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A practical implicit finite-difference method: examples from seismic modelling

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Abstract

We derive explicit and new implicit finite-difference formulae for derivatives of arbitrary order with any order of accuracy by the plane wave theory where the finite-difference coefficients are obtained from the Taylor series expansion. The implicit finite-difference formulae are derived from fractional expansion of derivatives which form tridiagonal matrix equations. Our results demonstrate that the accuracy of a $(2N + 2)$th-order implicit formula is nearly equivalent to that of a $(6N + 2)$th-order explicit formula for the first-order derivative, and $(2N + 2)$th-order implicit formula is nearly equivalent to $(4N + 2)$th-order explicit formula for the second-order derivative. In general, an implicit method is computationally more expensive than an explicit method, due to the requirement of solving large matrix equations. However, the new implicit method only involves solving tridiagonal matrix equations, which is fairly inexpensive. Furthermore, taking advantage of the fact that many repeated calculations of derivatives are performed by the same difference formula, several parts can be precomputed resulting in a fast algorithm. We further demonstrate that a $(2N + 2)$th-order implicit formulation requires nearly the same memory and computation as a $(2N + 4)$th-order explicit formulation but attains the accuracy achieved by a $(6N + 2)$th-order explicit formulation for the first-order derivative and that of a $(4N + 2)$th-order explicit method for the second-order derivative when additional cost of visiting arrays is not considered. This means that a high-order explicit method may be replaced by an implicit method of the same order resulting in a much improved performance. Our analysis of efficiency and numerical modelling results for acoustic and elastic wave propagation validates the effectiveness and practicality of the implicit finite-difference method.

Keywords: implicit finite-difference formulae, explicit finite-difference formulae, any order accuracy, any order derivative, plane wave theory, tridiagonal matrix equations, precision comparison, acoustic wave, elastic wave, seismic wave, numerical modelling

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Many scientific and engineering problems involve numerically solving partial differential equations. A variety of difference techniques, such as the finite-difference (FD), the pseudospectral (PS) and the finite-element (FM) methods, have been developed. However, because of the straightforward implementation, requiring small memory and computation time, the FD is the most popular and has been widely utilized in seismic modelling (Kelly *et al* 1976, Dablain 1986, Virieux 1986, Igel *et al* 1995, Etgen and O'Brien 2007, Bansal and Sen 2008) and migration (Claerbout 1985, Larner and Beasley 1987, Li 1991, Ristow and Ruhl 1994, Zhang *et al* 2000, Fei and Liner 2008). In order to improve the efficiency, the accuracy and the stability of a FDM in numerical modelling, several variants of FD methods have been developed.

A conventional FD needs a fixed number of grid points per wavelength in any one layer. In fact, a coarse mesh can be used in the high-velocity layer for its large wavelength. Therefore, variable grid schemes are proposed to significantly reduce computational time and memory requirements. When there is an abrupt transition from the adaptive region of a coarse mesh to a much finer mesh, large amplitude artificial reflections from the adaptive zone may occur. To overcome these problems, the scheme of interpolating the field variables in the adaptive region has been developed (Wang and Schuster 1996, Hayashi and Burns 1999). Other advanced methods include the PS-2 method for regular grids (Zahradník and Priolo 1995) and a simple case of so-called rectangular irregular grids. This method is developed further and applied to both nonplanar topography and internal discontinuities (Opršal and Zahradník 1999).

To save computational cost, besides optimizing mesh sizes according to the local parameters, different temporal sampling in different parts of the numerical grid is introduced by Falk *et al* (1996). Since the method is restricted to ratios of time steps between the different domains of $2n$, a new method is proposed to handle any positive integer ratio and does not depend on the time-step ratio by Tessmer (2000).

To improve the modelling accuracy of the first-order elastic and viscoelastic wave equations, staggered-grid FD schemes that involve defining different components of one physical parameter at different staggered points are usually applied to compute the derivatives in the equations (Virieux 1986, Levander 1988, Robertsson *et al* 1994, Graves 1996). However, boundary conditions of the elastic wave field at a free surface, i.e. the high-contrast discontinuity between vacuum and rock, must be defined in the FD algorithm (Robertsson 1996, Graves 1996, Opršal and Zahradník 1999, Saenger and Bohlen 2004). To avoid this problem, a rotated staggered-grid technique (Gold *et al* 1997, Saenger *et al* 2000) is presented where high contrast discontinuities can be incorporated without using explicit boundary conditions and without averaging elastic moduli. A velocity–stress rotated staggered-grid algorithm is used to simulate seismic waves in an elastic and viscoelastic model with 3D topography of the free surface (Saenger and Bohlen 2004). The accuracy for modelling Rayleigh waves utilizing the standard staggered-grid and the rotated staggered-grid method is also investigated by Bohlen and Saenger (2006).

A conventional method uses FD operators with low-order accuracy to calculate space derivatives; therefore, it needs small processor memory and less computation time, but leads to low accuracy results. High-order FD schemes are developed to improve the accuracy of the conventional finite-difference method. The FD scheme with any order accuracy has been derived for the first-order derivatives and used to solve the wave equations (Dablain 1986, Fornberg 1987, Crase 1990, Visbal and Gaitonde 2001, Hestholm 2007). The FD coefficients are determined by the Taylor series expansion (Dablain 1986) or by an optimization (Fornberg 1987). Using the Taylor series expansion also, the FD method with any even-order accuracy is presented for any order derivatives (Liu *et al* 1998) and utilized to simulate wave propagation in two-phase anisotropic media (Liu and Wei 2008).

However, most of these methods make use of the explicit finite-difference method (EFDM). Some development on the implicit finite-difference method (IFDM) has also been reported in the literature. To yield good modelling results, implicit finite-difference formulae are skilfully derived for the elastic wave equation (Emerman *et al* 1982). These formulae express the value of a variable at some point at a future time in terms of the value of the variable at that point and at its neighbouring points at present time, past times and future times. An IFDM for time derivatives has also been implemented in seismic migration algorithms (Ristow and Ruhl 1997, Shan 2007, Zhang and Zhang 2007).

Here, we focus on the space derivative calculation by a FDM. In our formulation, an EFDM directly calculates the derivative value at some point in terms of the function values at that point and at its neighbouring points. However, an IFDM expresses the derivative value at some point in terms of the function values at that point and at its neighbouring points and the derivative values at its neighbouring points. For example, a compact finite-difference method (CFDM) is one such IFDM (Lele 1992). In areas other than geophysics and seismology, several variants of the IFDM have been widely studied (Ekaterinaris 1999, Meitz and Fasel 2000, Lee and Seo 2002, Nihei and Ishii 2003). Zhang and Chen (2006) proposed a new numerical method, named the traction image method, to accurately and efficiently implement the traction-free boundary conditions in finite-difference simulation in the presence of surface topography. In this method, the physical traction-free boundary conditions provide a constraint on the derivatives of the velocity components along the free surface, which leads to a solution to calculate the derivative of the velocity components by a compact scheme.

In this paper, we derive both explicit and implicit finite-difference formulae with even-order accuracy for any order derivative. Further, we develop a practical IFDM and demonstrate its efficiency and applicability with some numerical results.

2. Implicit finite difference with fourth-order accuracy for second derivative

A second-order central difference operator for a function $p(x)$ is expressed as

$$\frac{\delta^2 p}{\delta x^2} = \frac{p(x+h) + p(x-h) - 2p(x)}{h^2}, \tag{2.1}$$

where x is a real variable and h is a small value.

Then,

$$\frac{\partial^2 p}{\partial x^2} = \lim_{h\to 0} \frac{\delta^2 p}{\delta x^2}. \tag{2.2}$$

According to the plane wave theory, we let

$$p = p_0 \,\mathrm{e}^{\mathrm{i}kx}, \tag{2.3}$$

where p_0 is a constant value, $\mathrm{i} = \sqrt{-1}$, k represents the wavenumber; then

$$\frac{\partial^2 p}{\partial x^2} = -k^2 p, \tag{2.4}$$

and

$$\frac{\delta^2 p}{\delta x^2} = \frac{p_0\,\mathrm{e}^{\mathrm{i}k(x+h)} + p_0\,\mathrm{e}^{\mathrm{i}k(x-h)} - 2p}{h^2} = \frac{-4\sin^2(kh/2)}{h^2}p. \tag{2.5}$$

To make $\frac{\delta^2 p}{\delta x^2}$ approach $\frac{\partial^2 p}{\partial x^2}$, a conventional EFDM lets $-\frac{4\sin^2(kh/2)}{h^2}$ approach $-k^2$. It is certain that $\frac{-4\sin^2(kh/2)}{h^2} \to -k^2$ when $h \to 0$.

Suggested by the idea of series expansion, the following expression is introduced by adding higher-order terms to approach $\frac{\partial^2 p}{\partial x^2}$ better:

$$\frac{\partial^2 p}{\partial x^2} \approx \frac{\delta^2 p}{\delta x^2} - bh^2\frac{\delta^4 p}{\delta x^4}, \tag{2.6}$$

where b is an adjustable constant. This expression can be rewritten as follows (Claerbout 1985):

$$\frac{\partial^2 p}{\partial x^2} \approx \frac{\frac{\delta^2 p}{\delta x^2}}{1 + bh^2\frac{\delta^2}{\delta x^2}}. \tag{2.7}$$

Substituting equations (2.3) into (2.7) and simplifying, we have

$$-k^2 \approx \frac{-\frac{4\sin^2(kh/2)}{h^2}}{1 - 4b\sin^2(kh/2)}. \tag{2.8}$$

If we substitute $\alpha = kh/2$, equation (2.8) reduces to

$$\frac{\sin^2\alpha}{1 - 4b\sin^2\alpha} \approx \alpha^2, \tag{2.9}$$

that is

$$\sin^2\alpha \approx \alpha^2(1 - 4b\sin^2\alpha). \tag{2.10}$$

Using a Taylor's series expansion for $\sin\alpha$ on both sides of the equation, we can write

$$\left(\alpha - \tfrac{1}{6}\alpha^3 + \cdots\right)^2 \approx \alpha^2\left[1 - 4b\left(\alpha - \tfrac{1}{6}\alpha^3 + \cdots\right)^2\right]. \tag{2.11}$$

Comparing the coefficients of α^4 in equation (2.11), we get

$$b = \tfrac{1}{12}. \tag{2.12}$$

For the Nyquist spatial frequency (maximum frequency), we have

$$kh = \pi, \qquad \alpha = \frac{\pi}{2}, \tag{2.13}$$

b is obtained from equation (2.9):

$$b = \frac{1}{4} - \frac{1}{\pi^2} \approx \frac{1}{6.726}. \tag{2.14}$$

Now if we let

$$\int_0^{\pi/2} \sin^2\alpha \,\mathrm{d}\alpha = \int_0^{\pi/2} \alpha^2(1 - 4b\sin^2\alpha)\,\mathrm{d}\alpha, \tag{2.15}$$

we have

$$b = \frac{\pi^2 - 6}{2\pi^2 + 12} \approx \frac{1}{8.202}. \tag{2.16}$$

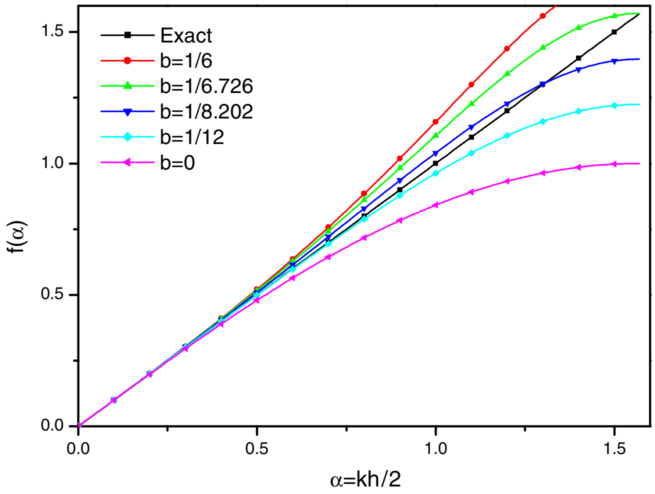


Figure 1. Plot of $f(\alpha)$ against α for different b values.

Thus, using three different approximations, we obtain three different values of b given by equations (2.12), (2.14) and (2.16). Further, Claerbout (1985) suggested the following value of b to fit over a wide range:

$$b = \tfrac{1}{6}. \tag{2.17}$$

Zhu and Wei (2006) used the best approximation method to estimate a b value in a certain area; therefore, b varies with the area in their formulation.

