Existence of a second range of stability of optimally accurate finite-difference schemes for numerically solving the wave equation

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1 Introduction

Explicit time-domain finite difference (FD) schemes are widely used in many fields of science and engineering to solve the wave equation. A standard result that can be found in almost all textbooks is the existence of an upper limit on the size of the time step Δt; if this limit is exceeded schemes become unstable. Considering the case of elastic wave propagation, let us define the Courant number to be

$$C^2 = \beta^2\, \Delta t^2 / \Delta x^2, \tag{1}$$

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where

$$\beta = \sqrt{\mu/\rho} \tag{2}$$

is the velocity of wave propagation, Δx is the spatial grid interval, μ is the elastic modulus, and ρ the density. Using the above notation we can write the usual textbook stability condition as

$$C \le C_1, \tag{3}$$

where the value of the stability limit C_1 depends on the nature of the particular FD scheme. In the usual case instability occurs whenever $C > C_1$.

We have developed two optimally accurate time-domain predictor-corrector FD schemes for numerically solving the wave equation; these schemes are $O(2,4)$ and $O(2,2)$ (second order in time, and respectively fourth order and second order in space). We discuss these schemes in detail below. An analysis of the stability of these schemes (below) demonstrates a remarkable, and, to our knowledge, previously unreported, stability behavior. We found that eq. (3) applies, but that these two schemes are not unstable for all $C > C_1$. We found that for these schemes instability occurs for the range

$$C_1 < C < C_2, \tag{4}$$

but that as the time step increases further, once again stability occurs for the range

$$C_2 \le C \le C_3. \tag{5}$$

Finally, as the time step increases still further, instability occurs for all

$$C_3 < C, \tag{6}$$

where

$$0 < C_1 < C_2 \le C_3. \tag{7}$$

We derive the particular values of C_1, C_2, and C_3 below, and confirm the existence of the additional ranges of stability and instability through numerical experiments.

2 Optimally accurate FD schemes

It is desirable for FD methods to be accurate and efficient. Our group developed a general criterion for optimally accurate numerical operators for solving the wave equation in arbitrarily heterogeneous media[1]. This criterion was derived by a formal analysis of the error of the numerical solution using an eigenfunction expansion, but it is not necessary to know the actual numerical values of the eigenfrequencies and eigenfunctions to use this criterion to derive optimally accurate numerical operators.

We used the above criterion to derive optimally accurate $O(2,2)$ (second order accuracy in time and space) time-domain finite-difference (FD) schemes for one-dimensional (1-D) media[2], and for 2-D and 3-D media[3]. These schemes are predictor-corrector schemes, in which a conventional FD scheme (the predictor) is used to extrapolate the wavefield to the next time step, followed by a second calculation (the corrector) to eliminate the lowest order error of the predictor. The implementation of the predictor-corrector scheme differs greatly from the Lax-Wendroff FD scheme[4] but we have shown that these two types of schemes are essentially equivalent[5].

The general criterion for optimally accurate operators[1] is not limited to $O(2,2)$ schemes, but can also be used to derive optimally accurate schemes of various other types. We recently used this criterion to derive an optimally accurate $O(2,4)$ (second order in time and fourth order in space) FD scheme for a one-dimensional heterogeneous medium as part of a study in which we compare the cost-performance ratios of various optimally accurate schemes[6]. We show here that some of the numerical schemes we derived in that and earlier studies have two distinct ranges of the time-step Δt for which stable solutions are obtained.

3 Optimally accurate FD schemes for 1-D homogeneous media

In this paper, for simplicity we consider only a homogeneous 1-D medium with periodic boundary conditions. We discretize and solve the 1-D elastic equation of motion:

$$\mu \frac{\partial^2 u(x,t)}{\partial x^2} - \rho \frac{\partial^2 u(x,t)}{\partial t^2} = -f(x,t), \tag{8}$$

where x and t are the spatial and temporal coordinates, u is the displacement, and f the external force.

We first analyze the stability of the $O(2,4)$ scheme. Omitting the force term for simplicity, we write the predictor step as

$$\tilde{c}_n^{N+1} - 2c_n^N + c_n^{N-1} = C^2 \mathbf{L}^{(2)} \mathbf{c}_n^N, \tag{9}$$

where c_n^N and c_n^{N-1} are the corrected values of the displacement at the nth node at the present (Nth) and past ($N-1$th) time steps, $\tilde{c}_n^{N+1}$ is the uncorrected value of the displacement at the nth node at the future ($N+1$th) time step.

