

A stability formula for Lax-Wendroff methods with fourth-order in time and general-order in space for the scalar wave equation

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ABSTRACT

Based on the formula for stability of finite-difference methods with second-order in time and general-order in space for the scalar wave equation, I obtain a stability formula for Lax-Wendroff methods with fourth-order in time and general-order in space. Unlike the formula for methods with second-order in time, this formula depends on two parameters: one parameter is related to the weights for approximations of second spatial derivatives; the other parameter is related to the weights for approximations of fourth spatial derivatives. When discretizing the mixed derivatives properly, the formula can be generalized to the case where the spacings in different directions are different. This formula can be useful in high-accuracy seismic modeling using the scalar wave equation on rectangular grids, which involves both high-order spatial discretizations and high-order temporal approximations. I also prove the instability of methods obtained by applying high-order finite-difference approximations directly to the second temporal derivative, and this result solves the “Bording’s conjecture.”

INTRODUCTION

Finite-difference methods are a useful tool for seismic modeling, imaging, and inversion. A condition for applicability of these methods is that they must be stable. Therefore, a formula for stability of finite-difference methods would be very helpful. Based on the well-known von Neumann method for analyzing stability, Lines et al. (1999) obtained a stability formula of

finite-difference methods with second-order in time and general-order in space for the scalar wave equation. The resulting formula depends only on one parameter, which is the sum of absolute values of weights of the finite-difference approximations for second spatial derivatives.

To achieve a balance between the accuracy of spatial discretizations and that of temporal discretizations, it is desirable to develop high-order temporal approximations. To this aim, a natural approach is to apply directly high-order finite-difference discretizations to the second temporal derivative. However, this approach does not work because the resulting finite-difference methods are unstable (see Appendix A). The “Bording’s conjecture” was raised in Lines et al. (1999), which is a stability formula for finite-difference methods with general-order in time and general-order in space. Because applying high-order finite-difference approximations to the second temporal derivative directly leads to instability, the “Bording’s conjecture” holds only for second-order finite-difference approximation of the second temporal derivative. To obtain high-order temporal approximations, one still uses second-order finite-difference approximation of the second temporal derivative, but at the same time needs to replace the high-order temporal derivatives (the errors caused by the second-order finite-difference approximation of the second temporal derivative) by spatial derivatives via the wave equation. This method is called the Lax-Wendroff method (Dablain, 1986; Carcione et al., 2002; Chen, 2007, 2009).

In this paper, I will generalize the stability formula obtained in Lines et al. (1999) for the scalar wave equation and derive a formula for stability of Lax-Wendroff methods with fourth-order in time and general-order in space. This is followed by (1) a description of the relationship between new and old formulas, (2) the generalization to the case where spacings in different directions are different, and (3) the approximation of the mixed fourth spatial derivatives. Finally, based on this new formula, some stability limits are tabulated and compared.

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STABILITY FORMULA FOR LAX-WENDROFF METHODS WITH FOURTH-ORDER IN TIME

The 3D acoustic wave equation is

$$\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{1}{c^2} \frac{\partial^2}{\partial t^2}, \quad (1)$$

where (p, u, v) is the pressure wavefield and (u, v, w) is the velocity. First, I consider a finite-difference method with second-order in time and general-order in space:

$$\frac{p_{i,j,k}^{n+1} - 2p_{i,j,k}^n + p_{i,j,k}^{n-1}}{\Delta t^2} = \frac{1}{c^2} \sum_{\ell=-\infty}^{\infty} \left(\frac{1}{\Delta x^\ell} p_{i+\ell, j, k}^n + \frac{2}{\Delta x^\ell} p_{i, j+\ell, k}^n + \frac{3}{\Delta x^\ell} p_{i, j, k+\ell}^n \right), \quad (2)$$