Recall that our goal is to satisfy equation (2.9). Thus, to examine the accuracy of these formulae, we examine the following function:

$$f(\alpha) = \sqrt{\frac{\sin^2\alpha}{1 - 4b\sin^2\alpha}}. \tag{2.18}$$

We evaluate the above equation for different values of b to examine how closely it approximates α for a range of α values. We consider positive values of α only since $f(\alpha)$ in formula (2.9) is symmetrical about zero. When calculating $f(\alpha)$, α only ranges from 0 to $\pi/2$, because kh is equal to π at the Nyquist frequency. The function $f(\alpha)$ against α for different b values is shown in figure 1. From this figure, it is seen that $f(\alpha)$ with $b = 1/12$ approaches the true values of $f(\alpha)$ when α varies from 0 to 0.7, which indicates that the b value from the Taylor series expansion provides the highest precision for a small range of α.

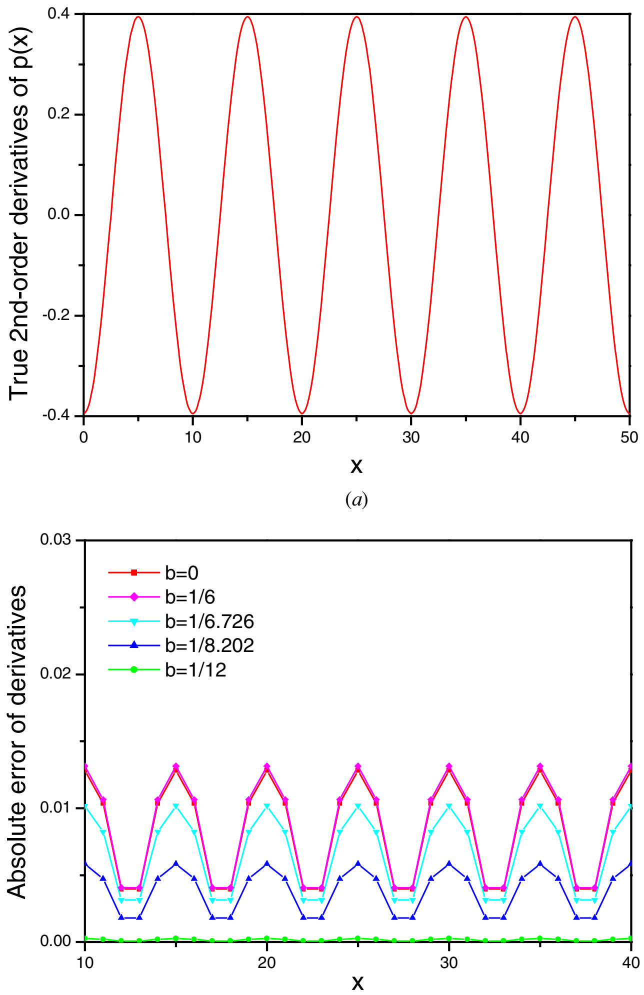
Next, we use formula (2.7) to calculate second derivatives. Let

$$q = \frac{\partial^2 p}{\partial x^2}. \tag{2.19}$$

Then, the following formula for second derivatives is obtained from equation (2.7):

$$q + bh^2\frac{\delta^2 q}{\delta x^2} \approx \frac{\delta^2 p}{\delta x^2}. \tag{2.20}$$

Using the second difference operator (2.1), formula (2.20) reduces to the following form:



(*a*)

(*b*)

Figure 2. An example testing the accuracy of EFDM and IFDM with different b values. (*a*) True second-order derivatives $q(x)$ of $p(x)$. (*b*) Absolute error between calculated and true derivatives by different b values.

$$bq(x+h)+bq(x-h)+(1-2b)q(x) = \frac{p(x+h)+p(x-h)-2p(x)}{h^2}. \tag{2.21}$$

Note that equation (2.21) is an explicit finite-difference formula when $b = 0$; it is an implicit formula for $b \neq 0$.

An example of calculating the second-order derivatives $q(x)$ by equation (2.21) is shown in figure 2, where $p(x) = \cos(\pi x/5)$, $h = 1$. The details of the algorithm are shown in section 6. Figure 2(*a*) shows the second-order derivatives of $p(x)$, and figure 2(*b*) illustrates absolute errors between the calculated derivatives with different b values and the true derivatives. This figure also indicates that the b value derived from the Taylor series expansion ($b = 1/12$) produces the second derivatives with the highest precision.

Our numerical results in the preceding paragraphs demonstrate that the Taylor series expansion method must be used to calculate the b value. Next, we derive explicit and implicit finite-difference formulae with even-order accuracy for any order derivative based on this idea.

3. Explicit finite-difference formulae with even-order accuracy

3.1. Even-order accurate finite-difference formula for the (2K − 1)th-order derivative

An explicit finite-difference formula for the $(2K-1)$th-order derivative is defined as follows (Dablain 1986):

$$\frac{\partial^{2K-1} p}{\partial x^{2K-1}} \approx \frac{\delta^{2K-1} p}{\delta x^{2K-1}} = \frac{1}{h^{2K-1}} \sum_{m=-M}^{M} c_m\, p(x+mh), \tag{3.1}$$

where $M = N + K - 1$, N and K are positive integers, N is related to the order of the approximation, c_m is an odd discrete sequence due to the centred finite difference and $c_0 = 0$.

Now we substitute $p = p_0\, \mathrm{e}^{\mathrm{i}kx}$ into formula (3.1) and simplify it to obtain

$$(-1)^{K-1} 2^{2K-2} \alpha^{2K-1} \approx \sum_{m=1}^{M} c_m \sin(2m\alpha), \tag{3.2}$$

where $\alpha = kh/2$.

Using the Taylor series expansion, we have

$$\sum_{m=1}^{M} c_m \sin(2m\alpha) = \sum_{n=1}^{\infty}\left[\frac{(-1)^{n-1}2^{2n-1}}{(2n-1)!}\sum_{m=1}^{M}\left(m^{2n-1}c_m\right)\alpha^{2n-1}\right]. \tag{3.3}$$

Comparing the coefficients of α for the first M terms of equation (3.2) with those of equation (3.3), we obtain

$$\frac{(-1)^{n-1}2^{2n-1}}{(2n-1)!}\sum_{m=1}^{M}\left(m^{2n-1}c_m\right) = \begin{cases}(-1)^{K-1}2^{2K-2} & (n = K)\\ 0 & (n \neq K).\end{cases} \tag{3.4}$$

Equations (3.4) can be rewritten in the following matrix form:

$$\begin{bmatrix} (1^2)^0 & (2^2)^0 & \cdots & (M^2)^0 \\ \vdots & \vdots & \vdots & \vdots \\ (1^2)^{K-2} & (2^2)^{K-2} & \cdots & (M^2)^{K-2} \\ (1^2)^{K-1} & (2^2)^{K-1} & \cdots & (M^2)^{K-1} \\ (1^2)^{K} & (2^2)^{K} & \cdots & (M^2)^{K} \\ \vdots & \vdots & \vdots & \vdots \\ (1^2)^{M-1} & (2^2)^{M-1} & \cdots & (M^2)^{M-1} \end{bmatrix} \begin{bmatrix} c_1 \\ 2c_2 \\ \vdots \\ Mc_M \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ (2K-1)!/2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{3.5}$$

Table 1. Coefficients of explicit difference for the first-order derivative.

Order of accuracy	c_1	c_2	c_3	c_4	c_5	c_6	c_7
2	1/2						
4	2/3	−1/12					
6	3/4	−3/20	1/60				
8	4/5	−1/5	4/105	−1/280			
10	5/6	−5/21	5/84	−5/504	1/1260		
12	6/7	−15/56	5/63	−1/56	1/385	−1/5544	
14	7/8	−7/24	7/72	−7/264	7/1320	−7/10 296	1/24 024

The coefficient matrix is a Vandermonde matrix. The c_m ($m = 1, 2, \ldots, M$) values are obtained by solving the system of equations, which are identical to those obtained using another method by Liu *et al* (1998) and Liu and Wei (2008).

The absolute error of the finite-difference formula, derived from equation (3.2), is

$$e_N = \left| \sum_{n=M+1}^{\infty} \left[\frac{(-1)^{n-1} 2^{2n-1}}{(2n-1)!} \sum_{m=1}^{M} \left(m^{2n-1} c_m\right) \frac{2\alpha^{2n-1}}{h^{2K-1}} \right] \right|$$
$$= \left| \sum_{n=M+1}^{\infty} \left[\frac{(-1)^{n-1}}{(2n-1)!} \sum_{m=1}^{M} \left(m^{2n-1} c_m\right) 2k^{2n-1} h^{2n-2K} \right] \right|. \quad (3.6)$$

The minimum power of h in the error function is $2M + 2 - 2K$; therefore, the finite-difference formula (3.1) has $(2M + 2 - 2K)$th-order accuracy.

When $K = 1$, for the first-order derivative, $M = N$; its difference coefficients are simplified to the following:

$$c_m = \frac{(-1)^{m+1}}{2m} \prod_{1 \leqslant i \leqslant N, i \neq m} \left| \frac{i^2}{m^2 - i^2} \right|. \quad (3.7)$$

These coefficients are equivalent to those obtained by Fornberg (1987), Liu *et al* (1998) and Liu and Wei (2008). Table 1 lists the difference coefficients for orders up to 14.

3.2. Even-order accurate finite-difference formula for the (2K)th-order derivative

An explicit finite-difference formula for the $(2K)$th-order derivative is defined as

$$\frac{\partial^{2K} p}{\partial x^{2K}} \approx \frac{\delta^{2K} p}{\delta x^{2K}} = \frac{1}{h^{2K}} \sum_{m=-M}^{M} c_m p(x + mh), \quad (3.8)$$

where $M = N + K - 1$, c_m is an even discrete sequence due to the centred finite-difference scheme used here.

Substituting $p = p_0 \mathrm{e}^{\mathrm{i}kx}$ into equation (3.8) and simplifying it, we obtain

$$(-1)^K 2^{2K-1} \alpha^{2K} \approx \frac{1}{2} c_0 + \sum_{m=1}^{M} c_m \cos(2m\alpha). \quad (3.9)$$

Using the Taylor series expansion, we have

$$\frac{1}{2} c_0 + \sum_{m=1}^{M} c_m \cos(2m\alpha)$$
$$= \frac{1}{2} c_0 + \sum_{m=1}^{M} c_m + \sum_{n=1}^{\infty} \left[\frac{(-1)^n 2^{2n}}{(2n)!} \sum_{m=1}^{M} \left(m^{2n} c_m\right) \alpha^{2n} \right]. \quad (3.10)$$

Comparing α coefficients of equation (3.9) with those of equation (3.10) for the first M items, we get

$$\frac{1}{2} c_0 + \sum_{m=1}^{M} c_m = 0, \quad (3.11a)$$

$$\frac{(-1)^n 2^{2n}}{(2n)!} \sum_{m=1}^{M} \left(m^{2n} c_m\right) = \begin{cases} (-1)^K 2^{2K-1} & (n = K) \\ 0 & (n \neq K). \end{cases} \quad (3.11b)$$

We can rewrite equations (3.11*b*) in the following matrix form:

$$\begin{bmatrix} (1^2)^0 & (2^2)^0 & \cdots & (M^2)^0 \\ \vdots & \vdots & \vdots & \vdots \\ (1^2)^{K-2} & (2^2)^{K-2} & \cdots & (M^2)^{K-2} \\ (1^2)^{K-1} & (2^2)^{K-1} & \cdots & (M^2)^{K-1} \\ (1^2)^{K} & (2^2)^{K} & \cdots & (M^2)^{K} \\ \vdots & \vdots & \vdots & \vdots \\ (1^2)^{M-1} & (2^2)^{M-1} & \cdots & (M^2)^{M-1} \end{bmatrix} \begin{bmatrix} c_1 \\ 2^2 c_2 \\ \vdots \\ M^2 c_M \end{bmatrix}$$
$$= \begin{bmatrix} 0 \\ \vdots \\ 0 \\ (2K)!/2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \quad (3.12)$$

Its coefficient matrix is also a Vandermonde matrix. The c_m ($m = 1, 2, \ldots, M$) are obtained by solving these equations, which are identical to those derived by Liu *et al* (1998, 2008).