The operator on the r.h.s. of eq. (9) and an operator which is used in the corrector step are defined respectively as follows:

$$\mathbf{L}^{(2)} = \frac{1}{12}\Big(-1,\ 16,\ -30,\ 16,\ -1\Big) \tag{10}$$

$$\mathbf{L}^{(4)} = \frac{1}{90}\Big(-1,\ 4,\ -6,\ 4,\ -1\Big). \tag{11}$$

When these operators act on a vector we obtain:

$$\mathbf{L}\mathbf{c}_n^N = \sum_{j=-2}^{2} L_j c_{n+j}^N. \tag{12}$$

Using the above definitions, the correction term and the corrected value of the displacement at the next time step are respectively:

$$\delta c_n^{N+1} = -\left(\mathbf{L}^{(4)}\tilde{\mathbf{c}}_n^{N+1} - 2\mathbf{L}^{(4)}\mathbf{c}_n^N + \mathbf{L}^{(4)}\mathbf{c}_n^{N-1}\right) + \frac{C^2}{12}\left(\mathbf{L}^{(2)}\tilde{\mathbf{c}}_n^{N+1} - 2\mathbf{L}^{(2)}\mathbf{c}_n^N + \mathbf{L}^{(2)}\mathbf{c}_n^{N-1}\right) \tag{13}$$

$$c_n^{N+1} = \tilde{c}_n^{N+1} + \delta c_n^{N+1}. \tag{14}$$

To evaluate the stability of the above scheme we sum the l.h.s. and r.h.s. of eqs. (9) and (13) to obtain:

$$c_n^{N+1} - 2c_n^N + c_n^{N-1} = C^2\mathbf{L}^{(2)}\mathbf{c}_n^N - C^2\mathbf{L}^{(4)}\mathbf{L}^{(2)}\mathbf{c}_n^N + \frac{C^4}{12}\mathbf{L}^{(2)}\mathbf{L}^{(2)}\mathbf{c}_n^N, \tag{15}$$

where $\mathbf{L}^{(2)}\mathbf{L}^{(2)}$ and $\mathbf{L}^{(4)}\mathbf{L}^{(2)}$ are convolutions of the respective operators. The stability limit is evaluated by a Von Neumann stability analysis in which a harmonic solution of the form

$$c_{n+m}^{N+l} = \exp\left(\mathrm{i} l\omega\Delta t\right)\exp\left(\mathrm{i} mk\Delta x\right), \tag{16}$$

where $\mathrm{i} = \sqrt{-1}$, m and l are spatial and temporal indices respectively, ω is the frequency, and k is the wavenumber, is substituted into eq. (15).

We define the following variables:

$$\begin{aligned}
A &= \cos(\omega\Delta t)\\
E &= \cos(k\Delta x)\\
F &= \cos(2k\Delta x) = 2E^2 - 1\\
G &= \cos(3k\Delta x) = 4E^3 - 3E\\
H &= \cos(4k\Delta x) = 8E^4 - 8E^2 + 1.
\end{aligned} \tag{17}$$

Omitting details, we obtain

$$\begin{aligned}
A = 1 &+ \frac{C^2}{12}(-15 + 16E - F)\\
&- \frac{C^2}{1080}(155 - 236E + 100F - 20G + H)\\
&+ \frac{C^4}{1728}(707 - 992E + 316F - 32G + H).
\end{aligned} \tag{18}$$

The stability condition is that A should be real and that

$$-1 \leq A \leq 1 \quad \text{for all} \quad -1 \leq E \leq 1. \tag{19}$$

The values of A for various values of E are shown in Fig. 1 (left panel). It is clear (and can be verified analytically) that there are two regions for which eq. (19) is satisfied. The first is

$$0 \leq C \leq \sqrt{(53 - \sqrt{109})/40} \approx 1.0315, \tag{20}$$

and the second is

$$1.2593 \approx \sqrt{(53 + \sqrt{109})/40} \leq C \leq \sqrt{53/20} \approx 1.6279. \tag{21}$$

On the other hand, for values of C lying between the respective stability ranges, namely

$$1.0315 \approx \sqrt{(53 - \sqrt{109})/40} < C < \sqrt{(53 + \sqrt{109})/40} \approx 1.2593, \tag{22}$$