where $\Delta x^\ell \approx (\Delta x, \Delta x, \Delta x, \Delta x)$, Δx^ℓ ,

where

$$\begin{aligned}
 \mathcal{D} = & 1 + \frac{2\Delta^2}{2} \sum_{\ell=-} \left(\binom{1}{\ell} i\ell\kappa + \binom{2}{\ell} i\ell\kappa + \binom{3}{\ell} i\ell\kappa \right) \\
 & + \frac{4\Delta^4}{24} \sum_{\ell=-} \left(\binom{4}{\ell} i\ell\kappa + \binom{5}{\ell} i\ell\kappa + \binom{6}{\ell} i\ell\kappa \right) \\
 & + \frac{4\Delta^4}{24} \sum_{\ell=-1}^1 \sum_{\ell=-1}^1 2 \left(\binom{7}{\ell} i(\ell\kappa + \kappa) + \binom{8}{\ell} i(\ell\kappa + \kappa) \right. \\
 & \left. + \binom{9}{\ell} i(\ell\kappa + \kappa) \right), \tag{9}
 \end{aligned}$$

where i is the unit of imaginary numbers, κ , κ , and κ are wavenumbers in the x , y , and z directions, respectively, and Δ is the Fourier amplitude at a particular step.

The stability is guaranteed if the moduli of the roots of equation 8 are less than or equal to unity. This requires $|\mathcal{D}| \leq 1$. Using equation 9, one can obtain

$$\left| \tilde{\mathcal{D}}^2 + \frac{\tilde{\mathcal{D}}}{12} \right| \leq 4,$$

where $\tilde{\mathcal{D}}$ is the same as in equation 3, and

$$\begin{aligned}
 \tilde{\mathcal{D}} = & \sum_{\ell=-} \left(\binom{1}{\ell} i\ell\kappa + \binom{2}{\ell} i\ell\kappa + \binom{3}{\ell} i\ell\kappa \right), \\
 \tilde{\mathcal{D}} = & \sum_{\ell=-} \left(\binom{4}{\ell} i\ell\kappa + \binom{5}{\ell} i\ell\kappa + \binom{6}{\ell} i\ell\kappa \right) \\
 & + \sum_{\ell=-1}^1 \sum_{\ell=-1}^1 2 \left(\binom{7}{\ell} i(\ell\kappa + \kappa) + \binom{8}{\ell} i(\ell\kappa + \kappa) \right. \\
 & \left. + \binom{9}{\ell} i(\ell\kappa + \kappa) \right). \tag{10}
 \end{aligned}$$

Using the triangle inequality regarding the sum of complex numbers, one can further obtain

$$\tilde{\mathcal{D}}^2 + \frac{\tilde{\mathcal{D}}}{12} \leq 4,$$

where

$$\begin{aligned}
 & = \sum_{\ell=-} (|\binom{1}{\ell}| + |\binom{2}{\ell}| + |\binom{3}{\ell}|), \\
 & = \sum_{\ell=-} (|\binom{4}{\ell}| + |\binom{5}{\ell}| + |\binom{6}{\ell}|) \\
 & + \sum_{\ell=-1}^1 \sum_{\ell=-1}^1 2 (|\binom{7}{\ell}| + |\binom{8}{\ell}| + |\binom{9}{\ell}|). \tag{11}
 \end{aligned}$$

The number $\tilde{\mathcal{D}}$ represents the sum of absolute values of weights for approximations of the fourth spatial derivatives (mixed derivatives are counted twice).

From inequality (11), one has

$$\tilde{\mathcal{D}}^2 \leq \frac{24}{3 + \sqrt{9^2 + 12}}. \tag{12}$$

Finally, one obtains

$$\leq \frac{2\sqrt{6}}{\sqrt{3 + \sqrt{9^2 + 12}}}. \tag{13}$$

The inequality 13 is the stability formula for the finite-difference method 7

In principle, the stability formulas for higher-order temporal discretizations can be obtained in the same way by considering more terms in equation 4. For example, for a Lax-Wendroff method with sixth-order in time and general-order in space, its stability formula depends on three parameters that correspond to the sum of absolute values of weights for approximations of second spatial derivatives, fourth spatial derivatives, and sixth spatial derivatives, respectively. Of course, the formula is very complicated.

