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Optimally accurate second order time-domain finite difference scheme for computing synthetic seismograms in 2-D and 3-D media

Nozomu Takeuchi *, Robert J. Geller

Department of Earth and Planetary Physics, Faculty of Science, Tokyo University, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-0033, Japan

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Abstract

We previously presented an optimally accurate time-domain finite difference method (FDM) scheme for computing synthetic seismograms for one-dimensional (1-D) problems [Geller, R.J., Takeuchi, N., 1998. Optimally accurate second-order time domain finite difference scheme for the elastic equation of motion: 1-D case. Geophys. J. Int. 135, 48–62]. This scheme was derived on the basis of a general criterion for optimally accurate numerical operators obtained by Geller and Takeuchi [Geller, R.J., Takeuchi, N., 1995. A new method for computing highly accurate DSM synthetic seismograms. Geophys. J. Int. 123, 449–470]. In this paper, we derive optimally accurate time-domain FDM operators for 2-D and 3-D problems following the same basic approach. A numerical example shows that synthetics for a 2-D P-SV problem computed using the modified scheme are 30 times more accurate than synthetics computed using a conventional FDM scheme, at a cost of only 3.5 times as much CPU time. This means that the CPU time required to compute synthetics of any specified accuracy using the modified scheme is only 1/47 that required to achieve the same accuracy using the conventional scheme; the memory required by the modified scheme is 1/18 that of the conventional scheme. We have not conducted computational experiments for the 3-D case, but we estimate that the CPU time advantage of the modified scheme will be a factor of over 100. The stability condition (maximum time step for a given spatial grid interval) for the various modified schemes is roughly equal to that for the corresponding conventional scheme.

Keywords: Synthetic seismograms; Finite difference method; Numerical accuracy

1. Introduction

Waveform inversion is a promising approach to inversion for three-dimensional (3-D) Earth structure, but requires the ability to make accurate and efficient calculation of synthetic seismograms. Whether synthetics should be computed in the frequency domain or the time domain depends on the

* Corresponding author. Present address: Earthquake Research Institute, Tokyo University, Yayoi 1-1-1, Bunkyo-ku, Tokyo 113-0032, Japan. Fax: +81-3-3812-9417; e-mail: takeuchi@eri.u-tokyo.ac.jp

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nature of each problem and dataset. It is therefore desirable to develop accurate and efficient computational methods for both the time domain and the frequency domain.

We previously derived optimally accurate [1] operators (modified operators) for computation of synthetics in the frequency domain (Cummins et al., 1994, 1997; Geller and Takeuchi, 1995; Takeuchi et al., 1996) using the Direct Solution Method (DSM; Geller and Ohminato, 1994). These modified operators were derived on the basis of a general criterion that must be approximately satisfied by optimally accurate modified operators (Eq. 2.20 of Geller and Takeuchi, 1995). This criterion can also be applied to derive optimally accurate modified operators for finite difference method (FDM) computations in the time domain. We previously derived modified time domain FDM operators for a 1-D problem (Geller and Takeuchi, 1998). In this paper, we use the same approach to derive modified time-domain FDM operators for 2-D and 3-D problems. (Note that the derivations in the present paper are not intended to be self-contained; see Geller and Takeuchi, 1995, 1998, for basic results.) Using these accurate and efficient synthetics together with algorithms for waveform inversion (Tarantola, 1984; Geller and Hara, 1993; Takeuchi et al., 2000) can contribute to improving our understanding of Earth structure.

Many works (we do not cite particular examples here) have attempted to derive more accurate FDM operators by redefining the operators for spatial differentiation to minimize numerical dispersion of the P- and S-velocities. Such efforts have not in general met with notable success. However, the Lax–Wendroff (LW) scheme (Lax and Wendroff, 1964) is one proposed scheme that has been viewed as promising by some workers. The details of the LW scheme and its relation to our approach are discussed below in Section 5 and elsewhere in this volume by Mizutani et al. (2000). It is shown that the LW scheme is similar to the scheme presented in this paper and by Geller and Takeuchi (1998), but that our approach appears advantageous, due to greater ease of application. Also, to our knowledge, it has never been rigorously established that the fourth order operators required by the LW scheme actually exist for general heterogeneous media in 2-D or 3-D.

Previous workers have generally evaluated proposed computational schemes by presenting theoretical derivations or conducting numerical tests for the case of a homogeneous medium, using the numerical dispersion of the phase velocity as the criterion for evaluating accuracy. However, seismologists use computational methods to study wave propagation in heterogeneous models that approximate the actual Earth, which is highly heterogeneous. It is therefore essential to evaluate the accuracy and performance of computational schemes for the case of heterogeneous models.

In contrast to previous studies, the derivations in this paper are based on the general results derived by Geller and Takeuchi (1995; 1998) for minimizing the error of schemes for computing synthetic seismograms. We thus can systematically derive optimally accurate operators (for a given order of operator and grid spacing) for heterogeneous media in 2-D or 3-D. The modified FDM operators derived in this paper optimally minimize the numerical dispersion of the P- and S-velocities as an indirect consequence of their minimizing the error of the synthetic seismograms (see Geller and Takeuchi, 1995, 1998). However, for technical reasons, it would have been extremely difficult to derive the operators presented in this paper directly on the basis of minimizing numerical dispersion of P- and S-wave velocities.

2. Modified operators for homogeneous 2-D SH problem

In this section, we derive modified FDM operators for the 2-D SH problem in a homogeneous medium. This is the simplest 2-D case, but other applications are basically similar. The extension to the inhomogeneous case is similar to that for the frequency domain problem (Geller and Takeuchi, 1995) or for the 1-D time domain problem (Geller and Takeuchi, 1998). The derivation of optimally accurate operators for the homogeneous 2-D P-SV problem (Section 3) is also straightforward. Modified operators for the heterogeneous 2-D P-SV and SH

[1] ‘‘Optimally accurate’’ operators yield the greatest attainable accuracy for a particular type of scheme (e.g., second order finite difference) for some particular grid spacing.

problems and for a general 3-D heterogeneous medium are presented in Appendix A.

2.1. Conventional operators

We consider 2-D Cartesian coordinates (x, z). The strong form of the time domain equation of motion (see Geller and Ohminato, 1994 for a discussion of the strong and weak forms) for the 2-D homogeneous SH problem is as follows:

$$\rho\frac{\partial^2 u}{\partial t^2} - \mu\frac{\partial^2 u}{\partial x^2} - \mu\frac{\partial^2 u}{\partial z^2} = f, \tag{1}$$

where t is the time, u is the displacement, ρ is the density, μ is the rigidity, and f is the external force. The discretized equation of motion can be expressed as follows:

$$\left(A_{p'r'N'prN} - K^{(1)}_{p'r'N'prN} - K^{(3)}_{p'r'N'prN}\right)c_{prN} = f_{p'r'N'}, \tag{2}$$

where c_{prN} and $f_{p'r'N'}$ are the discretized displacement and discretized external force, and $A_{p'r'N'prN}$, $K^{(1)}_{p'r'N'prN}$ and $K^{(3)}_{p'r'N'prN}$ are respectively the discretized operators for temporal differentiation $(\rho(\partial^2/\partial t^2))$, the second derivative in the x-direction $(\mu(\partial^2/\partial x^2))$ and the second derivative in the z-direction $(\mu(\partial^2/\partial z^2))$. Throughout this paper, the indices p, q, r and p', q', r' denote the x-, y- and z-grids, respectively (q and q' are used only for 3-D problems), and the indices N and N' denote the temporal grids. Summation over repeated indices (p, r, N in this case) is implied. For simplicity, we consider homogeneous grid spacing. The displacement and the external force are discretized as follows:

$$c_{prN} = u(p\Delta x, r\Delta z, N\Delta t),$$
$$f_{p'r'N'} = f(p'\Delta x, r'\Delta z, N'\Delta t), \tag{3}$$

where Δx, Δz and Δt are the spatial and temporal grid intervals.

Here, we consider second order FDM operators in time and space. Unlike some previous workers (e.g., Alterman and Karal, 1968), we define boundary elements without using pseudo nodes. We present operators for a scheme in which displacement is the only variable, rather than a staggered grid scheme (e.g., Virieux, 1986) where velocity and stress are independent variables. A free surface is a natural boundary condition (see Geller and Ohminato, 1994), and is therefore automatically satisfied by the weak-form FDM solution without its having to be imposed explicitly.

The elements of the conventional operators are as follows:

$$\mathbf{A} = \left(\frac{\rho}{\Delta t^2}\right) \times \begin{array}{|c|c|} \hline t+\Delta t & \begin{array}{c|ccc} z+\Delta z & & & \\ z & & 1 & \\ z-\Delta z & & & \\ \hline & x-\Delta x & x & x+\Delta x \end{array} \\ \hline t & \begin{array}{c|ccc} z+\Delta z & & & \\ z & & -2 & \\ z-\Delta z & & & \\ \hline & x-\Delta x & x & x+\Delta x \end{array} \\ \hline t-\Delta t & \begin{array}{c|ccc} z+\Delta z & & & \\ z & & 1 & \\ z-\Delta z & & & \\ \hline & x-\Delta x & x & x+\Delta x \end{array} \\ \hline \end{array} \tag{4}$$

$$\mathbf{K}^{(1)} = \left(\frac{\mu}{\Delta x^2}\right) \times \qquad (5)$$

		$x-\Delta x$	x	$x+\Delta x$
$t+\Delta t$	$z+\Delta z$			
	z			
	$z-\Delta z$			
t	$z+\Delta z$			
	z	1	-2	1
	$z-\Delta z$			
$t-\Delta t$	$z+\Delta z$			
	z			
	$z-\Delta z$			

$$\mathbf{K}^{(3)} = \left(\frac{\mu}{\Delta z^2}\right) \times \qquad (6)$$

		$x-\Delta x$	x	$x+\Delta x$
$t+\Delta t$	$z+\Delta z$			
	z			
	$z-\Delta z$			
t	$z+\Delta z$		1	
	z		-2	
	$z-\Delta z$		1	
$t-\Delta t$	$z+\Delta z$			
	z			
	$z-\Delta z$			

The above operators are expressed using the following difference stencil:

(7)

		$x-\Delta x$	x	$x+\Delta x$
$t+\Delta t$	$z+\Delta z$	$A_{p'r'N'(p'-1)(r'+1)(N'+1)}$	$A_{p'r'N'p'(r'+1)(N'+1)}$	$A_{p'r'N'(p'+1)(r'+1)(N'+1)}$
	z	$A_{p'r'N'(p'-1)r'(N'+1)}$	$A_{p'r'N'p'r'(N'+1)}$	$A_{p'r'N'(p'+1)r'(N'+1)}$
	$z-\Delta z$	$A_{p'r'N'(p'-1)(r'-1)(N'+1)}$	$A_{p'r'N'p'(r'-1)(N'+1)}$	$A_{p'r'N'(p'+1)(r'-1)(N'+1)}$
t	$z+\Delta z$	$A_{p'r'N'(p'-1)(r'+1)N'}$	$A_{p'r'N'p'(r'+1)N'}$	$A_{p'r'N'(p'+1)(r'+1)N'}$
	z	$A_{p'r'N'(p'-1)r'N'}$	$A_{p'r'N'p'r'N'}$	$A_{p'r'N'(p'+1)r'N'}$
	$z-\Delta z$	$A_{p'r'N'(p'-1)(r'-1)N'}$	$A_{p'r'N'p'(r'-1)N'}$	$A_{p'r'N'(p'+1)(r'-1)N'}$
$t-\Delta t$	$z+\Delta z$	$A_{p'r'N'(p'-1)(r'+1)(N'-1)}$	$A_{p'r'N'p'(r'+1)(N'-1)}$	$A_{p'r'N'(p'+1)(r'+1)(N'-1)}$
	z	$A_{p'r'N'(p'-1)r'(N'-1)}$	$A_{p'r'N'p'r'(N'-1)}$	$A_{p'r'N'(p'+1)r'(N'-1)}$
	$z-\Delta z$	$A_{p'r'N'(p'-1)(r'-1)(N'-1)}$	$A_{p'r'N'p'(r'-1)(N'-1)}$	$A_{p'r'N'(p'+1)(r'-1)(N'-1)}$

As shown by Geller and Takeuchi (1995), there are two types of operator error (basic error and boundary error), but only the basic error has an important effect on the solution error (the error of the synthetic seismograms). We therefore discuss only non-boundary elements and the basic error, and omit discussion of the difference stencils for boundary elements and the boundary error. The complete definitions of the operators, including boundary elements, are given in Appendix B. The conventional operators (Eqs. (4)–(6)) have the following basic error (Throughout this paper errors are stated only to lowest order.):

$$\left(\delta A_{p'r'N'prN} - \delta K^{(1)}_{p'r'N'prN} - \delta K^{(3)}_{p'r'N'prN}\right) c_{pqN} = \left(\frac{\Delta t^2}{12}\frac{\partial^2}{\partial t^2}\right)\rho\frac{\partial^2 u}{\partial t^2} - \left(\frac{\Delta x^2}{12}\frac{\partial^2}{\partial x^2}\right)\mu\frac{\partial^2 u}{\partial x^2} - \left(\frac{\Delta z^2}{12}\frac{\partial^2}{\partial z^2}\right)\mu\frac{\partial^2 u}{\partial z^2}. \quad (8)$$

The criterion for optimally accurate operators is that their basic error should be zero when the operand, u, is an eigensolution. However, as the basic error in Eq. (8) does not vanish when the operand is an eigensolution, the conventional operators do not satisfy the general criterion for optimal accuracy (see Geller and Takeuchi, 1995, 1998 for details).

2.2. Stability condition for unmodified operators

The standard method for estimating the stability condition (maximum time step) is to substitute a plane wave solution into the discretized equation of motion and derive the condition on Δt in order for the numerical solution not to have an eigenfrequency with a negative imaginary part (e.g., Richtmyer and Morton, 1967; Alterman and Loewenthal, 1970). This method is rigorous only for an infinite homogeneous medium. The stability conditions for a heterogeneous bounded medium can be rigorously obtained numerically (Geller and Takeuchi, 1998) by solving a generalized eigenvalue problem (Golub and Van Loan, 1989). In general, such numerical estimates show that the stability limit for a heterogeneous bounded medium is roughly equal to the minimum value of the stability limit (as estimated using the standard methods for a homogeneous unbounded medium).

We now derive the stability condition for the conventional operators for the homogeneous 2-D SH problem. We assume $\exp(i\omega N\Delta t)$ time dependence for the eigensolutions:

$$c_{prN} = c_{pr}\exp(i\omega N\Delta t), \quad (9)$$

where ω is angular frequency, $i = \sqrt{-1}$, and c_{pr} is the displacement in the frequency domain at $x = p\Delta x$ and $z = r\Delta z$ $(0 \le p \le N_x,\ 0 \le r \le N_z)$. For simplicity, we consider the case for which $\Delta x = \Delta z$. The Fourier transform of Eq. (2) is as follows:

$$\left(\mathbf{H}^{(1)} + \mathbf{H}^{(3)}\right)\boldsymbol{c} = \frac{2}{\Delta t^2}(1 - \cos\omega\Delta t)\mathbf{T}\boldsymbol{c}. \quad (10)$$

For the 1-D case, it is easy to write the explicit form of the matrices in the counterpart of Eq. (10); see Eqs. (30) and (31) of Geller and Takeuchi (1998). However, for the 2-D or 3-D cases, it is necessary to map the subscripts for the x- and z-grids into a single index in order to write the matrices in Eq. (10); this mapping should be chosen to minimize the bandwidth of the matrices in Eq. (10) (see Appendix A4 of Geller and Ohminato, 1994 for details). The elements of the matrices in Eq. (10) for a typical interior grid point are shown below in Eqs. (11)–(13); note, however, that these elements are not contiguous in the actual mapped matrices. Also, we do not show explicitly the elements for grid points on exterior boundaries or corners.

$$\mathbf{T} = \rho \times \begin{array}{|c|ccc|} \hline z+\Delta z & & & \\ z & & 1 & \\ z-\Delta z & & & \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline \end{array} \quad (11)$$

$$\mathbf{H}^{(1)} = \frac{\mu}{\Delta x^2} \times \begin{array}{|c|ccc|} \hline z+\Delta z & & & \\ z & -1 & 2 & -1 \\ z-\Delta z & & & \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline \end{array} \quad (12)$$

$$\mathbf{H}^{(3)} = \frac{\mu}{\Delta z^2} \times \begin{array}{|c|ccc|} \hline z+\Delta z & & -1 & \\ z & & 2 & \\ z-\Delta z & & -1 & \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline \end{array} \quad (13)$$

On the other hand, we can define the following generalized eigenvalue problem:

$$(\mathbf{H}^{(1)}+\mathbf{H}^{(3)})\boldsymbol{c}=\lambda\mathbf{T}\boldsymbol{c}, \tag{14}$$

where λ is the eigenvalue. The elements of the (l,n)th eigenvector of Eq. (14) for the matrices for a homogeneous medium (Eqs. (11)–(13)) are

$$\boldsymbol{c}^{(\mathrm{ln})}=\left(c_{pr}^{(\mathrm{ln})}\right)=\left(\cos\frac{pl\pi}{N_x}\right)\left(\cos\frac{rn\pi}{N_z}\right), \tag{15}$$

and the corresponding eigenvalues are given by:

$$\lambda_{\mathrm{ln}}=\frac{2V_{\mathrm{s}}^{2}(2-cl-cn)}{\Delta z^{2}} \tag{16}$$

where

$$cl=\cos\frac{l\pi}{N_x},\quad cn=\cos\frac{n\pi}{N_z}. \tag{17}$$

The maximum eigenvalue, $\lambda_{\max}$, of this eigenvalue problem is $\lambda_{\max}=8V_{\mathrm{s}}^{2}/\Delta z^{2}$ (V_{s} is the S-wave velocity; $V_{\mathrm{s}}=\sqrt{\mu/\rho}$) when $cl=cn=-1$ in Eq. (16). Following the same approach as for the 1-D problem (Geller and Takeuchi, 1998), we derive the following stability condition for the 2-D SH conventional operators:

$$\Delta t\leq\frac{\Delta z}{\sqrt{2}\,V_{\mathrm{s}}}. \tag{18}$$

This is the well-known Courant stability condition for this problem. Omitting the derivation, the stability limit for the case when $\Delta x\neq\Delta z$ is

$$\Delta t\leq\frac{\Delta x\Delta z}{V_{\mathrm{s}}\sqrt{\Delta x^{2}+\Delta z^{2}}}. \tag{19}$$

2.3. Standard modified operators

In contrast to the 1-D problem (Geller and Takeuchi, 1998), there are several possible formulations of the modified operators for the 2-D problem. In this section, we derive the explicit elements of the simplest possible form of the modified operators, which we call the standard modified operators. We also derive the stability condition for the standard modified operators.