The absolute error of the finite-difference formula, derived from equation (3.9), is

$$e_N = \left| \sum_{n=M+1}^{\infty} \left[\frac{(-1)^n 2^{2n}}{(2n)!} \sum_{m=1}^{M} \left(m^{2n} c_m\right) \frac{2\alpha^{2n}}{h^{2K}} \right] \right|$$
$$= \left| \sum_{n=M+1}^{\infty} \left[\frac{(-1)^n}{(2n)!} \sum_{m=1}^{M} \left(m^{2n} c_m\right) 2k^{2n} h^{2n-2K} \right] \right|. \quad (3.13)$$

The minimum power of h in the error function is $2M + 2 - 2K$; therefore, the finite-difference formula (3.8) has $(2M + 2 - 2K)$th-order accuracy.

Table 2. Coefficients of explicit difference for the second-order derivative.

Order of accuracy	c_0	c_1	c_2	c_3	c_4	c_5	c_6
2	-2	1					
4	$-5/2$	4/3	$-1/12$				
6	$-49/18$	3/2	$-3/20$	1/90			
8	$-205/72$	8/5	$-1/5$	8/315	$-1/560$		
10	$-5269/1800$	5/3	$-5/21$	5/126	$-5/1008$	1/3150	
12	$-5369/1800$	12/7	$-15/56$	10/189	$-1/112$	2/1925	$-1/16\,632$

When $K = 1$, for the second-order derivative, $M = N$, its difference coefficients are simplified as

$$c_m = \frac{(-1)^{m+1}}{m^2} \prod_{1\leqslant i\leqslant N, i\neq m} \left|\frac{i^2}{m^2 - i^2}\right|, \tag{3.14}$$

where c_0 is computed by equation (3.11*a*). These coefficients are equivalent to those obtained by Liu *et al* (1998) and Liu and Wei (2008). Table 2 lists the difference coefficients for orders up to 12.

4. Implicit finite-difference formulae with even-order accuracy

4.1. Even-order accurate finite-difference formula for the (2K − 1)th-order derivative

An implicit finite-difference formula for the $(2K-1)$th-order derivative is defined as follows:

$$\frac{\partial^{2K-1}p}{\partial x^{2K-1}} \approx \frac{\frac{\delta^{2K-1}p}{\delta x^{2K-1}}}{1 + bh^2\frac{\delta^2}{\delta x^2}} = \frac{\frac{1}{h^{2K-1}}\sum_{m=-M}^{M} c_m\, p(x+mh)}{1 + bh^2\frac{\delta^2}{\delta x^2}}, \tag{4.1}$$

where $M = N + K - 1$, c_m is an odd discrete sequence due to the centred finite difference, $c_0 = 0$. The difference operator in the denominator is a second-order centred finite-difference stencil.

Substituting $p = p_0\,\mathrm{e}^{ikx}$ and $\alpha = kh/2$ into equation (4.1) and simplifying it, we obtain

$$(-1)^{K-1}2^{2K-2}\alpha^{2K-1} \approx \frac{\sum_{m=1}^{M} c_m \sin(2m\alpha)}{1 - 4b\sin^2\alpha}. \tag{4.2}$$

Using the Taylor series expansion, we have

$$\sum_{n=1}^{\infty}\left[\frac{(-1)^{n-1}2^{2n-1}}{(2n-1)!}\sum_{m=1}^{M}\left(m^{2n-1}c_m\right)\alpha^{2n-1}\right] \approx (-1)^{K-1}2^{2K-2}\alpha^{2K-1}\left[1 + 2b\sum_{n=1}^{\infty}\frac{(-1)^n 2^{2n}}{(2n)!}\alpha^{2n}\right]. \tag{4.3}$$

Comparing the coefficients of α for the first $M + 1$ items of equation (4.2) with those of equation (4.3), we obtain

$$\frac{(-1)^{n-1}2^{2n-1}}{(2n-1)!}\sum_{m=1}^{M}\left(m^{2n-1}c_m\right) = \begin{cases} 0 & (1 \leqslant n < K) \\ (-1)^{K-1}2^{2K-2} & (n = K) \\ \dfrac{(-1)^{n-1}2^{2n-1}}{(2n-2K)!}b & (K < n \leqslant M+1). \end{cases} \tag{4.4}$$

We can rewrite equations (4.4) in the following matrix form:

$$\begin{bmatrix} (1^2)^0 & (2^2)^0 & \cdots & (M^2)^0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (1^2)^{K-2} & (2^2)^{K-2} & \cdots & (M^2)^{K-2} & 0 \\ (1^2)^{K-1} & (2^2)^{K-1} & \cdots & (M^2)^{K-1} & 0 \\ (1^2)^{K} & (2^2)^{K} & \cdots & (M^2)^{K} & -\frac{(2K+1)!}{2!} \\ (1^2)^{K+1} & (2^2)^{K+1} & \cdots & (M^2)^{K+1} & -\frac{(2K+3)!}{4!} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (1^2)^{M} & (2^2)^{M} & \cdots & (M^2)^{M} & -\frac{(2M+1)!}{(2M-2K+2)!} \end{bmatrix} \times \begin{bmatrix} 1c_1 \\ 2c_2 \\ \vdots \\ Mc_M \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ (2K-1)!/2 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{4.5}$$

The c_m $(m = 1, 2, \ldots, M)$ and b values are obtained by solving these equations.

The absolute error of the finite-difference formula, derived from equation (4.2), is

$$\begin{aligned} e_N &= \left|\sum_{n=M+2}^{\infty}\left[\frac{(-1)^{n-1}2^{2n-1}}{(2n-1)!}\sum_{m=1}^{M}\left(m^{2n-1}c_m\right)\frac{2\alpha^{2n-1}}{h^{2K-1}}\right] - \sum_{n=M+2-K}^{\infty}\frac{(-1)^{n+K-1}2^{2n+2K-1}b}{(2n)!}\alpha^{2n+2K-1}\frac{2}{h^{2K-1}}\right| \\ &= \left|\sum_{n=M+2}^{\infty}\left[2(-1)^{n-1}k^{2n-1}\left(\sum_{m=1}^{M}\left(m^{2n-1}c_m\right)/(2n-1)! - b/(2n-2K)!\right)h^{2n-2K}\right]\right|. \end{aligned} \tag{4.6}$$

The minimum power of h in the error function is $(2M + 4 - 2K)$; therefore, the finite-difference formula (4.1) has $(2M + 4 - 2K)$th-order accuracy.

Table 3. Coefficients of implicit difference for the first-order derivative.

Order of accuracy	b	c_1	c_2	c_3	c_4	c_5	c_6
4	1/6	1/2					
6	1/5	7/15	1/60				
8	3/14	25/56	1/35	−1/840			
10	2/9	13/30	1/27	−1/378	1/7560		
12	5/22	14/33	10/231	−5/1232	1/2772	−1/55 440	
14	3/13	38/91	5/104	−5/936	1/1560	−1/17 160	1/360 360

When $K = 1$ and $N = 2$, equation (4.5) becomes

$$\begin{bmatrix} 1 & 1 & 0 \\ 1 & 4 & -3 \\ 1 & 16 & -5 \end{bmatrix} \begin{bmatrix} 1c_1 \\ 2c_2 \\ b \end{bmatrix} = \begin{bmatrix} 1/2 \\ 0 \\ 0 \end{bmatrix}.$$

Solving the above equation, we get $c_1 = 7/15$, $c_2 = 1/60$ and $b = 1/5$. The implicit difference scheme based on these three coefficients is equivalent to a sixth-order compact finite-difference tridiagonal scheme for the first-order derivative (Lele 1992). The finite-difference coefficients for the first-order derivative with orders up to 14 are listed in table 3.

4.2. *Even-order accurate finite-difference formula for the (2K)th-order derivative*

An implicit finite-difference formula for the (2K)th-order derivative is defined as follows:

$$\frac{\partial^{2K} p}{\partial x^{2K}} \approx \frac{\frac{\delta^{2K} p}{\delta x^{2K}}}{1 + bh^2 \frac{\delta^2}{\delta x^2}} = \frac{\frac{1}{h^{2K}} \sum_{m=-M}^{M} c_m p(x + mh)}{1 + bh^2 \frac{\delta^2}{\delta x^2}}, \tag{4.7}$$

where $M = N + K - 1$, and c_m is an even discrete sequence due to the centred finite difference. The difference operator in the denominator is a second-order centred finite-difference stencil.

Substituting $p = p_0\, \mathrm{e}^{\mathrm{i}kx}$ into equation (4.7) and simplifying it, we get

$$(-1)^K 2^{2K-1} \alpha^{2K} \approx \frac{\frac{1}{2} c_0 + \sum_{m=1}^{M} c_m \cos(2m\alpha)}{1 - 4b \sin^2 \alpha}. \tag{4.8}$$

Using the Taylor series expansion yields

$$\frac{1}{2} c_0 + \sum_{m=1}^{M} c_m + \sum_{n=1}^{\infty} \left[\frac{(-1)^n 2^{2n}}{(2n)!} \sum_{m=1}^{M} (m^{2n} c_m) \alpha^{2n} \right] \approx (-1)^K 2^{2K-1} \alpha^{2K} \left[1 + 2b \sum_{n=1}^{\infty} \frac{(-1)^n 2^{2n}}{(2n)!} \alpha^{2n} \right]. \tag{4.9}$$

Comparing α coefficients of equation (4.8) with those of equation (4.9), we obtain

$$c_0 = -2 \sum_{m=1}^{M} c_m, \tag{4.10a}$$

$$(-1)^n \frac{2^{2n}}{(2n)!} \sum_{m=1}^{M} (m^{2n} c_m) = \begin{cases} 0 & (1 \leqslant n < K) \\ (-1)^K 2^{2K-1} & (n = K) \\ \frac{(-1)^n 2^{2n}}{(2n-2K)!} b & (K < n \leqslant M+1) \end{cases}. \tag{4.10b}$$

Rewrite equations (4.10b) as follows:

$$\begin{bmatrix} (1^2)^0 & (2^2)^0 & \cdots & (M^2)^0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (1^2)^{K-2} & (2^2)^{K-2} & \cdots & (M^2)^{K-2} & 0 \\ (1^2)^{K-1} & (2^2)^{K-1} & \cdots & (M^2)^{K-1} & 0 \\ (1^2)^{K} & (2^2)^{K} & \cdots & (M^2)^{K} & -\frac{(2K+2)!}{2!} \\ (1^2)^{K+1} & (2^2)^{K+1} & \cdots & (M^2)^{K+1} & -\frac{(2K+4)!}{4!} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (1^2)^{M} & (2^2)^{M} & \cdots & (M^2)^{M} & -\frac{(2M+2)!}{(2M+2-2K)!} \end{bmatrix} \times \begin{bmatrix} 1^2 c_1 \\ 2^2 c_2 \\ \vdots \\ M^2 c_M \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ (2K)!/2 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{4.11}$$

The c_m ($m = 1, 2, \ldots, M$) and b values are obtained by solving these equations.

The absolute error of the finite-difference formula, derived from equation (4.8), is

$$\begin{aligned} e_N &= \left| \sum_{n=M+2}^{\infty} \left[\frac{(-1)^n 2^{2n}}{(2n)!} \sum_{m=1}^{M} (m^{2n} c_m) \alpha^{2n} \right] \frac{2}{h^{2K}} - \sum_{n=M+2-K}^{\infty} \frac{(-1)^{n+K} 2^{2n+2K} b}{(2n)!} \alpha^{2n+2K} \frac{2}{h^{2K}} \right| \\ &= \left| \sum_{n=M+2}^{\infty} \left[2(-1)^n k^{2n} \left(\sum_{m=1}^{M} (m^{2n} c_m)/(2n)! - b/(2n-2K)! \right) h^{2n-2K} \right] \right|. \end{aligned} \tag{4.12}$$

Table 4. Coefficients of implicit difference for the second-order derivative.

Order of accuracy	b	c_0	c_1	c_2	c_3	c_4	c_5
4	1/12	−2	1				
6	2/15	−17/10	4/5	1/20			
8	9/56	−751/504	21/32	51/560	−23/10 080		
10	8/45	−4361/3240	1126/2025	247/2025	−74/14 175	43/226 800	
12	25/132	−90 552/72 869	4595/9504	55/378	−155/19 008	5/9504	−23/1108 800

The minimum power of h in the error function is $(2M + 4 - 2K)$; therefore, the finite-difference formula (4.7) has $(2M + 4 - 2K)$th-order accuracy. The finite-difference coefficients for the second-order derivative with orders up to 14 are listed in table 4.