SOME NOTES ON STABILITY FORMULA 13

Relationship between formulas 3 and 13

Clearly, the formula 13 can be rewritten as

$$\leq \frac{2}{\sqrt{\tilde{\mathcal{D}}}}, \tag{14}$$

where

$$= \frac{2}{2} + \frac{2}{2} \sqrt{1 + \frac{4}{3^2}}. \tag{15}$$

One can readily see that $\tilde{\mathcal{D}} > 3$. Therefore, for the same order of spatial accuracy, the stability limit of the finite-difference method with fourth-order in time is smaller than that of the finite-difference method with second-order in time. This is because the method with fourth-order in time involves approximations of fourth derivatives, which constitute the parameter $\tilde{\mathcal{D}}$. When $\tilde{\mathcal{D}} = 0$, the formula 13 reduces to the formula 3. Therefore, the formula 13 can be regarded as a generalization of the formula 3.

Generalization to the case where Δx , Δy , and Δz are different

From the derivation of formula 13, one can readily see that the formula 13 can be generalized to

$$\tilde{\mathcal{D}} \equiv \frac{\Delta}{\tilde{\mathcal{D}}} \leq \frac{2\sqrt{6}}{\sqrt{3 + \sqrt{9^2 + 12}}}, \tag{16}$$

where

$$\tilde{\mathcal{D}} = \sqrt{\frac{1}{\frac{1}{3} \left(\frac{1}{\Delta^2} + \frac{1}{\Delta^2} + \frac{1}{\Delta^2} \right)}}, \tag{17}$$

if the following conditions are satisfied:

$$\sum_{\ell=-} |\binom{1}{\ell}| = \sum_{\ell=-} |\binom{2}{\ell}| = \sum_{\ell=-} |\binom{3}{\ell}|, \tag{18}$$

$$\sum_{\ell=-} |\binom{4}{\ell}| = \sum_{\ell=-} |\binom{5}{\ell}| = \sum_{\ell=-} |\binom{6}{\ell}|, \tag{19}$$

Table 1. Weights of some approximations for second derivatives $\partial^2 p / \partial x^2$, $\partial^2 p / \partial y^2$, and $\partial^2 p / \partial z^2$.

	-5	-4	-3	-2	-1	0	1	2	3	4	5
Fourth-order				-1/12	4/3	-5/2	4/3	-1/12			
Sixth-order			1/90	-3/20	3/2	-49/18	3/2	-3/20	1/90		
Eighth-order		-1/560	8/315	-1/5	8/5	-205/72	8/5	-1/5	8/315	-1/560	
Tenth-order	1/3150	-5/1008	5/126	-5/21	5/3	-5269/1800	5/3	-5/21	5/126	-5/1008	1/3150

Table 2. Weights of fourth-order approximations for fourth derivatives $\partial^4 p / \partial x^4$, $\partial^4 p / \partial y^4$, and $\partial^4 p / \partial z^4$.

	-3	-2	-1	0	1	2	3
	-1/6	2	-13/2	28/3	-13/2	2	-1/6

Table 3. Weights of fourth-order approximations for the mixed fourth derivatives $\partial^4 p / \partial x^2 \partial y^2$, $\partial^4 p / \partial x^2 \partial z^2$, and $\partial^4 p / \partial y^2 \partial z^2$ obtained with the first method.

	-2	-1	0	1	2
-2	1/144	-1/9	5/24	-1/9	1/144
-1	-1/9	16/9	-10/3	16/9	-1/9
0	5/24	-10/3	25/4	-10/3	5/24
1	-1/9	16/9	-10/3	16/9	-1/9
2	1/144	-1/9	5/24	-1/9	1/144

Table 4. Weights of fourth-order approximations for the mixed fourth derivatives $\partial^4 p / \partial x^2 \partial y^2$, $\partial^4 p / \partial x^2 \partial z^2$, and $\partial^4 p / \partial y^2 \partial z^2$ obtained with the second method.