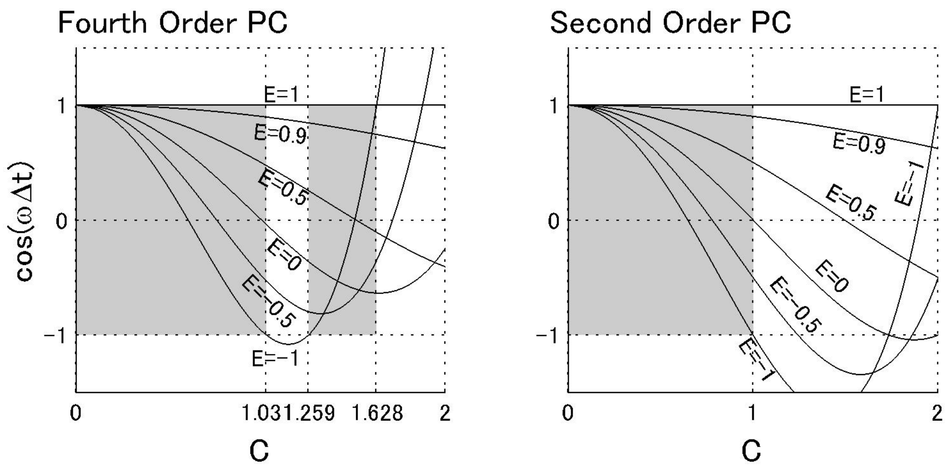

Fig. 1. (Left) Stability for the optimally accurate $O(2,4)$ FD scheme (shaded areas) is achieved when $A = \cos(\omega\Delta t)$ lies between -1 and 1 for all relevant values of $E = \cos k\Delta x$. The second region of stability (shaded area at right, $1.2593 \leq C \leq 1.6279$) is separated from the primary region of stability by a region of instability from $1.0315 < C < 1.2593$. (Right) Stability for the optimally accurate $O(2,2)$ FD scheme. The "classic" region of stability (shaded) is $0 \leq C \leq 1$, but stability is also obtained for the singular point $C = 2$.

the FD scheme will be unstable.

The stability range indicated by eq. (20) would normally be regarded as "the" stability range of the $O(2,4)$ scheme. To our knowledge the existence of a second range of stability (eq. 21 for the scheme considered here) has not been previously pointed out, and, in any case, its existence is certainly not widely known.

The classic CFL result[7] states that an FD scheme cannot converge to the analytic solution if the analytic domain of dependence is not contained in the numerical domain of dependence. From eq. (15) we see that CFL therefore requires $C \leq 4$ for the $O(2,4)$ predictor–corrector scheme considered above. Eq. (21) is thus fully consistent with CFL.

In order to confirm that the ranges in eqs. (20) and (21) are stable, and that values outside these ranges are unstable, we conduct the following numerical experiments (left and center panels of Fig. 2). We use the $O(2,4)$ predictor-corrector scheme to compute synthetic seismograms (numerical solutions of the time-dependence of the wavefield) for a homogeneous medium with a length of 1 km, and a seismic wave velocity $\beta = 1$ km/s, with periodic boundary conditions. The source is an optimally accurate point force, which is a point force "smeared out" in space and time using the following weights:

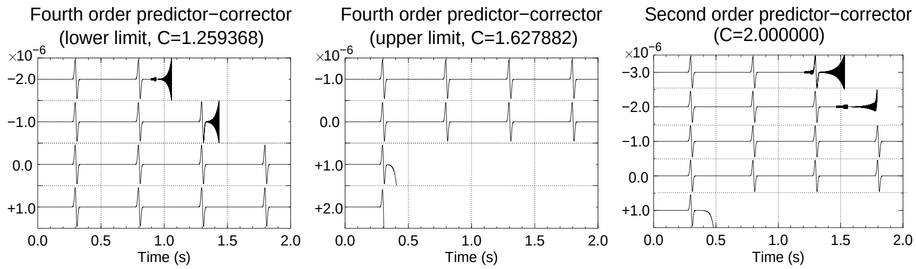

Fig. 2. Numerical solutions for values of C in the vicinity of the lower limit (left panel) and upper limit (center panel) of the second stability region for the optimally accurate $O(2,4)$ scheme, and (right panel) in the vicinity of the singular stability point $C = 2$ for the optimally accurate $O(2,2)$ scheme. The value of C used for each trace is the sum of the value in the left hand column (e.g. -2×10^{-6} for the top trace in the left panel) and the value shown at the top of the panel (e.g., $C = 1.259368$ for the left panel). The left and center panels show that stable waveforms are obtained for values of C inside the second stability region (eq. 21), but that solutions for values of C immediately outside that region are unstable. The right panel demonstrates that $C = 2$ is a singular point of stability.