Modified operators $\mathbf{A}'$, $\mathbf{K}^{(1)'}$ and $\mathbf{K}^{(3)'}$ satisfying the general criterion for optimal accuracy (Geller and Takeuchi, 1995) should, rather than Eq. (8), instead have the following basic error:

$$\begin{aligned}&\left(\delta A'_{p'r'N'prN}-\delta K^{(1)'}_{p'r'N'prN}-\delta K^{(3)'}_{p'r'N'prN}\right)c_{prN}\\&=\left(\frac{\Delta t^{2}}{12}\frac{\partial^{2}}{\partial t^{2}}+\frac{\Delta x^{2}}{12}\frac{\partial^{2}}{\partial x^{2}}+\frac{\Delta z^{2}}{12}\frac{\partial^{2}}{\partial z^{2}}\right)\\&\quad\times\left[\rho\frac{\partial^{2}u}{\partial t^{2}}-\mu\frac{\partial^{2}u}{\partial x^{2}}-\mu\frac{\partial^{2}u}{\partial z^{2}}\right].\end{aligned} \tag{20}$$

The r.h.s. of Eq. (20) will vanish when the operand is an eigensolution, as the bracketed term is the homogeneous equation of motion. Operators having the basic error given by Eq. (20) thus satisfy the general criterion for optimal accuracy.

We now derive modified operators that have the basic error specified by Eq. (20). Consider the time derivative operator $\mathbf{A}$. The basic error for the conventional time derivative operator $\mathbf{A}$ (Eq. (4)) has the desired basic error (specified by Eq. (20)) proportional to Δt^{2}:

$$\delta A_{p'r'N'prN}c_{prN}=\left(\frac{\Delta t^{2}}{12}\frac{\partial^{2}}{\partial t^{2}}\right)\rho\frac{\partial^{2}u}{\partial t^{2}} \tag{21}$$

(see Eq. (8)), but it has no error proportional to Δx^{2} or Δz^{2}. In contrast, the modified operator $\mathbf{A}'$ should have the following basic error which is dependent on Δx^{2} and Δz^{2} as well as Δt^{2}:

$$\begin{aligned}&\delta A'_{p'r'N'prN}c_{prN}\\&=\left(\frac{\Delta t^{2}}{12}\frac{\partial^{2}}{\partial t^{2}}+\frac{\Delta x^{2}}{12}\frac{\partial^{2}}{\partial x^{2}}+\frac{\Delta z^{2}}{12}\frac{\partial^{2}}{\partial z^{2}}\right)\rho\frac{\partial^{2}u}{\partial t^{2}}\end{aligned} \tag{22}$$

(see Eq. (20)). Note that this desired basic error for the modified operator is obtained by having all of the derivatives in the parentheses in Eq. (20) operate on the first term in the square brackets. In other words, we smear out the conventional operator $\mathbf{A}$ in the x- and z-directions to obtain the modified operator $\mathbf{A}'$, as shown below. The explicit form of the modified operator $\mathbf{A}'$ is as follows:

$$\mathbf{A}' = \left(\frac{\rho}{144\Delta t^2}\right) \times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|ccc|}\hline z+\Delta z & 1 & 10 & 1 \\ z & 10 & 100 & 10 \\ z-\Delta z & 1 & 10 & 1 \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline\end{array} \\ \hline t & \begin{array}{|c|ccc|}\hline z+\Delta z & -2 & -20 & -2 \\ z & -20 & -200 & -20 \\ z-\Delta z & -2 & -20 & -2 \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline\end{array} \\ \hline t-\Delta t & \begin{array}{|c|ccc|}\hline z+\Delta z & 1 & 10 & 1 \\ z & 10 & 100 & 10 \\ z-\Delta z & 1 & 10 & 1 \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline\end{array} \\ \hline\end{array} \qquad (23)$$

We derive the modified operators $\mathbf{K}^{(1)'}$ and $\mathbf{K}^{(3)'}$ in a similar fashion from Eq. (20), by having all of the operators in the parentheses in Eq. (20) operate on the second and third terms in the square brackets, respectively.

$$\mathbf{K}^{(1)'} = \left(\frac{\mu}{144\Delta x^2}\right) \times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|ccc|}\hline z+\Delta z & 1 & -2 & 1 \\ z & 10 & -20 & 10 \\ z-\Delta z & 1 & -2 & 1 \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline\end{array} \\ \hline t & \begin{array}{|c|ccc|}\hline z+\Delta z & 10 & -20 & 10 \\ z & 100 & -200 & 100 \\ z-\Delta z & 10 & -20 & 10 \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline\end{array} \\ \hline t-\Delta t & \begin{array}{|c|ccc|}\hline z+\Delta z & 1 & -2 & 1 \\ z & 10 & -20 & 10 \\ z-\Delta z & 1 & -2 & 1 \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline\end{array} \\ \hline\end{array} \qquad (24)$$

$$
\mathbf{K}^{(3)'} = \left(\frac{\mu}{144\Delta z^2}\right) \times
\begin{array}{|c|c|}
\hline
t+\Delta t & \begin{array}{|c|ccc|}
\hline
z+\Delta z & 1 & 10 & 1 \\
z & -2 & -20 & -2 \\
z-\Delta z & 1 & 10 & 1 \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array} \\
\hline
t & \begin{array}{|c|ccc|}
\hline
z+\Delta z & 10 & 100 & 10 \\
z & -20 & -200 & -20 \\
z-\Delta z & 10 & 100 & 10 \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array} \\
\hline
t-\Delta t & \begin{array}{|c|ccc|}
\hline
z+\Delta z & 1 & 10 & 1 \\
z & -2 & -20 & -2 \\
z-\Delta z & 1 & 10 & 1 \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array} \\
\hline
\end{array}
\quad (25)
$$

We refer to the operators in Eqs. (23)–(25) as the standard modified operators. Other possible definitions are discussed in Section 2.4.

Next, we derive the stability conditions for the standard modified operators. The Fourier transformed discretized equation of motion for the standard modified operators is as follows:

$$
\left(\frac{5}{6} + \frac{1}{6}\cos\omega\Delta t\right)\left(\mathbf{H}^{(1)'} + \mathbf{H}^{(3)'}\right)\boldsymbol{c} = \frac{2}{\Delta t^2}(1 - \cos\omega\Delta t)\mathbf{T}'\boldsymbol{c}, \quad (26)
$$

where the matrix elements for the interior grid points are as follows:

$$
\mathbf{T}' = \left(\frac{\rho}{144}\right) \times
\begin{array}{|c|ccc|}
\hline
z+\Delta z & 1 & 10 & 1 \\
z & 10 & 100 & 10 \\
z-\Delta z & 1 & 10 & 1 \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array}
\quad (27)
$$

$$
\mathbf{H}^{(1)'} = \left(\frac{\mu}{12\Delta x^2}\right) \times
\begin{array}{|c|ccc|}
\hline
z+\Delta z & -1 & 2 & -1 \\
z & -10 & 20 & -10 \\
z-\Delta z & -1 & 2 & -1 \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array}
\quad (28)
$$

$$
\mathbf{H}^{(3)'} = \left(\frac{\mu}{12\Delta z^2}\right) \times
\begin{array}{|c|ccc|}
\hline
z+\Delta z & -1 & 2 & -1 \\
z & -10 & 20 & -10 \\
z-\Delta z & -1 & 2 & -1 \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array}
\quad (29)
$$

On the other hand, we can define the following eigenvalue problem:

$$(\mathbf{H}^{(1)'} + \mathbf{H}^{(3)'})\boldsymbol{c} = \lambda' \mathbf{T}' \boldsymbol{c}, \tag{30}$$

where λ' is an eigenvalue. The (l,n)th eigenvector of Eq. (30) for the matrices Eqs. (27)–(29) is given by Eq. (15), and the corresponding eigenvalue is:

$$\lambda'_{ln} = \frac{12V_s^2}{\Delta z^2}\left(\frac{1-cl}{5+cl} + \frac{1-cn}{5+cn}\right), \tag{31}$$

where cl and cn are defined in Eq. (17). We can see that the maximum eigenvalue of Eq. (30) is $\lambda'_{\max} = 12V_s^2/\Delta x^2$ when

$$cl = cn = -1$$

in Eq. (31). From the above relations, we can find that the stability condition for the above modified operators (Eqs. (23)–(25)) is

$$\Delta t \le \frac{\Delta x}{\sqrt{2}\,V_s}. \tag{32}$$

This is the same condition as that for the conventional operators of Eq. (18). Omitting the derivation, the stability limit for the case when $\Delta x \neq \Delta z$ is

$$\Delta t \le \frac{\Delta x \Delta z}{V_s\sqrt{\Delta x^2 + \Delta z^2}}, \tag{33}$$

which is also the same as Eq. (19).

2.4. Non-standard modified operators

We consider below which other definitions of the modified operators are possible and what their stability conditions are. For the homogeneous 2-D SH problem, the definitions of the modified operators for $\mathbf{K}^{(1)}$ and $\mathbf{K}^{(3)}$ are unique (Eqs. (24) and (25)), but there are various possibilities for the modified operator $\mathbf{A}'$. The modified operator with the smallest number of non-zero elements is as follows:

$$\mathbf{A}'' = \left(\frac{\rho}{12\Delta t^2}\right) \times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|ccc|}\hline z+\Delta z & & 1 & \\ z & 1 & 8 & 1 \\ z-\Delta z & & 1 & \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline\end{array} \\ \hline t & \begin{array}{|c|ccc|}\hline z+\Delta z & & -2 & \\ z & -2 & -16 & -2 \\ z-\Delta z & & -2 & \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline\end{array} \\ \hline t-\Delta t & \begin{array}{|c|ccc|}\hline z+\Delta z & & 1 & \\ z & 1 & 8 & 1 \\ z-\Delta z & & 1 & \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline\end{array} \\ \hline\end{array} \tag{34}$$

Any linear combination of Eqs. (23) and (24) with weights summing to one will satisfy Eq. (20), and all such operators are possible definitions of the modified operators for the second time derivative:

$$\mathbf{A}''' = \alpha\mathbf{A}' + (1-\alpha)\mathbf{A}'', \tag{35}$$

where α is an arbitrary constant.

Next, we derive the stability condition for a scheme using the non-standard modified operator $\mathbf{A}'''$ together with $\mathbf{K}^{(1)'}$ and $\mathbf{K}^{(3)'}$ (Eqs. (35), (24) and (25) respectively). First, we derive the stability condition when $\alpha = 0$ in Eq. (35), i.e., the stability condition for $\mathbf{A}''$ (Eq. (34)), $\mathbf{K}^{(1)'}$ and $\mathbf{K}^{(3)'}$. For simplicity, we assume $\Delta x = \Delta z$. The discretized equation of motion is:

$$\left(\frac{5}{6} + \frac{1}{6}\cos\omega\Delta t\right)(\mathbf{H}^{(1)'} + \mathbf{H}^{(3)'})\boldsymbol{c} = \frac{2}{\Delta t^2}(1-\cos\omega\Delta t)\mathbf{T}''\boldsymbol{c}, \tag{36}$$

where

$$\mathbf{T}'' = \left(\frac{\rho}{12}\right) \times \begin{array}{|c|ccc|} \hline z+\Delta z & & 1 & \\ z & 1 & 8 & 1 \\ z-\Delta z & & 1 & \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline \end{array} \tag{37}$$

and $\mathbf{H}^{(1)'}$ and $\mathbf{H}^{(3)'}$ are given in Eqs. (28) and (29).

On the other hand, we can define the eigenvalue problem

$$(\mathbf{H}^{(1)'} + \mathbf{H}^{(3)'})\boldsymbol{c} = \lambda\mathbf{T}''\boldsymbol{c} \tag{38}$$

The (l,n)th eigenvector of Eq. (38) for the matrices of Eqs. (28), (29) and (37) is given by Eq. (15), and the corresponding eigenvalue is:

$$\lambda''_{ln} = \frac{2V_s^2}{\Delta z^2}\,\frac{(1-cl)(5+cl)+(1-cn)(5+cn)}{4+cl+cn}, \tag{39}$$

where cl and cn are defined in Eq. (17). The maximum eigenvalue is $\lambda''_{\max} = 16V_s^2/\Delta z^2$. From these relations, we can see that the stability condition is

$$\Delta t \le \sqrt{\frac{3}{8}}\,\frac{\Delta z}{V_s}. \tag{40}$$

As compared to the stability condition for the conventional operators (Eq. (18)) or standard modified operators (Eq. (32)), the above condition is stricter by a factor of $\sqrt{3/2}$.

If we change the value of α in Eq. (35), we can achieve a laxer stability condition than that for the standard modified operators. In general, the (l,n)th corresponding eigenvalue for the non-standard modified operators Eqs. (28), (29) and (35) is:

$$\lambda'''_{ln} = \frac{12V_s^2}{\Delta z^2}\,\frac{(1-cl)(5+cl)+(5+cn)(1-cn)}{\alpha(5+cl)(5+cn)+6(1-\alpha)(4+cl+cn)}, \tag{41}$$

where cl and cn are defined in Eq. (17). We can derive the stability limit from the maximum value of Eq. (41) for any α. For example, if we set $\alpha = 5$ in Eq. (35), the stability condition becomes

$$\Delta t \le \frac{\Delta x}{V_s}, \tag{42}$$

which is larger by a factor of $\sqrt{2}$ than Eq. (18). Numerical experiments (see Section 5) confirm that the stability limits given by Eqs. (40) and (42) are accurate.