	-2	-1	0	1	2
-2		-1/12	1/6	-1/12	
-1	-1/12	5/3	-19/6	5/3	-1/12
0	1/6	-19/6	6	-19/6	1/6
1	-1/12	5/3	-19/6	5/3	-1/12
2		-1/12	1/6	-1/12	

$$\sum_{\ell=-1}^1 \sum_{\ell=-1}^1 \left| \frac{7}{\ell} \right| = \sum_{\ell=-1}^1 \sum_{\ell=-1}^1 \left| \frac{8}{\ell} \right| = \sum_{\ell=-1}^1 \sum_{\ell=-1}^1 \left| \frac{9}{\ell} \right|, \tag{20}$$

$$\sum_{\ell=-1}^1 \left| \frac{4}{\ell} \right| = \sum_{\ell=-1}^1 \sum_{\ell=-1}^1 \left| \frac{7}{\ell} \right|. \tag{21}$$

Conditions 18, 19, and 20 are easily satisfied because the weights for approximations of second and fourth derivatives are often chosen as the same for different spatial directions. For condition 21 to hold, care should be taken for the approximation of the mixed fourth derivatives.

Wu et al. (1996) once used the quantity $\tilde{\Delta}$, but did not name it. After analyzing its mathematical structure, I call $\tilde{\Delta}$ the root-harmonic-mean-square (rhms) spacing because the following expression:

$$\frac{1}{\frac{1}{3} \left(\frac{1}{\Delta^2} + \frac{1}{\Delta^2} + \frac{1}{\Delta^2} \right)} \tag{22}$$

is the harmonic mean of Δ^2 , Δ^2 , and Δ^2 .

Approximation of the mixed fourth derivatives

To facilitate the discussion and later calculation, I list the weights for some approximations of second derivatives $\frac{\partial^2}{\partial x^2}$, $\frac{\partial^2}{\partial y^2}$, and $\frac{\partial^2}{\partial z^2}$, and fourth derivatives $\frac{\partial^4}{\partial x^4}$, $\frac{\partial^4}{\partial y^4}$, and $\frac{\partial^4}{\partial z^4}$ in Table 1 and Table 2, respectively. For more details, see Fornberg (1996).

For the approximation of the mixed fourth derivatives, there are two methods: the first method is to use approximations of second derivatives in different directions twice; the second method is to derive the weights from a Taylor series expansion of functions in two variables. Table 3 and Table 4 list the weights of fourth-order approximations for the mixed fourth derivatives obtained with the first method and the second method, respectively. In terms of computational cost, the weights obtained with the second method are preferable because less grid points are used in the approximation. Furthermore, the sum of absolute values of weights for the second method is $\frac{80}{3}$ which is equal to the sum of absolute values of weights for the fourth-order approximation of the non-mixed fourth derivative, and thus the condition 21 is satisfied. On the other hand, the sum of absolute values of weights for the first method is $\frac{126}{9}$, and thus the condition 21 does not hold.

In equation 7, because there is a factor Δ^2 in the approximation of fourth spatial derivatives, the order of approximation of fourth spatial derivatives can be lower than that of second spatial derivatives. Table 5 lists the stability limits of equation 7 with fourth-order approximation for the fourth spatial derivatives (Tables 2 and 4) and different-order approximation for the second spatial derivatives (Table 1). To make a comparison, Table 6 lists the stability limits of equation 2 with different-order approximation for the second spatial derivatives (Table 1). For

Table 5. Stability limits ($\tilde{r}_{\max} = 2\sqrt{6}/\sqrt{3a + \sqrt{9a^2 + 12b}}$) of equation 7 with fourth-order approximation for the fourth spatial derivatives (Tables 2 and 4) and different-order approximation for the second spatial derivatives (Table 1).