5. Accuracy of implicit and explicit finite-difference formulae for the first and the second derivatives

5.1. Comparison of accuracy for the first-order derivative

Here we follow a development analogous to that used in equation (2.18). That is, our goal here is to examine how well we satisfy equations (3.2) and (4.2). Thus, for the first-order derivative, $K = 1$, $M = N$, let

$$f_{\mathrm{EFDM}}(\alpha) = \sum_{m=1}^{M} c_m \sin(2m\alpha), \tag{5.1}$$

$$f_{\mathrm{IFDM}}(\alpha) = \frac{\sum_{m=1}^{M} c_m \sin(2m\alpha)}{1 - 4b\sin^2\alpha}. \tag{5.2}$$

The difference coefficients of the EFDM for the first-order derivative are obtained from equation (3.7) and those of the IFDM from equation (4.5). Since the exact values of $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ are α, the calculated $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ are compared with α for different order numbers. Figures 3 and 4 show the accurate α, $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ with different order numbers determined by N; they indicate that the accuracy of the EFDM and IFDM increases with increasing order number. We note that for the same order number, the accuracy of the IFDM is better than that of the EFDM. We calculate both $f_{\mathrm{IFDM}}(\alpha)$ and $f_{\mathrm{EFDM}}(\alpha)$ with the order number ranging from 4 to 52 and from 2 to 160, respectively. Figure 5 shows $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ with nearly the same accuracy in each figure. We find that the accuracy of $(2N + 2)$th-order implicit formula is equivalent to that of $(6N + 2)$th-order explicit formula, which is also reported in table 5.

An example of calculating the first-order derivatives is shown in figure 6, where $p(x) = \cos(2\pi x/3)$, and $h = 1$. Figure 6(*a*) shows the exact first-order derivatives of $p(x)$, and figure 6(*b*) illustrates absolute errors between calculated derivatives with different order numbers and true derivatives. This figure indicates that the error of the IFDM with 6th-order accuracy is about the same as that of the EFDM with 14th-order accuracy, which agrees with table 5.

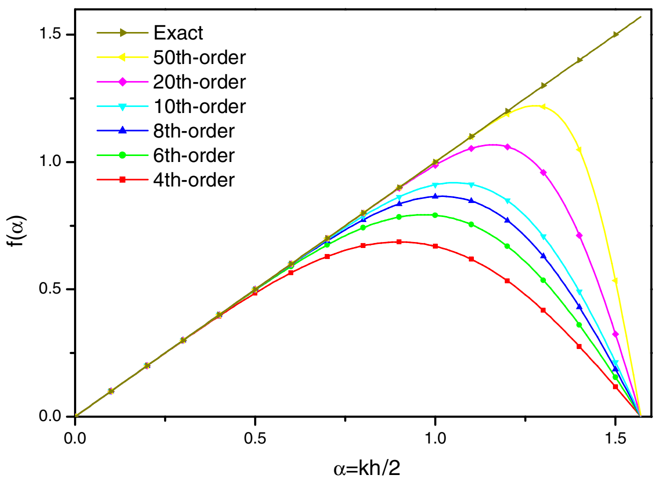


Figure 3. Plot of the exact α and $f_{\mathrm{EFDM}}(\alpha)$ of EFDM with different order numbers for the first-order derivative.

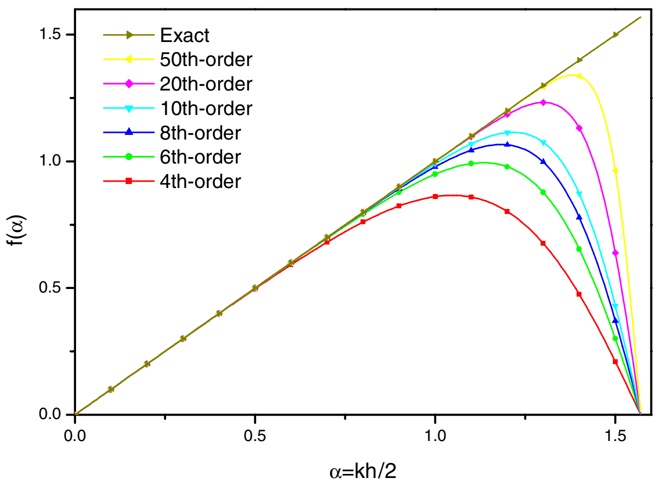


Figure 4. Plot of exact α and $f_{\mathrm{IFDM}}(\alpha)$ of IFDM with different order numbers for the first-order derivative.

5.2. Comparison of accuracy of the second-order derivative

Similar to the development reported in the previous section, for the second-order derivative, $K = 1$, $M = N$, let

$$f_{\mathrm{EFDM}}(\alpha) = \sqrt{-\frac{1}{4}c_0 - \frac{1}{2}\sum_{m=1}^{N} c_m \cos(2m\alpha)}, \tag{5.3}$$

$$f_{\mathrm{IFDM}}(\alpha) = \sqrt{\frac{-\frac{1}{4}c_0 - \frac{1}{2}\sum_{m=1}^{N} c_m \cos(2m\alpha)}{1 - 4b\sin^2\alpha}}. \tag{5.4}$$

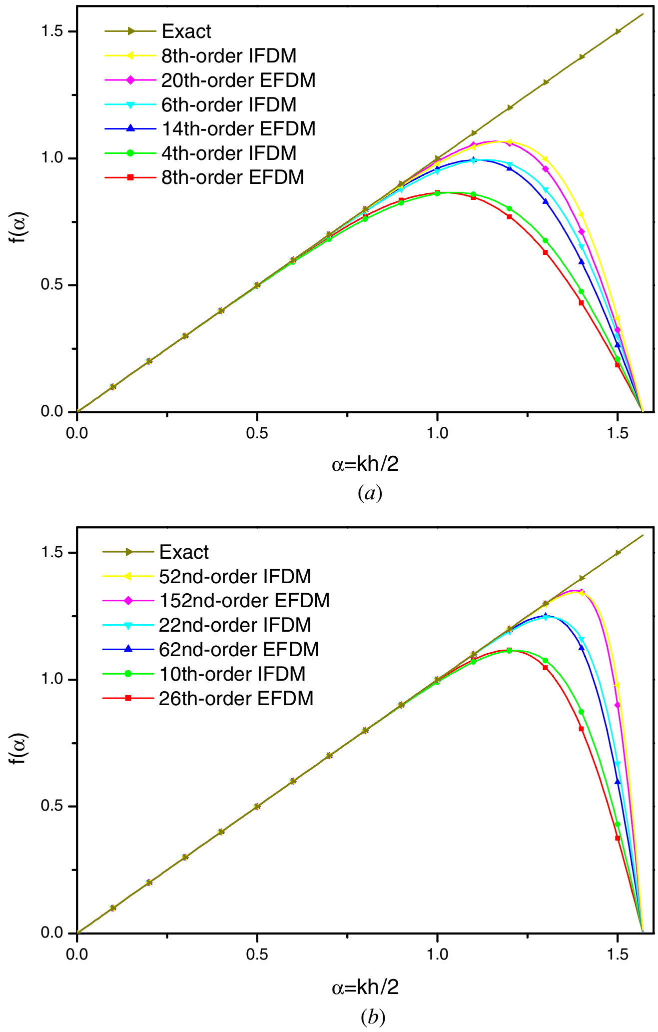


Figure 5. Plot of exact α, $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ with the same accuracy for the first-order derivative. (*a*) Implicit 4th, 6th, 8th and explicit 8th, 14th, 20th orders. (*b*) Implicit 10th, 22nd, 52nd and explicit 26th, 62nd, 152nd orders.

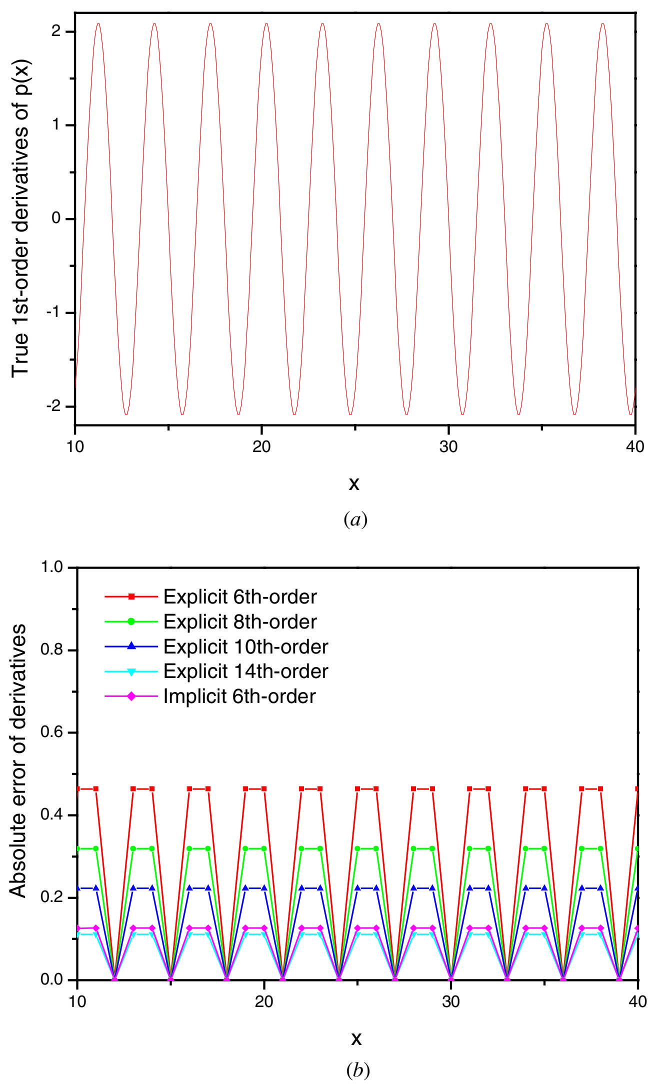


Figure 6. An example testing the accuracy of EFDM and IFDM with different order numbers for the first-order derivative. (*a*) True first-order derivatives of $p(x)$. (*b*) Absolute error between calculated and true derivatives by different order numbers.

Table 5. Order numbers of the IFDM and EFDM with the same accuracy for the first-order derivative.

Order number of the IFDM	Order number of the EFDM
4	8
6	14
8	20
10	26
22	62
52	152
$2N + 2$	$6N + 2$

The difference coefficients of the EFDM for the second-order derivative are obtained from equation (3.14), and those of the IFDM from equation (4.10). Since the exact values of $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ are α, the calculated $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ are compared with α for different order numbers. Figures 7 and 8 show the accurate α, $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ with different order numbers and suggest that the accuracy of the EFDM and IFDM increases with increasing order number. For the same order number, the precision of the IFDM is higher than that of the EFDM. It is obvious that both $f_{\mathrm{IFDM}}(\alpha)$ and $f_{\mathrm{EFDM}}(\alpha)$ are increasing functions and their values are not greater than α when α varies from 0 to $\pi/2$; therefore, an error function is introduced as follows to quantitatively evaluate their accuracies:

$$e_f = \frac{1}{n+1} \sum_{\alpha=0,\Delta\alpha,2\Delta\alpha,\ldots,n\Delta\alpha} |\alpha - f(\alpha)|. \tag{5.5}$$

Errors of $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ are calculated and shown in figure 9; where $\Delta\alpha = 0.001$ and $n = 1570$. This figure shows that the error of the IFDM is less than that of the EFDM for the same order number. Letting the (N_{E})th-order EFDM have the same error as the (N_{I})th-order IFDM, we find the relationship between N_{E} and N_{I}, that is the $(4N + 2)$th-order EFDM for $2N + 2 < 14$, the $(4N + 4)$th-order EFDM for $2N + 2 < 26$, the $(4N + 6)$th-order EFDM for $2N + 2 < 38$, the $(4N + 8)$th-order EFDM for $2N + 2 < 50$ and the $(4N + 10)$th-order EFDM for $2N + 2 < 60$ have nearly the same errors as the $(2N + 2)$th-order IFDM. These relationships are also shown in table 6.