3. Modified operators for homogeneous 2-D P-SV problem

In this section, we derive the modified operators for the 2-D homogeneous P-SV problem. The equation of motion is as follows:

$$\begin{bmatrix} \rho\frac{\partial^2}{\partial t^2} - (\lambda+2\mu)\frac{\partial^2}{\partial x^2} - \mu\frac{\partial^2}{\partial z^2} & -\lambda\frac{\partial^2}{\partial x\partial z} - \mu\frac{\partial^2}{\partial z\partial x} \\ -\lambda\frac{\partial^2}{\partial z\partial x} - \mu\frac{\partial^2}{\partial x\partial z} & \rho\frac{\partial^2}{\partial t^2} - \mu\frac{\partial^2}{\partial x^2} - (\lambda+2\mu)\frac{\partial^2}{\partial z^2} \end{bmatrix}\begin{bmatrix} u_x \\ u_z \end{bmatrix} = \begin{bmatrix} f_x \\ f_z \end{bmatrix}, \tag{43}$$

where u_x, u_z, f_x and f_z are the x- and z-components of the displacement and external force, respectively, and λ and μ are the Lamé constants. The discretized equation of motion using the modified operators is as follows:

$$\left(A'_{p'r'N'\gamma'prN\gamma} - K'_{p'r'N'\gamma'prN\gamma}\right)c_{prN\gamma} = f_{p'r'N'\gamma'}, \quad (44)$$

where $c_{prN\gamma}$ and $f_{p'r'N'\gamma'}$ are the discretized vector displacement and vector external force, and $A'_{p'r'N'\gamma'prN\gamma}$ and $K'_{p'r'N'\gamma'prN\gamma}$ are the modified operators for temporal and spatial differential operations, respectively. The indices $\gamma = 1$ or $\gamma' = 1$ denote the x-component, and $\gamma = 3$ or $\gamma' = 3$ denote the z-component. The displacement and the body force are discretized as follows:

$$\begin{aligned} c_{prN1} &= u_x(p\Delta x, r\Delta z, N\Delta t), \\ c_{prN3} &= u_z(p\Delta x, r\Delta z, N\Delta t), \\ f_{p'r'N'1} &= f_x(p'\Delta x, r'\Delta z, N'\Delta t), \\ f_{p'r'N'3} &= f_z(p'\Delta x, r'\Delta z, N'\Delta t). \end{aligned} \quad (45)$$

Because the modified operators $A'_{p'r'N'\gamma'prN\gamma}$, $K'_{p'r'1\gamma'prN1}$ and $K'_{p'r'N'3prN3}$ are the second derivative operators in the t-, x- and z-directions, they can be defined in a similar fashion as for the SH case.

$$A'_{p'r'\gamma'N'prN\gamma} = \delta_{\gamma'\gamma}\, A'_{p'r'N'prN} \quad (46)$$

$$\begin{aligned} K'_{p'r'N'1prN1} &= K^{(2)'}_{p'r'N'prN} + K^{(3)'}_{p'r'N'prN} \\ K'_{p'r'N'3prN3} &= K^{(1)'}_{p'r'N'prN} + K^{(4)'}_{p'r'N'prN} \end{aligned} \quad (47)$$

where $\delta_{\gamma'\gamma}$ is a Kronecker delta, $A'_{p'r'N'prN}$, $K^{(1)'}_{p'r'N'prN}$ and $K^{(3)'}_{p'r'N'prN}$ are given by Eqs. (23)–(25), and $K^{(2)'}_{p'r'N'prN}$ and $K^{(4)'}_{p'r'N'prN}$ are obtained by replacing μ in Eqs. (24) and (25) by $(\lambda + 2\mu)$.

Next, we define the modified operators $K'_{p'r'N'1prN3}$ and $K'_{p'r'N'3prN1}$, which approximate the mixed differential operators in the x- and z-directions. If we define modified operators $K^{(5)'}_{p'r'N'prN}$ and $K^{(6)'}_{p'r'N'prN}$ for the operators $\lambda(\partial^2/\partial x\partial z)$ and $\mu(\partial^2/\partial x\partial z)$, we have:

$$\begin{aligned} K'_{p'r'N'1prN3} &= K^{(5)'}_{p'r'N'prN} + K^{(6)'}_{prNp'r'N'}, \\ K'_{p'r'N'3prN1} &= K^{(5)'}_{prNp'r'N'} + K^{(6)'}_{p'r'N'prN} \end{aligned} \quad (48)$$

Note that the order of the indices $p'r'N'$ and prN are reversed in some of the above operators. We begin by deriving $K^{(5)'}_{p'r'N'prN}$. As $K^{(6)'}_{p'r'N'prN}$ can be defined by replacing λ in $K^{(5)'}_{p'r'N'prN}$ by μ, a detailed derivation is unnecessary.

The conventional operator $K^{(5)}_{p'r'N'prN}$ for the 2-D homogeneous P-SV problem is given by

$$\mathbf{K}^{(5)} = \left(\frac{\lambda}{4\Delta x\Delta z}\right) \times \begin{array}{|c|c|} \hline t+\Delta t & \begin{array}{c|ccc} z+\Delta z & & & \\ z & & & \\ z-\Delta z & & & \\ \hline & x-\Delta x & x & x+\Delta x \end{array} \\ \hline t & \begin{array}{c|ccc} z+\Delta z & -1 & & 1 \\ z & & & \\ z-\Delta z & 1 & & -1 \\ \hline & x-\Delta x & x & x+\Delta x \end{array} \\ \hline t-\Delta t & \begin{array}{c|ccc} z+\Delta z & & & \\ z & & & \\ z-\Delta z & & & \\ \hline & x-\Delta x & x & x+\Delta x \end{array} \\ \hline \end{array} \quad (49)$$

The operator error of the above operator is

$$\delta K^{(5)}_{p'r'N'prN} c_{prN1} = \left(\frac{\Delta x^2}{6}\frac{\partial^2}{\partial x^2} + \frac{\Delta z^2}{6}\frac{\partial^2}{\partial z^2}\right)\lambda\frac{\partial^2 u_x}{\partial x\partial z}. \quad (50)$$

The error in Eq. (50) does not match the operator error desired for the modified operators, because it does not include an error proportional to Δt^2 and because the coefficients of the error proportional to Δx^2 and Δz^2 are $1/6$ rather than $1/12$. The operator error of $K^{(5)'}_{p'r'N'prN}$ should be as follows in order to match the operator error of the other modified operators to second order:

$$\delta K^{(5)'}_{p'r'N'prN} c_{prN1} = \left(\frac{\Delta t^2}{12} \frac{\partial^2}{\partial t^2} + \frac{\Delta x^2}{12} \frac{\partial^2}{\partial x^2} + \frac{\Delta z^2}{12} \frac{\partial^2}{\partial z^2} \right) \lambda \frac{\partial^2 u_x}{\partial x \partial z}. \tag{51}$$

As noted by Geller and Takeuchi (1995), a modified first-order derivative operator having the above basic error must be defined using a four-point stencil rather than a three-point stencil. The explicit form of the modified operator is either of the following:

$$-\frac{5}{12} u(x - \Delta x) - \frac{3}{12} u(x) + \frac{9}{12} u(x + \Delta x) - \frac{1}{12} u(x + 2\Delta x) = \left(1 + \frac{\Delta x^2}{12} \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) \frac{\mathrm{d}u}{\mathrm{d}x}, \tag{52}$$

$$\frac{1}{12} u(x - 2\Delta x) - \frac{9}{12} u(x - \Delta x) + \frac{3}{12} u(x) + \frac{5}{12} u(x + \Delta x) = \left(1 + \frac{\Delta x^2}{12} \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) \frac{\mathrm{d}u}{\mathrm{d}x} \tag{53}$$

The above two definitions are equivalent; in the frequency domain DSM formulations, we choose the definition that does not increase the bandwidth of the total matrix operators (see Geller and Takeuchi, 1995). This is because we solve a global system of simultaneous linear equations in the frequency domain DSM formulation, and it is important to minimize the bandwidth of the matrices to optimize computational efficiency. In the time-domain FDM, we do not solve global system of simultaneous linear equations. We instead multiply the matrices $(\mathbf{A}' - \mathbf{K}')$ by the displacement vector $(\boldsymbol{c})$ to take local finite differences. Thus minimizing the number of non-zero elements (rather than minimizing the bandwidth) is critical. Both Eqs. (52) and (53) have an equal number of non-zero elements, and both definitions are equivalent in terms of computational efficiency. Here we choose Eq. (52).

The simplest way to define modified operator whose operator error is given by Eq. (51) is

1. define a first order derivative operator in the x-direction like Eq. (52);
2. define a first order derivative operator in the z-direction like Eq. (52);
3. define an identity operator whose operator error is $(\Delta t^2/12)(\partial^2/\partial t^2)$ by smearing out the elements in the t-direction.

and then combine 1–3. The resulting modified operator $\mathbf{K}^{(5)'}$ is as follows:

$$\mathbf{K}^{(5)'} = \left(\frac{\lambda}{1728 \Delta x \Delta z}\right) \times \begin{array}{|c|c|}
\hline
t + \Delta t & \begin{array}{c|cccc}
z + 2\Delta z & 5 & 3 & -9 & 1 \\
z + \Delta z & -45 & -27 & 81 & -9 \\
z & 15 & 9 & -27 & 3 \\
z - \Delta z & 25 & 15 & -45 & 5 \\
\hline
 & x - \Delta x & x & x + \Delta x & x + 2\Delta x
\end{array} \\
\hline
t & \begin{array}{c|cccc}
z + 2\Delta z & 50 & 30 & -90 & 10 \\
z + \Delta z & -450 & -270 & 810 & -90 \\
z & 150 & 90 & -270 & 30 \\
z - \Delta z & 250 & 150 & -450 & 50 \\
\hline
 & x - \Delta x & x & x + \Delta x & x + 2\Delta x
\end{array} \\
\hline
t - \Delta t & \begin{array}{c|cccc}
z + 2\Delta z & 5 & 3 & -9 & 1 \\
z + \Delta z & -45 & -27 & 81 & -9 \\
z & 15 & 9 & -27 & 3 \\
z - \Delta z & 25 & 15 & -45 & 5 \\
\hline
 & x - \Delta x & x & x + \Delta x & x + 2\Delta x
\end{array} \\
\hline
\end{array} \tag{54}$$

The results in this section combined with those in Section 2 give all of the modified operators needed for the homogeneous 2-D P-SV problem. The extension of this derivation to the inhomogeneous case is straightforward. The explicit form of the operators is given in Appendix C.

The eigenvalue and stability condition cannot be derived analytically even for the homogeneous case, because complex P-SV coupling occurs at the boundary. But the stability condition can be expressed as a small perturbation with respect to the condition for unbounded (or periodic) medium which can be derived analytically. This is very similar to the stability condition for the inhomogeneous medium (see Geller and Takeuchi, 1998). The stability condition for the homogeneous 2-D P-SV conventional operators is

$$\Delta t \le \frac{\Delta x}{\sqrt{V_p^2 + V_s^2}} + \epsilon \tag{55}$$

for the case of $\Delta x = \Delta z$, where V_p and V_s are P and S wave velocities and ϵ is a small number which may be either positive or negative. The stability limit for the homogeneous 2-D P-SV modified operators is

$$\Delta t \le \frac{\sqrt{6}\,\Delta x}{\sqrt{6\left(V_p^2 + V_s^2\right) + \left(V_p^2 - V_s^2\right)}} + \epsilon. \tag{56}$$

But in all cases

$$\frac{\sqrt{6}\,\Delta x}{\sqrt{6\left(V_p^2 + V_s^2\right) + \left(V_p^2 - V_s^2\right)}} \le \sqrt{\frac{6}{7}}\,\frac{\Delta x}{\sqrt{V_p^2 + V_s^2}} = 0.926\frac{\Delta x}{\sqrt{V_p^2 + V_s^2}}. \tag{57}$$

For a Poisson solid, for which $\lambda = \mu$ and thus $V_p^2 = 3V_s^2$, we have

$$\frac{\Delta t_{\max}(\text{modified})}{\Delta t_{\max}(\text{conventional})} = \sqrt{\frac{12}{13}} \approx 0.961. \tag{58}$$

Eqs. (57) and (58) thus show that the stability limit for the modified operators is not appreciably less than that of the conventional operators. Numerical tests (not presented in this paper) confirm the above results.

4. Predictor–corrector scheme using modified operators

Note that in this section, $\boldsymbol{\delta}\mathbf{A}$ and $\boldsymbol{\delta}\mathbf{K}$ denote the difference between the modified and conventional operators rather than the error of the operators $\mathbf{A}$ and $\mathbf{K}$. In this section, we present a computational scheme using the modified operators. We presented a computational scheme for the 1-D problem in our previous paper (Geller and Takeuchi, 1998, Section 4), but the scheme presented below is more efficient for 2-D or 3-D problems.

The FDM equation of motion using the modified operators $\mathbf{A}'$ and $\mathbf{K}'$ can be written as follows:

$$(\mathbf{A}' - \mathbf{K}')\,\boldsymbol{c} = \boldsymbol{f}. \tag{59}$$

In general, solving Eq. (59) directly yields an implicit scheme, because the modified operator $(\mathbf{A}' - \mathbf{K}')$ has multiple non-zero elements for time $t + \Delta t$ (see Eqs. (23)–(25) for the homogeneous 2-D SH problem and Eqs. (23)–(25) and (54) for the homogeneous 2-D P-SV problem).

To avoid the need to use an implicit scheme, Geller and Takeuchi (1998) use a predictor–corrector scheme for the 1-D problem. First, they solve the discretized equation of motion using the conventional operators $\mathbf{A}$ and $\mathbf{K}$, and predict the wavefield at the next time step:

$$(\mathbf{A} - \mathbf{K})\,\boldsymbol{c}^0 = \boldsymbol{f}. \tag{60}$$

As there is only one non-zero element for time $t + \Delta t$ in each of the equations for the conventional operators (see Eqs. (4)–(6) for the homogeneous 2-D SH problem and Eqs. (4)–(6) and (49) for the homogeneous 2-D P-SV problem), Eq. (60) can, as is well known, be solved using an explicit scheme. Next, they solve the following equation for the correction, $\boldsymbol{\delta c}$:

$$(\mathbf{A} - \mathbf{K})\,\boldsymbol{\delta c} = -(\boldsymbol{\delta}\mathbf{A} - \boldsymbol{\delta}\mathbf{K})\,\boldsymbol{c}^0, \tag{61}$$

where

$$\boldsymbol{\delta}\mathbf{A} = \mathbf{A}' - \mathbf{A},\ \boldsymbol{\delta}\mathbf{K} = \mathbf{K}' - \mathbf{K}. \tag{62}$$

Finally, they add the predicted wavefield and the correction to obtain the final value of the wavefield:

$$\boldsymbol{c} = \boldsymbol{c}^0 + \boldsymbol{\delta c}. \tag{63}$$

However, Eq. (61) is not efficient for 2-D or 3-D problems, because $\boldsymbol{\delta}\mathbf{A}$ and $\boldsymbol{\delta}\mathbf{K}$ do not have a simple form for these cases. We obtain a more computationally efficient scheme by substituting Eq. (62) into Eq. (61):

$$(\mathbf{A}-\mathbf{K})\boldsymbol{\delta c} = -(\mathbf{A}'-\mathbf{K}')\boldsymbol{c}^0 + (\mathbf{A}-\mathbf{K})\boldsymbol{c}^0, \tag{64}$$

and then substituting Eq. (60) into Eq. (64). The resulting equation is as follows:

$$(\mathbf{A}-\mathbf{K})\boldsymbol{\delta c} = -(\mathbf{A}'-\mathbf{K}')\boldsymbol{c}^0 + \boldsymbol{f}. \tag{65}$$

Eq. (65) is more efficient than Eq. (61) because the forms of $\mathbf{A}'$ and $\mathbf{K}'$ are simpler than $\boldsymbol{\delta}\mathbf{A}$ and $\boldsymbol{\delta}\mathbf{K}$. Almost all of the elements of $\boldsymbol{f}$ will be zero for most applications.

5. Relation between optimally accurate scheme and LW scheme

LW schemes (Lax and Wendroff, 1964) are frequently referred to as highly accurate schemes because of the apparent higher order accuracy of the temporal and spatial derivative operators. However, such statements are based on the apparent accuracy of the numerical operators rather than the accuracy of the numerical solutions. Furthermore, such statements are based on formal accuracy estimates for a homogeneous medium, whereas what one really wants to know is the accuracy of the solutions obtained using LW schemes for a heterogeneous medium. We consider this question in this section, and also discuss the relation between our scheme and LW schemes. We rely in part here on the conclusions reached by Mizutani et al. (2000) for the 1-D case.

Mizutani et al. (2000) showed that the LW scheme for the 1-D case satisfies the condition for optimal accuracy (Geller and Takeuchi, 1995). However, they also pointed out that the solution error of what is frequently referred to as the $O(\Delta t^4,\Delta z^4)$ LW scheme is actually only second order, and that this scheme is essentially equivalent to the optimally accurate scheme of Geller and Takeuchi (1998). They concluded that our optimally accurate scheme seems to be somewhat preferable to the LW scheme because of (i) the greater locality of the stencil, which ensures greater efficiency for massive parallel computations, and (ii) the greater ease of formulating and programming the scheme for a general heterogeneous medium, especially for boundary elements.