	1D	2D	3D
Fouth-order	$= 16/3, = 80/3$ $\tilde{r}_{\max} \approx 0.7746$	$= 32/3, = 320/3$ $\tilde{r}_{\max} \approx 0.5477$	$= 16, = 720/3$ $\tilde{r}_{\max} \approx 0.4472$
Sixth-order	$= 272/45, = 80/3$ $\tilde{r}_{\max} \approx 0.7419$	$= 544/45, = 320/3$ $\tilde{r}_{\max} \approx 0.5246$	$= 272/15, = 720/3$ $\tilde{r}_{\max} \approx 0.4283$
Eighth-order	$= 2048/315, = 80/3$ $\tilde{r}_{\max} \approx 0.7225$	$= 4096/315, = 320/3$ $\tilde{r}_{\max} \approx 0.5109$	$= 2048/105, = 720/3$ $\tilde{r}_{\max} \approx 0.4172$
Tenth-order	$= 42983/6300, = 80/3$ $\tilde{r}_{\max} \approx 0.7079$	$= 42983/3150, = 320/3$ $\tilde{r}_{\max} \approx 0.5018$	$= 42983/2100, = 720/3$ $\tilde{r}_{\max} \approx 0.4097$

Table 6. Stability limits ($\tilde{r}_{\max} = 2/\sqrt{a}$) of equation 2 with different-order approximation for the second spatial derivatives (Table 1).

	1D	2D	3D
Fouth-order	$= 16/3$ $\tilde{r}_{\max} \approx 0.8660$	$= 32/3$ $\tilde{r}_{\max} \approx 0.6124$	$= 16$ $\tilde{r}_{\max} \approx 0.5$
Sixth-order	$= 272/45$ $\tilde{r}_{\max} \approx 0.8135$	$= 544/45$ $\tilde{r}_{\max} \approx 0.5752$	$= 272/15$ $\tilde{r}_{\max} \approx 0.4697$
Eighth-order	$= 2048/315$ $\tilde{r}_{\max} \approx 0.7844$	$= 4096/315$ $\tilde{r}_{\max} \approx 0.5546$	$= 2048/105$ $\tilde{r}_{\max} \approx 0.4529$
Tenth-order	$= 42983/6300$ $\tilde{r}_{\max} \approx 0.7657$	$= 42983/3150$ $\tilde{r}_{\max} \approx 0.5414$	$= 42983/2100$ $\tilde{r}_{\max} \approx 0.4421$

completeness, the corresponding stability limits for 1D and 2D versions of equations 7 and 2 are also included. In Tables 5 and 6, the stability limits both decrease with increasing orders and increasing dimensionality. The stability limits in Table 5 are smaller than the corresponding ones in Table 6, which demonstrates the theoretical comparison between formulas 3 and 13.

CONCLUSIONS

In this paper, a formula for stability of Lax-Wendroff methods with fourth-order of temporal accuracy and general-order of spatial accuracy is obtained. This formula depends on two parameters: one is the sum of absolute values of weights of the finite-difference operators for second spatial derivatives; the other is the sum of absolute values of weights of the finite-difference operators for fourth spatial derivatives. Compared with their counterparts with second-order in time, the finite-difference methods with fourth-order in time have smaller stability limits due to the additional weights from approximations of the fourth derivatives. Fortunately, the difference between these two stability limits are small, particularly for 3D high-order methods. When the sums of absolute values of weights for approximations of second derivatives and fourth derivatives in different spatial directions equal each other, respectively, the stability formula can be extended to accommodate different directional spacings.

I also prove that methods, which are obtained by applying high-order finite-difference approximations directly to the second temporal derivative, are unstable. Based on this result, a conclusion can be drawn that the ‘‘Bording’s conjecture’’ does not hold for direct fourth-order and higher-order finite-difference approximations for the second temporal derivative.