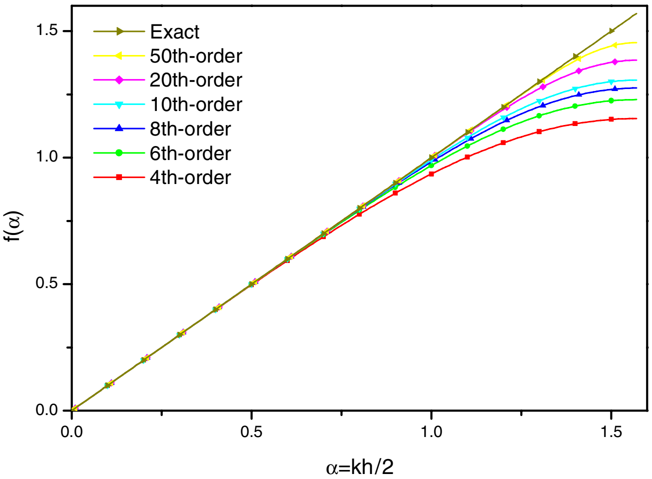


Figure 7. Plot of exact α and $f_{\mathrm{EFDM}}(\alpha)$ of EFDM with different order numbers for the second-order derivative.

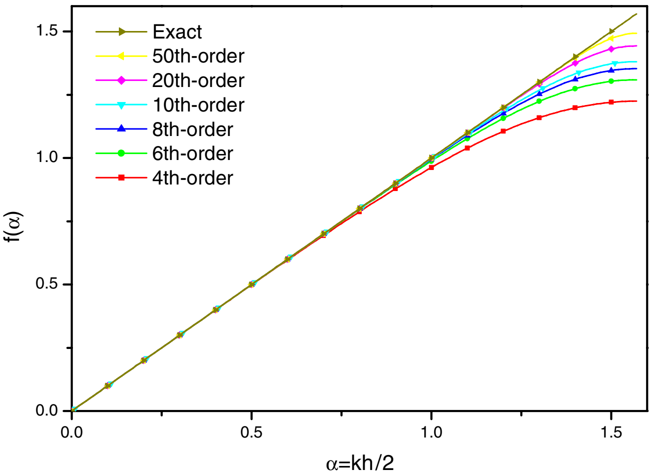


Figure 8. Plot of exact α and $f_{\mathrm{IFDM}}(\alpha)$ of IFDM with different order numbers for the second-order derivative.

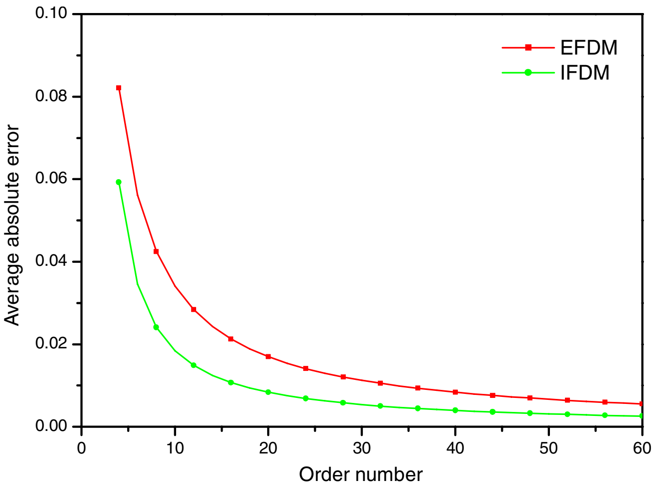


Figure 9. Errors of EFDM and IFDM for different order numbers.

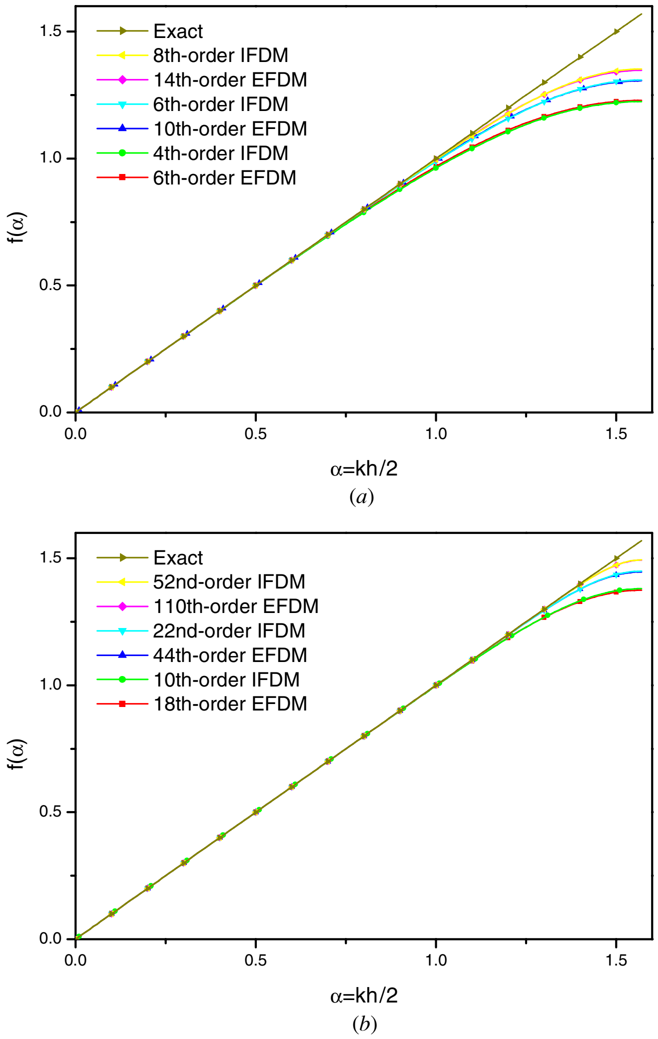


Figure 10. Plot of exact α, $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ with the same accuracy for the second-order derivative. (*a*) Implicit 4th, 6th, 8th and explicit 6th, 10th, 14th orders. (*b*) Implicit 10th, 22nd, 52nd and explicit 18th, 44th, 110th orders.

Table 6. Order numbers of the IFDM and EFDM with the same accuracy for the second-order derivative.

Order number of the IFDM	Order number of the EFDM
$2N+2$: 4–12	$4N+2$: 6–22
$2N+2$: 14–24	$4N+4$: 28–48
$2N+2$: 26–36	$4N+6$: 54–74
$2N+2$: 38–48	$4N+8$: 80–100
$2N+2$: 50–58	$4N+10$: 106–122

We calculate both $f_{\mathrm{IFDM}}(\alpha)$ and $f_{\mathrm{EFDM}}(\alpha)$ with the order number varying from 4 to 52 and from 4 to 110, respectively. Figure 10 shows $f_{\mathrm{EFDM}}(\alpha)$ and $f_{\mathrm{IFDM}}(\alpha)$ with nearly the same accuracy in each figure. It is found that the accuracy of $(2N+2)$th-order implicit formulae is equivalent to or greater than that of $(4N+2)$th-order explicit formulae, which is also shown in table 6.

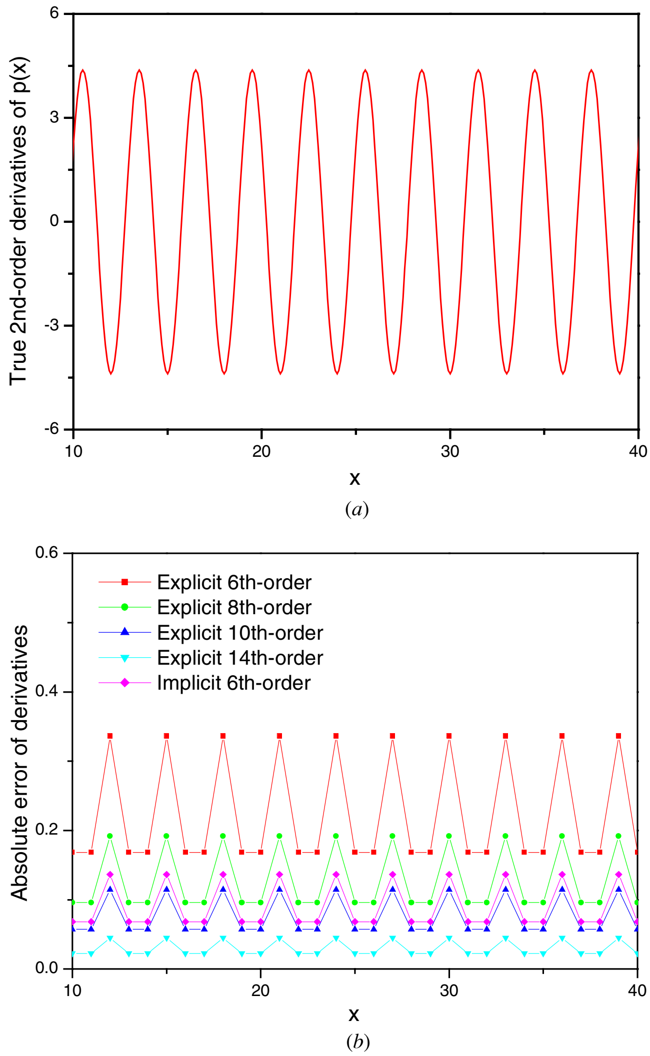


Figure 11. An example testing the accuracy of EFDM and IFDM with different order numbers for the second-order derivative. (*a*) True second-order derivatives of $p(x)$. (*b*) Absolute error between calculated and true derivatives by different order numbers.

An example of calculating the second-order derivatives is illustrated in figure 11, where $p(x) = \cos(2\pi x/3)$, and $h = 1$. Figure 11(*a*) plots the exact second-order derivatives of $p(x)$, and figure 11(*b*) illustrates absolute errors between calculated derivatives with different order numbers and true derivatives. This figure indicates that the error of the IFDM with sixth-order accuracy is approximately the same as that of the EFDM with tenth-order accuracy, which is in accord with table 6.

6. Implicit finite-difference method

6.1. Tridiagonal matrix equations of the IFDM for the first-order derivative

Let $q = \partial p/\partial x$ and use equation (4.1), an implicit finite-difference formula of $(2N + 2)$th-order for the first-order derivative is expressed as

$$bq(x-h) + (1-2b)q(x) + bq(x+h)$$

$$= \frac{\sum_{m=1}^{N} c_m\,[p(x+mh) - p(x-mh)]}{h}. \tag{6.1}$$

This formula reduces to a $(2N)$th-order explicit finite-difference formula when $b = 0$. For an implicit scheme, $b \neq 0$, let

$$a = \frac{1}{b} - 2, \tag{6.2a}$$

$$r(x) = \frac{\sum_{m=1}^{N} c_m[p(x+mh) - p(x-mh)]}{bh}. \tag{6.2b}$$

Then

$$q(x-h) + aq(x) + q(x+h) = r(x). \tag{6.3}$$

In the $(2N + 2)$th-order implicit finite difference, $2N$ points are involved in equation (6.2*b*). For a known sequence (p_1, p_2, ... , p_L), derivatives (q_1, q_2, ... , q_L) are calculated as follows: q_{N+1}, q_{N+2}, ... , q_{L-N} are computed by centred finite-difference formulae given by

$$q_{j-1} + a_N q_j + q_{j+1} = r_j \quad (j = N+1, N+2, \ldots, L-N), \tag{6.4}$$

where

$$q_j = q(jh), \tag{6.5a}$$

$$a_N = \frac{1}{b_N} - 2, \tag{6.5b}$$

$$r_j = \frac{\sum_{m=1}^{N} c_{N,m}(p_{j+m} - p_{j-m})}{b_N h}. \tag{6.5c}$$

From equations (6.4) and (6.5*c*), it can be observed that when $j = 2, 3, \ldots, N$, only $2j - 2$ points can be used in equation (6.5*c*) to maintain central finite difference and reach $(2j)$th-order accuracy, less than $(2N + 2)$th-order accuracy. There are two ways to maintain $(2N + 2)$th-order accuracy. One way is to assume that the known sequence (p_1, p_1, ... ,p_L) is periodic. The other way is to use non-centred finite difference with the $(2N + 2)$th-order accuracy. However, the stability condition of non-centred finite difference is more restrictive than that of centred finite difference for a sequence with higher wavenumbers. Therefore, when the sequence is non-periodic, $q_2, q_3, \ldots, q_N$ are calculated by centred finite difference, so are $q_{L-1}, q_{L-2}, \ldots, q_{L-N+1}$, that is

$$q_{j-1} + a_{j-1}q_j + q_{j+1} = r_j \qquad (j = 2, 3, \ldots, N), \tag{6.6a}$$

$$q_{j-1} + a_{L-j}q_j + q_{j+1} = r_j$$
$$(j = L-N+1, L-N+2, \ldots, L-1), \tag{6.6b}$$

where

$$a_j = \frac{1}{b_j} - 2 \qquad (j = 1, 2, \ldots, N-1), \tag{6.7a}$$

$$r_j = \frac{\sum_{m=1}^{j-1} c_{j-1,m}(p_{j+m} - p_{j-m})}{b_{j-1}h} \qquad (j = 2, 3, \ldots, N), \tag{6.7b}$$

$$r_j = \frac{\sum_{m=1}^{L-j} c_{L-j,m}(p_{j+m} - p_{j-m})}{b_{L-j}h}$$

$$(j = L - N + 1, L - N + 2, \ldots, L - 1) \qquad (6.7c)$$

and $c_{j,1}$, $c_{j,2}$, ..., $c_{j,j}$ and b_j are the finite-difference coefficients of the $(2j+2)$th-order implicit difference formula.