In this section, we evaluate the operator error and solution error of the $O(\Delta t^4,\Delta z^4)$ LW scheme for a general 3-D heterogeneous and anisotropic medium, and show that the conclusion of Mizutani et al. (2000) applies in general. There are some variations among proposed LW schemes. Here, we consider one widely cited so-called $O(\Delta t^4,\Delta z^4)$ LW scheme (Dablain, 1986):

$$\boldsymbol{a}^N = \mathbf{T}^{-1}\left[\mathbf{H}^{4\text{th}}\boldsymbol{c}^N + \boldsymbol{f}^N\right] \tag{66}$$

$$\boldsymbol{b}^N = \mathbf{T}^{-1}\left[\mathbf{H}(\mathbf{T}^{-1}\mathbf{H}\boldsymbol{c}^N)\right] \tag{67}$$

$$\boldsymbol{c}^{N+1} = 2\boldsymbol{c}^N - \boldsymbol{c}^{N-1} + \Delta t^2\boldsymbol{a}^N + \frac{\Delta t^4}{12}\boldsymbol{b}^N, \tag{68}$$

where $\boldsymbol{c}^N$, $\boldsymbol{a}^N$ and $\boldsymbol{b}^N$ are, respectively, the discretized wavefields for u_i, $\partial^2 u_i/\partial t^2$ and $\partial^4 u_i/\partial t^4$ at the Nth time step, $\boldsymbol{f}^N$ is the discretized force term for f_i at the Nth time step, $\mathbf{T}$ and $\mathbf{H}$ are the spatially dependent parts of the second-order conventional temporal and spatial derivative operators ($\mathbf{A}$ and $\mathbf{K}$, respectively) for a 3-D heterogeneous and anisotropic medium, and $\mathbf{H}^{4\text{th}}$ is the spatially dependent part of the fourth-order spatial derivative operator $\mathbf{K}^{4\text{th}}$ for a 3-D medium.

To estimate the operator error we derive the discretized equation of motion for the LW scheme given by Eqs. (66)–(68) in a form similar to that of Eq. (2) or Eq. (44). Substituting Eqs. (66) and (67) into Eq. (68) and multiplying both sides by $\mathbf{T}/\Delta t^2$, we obtain

$$\mathbf{T}\left(\frac{\boldsymbol{c}^{N+1} - 2\boldsymbol{c}^N + \boldsymbol{c}^{N-1}}{\Delta t^2}\right) - \mathbf{H}^{4\text{th}}\boldsymbol{c}^N - \frac{\Delta t^2}{12}\mathbf{H}(\mathbf{T}^{-1}\mathbf{H}\boldsymbol{c}^N) = \boldsymbol{f}^N. \tag{69}$$

This can be transformed as follows:

$$\left(\mathbf{A} - \mathbf{K}^{4\text{th}} - \frac{\Delta t^2}{12}\boldsymbol{\rho}^{-1}\mathbf{K}\mathbf{K}\right)\boldsymbol{c} = \boldsymbol{f}, \tag{70}$$

where $\boldsymbol{\rho}^{-1}$ is an operator whose explicit elements are

$$(\boldsymbol{\rho}^{-1})_{p'q'r'N'pqrN} = \frac{1}{\rho_{pqr}}\delta_{p'p}\delta_{q'q}\delta_{r'r}\delta_{N'N}. \tag{71}$$

Thus, the equivalent discretized equation of motion is as follows:

$$(\mathbf{A} - \mathbf{K}^{\mathrm{LW}})\boldsymbol{c} = \boldsymbol{f}, \tag{72}$$

where

$$\mathbf{K}^{\mathrm{LW}} = \mathbf{K}^{4\mathrm{th}} + \frac{\Delta t^2}{12}\boldsymbol{\rho}^{-1}\mathbf{K}\mathbf{K}. \tag{73}$$

Using the Born approximation, we can derive the relation between the solution error $\boldsymbol{\delta c}$ and the error of the operators $\boldsymbol{\delta}\mathbf{A}$, $\boldsymbol{\delta}\mathbf{K}^{\mathrm{LW}}$ as follows:

$$(\mathbf{A}^{(0)} - \mathbf{K}^{(0)})\boldsymbol{\delta c} = -(\boldsymbol{\delta}\mathbf{A} - \boldsymbol{\delta}\mathbf{K}^{\mathrm{LW}})\boldsymbol{c}^{(0)}, \tag{74}$$

where $\mathbf{A}^{(0)}$ and $\mathbf{K}^{(0)}$ are exact operators, and $\boldsymbol{c}^{(0)}$ is the exact solution. We evaluate the operator error, i.e., the r.h.s. of Eq. (74). First, we evaluate the basic error of each term on the r.h.s. of Eq. (74) to second order:

$$\boldsymbol{\delta}\mathbf{A}\boldsymbol{c}^{(0)} = \frac{\Delta t^2}{12}\frac{\partial^2}{\partial t^2}\left(\rho\frac{\partial^2 u_i}{\partial t^2}\right) = \frac{\Delta t^2}{12}\boldsymbol{\rho}^{-1}\mathbf{A}^{(0)}\mathbf{A}^{(0)}\boldsymbol{c}^{(0)} \tag{75}$$

$$\delta\mathbf{K}^{\mathrm{LW}}\boldsymbol{c}^{(0)} = \frac{\Delta t^2}{12}\boldsymbol{\rho}^{-1}\mathbf{K}\mathbf{K}\boldsymbol{c}^{(0)} = \frac{\Delta t^2}{12}\boldsymbol{\rho}^{-1}\mathbf{K}^{(0)}\mathbf{K}^{(0)}\boldsymbol{c}^{(0)} \tag{76}$$

Substituting Eqs. (75) and (76) into the r.h.s. of Eq. (74), we evaluate the operator error as follows:

$$\begin{aligned}
-(\boldsymbol{\delta}\mathbf{A} - \boldsymbol{\delta}\mathbf{K}^{\mathrm{LW}})\boldsymbol{c}^{(0)}
&= -\frac{\Delta t^2}{12}\boldsymbol{\rho}^{-1}\mathbf{A}^{(0)}\mathbf{A}^{(0)}\boldsymbol{c}^{(0)} \\
&\quad + \frac{\Delta t^2}{12}\boldsymbol{\rho}^{-1}\mathbf{K}^{(0)}\mathbf{K}^{(0)}\boldsymbol{c}^{(0)} \\
&= -\frac{\Delta t^2}{12}\boldsymbol{\rho}^{-1}(\mathbf{A}^{(0)}\mathbf{A}^{(0)} - \mathbf{K}^{(0)}\mathbf{K}^{(0)})\boldsymbol{c}^{(0)} \\
&= -\frac{\Delta t^2}{12}\rho^{-1}\big[\mathbf{A}^{(0)}\mathbf{K}^{(0)} - \mathbf{K}^{(0)}\mathbf{A}^{(0)} \\
&\quad + (\mathbf{A}^{(0)} + \mathbf{K}^{(0)})(\mathbf{A}^{(0)} - \mathbf{K}^{(0)})\big]\boldsymbol{c}^{(0)} \\
&= -\frac{\Delta t^2}{12}\rho^{-1}(\mathbf{A}^{(0)} + \mathbf{K}^{(0)})(\mathbf{A}^{(0)} - \mathbf{K}^{(0)})\boldsymbol{c}^{(0)}.
\end{aligned} \tag{77}$$

As the r.h.s. of Eq. (77) is equal to zero when $\boldsymbol{c}^{(0)}$ is an eigensolution, the LW scheme is an optimally accurate scheme. However, we show below that the solution error of this optimally accurate scheme is second order rather than fourth order. We estimate the solution error of the LW scheme using the results of Geller and Takeuchi (1995; Section 6). From Eqs. (74) and (77), we obtain the following relation:

$$\begin{aligned}
&(\mathbf{A}^{(0)} - \mathbf{K}^{(0)})\boldsymbol{\delta c} \\
&\quad = -\frac{\Delta t^2}{12}\boldsymbol{\rho}^{-1}(\mathbf{A}^{(0)} + \mathbf{K}^{(0)})(\mathbf{A}^{(0)} - \mathbf{K}^{(0)})\boldsymbol{c}^{(0)}.
\end{aligned} \tag{78}$$

If we express Eq. (78) in the frequency domain using the normal mode basis normalized so that $\boldsymbol{\rho}$ is an identity matrix, we obtain

$$(\omega^2 - \omega_m^2)\delta c_m = -\frac{\Delta t^2}{12}(\omega^2 + \omega_m^2)(\omega^2 - \omega_m^2)c_m, \tag{79}$$

where ω_m is the eigenfrequency of the mth mode. Note that summation over repeated indices is not implied in Eq. (79). When ω is close to ω_m, we obtain the following relation:

$$\left|\frac{\delta c_m}{c_m}\right| = \frac{\Delta t^2}{12}(\omega^2 + \omega_m^2) \approx \frac{\omega^2\Delta t^2}{6}. \tag{80}$$

As shown by Geller and Takeuchi (1995), the r.h.s. of Eq. (80) is an estimate of the relative solution error. Thus, the expected solution error for the LW scheme is

$$\left|\frac{\boldsymbol{\delta c}}{\boldsymbol{c}^{(0)}}\right| \approx \frac{\omega^2\Delta t^2}{6} \tag{81}$$

for a harmonic source with angular frequency ω. On the other hand, the solution error of synthetic seismograms computed using our optimally accurate operators is as follows:

$$\left|\frac{\boldsymbol{\delta c}}{\boldsymbol{c}^{(0)}}\right| \approx \frac{\omega^2\Delta t^2 + |\boldsymbol{k}|^2\Delta z^2}{12}, \tag{82}$$

where $|\boldsymbol{k}|$ is a representative absolute value of the wavenumber. Comparing Eqs. (81) and (82), we see that the solution error for our optimally accurate scheme and the solution error for the LW scheme are roughly equal when both use the same grid spacing.

There are some additional questions regarding the LW scheme. In the above formulation, we assumed that $\mathbf{H}^{4th}$ and $\mathbf{K}^{4th}$ were exact to third order (i.e., that the lowest order non-zero error terms were fourth order) and thus make no contribution to the second-order error. But, in general, derivations of so-called higher order operators assume a homogeneous medium, and the accuracy of such operators, especially for boundary elements, is in question for a general heterogeneous medium with sharp internal discontinuities. To our knowledge, no rigorous derivation of higher order operators $\mathbf{H}^{4th}$ for general heterogeneous media has ever been published, and it is far from clear that they necessarily exist. Resolving this question is an important topic for future research. A quantitative comparison of performance between a rigorously derived LW scheme for such general heterogeneous media and our optimally accurate scheme is thus a topic for future research.

Some readers may question why the LW scheme has a second order basic error (r.h.s. of Eq. (77)), in view of the fact that it is frequently characterized as a ''higher order scheme.'' The explanation is as follows. This error is caused by the approximation used in Eq. (67), which is the equation to evaluate $\partial^4 u_i/\partial t^4$ in discretized form. The exact evaluation is as follows:

$$\begin{aligned}\frac{\partial^4 u_i}{\partial t^4} &= \frac{1}{\rho}\left\{\left(C_{ijkl}\frac{\partial^2 u_{k,l}}{\partial t^2}\right)_{,j} + \frac{\partial^2 f_i}{\partial t^2}\right\}\\ &= \frac{1}{\rho}\left\{\left[C_{ijkl}\left(\frac{1}{\rho}\left\{\left(C_{kj'k'l'}u_{k',l'}\right)_{,j'} + f_k\right\}\right)_{,l}\right]_{,j}\right.\\ &\quad\left. + \frac{\partial^2 f_i}{\partial t^2}\right\},\end{aligned} \tag{83}$$

where C_{ijkl} is the elastic constant. But Eq. (67) omits the f_k and $\partial^2 f_i/\partial t^2$ term. Because these terms have a second-order contribution, the net operator error is second order. Some LW schemes appear not to use this approximation, and thus their basic error for homogeneous media has higher order accuracy (e.g., Igel et al., 1995). But the extension of this result to heterogeneous media would require the assumption that $\mathbf{H}^{4th}$ is exactly fourth order, so a rigorous derivation of such operators, including the boundary errors, is another important research topic.

In summary, it seems questionable to characterize the LW scheme as a ''higher order scheme,'' since the solution error for the so-called $O(\Delta t^4, \Delta z^4)$ LW scheme analyzed above is second order optimally accurate. Furthermore, there seem to be problems in defining rigorously fourth order $\mathbf{H}^{4th}$ operators for general heterogeneous media with sharp internal discontinuities, especially for boundary elements.

6. Numerical examples

We compare the accuracy of synthetic seismograms computed using the conventional and modified operators for the 2-D heterogeneous P-SV problem. We consider a heterogeneous medium whose density ρ (g/cm^3), P-wave velocity V_p (km/s), and S-wave velocity V_s (km/s) at x (km) and z (km) are as follows:

$$\begin{aligned}&\rho(x,z) = 1 + x/1000\\ &V_p(x,z) = \sqrt{\frac{75 + 3x/40 + 5z/40}{1 + x/1000}} \qquad \begin{pmatrix}0 \le x \le 1000\\ 0 \le z \le 1000\end{pmatrix}\\ &V_s(x,z) = \sqrt{\frac{25 + x/40 + z/20}{1 + x/1000}}\,.\end{aligned} \tag{84}$$

A comparison of the error for synthetics computed using the conventional and the modified operators is shown in Fig. 1. We use a constant grid spacing ($\Delta x = \Delta z = 2$ km), and the length of the time series is 250 s. The source is a point single force ($f_x = f_z = 1$ N at $x = z = 500$ km) with a Ricker wavelet time history whose central frequency is 10 s. The receiver is at $(x,z) = (300, 500)$. The error at the receiver is plotted against the temporal grid spacing Δt normalized by the (nominal value of the) Courant limit for the conventional operators. The relative error is the ratio of the RMS of the residual $(u_i - u_i^{(0)})$ and the RMS of the exact solution $u_i^{(0)}$. Its explicit definition is as follows:

$$\text{Relative Error}\,(\%) = \sqrt{\frac{\int |u_i - u_i^{(0)}|^2 \mathrm{d}t}{\int |u_i^{(0)}|^2 \mathrm{d}t}} \times 100. \tag{85}$$

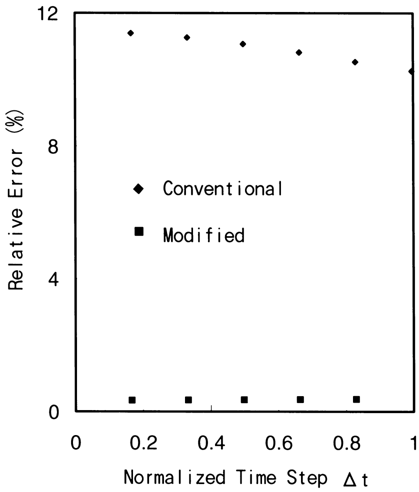

Fig. 1. A comparison of the error of the synthetic seismograms as a function of the temporal grid spacing. The temporal grid spacing is normalized by the nominal Courant limit (Alterman and Loewenthal, 1970). The diamonds and squares show the error at the receiver point using the conventional and modified operators, respectively.

The nominal Courant limit for the conventional operators for the inhomogeneous P-SV problem (when $\Delta x = \Delta z$) is as follows (e.g., Alterman and Loewenthal, 1970):

$$\Delta t_{\text{courant}} = \frac{\Delta x}{\sqrt{\left(V_{\text{p}}^2 + V_{\text{s}}^2\right)_{\max}}}. \tag{86}$$

However, as noted above and by Geller and Takeuchi (1998), the actual Courant limit for the conventional operators for a heterogeneous medium or for a finite but homogeneous medium is slightly different from the above limit, and the stability limit for the modified operators is slightly lower than that of the conventional operators. The nominal limit predicted by Eq. (86) is $\Delta t = 0.1206$ s, but we found that the actual limits for this case are $\Delta t = 0.121$ s and $\Delta t = 0.118$ s for the conventional and modified operators, respectively.

We found (see Fig. 2) that the accuracy of the synthetics computed using the modified operators is greatly improved (by about a factor of 30 times as compared to synthetics computed with the same spatial and temporal gridding for the conventional operators) for all values of the temporal grid spacing used in the numerical experiment. In contrast to Fig. 2a and c of Geller and Takeuchi (1998), there is not great improvement in the accuracy of the synthetics computed using the conventional operators for values of Δt near the Courant limit. This is an expected result, for reasons that were explained by Geller and Takeuchi (1998): for the homogeneous 1-D or 2-D

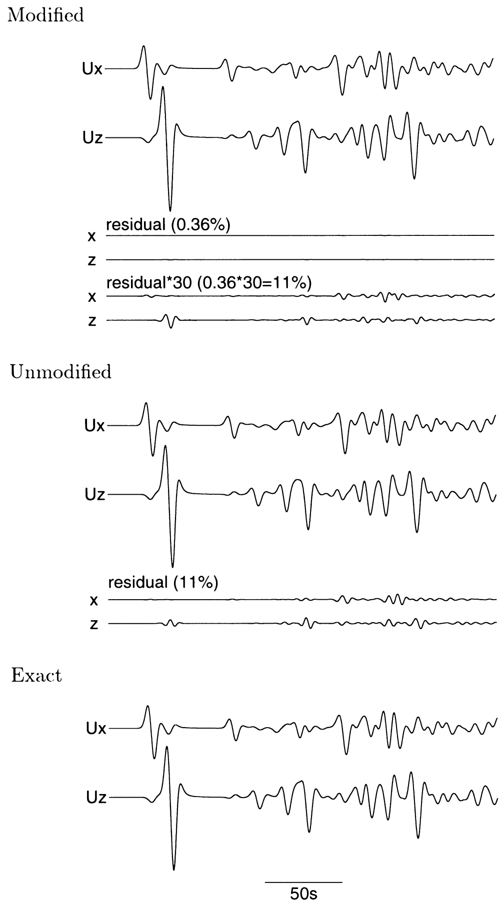

Fig. 2. A comparison of the waveforms and the residuals for P-SV synthetics in a heterogeneous medium computed using the modified and conventional operators. These are synthetics for the case when the temporal grid spacing normalized by the Courant limit is 0.5. The upper two traces show the x- and z-components of the synthetics, and the next two traces show the x- and z-components of the residuals (synthetic waveforms minus exact waveforms) for synthetics computed using the modified operators. $30\times$ enlargements of the residuals are also shown. The next four traces show the synthetics and residuals for synthetics computed using the conventional operators. The last two traces show the almost exact synthetics (synthetics computed by very fine grids). All traces are plotted using the same vertical scale.

