sqrt{-1}$ and

$$f_n = e^{i\omega t_n} \tag{6}$$

then

$$\frac{\mathrm{d}f_n}{\mathrm{d}t} = i\omega f_n \quad \text{and} \quad f'_n = i\omega' f_n \tag{7}$$

where ω' is the circular frequency calculated by the difference scheme, since f' is only an approximation of the time derivative. The relation between the approximate frequency ω' and the exact frequency can be found by substituting equation (6) into equation (2) and using equation (7). It is

$$\omega' h = -i \frac{(1-e^{-i\omega h}) + \frac{b}{2}(1-e^{-i2\omega h}) + \frac{c}{3}(1-e^{-i3\omega h})}{\alpha + \beta e^{-i\omega h} + \chi e^{-i2\omega h} + \delta e^{-3\omega h}}. \tag{8}$$

The amplitude and the phase angle of $h\omega'$ are plotted in Figs. 1 and 2 as function of $h\omega$. The physical meaning of $h\omega$ can be interpreted as a dimensionless time step normalized by the maximum frequency that the numerical mode must accurately predict. The time step, $h\omega$ of the explicit methods such as FE, AB2 and AB3 can be set no more than 0.4. Among them, AB2 is the least accurate one and its time step should not be larger than 0.3. Since the shortest period $T_{\min} = 2\pi/\omega_{\max}$, h cannot be larger than 6% of $T_{\min}$. This is a rather severe restriction in transient computations. The acceptable value of $h\omega$ for implicit methods is about 0.5, slightly larger. On the other hand, CN and AB3 can generate spurious error of higher frequencies. This likely causes unstable computation.

Two spectral-like schemes are also plotted in Figs. 1 and 2. The explicit scheme (SE2) is a second-order scheme. The coefficients are determined from equations (3), (4) and three equations of (8) by forcing $\omega' = \omega = 2.8$, 3 and 3.2. They are:

$$b = -2.138 + i1.290, \quad c = 0.366 - i1.722,$$
$$\alpha = 0 \quad \beta = -0.330 + i0.285,$$
$$\chi = -0.569 - i0.573, \quad \delta = 0.126 - i0.144. \tag{9}$$

We found that the values of the determined coefficients are relatively insensitive to the selected collocation points, so we did not optimize the collocation points.

The implicit scheme (SI3) is third-order. Solving equations (3)–(5) and equation (8) at $\omega' = \omega = 3.2$, 3.4 and 3.6 results in:

$$b = -1.561 + i1.250, \quad c = 0.148 - i1.002,$$
$$\alpha = 0.088 + i0.060 \quad \beta = -0.279 + i0.529,$$
$$\chi = -0.549 - i0.238, \quad \delta = 0.032 - i0.105. \tag{10}$$

Clearly, the schemes (9) and (10) are accurate for $h\omega \leqslant 3.8$. This implies that the time step for these schemes can be taken as large as the half of $T_{\min}$. The formal order of the scheme is not a necessary measure of the accuracy of the difference scheme. The phase angle of the exact solution is zero. The plot of phase angle in Fig. 2 can be viewed as the phase error of the methods. The two proposed schemes (9) and (10) are free of phase error for substantial range of $h\omega$. It is worthy to note that the implicit scheme (10) can introduce spurious error of high frequency. Thus, the explicit scheme (9) is a more desirable scheme for time marching computation. Since it is a fourth time-step method, it requires one to know the initial conditions of the three previous time steps that will usually not present any difficulty in computation.

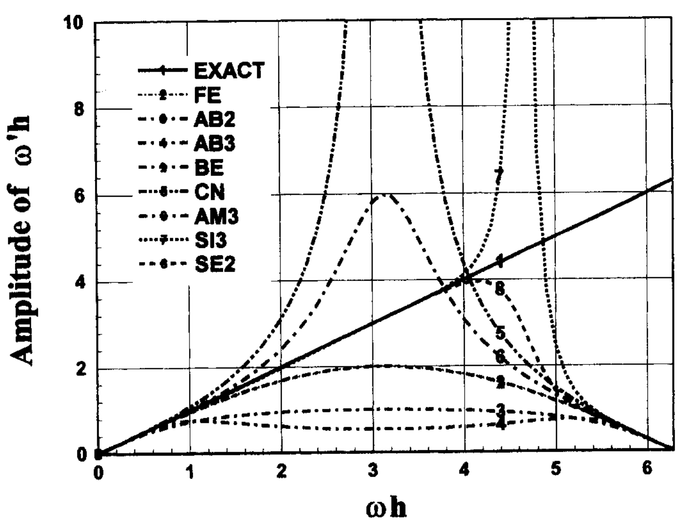

Fig. 1. Plot of modified frequency vs frequency.