Let

$$d_{j,m} = \frac{c_{j,m}}{b_j h}. \qquad (6.8)$$

Then

$$r_j = \begin{cases} \sum_{m=1}^{j-1} d_{j-1,m}(p_{j+m} - p_{j-m}) \\ \qquad (j = 2, 3, \ldots, N) \\ \sum_{m=1}^{N} d_{N,m}(p_{j+m} - p_{j-m}) \\ \qquad (j = N+1, N+2, \ldots, L-N) \\ \sum_{m=1}^{L-j} d_{L-j,m}(p_{j+m} - p_{j-m}) \\ \qquad (j = L-N+1, L-N+2, \ldots, L-1) \end{cases} . \qquad (6.9)$$

To complete the system, we write for the first and the last nodes, under the assumption of linear variation for p_0 and p_L,

$$a_0 q_1 + q_2 = r_1, \qquad (6.10a)$$

$$q_{L-1} + a_0 q_L = r_L, \qquad (6.10b)$$

where

$$a_0 = a_1 + 1, \qquad (6.11a)$$

$$r_1 = 2d_{1,1}(p_2 - p_1), \qquad (6.11b)$$

$$r_L = 2d_{1,1}(p_L - p_{L-1}). \qquad (6.11c)$$

Finally, the following tridiagonal matrix equations are formed, from formulae (6.4), (6.6*a*), (6.6*b*), (6.10*a*) and (6.10*b*), to calculate the derivatives

$$\begin{bmatrix} a_0 & 1 & & & & & & & & & & \\ 1 & a_1 & 1 & & & & & & & & & \\ & 1 & a_2 & 1 & & & & & & & & \\ & & \vdots & \vdots & \vdots & & & & & & & \\ & & & 1 & a_{N-1} & 1 & & & & & & \\ & & & & 1 & a_N & 1 & & & & & \\ & & & & & \vdots & \vdots & \vdots & & & & \\ & & & & & & 1 & a_N & 1 & & & \\ & & & & & & & 1 & a_{N-1} & 1 & & \\ & & & & & & & & \vdots & \vdots & \vdots & \\ & & & & & & & & & 1 & a_2 & 1 & \\ & & & & & & & & & & 1 & a_1 & 1 \\ & & & & & & & & & & & 1 & a_0 \end{bmatrix}$$

$$\times \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ \vdots \\ q_{L-2} \\ q_{L-1} \\ q_L \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \\ r_{L-2} \\ r_{L-1} \\ r_L \end{bmatrix}. \qquad (6.12)$$

Note that for the given order $2n$, the coefficients a_n and $d_{n,m}$, expressed by equations (6.7*a*) and (6.8), respectively, are constant and related to the coefficients $c_{n,m}$ and b_n, which can be obtained by solving equations (4.5).

6.2. Tridiagonal matrix equations of the IFDM for the second-order derivative

Letting $q = \partial^2 p/\partial x^2$ and using equation (4.7), an implicit finite-difference formula of $(2N+2)$th-order for the second-order derivative is denoted as

$$bq(x-h) + (1-2b)q(x) + bq(x+h)$$

$$= \frac{c_0 p(x) + \sum_{m=1}^{N} c_m [p(x-mh) + p(x+mh)]}{h^2}. \qquad (6.13)$$

For implicit format, $b \neq 0$, let

$$a = \frac{1}{b} - 2, \qquad (6.14a)$$

$$r(x) = \frac{c_0 p(x) + \sum_{m=1}^{N} c_m [p(x-mh) + p(x+mh)]}{bh^2}. \qquad (6.14b)$$

Then

$$q(x-h) + aq(x) + q(x+h) = r(x). \qquad (6.15)$$

We adopt a similar method for the first-order derivatives to calculate the second-order derivatives $(q_1, q_2, \ldots, q_L)$ of the known sequence $(p_1, p_2, \ldots, p_L)$. $q_{N+1}, q_{N+2}, \ldots, q_{L-N}$ are calculated by centred finite-difference formulae. When the sequence is non-periodic, both $q_2, q_3, \ldots, q_N$ and $q_{L-1}, q_{L-2}, \ldots, q_{L-N+1}$ are computed by centred finite differences with 4, 6, ..., $2N$th-order accuracies, respectively. Then, the same equations (6.4), (6.6*a*) and (6.6*b*) can also be obtained, but r_j and $d_{j,m}$ must be changed as follows:

$$r_j = \begin{cases} d_{j-1,0}p_m + \sum_{m=1}^{j-1} d_{j-1,m}(p_{j+m} + p_{j-m}) \\ \qquad (j = 2, 3, \ldots, N) \\ d_{N,0}p_m + \sum_{m=1}^{N} d_{N,m}(p_{j+m} + p_{j-m}) \\ \qquad (j = N+1, N+2, \ldots, L-N) \\ d_{L-j,0}p_m + \sum_{m=1}^{L-j} d_{L-j,m}(p_{j+m} + p_{j-m}) \\ \qquad (j = L-N+1, L-N+2, \ldots, L-1) \end{cases} \qquad (6.16a)$$

$$d_{j,m} = \frac{c_{j,m}}{b_j h^2}. \qquad (6.16b)$$

Two equations are added as follows under the assumption of quadratic variation for p_0 and p_L:

$$a_0 q_1 + q_2 = r_1, \qquad (6.17a)$$

$$q_{L-1} + a_0 q_L = r_L, \qquad (6.17b)$$

Table 7. Calculation amount comparison of $(2N)$th-order EFDM and $(2N+2)$th-order IFDM.

Operation	Operation times of $(2N)$th-order EFDM ($L \times K$)	Operation times of $(2N+2)$th-order IFDM ($L \times K$)
$\times$	N	$N+2$
+ or −	$2N$	$2N+2$
Visiting array elements	$4N$	$4N+8$

The length of the sequence is L; the derivatives of the sequence are calculated K times.

Table 8. Accuracy relationship between EFDM and IFDM under the condition of the same calculation amount for the first-order derivative.

N	$(2N+4)$th-order EFDM	$(2N+2)$th-order IFDM (costing the same calculation amount as $(2N+4)$th-order EFDM)	$(6N+2)$th-order EFDM (reaching the same accuracy as $(2N+2)$th-order IFDM)
1	6	4	8
2	8	6	14
8	20	18	50
18	40	38	110

Additional cost of visiting arrays, which may be dependent on computer configuration and programming language, is not considered here.

where

$$a_0 = a_1 + 1, \tag{6.18a}$$

$$r_1 = r_2, \tag{6.18b}$$

$$r_L = r_{L-1}. \tag{6.18c}$$

Then, the tridiagonal matrix equations, the same as equations (6.12), are formed to calculate derivatives.

6.3. A strategy to decrease the computation in solving the tridiagonal matrix equations

Assuming that the length of the sequence is L, conventional arithmetic for solving tridiagonal matrix equations needs approximately $3L$ multiplications, $2L$ divisions and $3L$ subtractions for real number operations, and needs to visit arrays $13L$ times (William *et al* 1992). In numerical modelling, calculating derivatives with the same implicit difference algorithm will be performed many times. Therefore, the same calculation involved in solving tridiagonal matrix equations can be pre-computed to decrease the computation time. Since the coefficient matrix of equations (6.12) is constant for a given order, the coefficient vectors involved in solving tridiagonal matrix equations are also constant and can be pre-computed. Thus, only $2L$ multiplications and subtractions and $8L$ visits to arrays are needed to solve the tridiagonal matrix equations.

6.4. Analysis of computational requirements and accuracy

First, we compare the computational requirements of the EFDM and IFDM. Since the derivative calculation is executed many times in a numerical modelling, the computation for difference coefficients can be ignored in the following analysis. Assuming that the length of the sequence is L, the derivatives of the sequence are calculated K times, and the $(2N)$th-order EFDM and $(2N+2)$th-order IFDM are adopted. Then, an EFDM requires nearly $N \times L \times K$ multiplications, $2N \times L \times K$ additions and $4N \times L \times K$ times for visiting array elements while an IFDM requires nearly $(N+2) \times L \times K$ multiplications, $(2N+2) \times L \times K$ additions or subtractions and $(4N+8) \times L \times K$ times for visiting array elements, as shown in table 7. Additional cost of visiting arrays may be dependent on computer configuration and programming language, and is not considered in the next discussion. Therefore, the $(2N+2)$th-order IFDM requires nearly the same computations as the $(2N+4)$th-order EFDM. Moreover, additional memory is needed only for saving $2L$ real numbers, which can be ignored.

Next, we discuss the EFDM and IFDM for the first- and the second-order derivatives. For the first-order derivatives, the $(2N+2)$th-order IFDM reaches the accuracy of the $(6N+2)$th-order EFDM. Therefore, for the same amount of computation, the $(2N+4)$th-order EFDM may be replaced by the $(2N+2)$th-order IFDM, which reaches the accuracy of the $(6N+2)$th-order EFDM. This relationship is also shown in table 8.

For the second-order derivatives, the accuracy relationship between the EFDM and IFDM under the condition of the same amount of computation is shown in table 9, which implies that a high-order EFDM may be replaced by an IFDM to augment the accuracy under the condition of not increasing the computation.

7. Dispersion and stability analyses

As an example, we perform dispersion analysis for 1D acoustic wave equation modelling by the EFDM and IFDM, respectively.

1D acoustic wave equation is

$$\frac{\partial^2 w}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 w}{\partial t^2}, \tag{7.1}$$

Table 9. Accuracy relationship between EFDM and IFDM under the condition of the same calculation amount for the second-order derivative.