SH problems, the basic error of the temporal derivatives and the basic error of the spatial derivatives fortuitously cancel at the Courant limit when the operand is an eigensolution. Even for heterogeneous 1-D or 2-D SH problems, the errors due to the temporal and spatial derivatives will approximately cancel if we choose an appropriately spatially varying grid spacing. However, for the 2-D P-SV problem (or general 3-D problem), P and S waves, which have different wavenumbers, exist simultaneously in the wavefield. The temporal and spatial errors will never cancel simultaneously for both types of waves using the conventional operators. Thus, using the modified operators is especially advantageous for the P-SV or 3-D problems.

Synthetics computed using the conventional and modified operators are shown in Fig. 2. We show synthetics for the case $\Delta t/\Delta t_{\mathrm{courant}} = 0.5$. The required CPU times were 3830 and 13 300 s (on an UltraSPARC, 170 MHz) for the conventional and modified operators, respectively. About 3.5 times more CPU time was required for the modified operators, but about 30 times improvement in the accuracy was obtained. Because the CPU time is proportional to the cube of the grid spacing, while the error is proportional to the square of the grid spacing, this means a $30^{3/2}/3.5 = 47$ times decrease in the CPU time required to obtain synthetics of any given accuracy using the modified operators rather than the conventional operators. We estimate that the advantage of the modified operators will be a factor of over 100 for 3-D problems (see Appendix D), but we have not yet confirmed this by numerical tests.

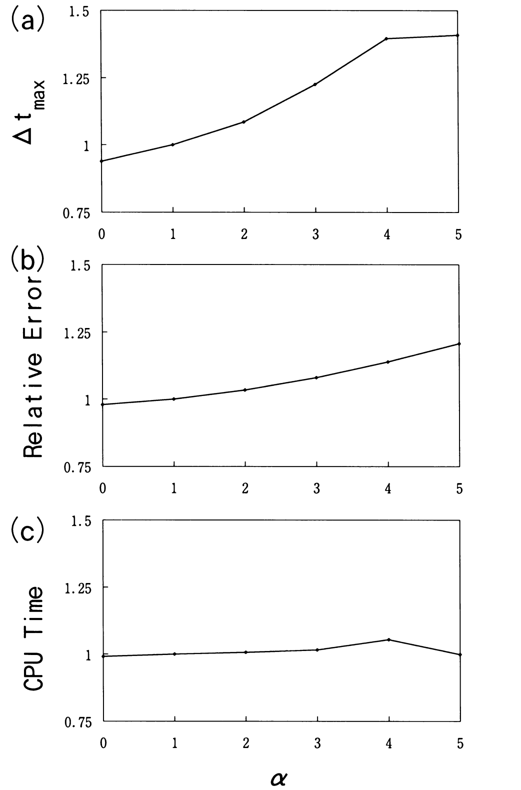

Fig. 3. (a) Stability limit for various values of α (see Eq. (35)). (b) relative error (for constant grid size) as a function of α. (c) CPU time (for constant grid size) as a function of α. Each plot is normalized by the results for the standard modified operators ($\alpha = 1$).

We conducted some simple numerical tests of the standard and non-standard modified operators (see Eqs. (23), (34) and (35), and accompanying discussions). The goal of these tests was to verify the general results on stability (e.g., Eqs. (41) and (42)) rather than to determine the optimum value of α to maximize computational efficiency. The latter remains a subject for future work. The calculations described in this paragraph were all carried out for $\Delta t \approx 0.7\Delta t_{\mathrm{max}}$(conventional). Fig. 3a shows the stability limit (verified through numerical experiment) for the alternative modified operators for various values of α (see Eqs. (35), (39)–(42)). Fig. 3b shows the variation of the relative accuracy as a function of α, normalized to the relative accuracy for the standard modified operators for the same grid size. Fig. 3c shows the CPU time, normalized to the CPU time for a scheme using the standard modified operators. Here, we consider the 2-D SH problem for the heterogeneous medium whose density and S wave velocity are given in Eq. (84). We use constant grid spacing ($\Delta x = \Delta z = 2$ km) for all cases.

We can see that the stability limit increases slightly, while the accuracy degrades slightly, as α increases. There is no significant difference in CPU time. The stability limit is essentially equal to the predicted value. The reason that the accuracy degrades for larger α is probably that higher order errors increase as α increases. There thus seems to be a trade-off between accuracy and the stability limit; the standard modified operators ($\alpha = 1$) appear to be a reasonable choice, but we have not yet ascertained the optimum value of α.

7. Conclusions and discussion

We derived modified time domain FDM operators for a general heterogeneous medium and confirmed that the accuracy of the synthetic seismograms computed using the modified operators was greatly improved as compared to the conventional FDM operators. We also confirmed that the CPU time required to achieve any given level of accuracy was greatly reduced by using the modified operators. In this paper we considered an isotropic and elastic medium, but extension to an anisotropic medium should be straightforward. The extension the anelastic case (Emmerich and Korn, 1987) is an important future topic, but appears to be relatively straightforward.

In this paper, we presented operators for a medium without sharp internal discontinuities. Discontinuous boundaries coinciding with grid boundaries can be handled by ‘‘overlapping’’ the operators in a straightforward fashion (see Geller and Takeuchi, 1995). However, developing methods for accurate handling of discontinuities between nodes is an important topic for future research.

A variety of approaches exist for computing synthetic seismograms. These may effectively be separated into quasi-analytic methods (e.g., reflectivity: Fuchs and Müller, 1971, modal superposition: Takeuchi and Saito, 1972, the DSM, e.g., Takeuchi et al., 1996) and purely numerical methods (e.g., finite difference, finite element, pseudo-spectral). The choice between these two classes is depends on the nature of the problem. For example, the former class of methods is obviously more appropriate for a flat-layered medium. However, the distinction between analytic and numerical methods can become fuzzy. Consider, for example, a laterally homogeneous medium with arbitrary vertical heterogeneity. For such a medium, we would use separation of variables to break the problem up into a series of decoupled problems for each distinct wavenumber or harmonic, and then solve these decoupled 1-D problems numerically. On the other hand, for general arbitrarily heterogeneous media purely numerical methods will probably be preferable.

Suppose we have decided to use a purely numerical method, and are trying to decide which is best. Generally speaking, second-order FDM schemes have been considered inferior to fourth order (in space) FDM schemes or pseudo-spectral schemes. This view may be correct if consideration is limited to conventional second-order FDM schemes. However, the modified second order FDM schemes presented in this paper have significant advantages over other types of schemes. Memory access is more localized than in higher order FDM schemes, and much more localized than in pseudo-spectral schemes, which rely on FFT differentiation. This is a major advantage for applications on highly parallel machines. Also, pseudo-spectral methods have difficulty in handling sharp boundaries, while FDM schemes do not (Mizutani et al., 2000). Finally, it appears that nominally fourth order (or higher) FDM schemes may actually be of lower order accuracy due to boundary errors, and that the problem of boundary errors may preclude the possibility of developing modified operators for higher order FDM schemes along the lines used in this paper for the second order case. We therefore think that the modified second order FDM operators derived in this paper may well prove preferable for a broad general class of problems.

Acknowledgements

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Appendix A. Notation

For simplicity, we assume constant grid intervals Δx, Δy, Δz and Δt. We also assume the medium has no sharp internal discontinuities. We denote the displacement $u_{\gamma'}(p'\Delta x,\ q'\Delta y,\ r'\Delta z,\ N'\Delta t)$ and the external force $f_{\gamma'}(p'\Delta x,\ q'\Delta y,\ r'\Delta z,\ N'\Delta t)$ by $c^{N'}_{p'q'r'\gamma'}$ and $f^{N'}_{p'q'r'\gamma'}$, respectively ($\gamma'=1$, $\gamma'=2$ and $\gamma'=3$ denote the x-, y- and z-components, respectively), where $0 \le p' \le N_x$, $0 \le q' \le N_y$, and $0 \le r' \le N_z$. We denote the density $\rho(p'\Delta x,\ q'\Delta y,\ r'\Delta z)$, and the Lamé constants $\lambda(p'\Delta x,\ q'\Delta y,\ r'\Delta z)$ and $\mu(p'\Delta x,\ q'\Delta y,\ r'\Delta z)$ as $\rho_{p'q'r'}$, $\lambda_{p'q'r'}$ and $\mu_{p'q'r'}$, respectively. To express matrix elements and schemes in a compact form, we use the following simplified notations.

$$\rho_{000} = \rho_{p'q'r'}$$

$$\mu_{-00} = (\mu_{(p'-1)q'r'} + \mu_{p'q'r'})/2$$

$$\mu_{+00} = (\mu_{p'q'r'} + \mu_{(p'+1)q'r'})/2$$

$$\mu_{00-} = (\mu_{p'q'(r'-1)} + \mu_{p'q'r'})/2$$

$$\mu_{00+} = (\mu_{p'q'r'} + \mu_{(p'+1)q'(r'+1)})/2$$

The other type of notations like μ_{0-0}, λ_{-00}, etc. are defined in a similar fashion. For the 2-D SH and P-SV problem, we omit q' and its related indices (e.g., second index of λ_{-00}) because we assume homogeneous dependence in the y-direction. For the 2-D SH problem, only $\gamma'=2$ appears, so we further omit the index γ'. We denote replacement (like the equal sign in a Fortran program, as opposed to mathematical equality) by a left arrow ($\leftarrow$).

Appendix B. Explicit forms for heterogeneous 2-D SH problems

First, we show the explicit form of submatrices of modified operators (Eqs. (23)–(25) for homogeneous case) for heterogeneous medium using the stencils. We show the boundary elements also. Next, we show the total conventional and modified operators, and numerical scheme using these operators. In these discussions, we consider only non-boundary elements to show the required number of floating point operations clearly. Finally, we compare the number of floating point operators between our modified scheme and conventional scheme.

B.1. Submatrices of the modified operators

B.1.1. Non-boundary elements

First, we show the non-boundary elements of submatrices of modified operators. The explicit elements of $A'_{p'r'N'prN}$, $K^{(1)'}_{p'r'N'prN}$ and $K^{(3)'}_{p'r'N'prN}$ for $r' \neq 1,\ N_x$ and $q' \neq 1,\ N_z$ are as follows:

$$\mathbf{A}' = \left(\frac{\rho_{00}}{144\Delta t^2}\right) \times \begin{array}{|c|c|} \hline t+\Delta t & \begin{array}{|c|ccc|} \hline z+\Delta z & 1 & 10 & 1 \\ z & 10 & 100 & 10 \\ z-\Delta z & 1 & 10 & 1 \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline \end{array} \\ \hline t & \begin{array}{|c|ccc|} \hline z+\Delta z & -2 & -20 & -2 \\ z & -20 & -200 & -20 \\ z-\Delta z & -2 & -20 & -2 \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline \end{array} \\ \hline t-\Delta t & \begin{array}{|c|ccc|} \hline z+\Delta z & 1 & 10 & 1 \\ z & 10 & 100 & 10 \\ z-\Delta z & 1 & 10 & 1 \\ \hline & x-\Delta x & x & x+\Delta x \\ \hline \end{array} \\ \hline \end{array} \tag{87}$$

$$
\mathbf{K}^{(1)'} = \left(\frac{1}{144\Delta x^2}\right) \times
\begin{array}{|c|c|}
\hline
t+\Delta t &
\begin{array}{|c|ccc|}
\hline
z+\Delta z & \mu_{-0} & -(\mu_{-0}+\mu_{+0}) & \mu_{+0} \\
z & 10\mu_{-0} & -10(\mu_{-0}+\mu_{+0}) & 10\mu_{+0} \\
z-\Delta z & \mu_{-0} & -(\mu_{-0}+\mu_{+0}) & \mu_{+0} \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array} \\
\hline
t &
\begin{array}{|c|ccc|}
\hline
z+\Delta z & 10\mu_{-0} & -10(\mu_{-0}+\mu_{+0}) & 10\mu_{+0} \\
z & 100\mu_{-0} & -100(\mu_{-0}+\mu_{+0}) & 100\mu_{+0} \\
z-\Delta z & 10\mu_{-0} & -10(\mu_{-0}+\mu_{+0}) & 10\mu_{+0} \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array} \\
\hline
t-\Delta t &
\begin{array}{|c|ccc|}
\hline
z+\Delta z & \mu_{-0} & -(\mu_{-0}+\mu_{+0}) & \mu_{+0} \\
z & 10\mu_{-0} & -10(\mu_{-0}+\mu_{+0}) & 10\mu_{+0} \\
z-\Delta z & \mu_{-0} & -(\mu_{-0}+\mu_{+0}) & \mu_{+0} \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array} \\
\hline
\end{array}
\qquad (88)
$$

$$
\mathbf{K}^{(3)'} = \left(\frac{1}{144\Delta z^2}\right) \times
\begin{array}{|c|c|}
\hline
t+\Delta t &
\begin{array}{|c|ccc|}
\hline
z+\Delta z & \mu_{0-} & 10\mu_{0-} & \mu_{0-} \\
z & -(\mu_{0-}+\mu_{0+}) & -10(\mu_{0-}+\mu_{0+}) & -(\mu_{0-}+\mu_{0+}) \\
z-\Delta z & \mu_{0+} & 10\mu_{0+} & \mu_{0+} \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array} \\
\hline
t &
\begin{array}{|c|ccc|}
\hline
z+\Delta z & 10\mu_{0-} & 100\mu_{0-} & 10\mu_{0-} \\
z & -10(\mu_{0-}+\mu_{0+}) & -100(\mu_{0-}+\mu_{0+}) & -10(\mu_{0-}+\mu_{0+}) \\
z-\Delta z & 10\mu_{0+} & 100\mu_{0+} & 10\mu_{0+} \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array} \\
\hline
t-\Delta t &
\begin{array}{|c|ccc|}
\hline
z+\Delta z & \mu_{0-} & 10\mu_{0-} & \mu_{0-} \\
z & -(\mu_{0-}+\mu_{0+}) & -10(\mu_{0-}+\mu_{0+}) & -(\mu_{0-}+\mu_{0+}) \\
z-\Delta z & \mu_{0+} & 10\mu_{0+} & \mu_{0+} \\
\hline
 & x-\Delta x & x & x+\Delta x \\
\hline
\end{array} \\
\hline
\end{array}
\qquad (89)
$$

B.1.2. Boundary elements

Next, we show the boundary elements, the explicit elements of $A'_{p'r'N'prN}$, $K^{(1)'}_{p'r'N'prN}$ and $K^{(3)'}_{p'r'N'prN}$ for $p'=1$, $p'=N_x$, $r'=1$ or $r'=N_z$. The explicit elements for $p'=1$ and $r'\neq 1,\ N_z$ are as follows. The other boundary elements can be defined in a similar fashion.