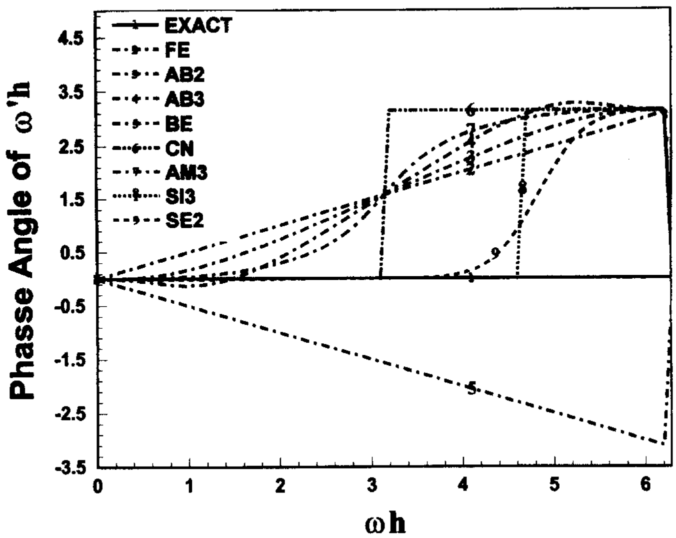

Fig. 2. Phase error.

Two proposed schemes are suitable for equations of complex variables resulted by spectral methods. In the next section, we will present a scheme for equations of real variable.

TIME ADVANCING SCHEME FOR FINITE-DIFFERENCE METHODS

Following the principle of the last section, the discretized form of equation (1), can be casted as

$$\frac{f_{n+2}-f_{n-2}}{4h}+a\frac{f_{n+1}-f_{n-1}}{2h}$$

$$=\alpha(f'_n+\beta(f'_{n+1}+f'_{n-1})+\chi(f'_{n+2}+f'_{n-2}). \quad (11)$$

Here, we assume that we know f_{n+1}, f_n, f_{n-1} and f_{n-2} in order to compute f_{n+2}. The expansion of the Taylor series leads to:

$$1+a = \alpha+2\beta+2\chi \quad \text{(second order)} \quad (12)$$

$$4+a = 6(\beta+4\chi) \quad \text{(fourth order)}. \quad (13)$$

The Fourier analysis gives

$$\omega' h = \frac{\frac{1}{2}\sin(2\omega h)+a\sin(\omega h)}{\alpha+2\beta\cos(\omega h)+2\chi\cos(2\omega h)}. \quad (14)$$

For fourth time-step methods, we will propose an implicit and an explicit scheme of second-order. From equation (12), we know that $a = \alpha+2\beta+2\chi-1$. The implicit scheme (IMP2) is obtained by solving equation (14) at $\omega' = \omega = 1$, 1.2 and 1.4, and is

$$\alpha = 1.794 \quad \beta = 0.848 \quad \chi = 0.064. \quad (15)$$

The explicit scheme (EXP2) is collocating at $\omega' = 1$ and 1.2, and is

$$\alpha = 0.286 \quad \beta = 0.085 \quad \chi = 0.$$

The plots of $h\omega'$ in Fig. 3 show that the implicit scheme is better and is accurate for $h\omega \leqslant 2$. The explicit scheme

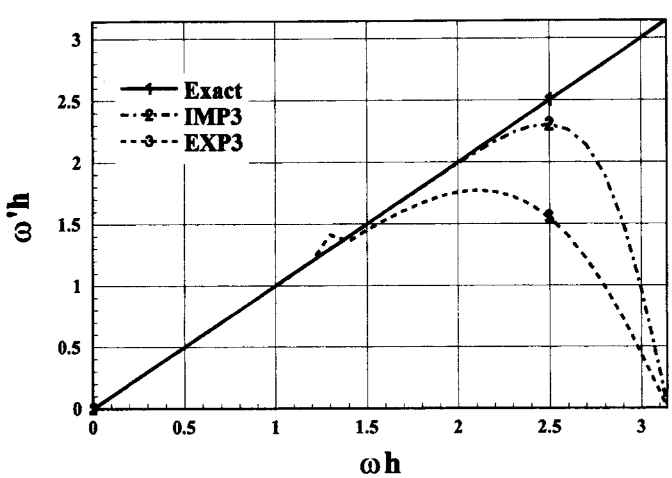

Fig. 3. Plot of modified frequency vs frequency.

is good for $h\omega \leqslant 1.2$. Both are considerably better than the commonly used Adams–Bash or Adams–Moulton marching schemes.

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