N	$(2N+4)$th-order EFDM	$(2N+2)$th-order IFDM (costing the same calculation amount as $(2N+4)$th-order EFDM)	$(4N+2)$th-order EFDM (reaching the same accuracy as $(2N+2)$th-order IFDM)
1	6	4	6
2	8	6	10
8	20	18	34
18	40	38	74

Additional cost of visiting arrays, which may be dependent on computer configuration and programming language, is not considered here.

where $w = w(x, t)$ is the wave field, and v is the velocity of the P-wave. In the modelling, the time derivatives are calculated by the following second-order centred FD:

$$\frac{\partial^2 w}{\partial t^2} = \frac{1}{\tau^2}\left[-2w_0^0 + \left(w_0^{-1} + w_0^1\right)\right], \tag{7.2}$$

where $w_m^n = w(x+mh, t+n\tau)$, τ is the time step and h is the grid size. The space derivatives are calculated by the following equation:

$$\frac{\partial^2 w}{\partial x^2} = \frac{\frac{1}{h^2}\left[a_0 w_0^0 + \sum_{m=1}^{N} a_m\left(w_{-m}^0 + w_m^0\right)\right]}{1 + bh^2\frac{\delta^2}{\delta x^2}}. \tag{7.3}$$

When $b = 0$, equation (7.3) represents an EFDM; otherwise it represents an IFDM. Substituting equations (7.2) and (7.3) into equation (7.1), we have

$$\begin{aligned}&\frac{v^2\tau^2}{h^2}\left[a_0 w_0^0 + \sum_{m=1}^{M} a_m\left(w_{-m}^0 + w_m^0\right)\right]\\ &= b\left[\left(w_{-1}^{-1} + w_{-1}^1\right) - 2w_{-1}^0 + \left(w_1^{-1} + w_1^1\right) - 2w_1^0\right]\\ &+(1-2b)\left[\left(w_0^{-1} + w_0^1\right) - 2w_0^0\right].\end{aligned} \tag{7.4}$$

7.1. Dispersion analysis

Using the plane wave theory, we let

$$w_m^n = \mathrm{e}^{\mathrm{i}[k(x+mh)-\omega(t+n\tau)]}. \tag{7.5}$$

Substituting equation (7.5) into (7.4) and simplifying it, we have

$$r^2\sum_{m=1}^{M} a_m \sin^2(m\alpha) = [1 - 4b\sin^2\alpha]\sin^2(\omega\tau/2), \tag{7.6}$$

where $r = v\tau/h$, and $\alpha = kh/2$. ω can be derived from equation (7.6), and then dispersion δ is defined as follows:

$$\delta = \frac{v_{FD}}{v} = \frac{\omega}{vk} = \frac{1}{r\alpha}\sin^{-1}\sqrt{\frac{r^2\sum_{m=1}^{M} a_m\sin^2(m\alpha)}{1 - 4b\sin^2\alpha}}. \tag{7.7}$$

If δ equals 1, there will be no dispersion. If δ is far from 1, a large dispersion will occur. Figure 12 shows dispersion curves by the PSM (pseudo spectral method), EFDM and IFDM. This figure demonstrates that

- PSM has the smallest dispersion,

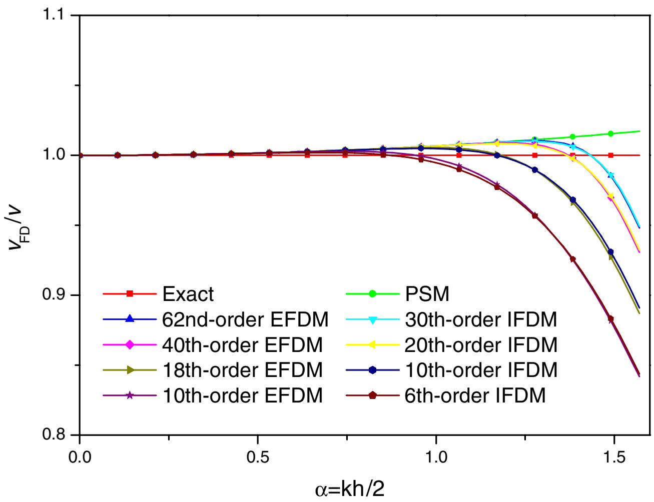


Figure 12. Plot of dispersion curves of 1D acoustic wave equation modelling by PSM, EFDM and IFDM; $v = 2000$ m s^{-1}, $\tau = 0.001$ s, $h = 10$ m.

- dispersion decreases with increasing FD order,
- the accuracy of the IFDM is higher than that of the EFDM for the same order and
- some higher-order EFDM and some lower-order IFDM have nearly the same dispersion curves. These relationships agree with table 6.

7.2. Stability analysis

The stability condition for 1D acoustic wave equation modelling by the $(2N)$th-order EFDM is (Liu *et al* 1998)

$$r \leqslant \left(\sum_{n=1}^{N_1} c_{2n-1}\right)^{-1/2}, \tag{7.8}$$

where $N_1 = \mathrm{int}[(N+1)/2]$, int is a function to get the integer part of a value.

When $N \to \infty$, this method approaches the PSM, and the stability condition becomes (Liu and Wei 2005)

$$r \leqslant 2/\pi. \tag{7.9}$$

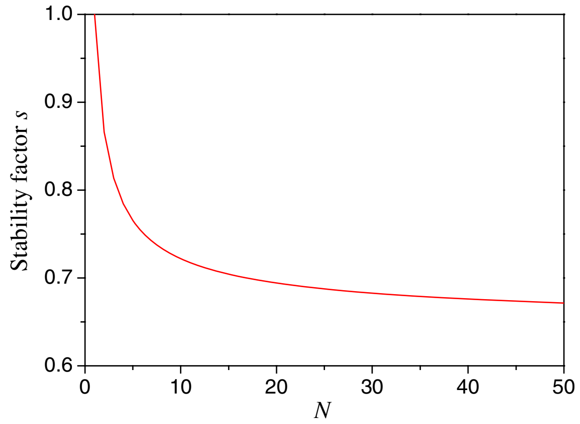


Figure 13. The variation of stability factor s with N for 1D acoustic wave equation modelling by (2N)th-order EFDM.

To calculate and analyse the stability of the finite differences, we define 1D stability factor s as follows according to equation (7.8):

$$s = \left(\sum_{n=1}^{N_1} c_{2n-1} \right)^{-1/2}. \tag{7.10}$$

We calculate the variation of s with N, which is shown in figure 13. From the figure, we can see that the area of r for stable recursion decreases with the increase of N. When $N \to \infty$, $s \to 2/\pi \approx 0.637$. Figures 12 and 13 demonstrate that the accuracy becomes higher and stability becomes stricter with the increase of the FD order.

Since some lower-order IFDM has the same accuracy as some higher-order EFDM, these two methods, used to calculate space derivatives, will result in the same space derivatives values and thus the same wave field values. Therefore, these two methods have nearly the same stability condition. We can obtain the stability condition of the IFDM from figure 13 by using table 6.

Here, we only discuss the dispersion and stability for 1D acoustic wave equation modelling. In fact, according to the above analyses, some higher-order EFDM and some lower-order IFDM, having the same accuracies when used to calculate space derivatives, the dispersion relation and stability condition should be nearly the same for acoustic or elastic wave equation modelling under the same discretization. Furthermore, the IFDM has greater accuracy and stricter stability condition than the EFDM for the same accuracy order.

8. Examples of numerical modelling

8.1. Numerical modelling of an acoustic wave equation

The EFDM and IFDM for the second-order derivative are used to perform numerical modelling of the following acoustic wave equation:

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial z^2} = \frac{1}{v} \frac{\partial^2 w}{\partial t^2}, \tag{8.1}$$

where $w = w(x, z, t)$ is the wave field, and v is the velocity of the P-wave. In the modelling, all the second-order space derivatives are calculated respectively by the EFDM with equations (3.8), and the IFDM with equations (6.12) determined by equations (6.16)–(6.18), the second-order time derivatives by the second-order EFDM. The physical model uses the parameters listed in table 10. Snapshots at 200 ms by the IFDM and EFDM with different order numbers are shown in figure 14. The figure indicates that the accuracy of a sixth-order IFDM is higher than that of a sixth-order EFDM and is equivalent to that of a tenth-order EFDM. These results are consistent with those listed in table 5.

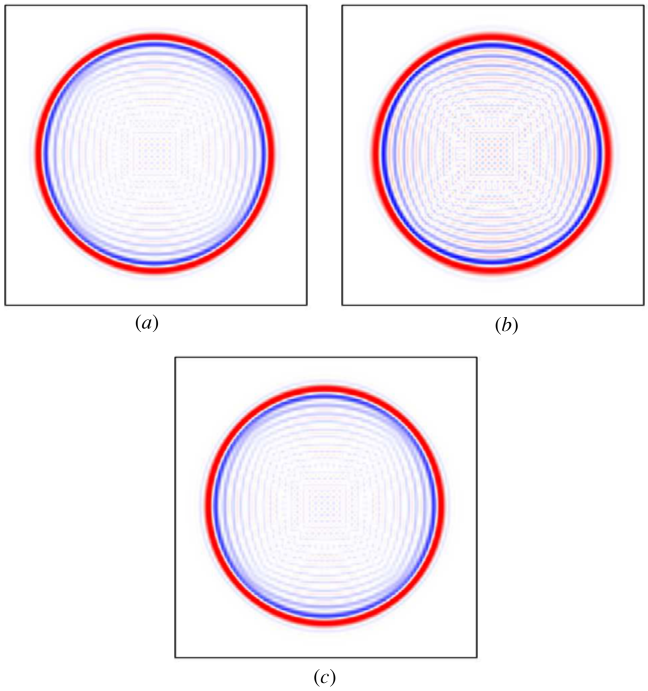


Figure 14. Snapshots of acoustic wave equation numerical modelling respectively by IFDM and EFDM with different order numbers. (*a*) Implicit 6th order. (*b*) Explicit 6th order. (*c*) Explicit 10th order.

Table 10. Homogeneous acoustic model and its modelling parameters.

Parameters	Values
Model size	1000 m × 1000 m
Model velocity	2000 m s^{-1}
Grid size	10 m × 10 m
Time step	1 ms
Source function	Sine signal of 50 Hz with one period length
Source location	In the middle of the model

8.2. Numerical modelling of elastic wave equations

The EFDM and IFDM for the first-order derivative are used to perform numerical modelling of the following elastic wave equations for the heterogeneous media (Virieux 1986):

$$\frac{\partial v_x}{\partial t} = \frac{1}{\rho} \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xz}}{\partial z} \right), \tag{8.2a}$$

$$\frac{\partial v_z}{\partial t} = \frac{1}{\rho} \left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{zz}}{\partial z} \right), \tag{8.2b}$$

Table 11. Homogeneous elastic model and its modelling parameters.

Parameters	Values
Model size	1000 m × 1000 m
Model P-wave velocity	2000 m s^{-1}
Model S-wave velocity	1000 m s^{-1}
Model density	1000 kg^3 m^{-3}
Grid size	10 m × 10 m
Time step	1 ms
P-wave source function	$e^{-0.25[(x-x_0)^2+(z-z_0)^2]}$
Source location	In the middle of the model

Table 12. SEG/EAGE salt model and its simulating parameters.

Parameters	Values
Model size	12 000 m × 4000 m
Model first layer	Ocean water
Grid size	20 m × 20 m
Time step	1 ms
P-wave source function	$e^{-0.25r^2}\cos(0.0335r)$, $r^2 = (x-x_0)^2 + (z-z_0)^2$.
Source location	$x_0 = 6000$, $z_0 = 20$
Receiver location	Ocean bottom

$$\frac{\partial \tau_{xx}}{\partial t} = (\lambda + 2u)\frac{\partial v_x}{\partial x} + \lambda \frac{\partial v_z}{\partial z}, \tag{8.2c}$$

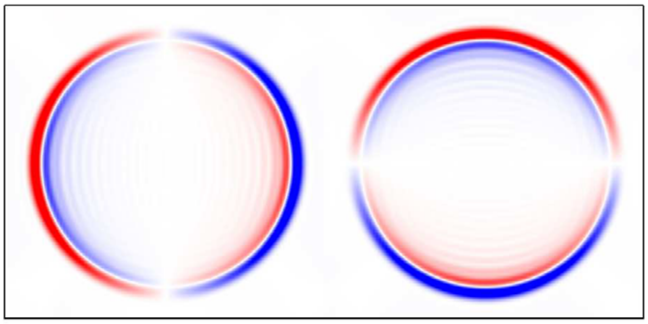
$$\frac{\partial \tau_{zz}}{\partial t} = \lambda \frac{\partial v_x}{\partial x} + (\lambda + 2u)\frac{\partial v_z}{\partial z}, \tag{8.2d}$$

$$\frac{\partial \tau_{zx}}{\partial t} = \mu\left(\frac{\partial v_z}{\partial x} + \frac{\partial v_x}{\partial z}\right). \tag{8.2e}$$

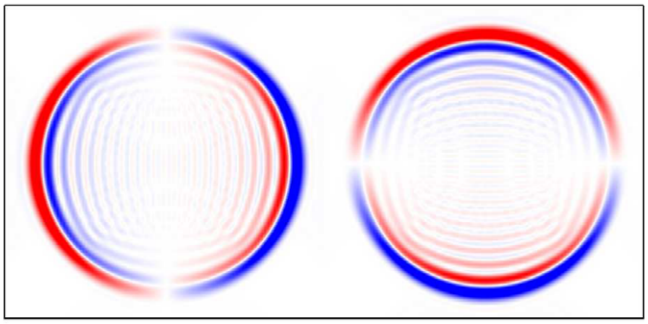
In these equations, (v_x, v_z) is the velocity vector, $(\tau_{xx}, \tau_{zz}, \tau_{xz})$ is the stress tensor, $\lambda(x, z)$ and $\mu(x, z)$ are Lamé coefficients and $\rho(x, z)$ is the density. In the modelling, the first-order space derivatives are calculated, respectively, by the EFDM with equation (3.1) and the IFDM with equation (6.12) determined by equations (6.4)–(6.11), the second-order time derivatives by the second-order EFDM. The physical model uses the parameters listed in table 11. The source function is added into both τ_{xx} and τ_{zz} at $t = 0$ to form the P-wave source. Snapshots at 200 ms respectively by the IFDM and EFDM with different order numbers are illustrated in figure 15. The figure demonstrates that the precision of the 6th-order IFDM is higher than that of the 6th-order EFDM and identical to that of the 14th-order EFDM.