$$\mathbf{A}' = \left(\frac{\rho_{00}}{144\Delta t^2}\right) \times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & 5 & 1 \\ z & 50 & 10 \\ z-\Delta z & 5 & 1 \\ \hline & x & x+\Delta x \\ \hline \end{array} \\ \hline t & \begin{array}{|c|cc|}\hline z+\Delta z & -10 & -2 \\ z & -100 & -20 \\ z-\Delta z & -10 & -2 \\ \hline & x & x+\Delta x \\ \hline \end{array} \\ \hline t-\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & 5 & 1 \\ z & 50 & 10 \\ z-\Delta z & 5 & 1 \\ \hline & x & x+\Delta x \\ \hline \end{array} \\ \hline \end{array} \tag{90}$$

$$\mathbf{K}^{(1)'} = \left(\frac{1}{144\Delta x^2}\right) \times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & -\mu_{+0} & \mu_{+0} \\ z & -10\mu_{+0} & 10\mu_{+0} \\ z-\Delta z & -\mu_{+0} & \mu_{+0} \\ \hline & x & x+\Delta x \\ \hline \end{array} \\ \hline t & \begin{array}{|c|cc|}\hline z+\Delta z & -10\mu_{+0} & 10\mu_{+0} \\ z & -100\mu_{+0} & 100\mu_{+0} \\ z-\Delta z & -10\mu_{+0} & 10\mu_{+0} \\ \hline & x & x+\Delta x \\ \hline \end{array} \\ \hline t-\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & -\mu_{+0} & \mu_{+0} \\ z & -10\mu_{+0} & 10\mu_{+0} \\ z-\Delta z & -\mu_{+0} & \mu_{+0} \\ \hline & x & x+\Delta x \\ \hline \end{array} \\ \hline \end{array} \tag{91}$$

$$\mathbf{K}^{(3)'} = \left(\frac{1}{144\Delta z^2}\right) \times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & 5\mu_{0+} & \mu_{0+} \\ z & -5(\mu_{0-}+\mu_{0+}) & -(\mu_{0-}+\mu_{0+}) \\ z-\Delta z & 5\mu_{0-} & \mu_{0-} \\ \hline & x & x+\Delta x \\ \hline \end{array} \\ \hline t & \begin{array}{|c|cc|}\hline z+\Delta z & 50\mu_{0+} & 10\mu_{0+} \\ z & -50(\mu_{0-}+\mu_{0+}) & -10(\mu_{0-}+\mu_{0+}) \\ z-\Delta z & 50\mu_{0-} & 10\mu_{0-} \\ \hline & x & x+\Delta x \\ \hline \end{array} \\ \hline t-\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & 5\mu_{0+} & \mu_{0+} \\ z & -5(\mu_{0-}+\mu_{0+}) & -(\mu_{0-}+\mu_{0+}) \\ z-\Delta z & 5\mu_{0-} & \mu_{0-} \\ \hline & x & x+\Delta x \\ \hline \end{array} \\ \hline \end{array} \tag{92}$$

Finally, we show the corner elements. The explicit elements for $p'=1$ and $r'=1$ are as follows. The other corner elements can be defined in a similar fashion.

$$\mathbf{A}' = \left(\frac{\rho_{00}}{144\Delta t^2}\right) \times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & 5 & 1 \\ z & 25 & 5 \\ \hline & x & x+\Delta x \\ \hline\end{array} \\ \hline t & \begin{array}{|c|cc|}\hline z+\Delta z & -10 & -2 \\ z & -50 & -10 \\ \hline & x & x+\Delta x \\ \hline\end{array} \\ \hline t-\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & 5 & 1 \\ z & 25 & 5 \\ \hline & x & x+\Delta x \\ \hline\end{array} \\ \hline\end{array} \tag{93}$$

$$\mathbf{K}^{(1)'} = \left(\frac{1}{144\Delta x^2}\right) \times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & -\mu_{+0} & \mu_{+0} \\ z & -5\mu_{+0} & 5\mu_{+0} \\ \hline & x & x+\Delta x \\ \hline\end{array} \\ \hline t & \begin{array}{|c|cc|}\hline z+\Delta z & -10\mu_{+0} & 10\mu_{+0} \\ z & -50\mu_{+0} & 50\mu_{+0} \\ \hline & x & x+\Delta x \\ \hline\end{array} \\ \hline t-\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & -\mu_{+0} & \mu_{+0} \\ z & -5\mu_{+0} & 5\mu_{+0} \\ \hline & x & x+\Delta x \\ \hline\end{array} \\ \hline\end{array} \tag{94}$$

$$\mathbf{K}^{(3)'} = \left(\frac{1}{144\Delta z^2}\right) \times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & 5\mu_{0+} & \mu_{0+} \\ z & -5\mu_{0+} & -\mu_{0+} \\ \hline & x & x+\Delta x \\ \hline\end{array} \\ \hline t & \begin{array}{|c|cc|}\hline z+\Delta z & 50\mu_{0+} & 10\mu_{0+} \\ z & -50\mu_{0+} & -10\mu_{0+} \\ \hline & x & x+\Delta x \\ \hline\end{array} \\ \hline t-\Delta t & \begin{array}{|c|cc|}\hline z+\Delta z & 5\mu_{0+} & \mu_{0+} \\ z & -5\mu_{0+} & -\mu_{0+} \\ \hline & x & x+\Delta x \\ \hline\end{array} \\ \hline\end{array} \tag{95}$$

B.2. Modified / conventional operators (non-boundary terms)

$$A_{p'r'N'prN} = \frac{\delta_{p'p}\delta_{r'r}}{\Delta t^2}\rho_{00}\left[\delta_{(N'+1)N} - 2\delta_{N'N} + \delta_{(N'-1)N}\right]$$

$$\begin{aligned} K_{p'r'N'prN} = {} & \frac{\delta_{r'r}\delta_{N'N}}{\Delta x^2}\left[\mu_{-0}\left(\delta_{(p'-1)p} - \delta_{p'p}\right) + \mu_{+0}\left(-\delta_{p'p} + \delta_{(p'+1)p}\right)\right] \\ & + \frac{\delta_{p'p}\delta_{N'N}}{\Delta z^2}\left[\mu_{0-}\left(\delta_{(r'-1)r} - \delta_{r'r}\right) + \mu_{0+}\left(-\delta_{r'r} + \delta_{(r'+1)r}\right)\right] \end{aligned}$$

$$A'_{p'r'N'prN} = \frac{\delta_{p'p}\,\delta_{r'r}}{\Delta t^2}\rho_{00}\left[\delta_{(N'+1)N} - 2\,\delta_{N'N} + \delta_{(N'-1)N}\right] \times\left[\frac{1}{12}\delta_{(p'-1)p} + \frac{10}{12}\delta_{p'p} + \frac{1}{12}\delta_{(p'+1)p}\right] \times\left[\frac{1}{12}\delta_{(r'-1)r} + \frac{10}{12}\delta_{r'r} + \frac{1}{12}\delta_{(r'+1)r}\right] \quad (96)$$

$$K_{p'r'N'prN} = \frac{\delta_{r'r}\,\delta_{N'N}}{\Delta x^2}\left[\mu_{-0}\left(\delta_{(p'-1)p} - \delta_{p'p}\right) + \mu_{+0}\left(-\delta_{p'p} + \delta_{(p'+1)p}\right)\right] \times\left[\frac{1}{12}\delta_{(N'-1)N} + \frac{10}{12}\delta_{N'N} + \frac{1}{12}\delta_{(N'+1)N}\right] \times\left[\frac{1}{12}\delta_{(r'-1)r} + \frac{10}{12}\delta_{r'r} + \frac{1}{12}\delta_{(r'+1)r}\right] + \frac{\delta_{p'p}\,\delta_{N'N}}{\Delta z^2}\left[\mu_{0-}\left(\delta_{(r'-1)r} - \delta_{r'r}\right) + \mu_{0+}\left(-\delta_{r'r} + \delta_{(r'+1)r}\right)\right] \times\left[\frac{1}{12}\delta_{(N'-1)N} + \frac{10}{12}\delta_{N'N} + \frac{1}{12}\delta_{(N'+1)N}\right] \times\left[\frac{1}{12}\delta_{(r'-1)r} + \frac{10}{12}\delta_{r'r} + \frac{1}{12}\delta_{(r'+1)r}\right] \quad (97)$$

B.3. Scheme using the modified operators

B.3.1. Prediction scheme

The values within the large braces ‘‘()’’ in this and all schemes hereafter are computed only once and stored, and thus do not require evaluation at each time step. Intermediate variables, $s^1_{p'r'}$ and $s^3_{p'r'}$, need not to be stored for every p' and r' simultaneously. If the p'-loop is inside the r'-loop, $s^1_{p'r'}$ is stored only for the current r' and $s^3_{p'r'}$ is stored only for $r'-1$, r' and $r'+1$. We assume the most of the force term elements are zero, and ignore their addition operations for all FLOPS counting hereafter.

$$s^1_{p'r'} = c^{N'}_{(p'-1)r'} - c^{N'}_{p'r'}$$
$$s^3_{p'r'} = c^{N'}_{p'(r'-1)} - c^{N'}_{p'r'}$$
$$c^{N'+1}_{p'r'} = 2\,c^{N'}_{p'r'} - c^{N'-1}_{p'r'} + \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{-0}}{\Delta x^2}\right) \times s^1_{p'r'} - \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{+0}}{\Delta x^2}\right) \times s^1_{(p'+1)r'} + \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{0-}}{\Delta z^2}\right) \times s^3_{p'r'} - \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{0+}}{\Delta z^2}\right) \times s^3_{p'(r'+1)}$$
$$c^{N'+1}_{p'r'} \leftarrow c^{N'+1}_{p'r'} + \left(\frac{\Delta t^2}{\rho_{00}}\right) f^{N'}_{p'r'} \quad (98)$$

$\boxed{\text{4 muls, 8 adds}}$

B.3.2. Correction scheme

Intermediate variables, $a^*_{p'r'}$, $c^*_{p'r'}$, $s^{1*}_{p'r'}$, $s^{3*}_{p'r'}$, $s^{1**}_{p'r'}$ and $s^{3**}_{p'r'}$, need not to be stored for every p' and r' simultaneously.

$$a^*_{p'r'} = c^{N'+1}_{p'r'} - 2\,c^{N'}_{p'r'} + c^{N'-1}_{p'r'},$$
$$c^*_{p'r'} = a^*_{p'r'} + 12\,c^{N'}_{p'r'}$$
$$s^{1*}_{p'r'} = c^*_{(p'-1)r'} - c^*_{p'r'}, \quad s^{3*}_{p'r'} = c^*_{p'(r'-1)} - c^*_{p'r'}$$
$$s^{1**}_{p'r'} = s^{1*}_{p'(r'-1)} + 10\,s^{1*}_{p'r'} + s^{1*}_{(p'+1)(r'+1)},$$
$$s^{3**}_{p'r'} = s^{3*}_{(p'-1)r'} + 10\,s^{3*}_{p'r'} + s^{3*}_{(p'+1)r'}$$
$$c^{N'+1}_{p'r'} \leftarrow c^{N'+1}_{p'r'} + \left(-\frac{1}{144}\right) \times \left\{\left[a^*_{(p'-1)(r'-1)} + a^*_{(p'-1)(r'+1)} + a^*_{(p'+1)(r'-1)} + a^*_{(p'+1)(r'+1)}\right] + 10\left[a^*_{(p'-1)r'} + a^*_{p'(r'-1)} + a^*_{p'(r'+1)} + a^*_{(p'+1)r'}\right] + 100\,a^*_{p'r'}\right\} + \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{-0}}{144\Delta x^2}\right) \times s^{1**}_{p'r'} - \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{+0}}{144\Delta x^2}\right) \times s^{1**}_{(p'+1)r'} + \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{0-}}{144\Delta z^2}\right) \times s^{3**}_{p'r'} - \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{0+}}{144\Delta z^2}\right) \times s^{3**}_{p'(r'+1)}$$
$$c^{N'+1}_{p'r'} \leftarrow c^{N'+1}_{p'r'} + \left(\frac{\Delta t^2}{\rho_{00}}\right) f^{N'}_{p'r'} \quad (99)$$

$\boxed{\text{10 muls, 23 adds}}$

B.3.3. Required floating point operations

The required number of floating point operations for the conventional scheme (prediction scheme) is 4 muls and 8 adds. On the other hand, the required number of floating point operations for the modified scheme (prediction and correction scheme) is 14 muls and 31 adds in total. (We assume the source is very localized and ignore the addition operations for source term. If this assumption is not valid, 1 and 2 more addition operations are required for conventional and modified scheme respectively. However, the required FLOPS are not essentially changed.) Thus, modified scheme required 3.5 times muls and 3.9 times adds. Numerical experiments which are not shown in this paper show the required CPU time using modified scheme is about 2.9 times as much as the CPU time using the conventional scheme (The reason of difference of the ratios between FLOPS and actual CPU time has not been specified.) About 36 times improvement in accuracy can be obtained at the cost of 2.9 times CPU time, so the required CPU time of modified scheme is about $1/74$ to achieve the same accuracy compared to conventional scheme.

Appendix C. Explicit forms for heterogeneous 2-D P-SV problems

First, we show the explicit form of submatrices of modified operators appearing for P-SV case only (Eq. (54) for homogeneous case) for the heterogeneous medium using the stencils. We show the boundary elements also. Next, we show the total conventional and modified operators, and numerical scheme using these operators. We restrict non-boundary elements to show the required number of floating point operations clearly. Finally, we compare the number of floating point operators between our modified scheme and conventional scheme.

C.1. Submatrices of the modified operators

C.1.1. Non-boundary elements

First, we show the non-boundary elements of submatrices of modified operators. The explicit elements of $K^{(5)'}_{p'r'pr}$ for $p' \neq 1,\ N_x-1,\ N_x$ and $q' \neq 1,\ N_z-1,\ N_z$ are as follows:

$$
\mathbf{K}^{(5)'} = \left(\frac{1}{1728\Delta x\Delta z}\right)
\times
\begin{array}{|c|c|}
\hline
t+\Delta t &
\begin{array}{|c|cccc|}
\hline
z+2\Delta z & 5\lambda_{(p'-1)r'} & 3\lambda_{p'r'} & -9\lambda_{(p'+1)r'} & \lambda_{(p'+2)r'} \\
z+\Delta z & -45\lambda_{(p'-1)r'} & -27\lambda_{p'r'} & 81\lambda_{(p'+1)r'} & -9\lambda_{(p'+2)r'} \\
z & 15\lambda_{(p'-1)r'} & 9\lambda_{p'r'} & -27\lambda_{(p'+1)r'} & 3\lambda_{(p'+2)r'} \\
z-\Delta z & 25\lambda_{(p'-1)r'} & 15\lambda_{p'r'} & -45\lambda_{(p'+1)r'} & 5\lambda_{(p'+2)r'} \\
\hline
 & x-\Delta x & x & x+\Delta x & x+2\Delta x \\
\hline
\end{array} \\
\hline
t &
\begin{array}{|c|cccc|}
\hline
z+2\Delta z & 50\lambda_{(p'-1)r'} & 30\lambda_{p'r'} & -90\lambda_{(p'+1)r'} & 10\lambda_{(p'+2)r'} \\
z+\Delta z & -450\lambda_{(p'-1)r'} & -270\lambda_{p'r'} & 810\lambda_{(p'+1)r'} & -90\lambda_{(p'+2)r'} \\
z & 150\lambda_{(p'-1)r'} & 90\lambda_{p'r'} & -270\lambda_{(p'+1)r'} & 30\lambda_{(p'+2)r'} \\
z-\Delta z & 250\lambda_{(p'-1)r'} & 150\lambda_{p'r'} & -450\lambda_{(p'+1)r'} & 50\lambda_{(p'+2)r'} \\
\hline
 & x-\Delta x & x & x+\Delta x & x+2\Delta x \\
\hline
\end{array} \\
\hline
t-\Delta t &
\begin{array}{|c|cccc|}
\hline
z+2\Delta z & 5\lambda_{(p'-1)r'} & 3\lambda_{p'r'} & -9\lambda_{(p'+1)r'} & \lambda_{(p'+2)r'} \\
z+\Delta z & -45\lambda_{(p'-1)r'} & -27\lambda_{p'r'} & 81\lambda_{(p'+1)r'} & -9\lambda_{(p'+2)r'} \\
z & 15\lambda_{(p'-1)r'} & 9\lambda_{p'r'} & -27\lambda_{(p'+1)r'} & 3\lambda_{(p'+2)r'} \\
z-\Delta z & 25\lambda_{(p'-1)r'} & 15\lambda_{p'r'} & -45\lambda_{(p'+1)r'} & 5\lambda_{(p'+2)r'} \\
\hline
 & x-\Delta x & x & x+\Delta x & x+2\Delta x \\
\hline
\end{array} \\
\hline
\end{array}
\tag{100}
$$

C.1.2. Boundary elements

Because the explicit elements of $\mathbf{K}^{(5)\prime}$ is a little complex especially for boundary elements, we first express $\mathbf{K}^{(5)\prime}$ in a general form and define boundary elements as a special case. $\mathbf{K}^{(5)\prime}$ can be expressed as follows

$$K^{(5)\prime}_{p'r'N'prN} = H^{\alpha}_{p'p}\lambda_{pr'}H^{\beta}_{r'r}\left(\frac{1}{12}\delta_{(N'+1)N} + \frac{10}{12}\delta_{N'N} + \frac{1}{12}\delta_{(N'-1)N}\right), \tag{101}$$

where

$$\mathbf{H}^{\alpha} = \frac{1}{12\Delta x}\begin{bmatrix} 5 & 8 & -1 & & & \\ -5 & -3 & 9 & -1 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & -5 & -3 & 9 & -1 \\ & & & -5 & -3 & 8 \\ & & & & -5 & -7 \end{bmatrix}. \tag{102}$$

$$\mathbf{H}^{\beta} = \frac{1}{12\Delta z}\begin{bmatrix} -7 & 8 & -1 & & & \\ -5 & -3 & 9 & -1 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & -5 & -3 & 9 & -1 \\ & & & -5 & -3 & 8 \\ & & & & -5 & 5 \end{bmatrix}. \tag{103}$$

$\mathbf{H}^{\alpha}$ and $\mathbf{H}^{\beta}$ are $N_x \times N_x$ and $N_z \times N_z$ matrices, respectively. Summation rule for repeated indicesis not applied in r.h.s. of Eq. (101).