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APPENDIX A

INSTABILITY OF METHODS OBTAINED BY APPLYING HIGH-ORDER FINITE-DIFFERENCE APPROXIMATIONS DIRECTLY TO THE SECOND TEMPORAL DERIVATIVE

One can obtain higher-temporal-accuracy versions of equation 2 by applying high-order finite-difference approximations directly to the second temporal derivative in equation 1. This results in

$$\sum_{\ell=-\infty}^{\infty} \binom{2}{\ell} \left(\frac{\Delta^2}{2} \sum_{\ell=-\infty}^{\infty} \left(\binom{1}{\ell} \frac{\Delta^2}{2} + \binom{2}{\ell} \frac{\Delta^2}{2} + \binom{3}{\ell} \frac{\Delta^2}{2} \right) \right), \quad (\text{A-1})$$

where $\Delta = \Delta t$ and $\Delta t \geq 2$. Equation A-1 has the temporal accuracy of $\mathcal{O}(\Delta^2)$.

Now I will prove that equation A-1 is unstable. Replacing Δt by $\Delta t e^{i\kappa \Delta t}$, substituting the expression $\Delta t = i(\kappa \Delta t + \kappa \Delta t + \kappa \Delta t)$ into equation A-1 and dividing the resulting equation by $i(\kappa + \kappa + \kappa)$, one obtains

$$2 + \frac{-1}{2} 2^{-1} + \dots + \frac{(0-)}{2} + \dots + \frac{-(-1)}{2} + 1 = 0, \quad (\text{A-2})$$

where

$$= \frac{2\Delta^2}{2} \sum_{\ell=-\infty}^{\infty} \left(\binom{1}{\ell} i\ell\kappa + \binom{2}{\ell} i\ell\kappa + \binom{3}{\ell} i\ell\kappa \right). \quad (\text{A-3})$$

Multiplying both sides of equation (A-2) by $1/2$ and using the fact that $\Delta t = \Delta t$ leads to

$$2 + \frac{-1}{2} 2^{-1} + \dots + \frac{(0-)}{2} + \dots + \frac{-(-1)}{2} + 1 = 0. \quad (\text{A-4})$$

The weights Δt have an analytical expression (Fornberg, 1996):

$$= \begin{cases} \frac{2(-1)^{+1}(-1)^2}{2^{+1}(-1)!(-1)!}, & = \pm 1, \pm 2, \dots, \pm \infty, \\ -2 \sum_{\ell=1}^{\infty} \frac{1}{2^\ell}, & = 0. \end{cases} \quad (\text{A-5})$$

Noting that $-1 \geq 1$ since $\Delta t \geq 2$, one obtains the coefficient of 2^{-1} in equation A-4 by using equation A-5:

$$\frac{-1}{2} = -2 \frac{2}{(-1)^2}. \quad (\text{A-6})$$

It follows from equation (A-6) that

$$\left| \frac{-1}{2} \right| > 2. \quad (\text{A-7})$$

Suppose that equation A-4 has 2 roots $\Delta t = 1, 2, \dots, 2$; then one obtains

$$\prod_{\ell=1}^2 \left(\frac{-1}{2} \right) = 2 + \frac{-1}{2} 2^{-1} + \dots + \frac{(0-)}{2} + \dots + \frac{-(-1)}{2} + 1. \quad (\text{A-8})$$

Note that every term of expansion of $\prod_{\ell=1}^2 \left(\frac{-1}{2} \right)$ is a product of 2 numbers (or $-$). Therefore, it follows from A-8 that

$$\frac{-1}{2} = \sum_{\ell=1}^2 \left(\frac{-1}{2} \right). \quad (\text{A-9})$$

Now I use the method of proof by contradiction. Suppose that the moduli of Δt are less than or equal to unity, i.e.,

$$|\Delta t| \leq 1, \quad \Delta t = 1, 2, \dots, 2. \quad (\text{A-10})$$

Then, it follows from A-9 and A-10 that

$$\left| \frac{-1}{2} \right| \leq \sum_{\ell=1}^2 |\Delta t| \leq 2. \quad (\text{A-11})$$

Inequality A-11 contradicts with inequality A-7. Therefore, there is at least one root of equation A-4 whose modulus is greater than one. This shows that equation A-1 is unstable.

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