$$\frac{1}{180} \times \begin{array}{|c|ccccc|} \hline & x-2\Delta x & x-\Delta x & x & x+\Delta x & x+2\Delta x \\ \hline t-\Delta t & & & 15 & & \\ t & -2 & 8 & 138 & 8 & -2 \\ t+\Delta t & & & 15 & & \\ \hline \end{array}, \tag{23}$$

which are chosen so that the error of the force term matches the errors of the other operators. Note that blank spaces in eq. (23) indicate zeros. The weighting scheme in eq. (23) is essentially perfect for a homogeneous medium and a source exactly at a grid point. We have derived accurate treatments of the source term for heterogeneous media or sources located between grid points[8], but a detailed discussion is beyond the scope of this paper.

The time dependence of the force is a “Ricker wavelet” (a function commonly used in seismological modeling studies), defined as follows]:

$$R(t) = (2\pi^2 f_c^2 t^2 - 1) \exp(-\pi^2 f_c^2 t^2), \tag{24}$$

where the characteristic frequency f_c has a value of 30 Hz. The source is located at $x_0 = 500$ m, and the receiver at $x = 250$ m.

As shown by the left and center panels of Fig. 2, the solution is stable for values of C within the second stability range (eq. 21), but unstable for values of C outside this range. Thus the above theoretical results are confirmed.

3.2 $O(2,2)$ scheme

We now investigate the possible existence of a second range of stability for the optimally accurate $O(2,2)$ scheme, for which eqs. (1), (9), and (13)–(15) hold without change, provided that the operators in eqs. (10) and (11) are redefined as follows:

$$\mathbf{L}^{(2)} = \begin{pmatrix} 1, & -2, & 1 \end{pmatrix} \tag{25}$$

$$\mathbf{L}^{(4)} = \frac{1}{12}\mathbf{L}^{(2)}, \tag{26}$$

and the limits of summation in eq. (12) are -1 to 1.

We substitute eq. (16) into eq. (15) to obtain the following dispersion relation (using eq. 17):

$$A = 1 + C^2(E-1) + (3 - 4E + F)\left(\frac{C^4}{12} - \frac{C^2}{12}\right). \tag{27}$$

As shown in Fig. 1 (right panel), and as can be analytically verified, the stability condition eq. (19) is satisfied in two cases. The first is the well known case of

$$0 \leq C \leq 1. \tag{28}$$

However, Fig. 1 (right panel) shows that for the singular point $C = 2$, the stability condition eq. (19) is also satisfied.

The weights for the point force for the optimally accurate $O(2,2)$ scheme are

$\frac{1}{12} \times$ (29)

	$x - \Delta x$	x	$x + \Delta x$
$t - \Delta t$		1	
t	1	8	1
$t + \Delta t$		1	

A numerical experiment (Fig. 2, right) shows that stable solutions are obtained for $C = 2$. We have not run these calculations to exceedingly long times; it is possible that accumulated round-off errors might eventually lead to instability.

Note that for the optimally accurate $O(2,2)$ scheme the CFL condition[7] requires $C \leq 2$, so the singular point ($C = 2$) of the second stability regime is exactly at the upper CFL limit.

4 Discussion

Normally as FD schemes become higher order the upper bound on C decreases. For example, a conventional $O(2,2)$ FD scheme (eq. 9 using eq. 25) must satisfy $C \leq 1$, while a conventional $O(2,4)$ FD scheme (eq. 9 using eq. 10) must satisfy $C \leq \sqrt{3/4} \approx 0.8660$. Eq. (20) is an exception to this general pattern.

Fig. 2 shows that all of the stable solutions are basically accurate. We omit a detailed discussion, but it should be noted that the error of the numerical solutions for the second region of stability of the optimally accurate $O(2,4)$ scheme is about an order of magnitude worse than that for the first region. The errors for the case $C = 2$ for the optimally accurate $O(2,2)$ scheme were smaller than those for $0 \leq C \leq 1$ in some cases, and worse in others.

Although the potential utility of the second range of stability in practical calculations remains to be seen, it is a fascinating and apparently heretofore unknown (certainly not widely known) mathematical phenomenon, which, having been found, is fully explained by the analyses presented above.

In this paper we considered only the case of an infinite 1-D homogeneous medium (or, equivalently, a 1-D medium with periodic boundary conditions). It should be possible to extend this work to heterogeneous media with free surface boundary conditions using the eigenproblem approaches from our work on other numerical schemes[2,3], but a detailed discussion is omitted.

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