Every boundary elements are defined by Eqs. (101)–(103), so we just show one example. The explicit elements for $p' = 1$ and $r' \neq 1,\ N_z - 1,\ N_z$ case is as follows:

$$\mathbf{K}^{(5)\prime} = \left(\frac{1}{1728\Delta x\Delta z}\right)$$

$$\times \begin{array}{|c|c|}\hline t+\Delta t & \begin{array}{|c|ccc|} z+2\Delta z & -5\lambda_{p'r'} & -8\lambda_{(p'+1)r'} & \lambda_{(p'+2)r'} \\ z+\Delta z & 45\lambda_{p'r'} & 72\lambda_{(p'+1)r'} & -9\lambda_{(p'+2)r'} \\ z & -15\lambda_{p'r'} & -24\lambda_{(p'+1)r'} & 3\lambda_{(p'+2)r'} \\ z-\Delta z & -25\lambda_{p'r'} & -40\lambda_{(p'+1)r'} & 5\lambda_{(p'+2)r'} \\ \hline & x & x+\Delta x & x+2\Delta x \\ \hline \end{array} \\ \hline t & \begin{array}{|c|ccc|} z+2\Delta z & -50\lambda_{p'r'} & -80\lambda_{(p'+1)r'} & 10\lambda_{(p'+2)r'} \\ z+\Delta z & 450\lambda_{p'r'} & 720\lambda_{(p'+1)r'} & -90\lambda_{(p'+2)r'} \\ z & -150\lambda_{p'r'} & -240\lambda_{(p'+1)r'} & 30\lambda_{(p'+2)r'} \\ z-\Delta z & -250\lambda_{p'r'} & -400\lambda_{(p'+1)r'} & 50\lambda_{(p'+2)r'} \\ \hline & x & x+\Delta x & x+2\Delta x \\ \hline \end{array} \\ \hline t-\Delta t & \begin{array}{|c|ccc|} z+2\Delta z & -5\lambda_{p'r'} & -8\lambda_{(p'+1)r'} & \lambda_{(p'+2)r'} \\ z+\Delta z & 45\lambda_{p'r'} & 72\lambda_{(p'+1)r'} & -9\lambda_{(p'+2)r'} \\ z & -15\lambda_{p'r'} & -24\lambda_{(p'+1)r'} & 3\lambda_{(p'+2)r'} \\ z-\Delta z & -25\lambda_{p'r'} & -40\lambda_{(p'+1)r'} & 5\lambda_{(p'+2)r'} \\ \hline & x & x+\Delta x & x+2\Delta x \\ \hline \end{array} \\ \hline \end{array} \tag{104}$$

C.2. Modified / conventional operators (non-boundary elements)

$$A_{p'r'N'\gamma'prN\gamma} = \frac{\delta_{p'p}\delta_{r'r}\delta_{\gamma'\gamma}}{\Delta t^2}\rho_{00}\left[\delta_{(N'+1)N} - 2\delta_{N'N} + \delta_{(N'-1)N}\right]$$

$$\begin{aligned} K_{p'r'N'1prN1} &= \frac{\delta_{p'p}\delta_{N'N}}{\Delta z^2}\left[\mu_{0-}\left(\delta_{(r'-1)r} - \delta_{r'r}\right) + \mu_{0+}\left(-\delta_{r'r} + \delta_{(r'+1)r}\right)\right] \\ &\quad + \frac{\delta_{r'r}\delta_{N'N}}{\Delta x^2}\left[(\lambda+2\mu)_{-0}\left(\delta_{(p'-1)p} - \delta_{p'p}\right) + (\lambda+2\mu)_{+0}\left(-\delta_{p'p} + \delta_{(p'+1)p}\right)\right] \end{aligned}$$

$$\begin{aligned} K_{p'r'N'3prN3} &= \frac{\delta_{r'r}\delta_{N'N}}{\Delta x^2}\left[\mu_{-0}\left(\delta_{(p'-1)p} - \delta_{p'p}\right) + \mu_{+0}\left(-\delta_{p'p} + \delta_{(p'+1)p}\right)\right] \\ &\quad + \frac{\delta_{p'p}\delta_{N'N}}{\Delta z^2}\left[(\lambda+2\mu)_{0-}\left(\delta_{(r'-1)r} - \delta_{r'r}\right) + (\lambda+2\mu)_{0+}\left(-\delta_{r'r} + \delta_{(r'+1)r}\right)\right] \end{aligned}$$

$$\begin{aligned} K_{p'r'N'1prN3} &= \frac{\delta_{N'N}}{\Delta x \Delta z}\left[-\frac{\lambda_{(p'-1)r'}}{2}\delta_{(p'-1)p} + \frac{\lambda_{(p'+1)r'}}{2}\delta_{(p'+1)p}\right] \times \left[-\frac{1}{2}\delta_{(r'-1)r} + \frac{1}{2}\delta_{(r'+1)r}\right] \\ &\quad + \frac{\delta_{N'N}}{\Delta x \Delta z}\left[-\frac{\mu_{p'(r'-1)}}{2}\delta_{(r'-1)r} + \frac{\mu_{p'(r'+1)}}{2}\delta_{(r'+1)r}\right] \times \left[-\frac{1}{2}\delta_{(p'-1)p} + \frac{1}{2}\delta_{(p'+1)p}\right] \end{aligned}$$

$$\begin{aligned} K_{p'r'N'3prN1} &= \frac{\delta_{N'N}}{\Delta x \Delta z}\left[-\frac{\mu_{(p'-1)r'}}{2}\delta_{(p'-1)p} + \frac{\mu_{(p'+1)r'}}{2}\delta_{(p'+1)p}\right] \times \left[-\frac{1}{2}\delta_{(r'-1)r} + \frac{1}{2}\delta_{(r'+1)r}\right] \\ &\quad + \frac{\delta_{N'N}}{\Delta x \Delta z}\left[-\frac{\lambda_{p'(r'-1)}}{2}\delta_{(r'-1)r} + \frac{\lambda_{p'(r'+1)}}{2}\delta_{(r'+1)r}\right] \times \left[-\frac{1}{2}\delta_{(p'-1)p} + \frac{1}{2}\delta_{(p'+1)p}\right] \end{aligned} \tag{105}$$

$$\begin{aligned} A'_{p'r'N'\gamma'prN\gamma} &= \frac{\delta_{\gamma'\gamma}}{\Delta t^2}\rho_{00}\left[\delta_{(N'+1)N} - 2\delta_{N'N} + \delta_{(N'-1)N}\right] \\ &\quad \times \left[\frac{1}{12}\delta_{(p'-1)p} + \frac{10}{12}\delta_{p'p} + \frac{1}{12}\delta_{(p'+1)p}\right] \times \left[\frac{1}{12}\delta_{(r'-1)r} + \frac{10}{12}\delta_{r'r} + \frac{1}{12}\delta_{(r'+1)r}\right] \end{aligned}$$

$$\begin{aligned} K'_{p'r'N'1prN1} &= \frac{1}{\Delta z^2}\left[\mu_{0-}\left(\delta_{(r'-1)r} - \delta_{r'r}\right) + \mu_{0+}\left(-\delta_{r'r} + \delta_{(r'+1)r}\right)\right] \\ &\quad \times \left[\frac{1}{12}\delta_{(p'-1)p} + \frac{10}{12}\delta_{p'p} + \frac{1}{12}\delta_{(p'+1)p}\right] \times \left[\frac{1}{12}\delta_{(N'-1)N} + \frac{10}{12}\delta_{N'N} + \frac{1}{12}\delta_{(N'+1)N}\right] \\ &\quad + \frac{1}{\Delta x^2}\left[(\lambda+2\mu)_{-0}\left(\delta_{(p'-1)p} - \delta_{p'p}\right) + (\lambda+2\mu)_{+0}\left(-\delta_{p'p} + \delta_{(p'+1)p}\right)\right] \\ &\quad \times \left[\frac{1}{12}\delta_{(r'-1)r} + \frac{10}{12}\delta_{r'r} + \frac{1}{12}\delta_{(r'+1)r}\right] \times \left[\frac{1}{12}\delta_{(N'-1)N} + \frac{10}{12}\delta_{N'N} + \frac{1}{12}\delta_{(N'+1)N}\right] \end{aligned}$$

$$
\begin{aligned}
K'_{p'r'N'3prN3}
&= \frac{1}{\Delta x^2}\Big[\mu_{-0}\big(\delta_{(p'-1)p}-\delta_{p'p}\big)\\
&\quad+\mu_{+0}\big(-\delta_{p'p}+\delta_{(p'+1)p}\big)\Big]\\
&\quad\times\left[\frac{1}{12}\delta_{(r'-1)r}+\frac{10}{12}\delta_{r'r}+\frac{1}{12}\delta_{(r'+1)r}\right]\\
&\quad\times\left[\frac{1}{12}\delta_{(N'-1)N}+\frac{10}{12}\delta_{N'N}+\frac{1}{12}\delta_{(N'+1)N}\right]\\
&\quad+\frac{1}{\Delta z^2}\Big[(\lambda+2\mu)_{0-}\big(\delta_{(r'-1)r}-\delta_{r'r}\big)\\
&\quad+(\lambda+2\mu)_{0+}\big(-\delta_{r'r}+\delta_{(r'+1)r}\big)\Big]\\
&\quad\times\left[\frac{1}{12}\delta_{(p'-1)p}+\frac{10}{12}\delta_{p'p}+\frac{1}{12}\delta_{(p'+1)p}\right]\\
&\quad\times\left[\frac{1}{12}\delta_{(N'-1)N}+\frac{10}{12}\delta_{N'N}+\frac{1}{12}\delta_{(N'+1)N}\right]\\
K'_{p'r'N'1prN3}
&= \frac{1}{\Delta x\Delta z}\times\left[-\frac{5\lambda_{(p'-1)r'}}{12}\delta_{(p'-1)p}\right.\\
&\quad-\frac{3\lambda_{p'r'}}{12}\delta_{p'p}+\frac{9\lambda_{(p'+1)r'}}{12}\delta_{(p'+1)p}\\
&\quad\left.-\frac{\lambda_{(p'+2)r'}}{12}\delta_{(p'+2)p}\right]\\
&\quad\times\left[-\frac{5}{12}\delta_{(r'-1)r}-\frac{3}{12}\delta_{r'r}\right.\\
&\quad\left.+\frac{9}{12}\delta_{(r'+1)r}-\frac{1}{12}\delta_{(r'+2)r}\right]\\
&\quad\times\left[\frac{1}{12}\delta_{(N'-1)N}+\frac{10}{12}\delta_{N'N}+\frac{1}{12}\delta_{(N'+1)N}\right]\\
&\quad+\frac{1}{\Delta x\Delta z}\times\left[\frac{\mu_{p'(r'-2)}}{12}\delta_{(r'-2)r}\right.\\
&\quad-\frac{9\mu_{p'(r'-1)}}{12}\delta_{(r'-1)r}\\
&\quad\left.+\frac{3\mu_{p'r'}}{12}\delta_{rr}+\frac{5\mu_{p'(r'+1)}}{12}\delta_{(r'+1)r}\right]\\
&\quad\times\left[\frac{1}{12}\delta_{(p'-2)p}-\frac{9}{12}\delta_{(p'-1)p}\right.\\
&\quad\left.+\frac{3}{12}\delta_{p'p}+\frac{5}{12}\delta_{(p'+1)p}\right]\\
&\quad\times\left[\frac{1}{12}\delta_{(N'-1)N}+\frac{10}{12}\delta_{N'N}+\frac{1}{12}\delta_{(N'+1)N}\right]\\
K'_{p'r'N'3prN1}
&= \frac{1}{\Delta x\Delta z}\times\left[-\frac{5\mu_{(p'-1)r'}}{12}\delta_{(p'-1)p}\right.\\
&\quad-\frac{3\mu_{p'r'}}{12}\delta_{p'p}+\frac{9\mu_{(p'+1)r'}}{12}\delta_{(p'+1)p}\\
&\quad\left.-\frac{\mu_{(p'+2)r'}}{12}\delta_{(p'+2)p}\right]\\
&\quad\times\left[-\frac{5}{12}\delta_{(r'-1)r}-\frac{3}{12}\delta_{r'r}\right.\\
&\quad\left.+\frac{9}{12}\delta_{(r'+1)r}-\frac{1}{12}\delta_{(r'+2)r}\right]\\
&\quad\times\left[\frac{1}{12}\delta_{(N'-1)N}+\frac{10}{12}\delta_{N'N}+\frac{1}{12}\delta_{(N'+1)N}\right]\\
&\quad+\frac{1}{\Delta x\Delta z}\times\left[\frac{\lambda_{p'(r'-2)}}{12}\delta_{(r'-2)r}\right.\\
&\quad-\frac{9\lambda_{p'(r'-1)}}{12}\delta_{(r'-1)r}+\frac{3\lambda_{p'r'}}{12}\delta_{r'r}\\
&\quad\left.+\frac{5\lambda_{p'(r'+1)}}{12}\delta_{(r'+1)r}\right]\\
&\quad\times\left[\frac{1}{12}\delta_{(p'-2)p}-\frac{9}{12}\delta_{(p'-1)p}\right.\\
&\quad\left.+\frac{3}{12}\delta_{p'p}+\frac{5}{12}\delta_{(p'+1)p}\right]\\
&\quad\times\left[\frac{1}{12}\delta_{(N'-1)N}+\frac{10}{12}\delta_{N'N}+\frac{1}{12}\delta_{(N'+1)N}\right]
\end{aligned}
\tag{106}
$$

C.3. Scheme using the modified operators

C.3.1. Prediction scheme

The values within large braces ‘‘()’’ are computed only once and stored, and thus do not require evaluation at each time step. Intermediate variables, $s^{11}_{p'r'}$, $s^{13}_{p'r'}$, $s^{31}_{p'r'}$, $s^{33}_{p'r'}$, $t^{11}_{p'r'}$, $t^{13}_{p'r'}$, $t^{31}_{p'r'}$ and $t^{33}_{p'r'}$, need not to be stored for every p' and r' simultaneously. If the p'-loop is inside the r'-loop, $s^{11}_{p'r'}$ is stored only for the current r' and $s^{11}_{p'r'}$ is stored only for $r'-2$, $r'-1$, r' and $r'+1$, for example.