8.3. Numerical modelling of the SEG/EAGE salt model

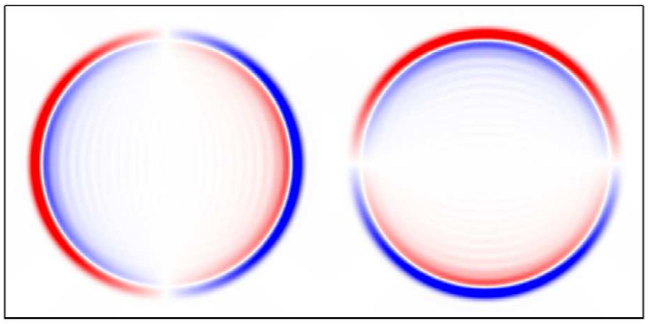
Finally, numerical modelling of the elastic wave equations (8.2*a*)–(8.2*e*), by the IFDM and EFDM with the same amount of computation, is utilized to simulate wave propagation in the SEG/EAGE salt model. The material parameters at the liquid–solid interface are represented by arithmetic averages from neighbouring grids (van Vossen *et al* 2002). Figure 16(*a*) shows the model and table 12 lists the model and its modelling parameters. The source function is added into both τ_{xx} and τ_{zz} at $t = 0$ to form the P-wave source. The 12th-order IFDM and 14th-order EFDM, having



(*a*)



(*b*)



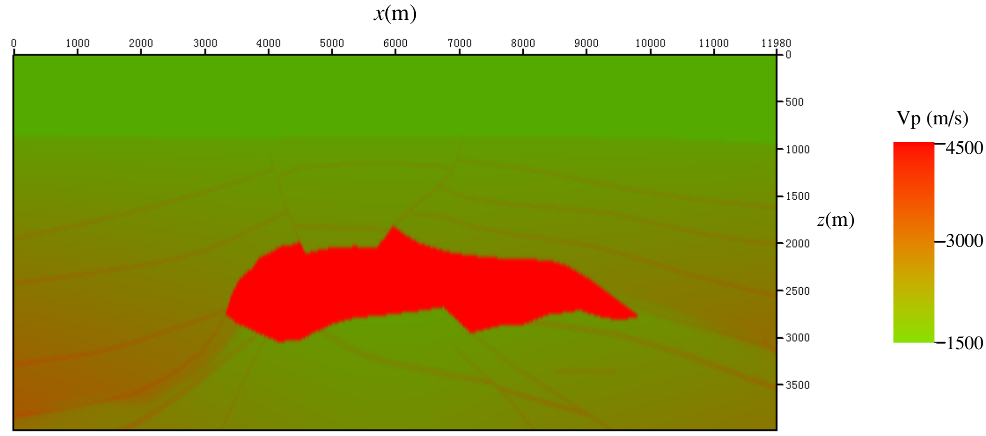
(*c*)

Figure 15. Snapshots of elastic wave equations numerical modelling respectively by IFDM and EFDM with different order numbers (left—x component; right—z component). (*a*) Implicit 6th order. (*b*) Explicit 6th order. (*c*) Explicit 14th order.

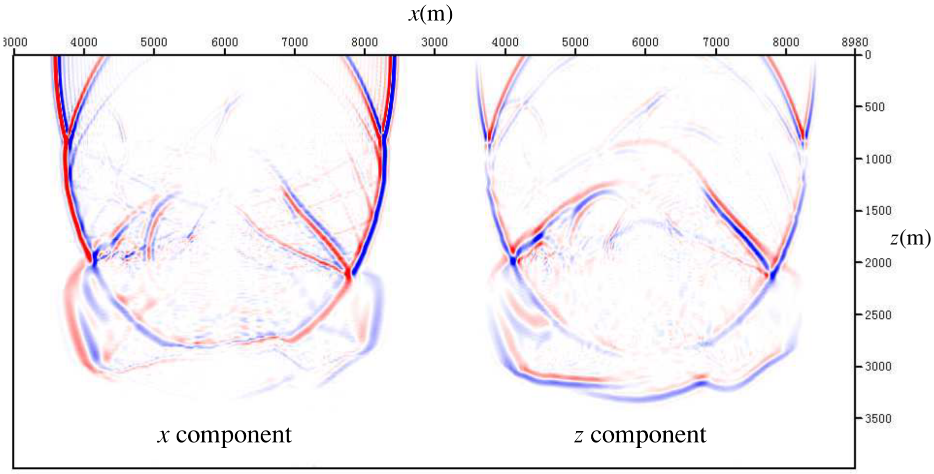
the same computation amounts, are utilized to simulate elastic wave propagation in the model. Snapshots and shot gathers are illustrated in figures 16(*b*)–(*e*), which indicate that the accuracy of the IFDM is higher than that of the EFDM.

9. Discussion and conclusions

The EFDM is most commonly used in seismic modelling due to its fast computational speed. An IFDM is usually considered expensive due to the requirement of solving a larger number of equations and is therefore not very popular. In this paper, we derive new formulae for space derivatives using the IFDM with any order accuracy for any order derivative. The new approach requires solving tridiagonal matrix equations only. Pre-computing parts of the operators is adopted to decrease the computation time for solving these equations. For calculating



(*a*)



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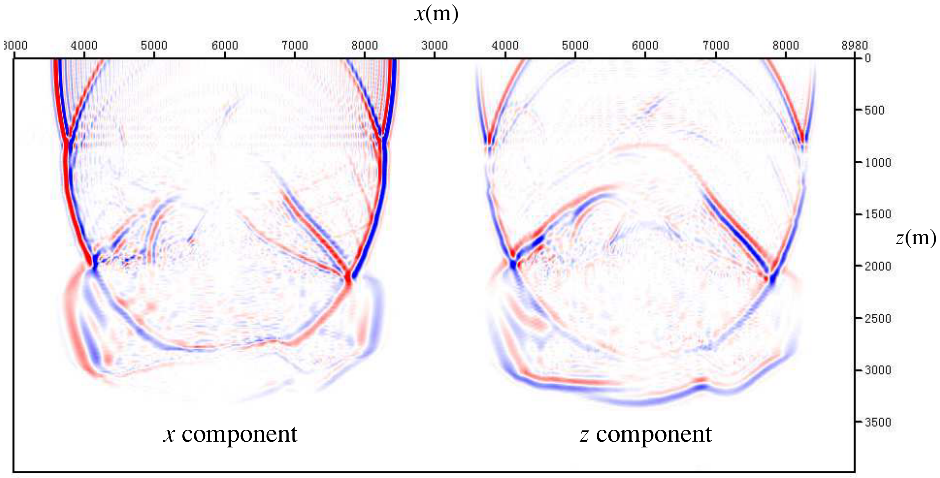
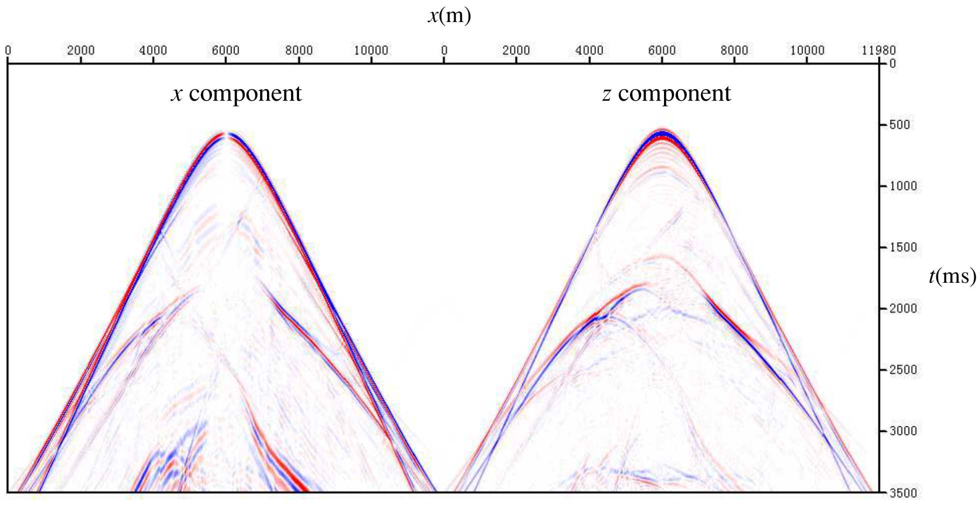


(*c*)

Figure 16. Numerical modelling results of SEG/EAGE salt model respectively by IFDM and EFDM with the same computation amount. (*a*) SEG/EAGE salt model of P-wave velocity. (*b*) Snapshots of x (left) and z (right) components at $t = 1600$ ms by 12th-order IFDM. (*c*) Snapshots of x (left) and z (right) components at $t = 1600$ ms by 14th-order EFDM. (*d*) OBC gather of x (left) and z (right) components by 12th-order IFDM. (*e*) OBC gather of x (left) and z (right) components by 14th-order EFDM.

derivatives with the same implicit difference formula many times, the $(2N + 2)$th-order implicit method requires nearly the same amount of computation and calculation memory as those required by a $(2N + 4)$th-order explicit method but attains the accuracy of $(6N + 2)$th-order explicit for the first-order derivative and $(4N + 2)$th-order explicit for the second-order



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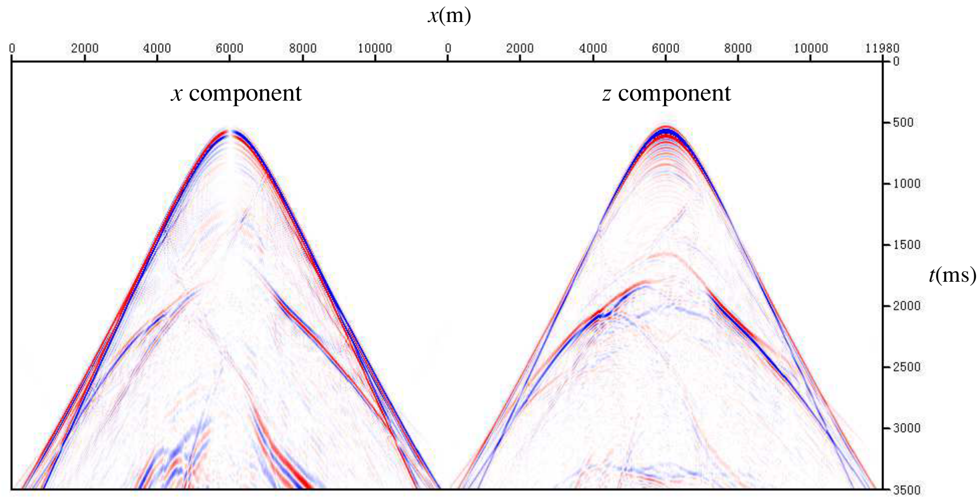

(*e*)

Figure 16. (Continued).

derivative when the additional cost of visiting arrays is not considered. A high-order explicit method may be replaced by a lower-order implicit method, which will improve the accuracy but not increase the computational cost.

As a final note, we discuss two issues. One is about the performance of the IFDM relative to the PSM. Although the PSM has the highest accuracy as the highest-order IFDM, the cost of the PSM is fixed and higher. However, the high-order IFDM provides the trade-off between accuracy and computational requirement. The second issue relates to temporal and spatial discretizations. Since second-order differencing for temporal discretizations and higher-order differencing or pseudospectral method for spatial discretizations will result in an imbalance between temporal and spatial accuracy, these discretizations are inefficient for long-time simulations when the source frequency is high. One valid method to solve this problem is to use spatial derivatives to replace high-order time derivatives (Dablain 1986), which depend on the wave equations.

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Note added in proof. During proof reading stage, we came across a paper by Kosloff *et al* (2008) who developed a new implicit numerical scheme for the solution of the constant density acoustic wave equation using standard grid finite difference. The scheme is based on recursive second-order derivative operators designed by fitting the spectrum at the specified wavenumbers and involves solution of tridiagonal linear system of equations. Our method is general in that we can treat elastic waves.

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