$$s^{11}_{p'r'} = c_{(p'-1)r'1} - c_{p'r'1}, \quad s^{13}_{p'r'} = c_{p'(r'-1)1} - c_{p'r'1}$$

$$s^{31}_{p'r'} = c_{(p'-1)r'3} - c_{p'r'3}, \quad s^{33}_{p'r'} = c_{p'(r'-1)3} - c_{p'r'3}$$

$$t^{11}_{p'r'} = c_{(p'+1)r'1} - c_{(p'-1)r'1},$$

$$t^{13}_{p'r'} = c_{p'(r'+1)1} - c_{p'(r'-1)1}$$

$$t^{31}_{p'r'} = c_{(p'+1)r'3} - c_{(p'-1)r'3},$$

$$t^{33}_{p'r'} = c_{p'(r'+1)3} - c_{p'(r'-1)3}$$

$$\begin{aligned}
c^{N'+1}_{p'r'1} &= 2c^{N'}_{p'r'1} - c^{N'-1}_{p'r'1} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}}\frac{(\lambda+2\mu)_{-0}}{\Delta x^2}\right)\times s^{11}_{p'r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}}\frac{(\lambda+2\mu)_{+0}}{\Delta x^2}\right)\times s^{11}_{(p'+1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{0-}}{\Delta z^2}\right)\times s^{13}_{p'r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{0+}}{\Delta z^2}\right)\times s^{13}_{p'(r'+1)} \\
&- \left(\frac{\Delta t^2}{\rho_{00}}\frac{\lambda_{(p'-1)r'}}{4\Delta x\Delta z}\right)\times t^{33}_{(p'-1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}}\frac{\lambda_{(p'+1)r'}}{4\Delta x\Delta z}\right)\times t^{33}_{(p'+1)r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{p'(r'-1)}}{4\Delta x\Delta z}\right)\times t^{31}_{p'(r'-1)} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{p'(r'+1)}}{4\Delta x\Delta z}\right)\times t^{31}_{p'(r'-1)}
\end{aligned}$$

$$c^{N'+1}_{p'r'1} \leftarrow c^{N'+1}_{p'r'1} + \left(\frac{\Delta t^2}{\rho_{00}}\right) f^{N'}_{p'r'1} \tag{107}$$

$$\begin{aligned}
c^{N'+1}_{p'r'3} &= 2c^{N'}_{p'r'3} - c^{N'-1}_{p'r'3} + \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{-0}}{\Delta x^2}\right)\times s^{31}_{p'r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{+0}}{\Delta x^2}\right)\times s^{31}_{(p'+1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}}\frac{(\lambda+2\mu)_{0-}}{\Delta z^2}\right)\times s^{33}_{p'r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}}\frac{(\lambda+2\mu)_{0+}}{\Delta z^2}\right)\times s^{33}_{p'(r'+1)} \\
&- \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{(p'-1)r'}}{4\Delta x\Delta z}\right)\times t^{13}_{(p'-1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}}\frac{\mu_{(p'+1)r'}}{4\Delta x\Delta z}\right)\times t^{13}_{(p'+1)r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}}\frac{\lambda_{p'(r'-1)}}{4\Delta x\Delta z}\right)\times t^{11}_{p'(r'-1)} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}}\frac{\lambda_{p'(r'+1)}}{4\Delta x\Delta z}\right)\times t^{11}_{p'(r'+1)}
\end{aligned}$$

$$c^{N'+1}_{p'r'1} \leftarrow c^{N'+1}_{p'r'1} + \left(\frac{\Delta t^2}{\rho_{00}}\right) f^{N'}_{p'r'1} \tag{108}$$

$$\boxed{\text{16 muls and 28 adds}}$$

C.3.2. Correction scheme

$$a^{*}_{p'r'1} = c^{N'+1}_{p'r'1} - 2c^{N'}_{p'r'1} + c^{N'-1}_{p'r'1},$$

$$a^{*}_{p'r'3} = c^{N'+1}_{p'r'3} - 2c^{N'}_{p'r'3} + c^{N'-1}_{p'r'3}$$

$$c^{*}_{p'r'1} = a^{*}_{p'r'1} + 12c^{N}_{p'r'1}, \quad c^{*}_{p'r'3} = a^{*}_{p'r'3} + 12c^{N}_{p'r'3}$$

$$s^{11*}_{p'r'} = c^{*}_{(p'-1)r'1} - c^{*}_{p'r'1}, \quad s^{13*}_{p'r'} = c^{*}_{p'(r'-1)1} - c^{*}_{p'r'1}$$

$$s^{31*}_{p'r'} = c^{*}_{(p'-1)r'3} - c^{*}_{p'r'3}, \quad s^{33*}_{p'r'} = c^{*}_{p'(r'-1)3} - c^{*}_{p'r'3}$$

$$t^{11*}_{p'r'} = s^{11*}_{(p'-1)r'} - 8s^{11*}_{p'r'} - 5s^{11*}_{(p'+1)r'}$$

$$t^{13*}_{p'r'} = -5s^{13*}_{p'r'} - 8s^{13*}_{p'(r'+1)} + s^{13*}_{p'(r'+2)}$$

$$t^{31*}_{p'r'} = s^{31*}_{(p'-1)r'} - 8s^{31*}_{p'r'} - 5s^{31*}_{(p'+1)r'}$$

$$t^{33*}_{p'r'} = -5s^{33*}_{p'r'} - 8s^{33*}_{p'(r'+1)} + s^{33*}_{p'(r'+2)}$$

$$
\begin{aligned}
c^{N'+1}_{p'r'1} \leftarrow c^{N'+1}_{p'r'1} &+ \left(-\frac{1}{144}\right) \\
&\times \Big\{ \left[a^{*}_{(p'-1)(r'-1)1} + a^{*}_{(p'-1)(r'+1)1} \right.\\
&\left. + a^{*}_{(p'+1)(r'-1)1} + a^{*}_{(p'+1)(r'+1)1} \right] \\
&+ 10\left[a^{*}_{(p'-1)r'1} + a^{*}_{p'(r'-1)1} + a^{*}_{p'(r'+1)1} \right.\\
&\left. + a^{*}_{(p'+1)r'1} \right] + 100\, a^{**}_{p'r'1} \Big\} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{(\lambda + 2\mu)_{-0}}{144 \Delta x^2} \right) \times s^{11**}_{p'r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}} \frac{(\lambda + 2\mu)_{+0}}{144 \Delta x^2} \right) \times s^{11**}_{(p'+1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{\mu_{0-}}{144 \Delta z^2} \right) \times s^{13**}_{p'r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}} \frac{\mu_{0+}}{144 \Delta z^2} \right) \times s^{13**}_{p'(r'+1)} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{-5\lambda_{(p'-1)r'}}{1728 \Delta x \Delta z} \right) \times t^{33*}_{(p'-1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{-3\lambda_{p'r'}}{1728 \Delta x \Delta z} \right) \times t^{33*}_{p'r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{9\lambda_{(p'+1)r'}}{1728 \Delta x \Delta z} \right) \times t^{33*}_{(p'+1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{-\lambda_{(p'+2)r'}}{1728 \Delta x \Delta z} \right) \times t^{*}_{(p'+2)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{\mu_{p'(r'-2)}}{1728 \Delta x \Delta z} \right) \times t^{31*}_{p'(r'-2)} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{-9\mu_{p'(r'-1)}}{1728 \Delta x \Delta z} \right) \times t^{31*}_{p'(r'-1)} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{3\mu_{p'r'}}{1728 \Delta x \Delta z} \right) \times t^{31*}_{p'r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{5\mu_{p'(r'+1)}}{1728 \Delta x \Delta z} \right) \times t^{31*}_{p'(r'+1)} \\
c^{N'+1}_{p'r'1} \leftarrow c^{N'+1}_{p'r'1} &+ \frac{\Delta t^2}{\rho_{00}} f^{N'}_{p'r'1}
\end{aligned}
\tag{109}
$$

$$
\begin{aligned}
c^{N'+1}_{p'r'3} \leftarrow c^{N'+1}_{p'r'3} &+ \left(-\frac{1}{144}\right) \\
&\times \Big\{ \left[a^{*}_{(p'-1)(r'-1)3} + a^{*}_{(p'-1)(r'+1)3} \right.\\
&\left. + a^{*}_{(p'+1)(r'-1)3} + a^{*}_{(p'+1)(r'+1)3} \right] \\
&+ 10\left[a^{*}_{(p'-1)r'3} + a^{*}_{p'(r'-1)3} + a^{*}_{p'(r'+1)3} \right.\\
&\left. + a^{*}_{(p'+1)r'3} \right] + 100\, a^{*}_{p'r'3} \Big\} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{\mu_{-0}}{144 \Delta x^2} \right) \times s^{31**}_{p'r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}} \frac{2\mu_{+0}}{144 \Delta x^2} \right) \times s^{31**}_{(p'+1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{(\lambda + 2\mu)_{0-}}{144 \Delta z^2} \right) \times s^{33**}_{p'r'} \\
&- \left(\frac{\Delta t^2}{\rho_{00}} \frac{(\lambda + 2\mu)_{0+}}{144 \Delta z^2} \right) \times s^{33**}_{p'(r'+1)} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{-5\mu_{(p'-1)r'}}{1728 \Delta x \Delta z} \right) \times t^{13*}_{(p'-1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{-3\mu_{p'r'}}{1728 \Delta x \Delta z} \right) \times t^{13*}_{p'r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{9\mu_{(p'+1)r'}}{1728 \Delta x \Delta z} \right) \times t^{13*}_{(p'+1)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{-\mu_{(p'+2)r'}}{1728 \Delta x \Delta z} \right) \times t^{13*}_{(p'+2)r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{\lambda_{p'(r'-2)}}{1728 \Delta x \Delta z} \right) \times t^{11*}_{p'(r'-2)} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{-9\lambda_{p'(r'-1)}}{1728 \Delta x \Delta z} \right) \times t^{11*}_{p'(r'-1)} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{3\lambda_{p'r'}}{1728 \Delta x \Delta z} \right) \times t^{11*}_{p'r'} \\
&+ \left(\frac{\Delta t^2}{\rho_{00}} \frac{5\lambda_{p'(r'+1)}}{1728 \Delta x \Delta z} \right) \times t^{11*}_{p'(r'+1)} \\
c^{N'+1}_{p'r'3} \leftarrow c^{N'+1}_{p'r'3} &+ \left(\frac{\Delta t^2}{\rho_{00}} \right) f^{N'}_{p'r'3}
\end{aligned}
\tag{110}
$$

$\boxed{\text{40 muls and 62 adds}}$

C.3.3. Required floating point operations

The required number of floating point operations for the conventional scheme (prediction scheme) is 16 muls and 28 adds. On the other hand, the required number of floating point operations for the modified scheme (prediction and correction scheme) is 56 muls and 90 adds in total. (We assume the source is very localized and ignore the addition operations for source term. If this assumption is not valid, 2 and 4 more addition operations are required for conventional and modified scheme respectively. However, the required FLOPS are not essentially changed.) Thus, modified scheme required 3.5 times muls and 3.2 times adds. Numerical experiments show the required CPU time using modified scheme is about 3.5 times as much as the CPU time using the conventional scheme. About 30 times improvement in accuracy can be obtained at the cost of 3.5 times CPU time, so the required CPU time for the modified scheme is about $1/47$ of that required by the conventional scheme to achieve any given accuracy.

Appendix D. Heterogeneous 3-D problem

Our method can be extended to a general 3-D heterogeneous medium. Here, we show a part of the modified operators. The others can be defined in a similar fashion. We have not yet used these operators in actual computations, but there should be no special difficulty.

$$
\begin{aligned}
&A'_{p'q'r'N'\gamma pqrN\gamma} \\
&= \frac{\delta_{\gamma'\gamma}}{\Delta t^2}\rho_{000}\left[\delta_{(N'+1)N} - 2\delta_{N'N} + \delta_{(N'-1)N}\right] \\
&\quad\times\left[\frac{1}{12}\delta_{(p'-1)p} + \frac{10}{12}\delta_{p'p} + \frac{1}{12}\delta_{(p'+1)p}\right] \\
&\quad\times\left[\frac{1}{12}\delta_{(q'-1)q} + \frac{10}{12}\delta_{q'q} + \frac{1}{12}\delta_{(q'+1)q}\right] \\
&\quad\times\left[\frac{1}{12}\delta_{(r'-1)r} + \frac{10}{12}\delta_{r'r} + \frac{1}{12}\delta_{(r'+1)r}\right]
\end{aligned}
$$

$$
\begin{aligned}
&K'_{p'q'r'N'1pqrN1} \\
&= \frac{1}{\Delta x^2}\Big[(\lambda+2\mu)_{-00}\big(\delta_{(p'-1)p} - \delta_{p'p}\big) \\
&\quad + (\lambda+2\mu)_{000}\big(-\delta_{p'p} + \delta_{(p'+1)p}\big)\Big] \\
&\quad\times\left[\frac{1}{12}\delta_{(q'-1)q} + \frac{10}{12}\delta_{q'q} + \frac{1}{12}\delta_{(q'+1)q}\right] \\
&\quad\times\left[\frac{1}{12}\delta_{(r'-1)r} + \frac{10}{12}\delta_{r'r} + \frac{1}{12}\delta_{(r'+1)r}\right] \\
&\quad\times\left[\frac{1}{12}\delta_{(N'-1)N} + \frac{10}{12}\delta_{N'N} + \frac{1}{12}\delta_{(N'+1)N}\right] \\
&\quad + \frac{1}{\Delta y^2}\Big[\mu_{0-0}\big(\delta_{(q'-1)q} - \delta_{q'p}\big) \\
&\quad + \mu_{0+0}\big(-\delta_{q'q} + \delta_{(q'+1)q}\big)\Big] \\
&\quad\times\left[\frac{1}{12}\delta_{(p'-1)p} + \frac{10}{12}\delta_{p'p} + \frac{1}{12}\delta_{(p'+1)p}\right] \\
&\quad\times\left[\frac{1}{12}\delta_{(r'-1)r} + \frac{10}{12}\delta_{r'r} + \frac{1}{12}\delta_{(r'+1)r}\right] \\
&\quad\times\left[\frac{1}{12}\delta_{(N'-1)N} + \frac{10}{12}\delta_{N'N} + \frac{1}{12}\delta_{(N'+1)N}\right] \\
&\quad + \frac{1}{\Delta z^2}\Big[\mu_{00-}\big(\delta_{(r'-1)r} - \delta_{r'r}\big) \\
&\quad + \mu_{00+}\big(-\delta_{r'r} + \delta_{(r'+1)r}\big)\Big] \\
&\quad\times\left[\frac{1}{12}\delta_{(p'-1)p} + \frac{10}{12}\delta_{p'p} + \frac{1}{12}\delta_{(p'+1)p}\right] \\
&\quad\times\left[\frac{1}{12}\delta_{(r'-1)r} + \frac{10}{12}\delta_{r'r} + \frac{1}{12}\delta_{(r'+1)r}\right] \\
&\quad\times\left[\frac{1}{12}\delta_{(N'-1)N} + \frac{10}{12}\delta_{N'N} + \frac{1}{12}\delta_{(N'+1)N}\right]
\end{aligned}
$$

$$
\begin{aligned}
&K'_{p'q'r'N'1pqrN2} \\
&= \frac{1}{\Delta x \Delta y}\times\Bigg[-\frac{5\lambda_{(p'-1)q'r'}}{12}\delta_{(p'-1)p'} \\
&\quad - \frac{3\lambda_{p'q'r'}}{12}\delta_{p'p} + \frac{9\lambda_{(p'+1)q'r'}}{12}\delta_{(p'+1)p} \\
&\quad - \frac{\lambda_{(p'+2)q'r'}}{12}\delta_{(p'+2)p}\Bigg]
\end{aligned}
$$

$$\times\left[-\frac{5}{12}\delta_{(q'-1)q}-\frac{3}{12}\delta_{q'q}+\frac{9}{12}\delta_{(q'+1)'q}-\frac{1}{12}\delta_{(q'+2)'q}\right]\times\left[\frac{1}{12}\delta_{(r'-1)r}+\frac{10}{12}\delta_{r'r}+\frac{1}{12}\delta_{(r'+1)r}\right]\times\left[\frac{1}{12}\delta_{(N'-1)N}+\frac{10}{12}\delta_{N'N}+\frac{1}{12}\delta_{(N'+1)N}\right]+\frac{1}{\Delta x\Delta y}\times\left[\frac{\mu_{p'(q'-2)r'}}{12}\delta_{(q'-2)q}-\frac{9\mu_{p'(q'-1)r'}}{12}\delta_{(q'-1)q}+\frac{3\mu_{p'q'r'}}{12}\delta_{q'q}+\frac{5\mu_{p'(q'+1)r'}}{12}\delta_{(q'+1)q}\right]\times\left[\frac{1}{12}\delta_{(p'-2)p}-\frac{9}{12}\delta_{(p'-1)p}+\frac{3}{12}\delta_{p'p}+\frac{5}{12}\delta_{(p'+1)p}\right]\times\left[\frac{1}{12}\delta_{(r'-1)r}-\frac{10}{12}\delta_{r'r}+\frac{1}{12}\delta_{(r'+1)r}\right]\times\left[\frac{1}{12}\delta_{(N'-1)N}+\frac{10}{12}\delta_{N'N}+\frac{1}{12}\delta_{(N'+1)N}\right]\tag{111}$$

D.1. Required floating point operations

We have not counted the number of floating point operations required for the 3-D heterogeneous problem, but we can make a rough estimate. For 1-D problems, our modified scheme required about 2 times as many floating point operations (or CPU time) as the conventional scheme (Geller and Takeuchi, 1998). For 2-D problems, we showed above that the required floating point operations (or CPU time) is about 3.5 times that of the conventional scheme. Because the ratio of required floating point operations will linearly increase as the dimension of the problem increases, the required CPU time will be about 5–8 times for the 3-D problem. On the other hand, the improvement in the accuracy will be independent of the dimension of the problems, and about 30 times improvement can be expected for 3-D problems. The solution error is proportional to the square of the grid spacing, and the required CPU time for 3-D problem is proportional to the fourth power of the number of grid intervals. This means that the required CPU time using the modified scheme is between $(30^{4/2}/5)$ and $(30^{4/2}/8)$, or roughly $1/100$ of that required by the conventional operators to achieve the same order accuracy for 3-D problems.

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