

# Optimally accurate second-order time-domain finite difference scheme for the elastic equation of motion: one-dimensional case

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## SUMMARY

We previously derived a general criterion for optimally accurate numerical operators for the calculation of synthetic seismograms in the frequency domain (Geller & Takeuchi 1995). We then derived modified operators for the Direct Solution Method (DSM) (Geller & Ohminato 1994) which satisfy this general criterion, thereby yielding significantly more accurate synthetics (for any given numerical grid spacing) without increasing the computational requirements (Cummins *et al.* 1994; Takeuchi, Geller & Cummins 1996; Cummins, Takeuchi & Geller 1997). In this paper, we derive optimally accurate time-domain finite difference (FD) operators which are second order in space and time using a similar approach. As our FD operators are local, our algorithm is well suited to massively parallel computers. Our approach can be extended to other methods (e.g. pseudo-spectral) for solving the elastic equation of motion. It might also be possible to extend this approach to equations other than the elastic equation of motion, including non-linear equations.

**Key words:** finite difference method, synthetic seismograms.

## 1 INTRODUCTION

Waveform inversion (e.g. Tarantola 1984; Geller & Hara 1993) is a promising approach for determining 3-D Earth structure, as it directly uses all of the information in the recorded seismograms. Practical applications of waveform inversion require efficient methods for computing synthetic seismograms. It is also important to be able to quantify the accuracy of the synthetics. Reliable advance estimates of the accuracy that will be attained for a given numerical scheme and grid size are particularly desirable.

Standard techniques of numerical analysis provide estimates of the error of discretized numerical operators rather than the error of the numerical solutions (i.e. synthetic seismograms) computed using these operators. For example, the error of the three-point central finite difference (FD) operator for the second derivative is well known to be the second term of the following Taylor series:

$$\frac{1}{\Delta z^2} [u(z - \Delta z) - 2u(z) + u(z + \Delta z)] = \frac{d^2 u}{dz^2} + \frac{\Delta z^2}{12} \frac{d^4 u}{dz^4} + \dots \quad (1)$$

The error of synthetic seismograms computed by schemes based on eq. (1) will thus also be proportional to  $\Delta z^2$ . However, this information is of little practical value unless the coefficient of  $\Delta z^2$  is also known.

Geller & Takeuchi (1995), cited hereafter as GT95, developed a method that uses an eigenfunction expansion to make formal estimates of the error of synthetic seismograms computed using a given numerical scheme. Their results allow numerical operators to be ‘tuned’ to produce optimally accurate numerical schemes of a given type and order. GT95 obtained the following estimate of the relative error of synthetics computed using an optimally accurate 1-D second-order FD scheme in the frequency domain:

$$\text{relative error} \approx \frac{k_z^2 \Delta z^2}{12}, \quad (2)$$

where  $k_z$  is the  $z$ -component of the wavenumber. Eq. (2) is almost exact for a homogeneous medium with a uniform grid spacing, and is a good approximation for a heterogeneous medium or a non-uniform grid spacing.

Numerical schemes of a given order are not generically equivalent. The new  $O(\Delta z^2, \Delta t^2)$  FD scheme presented in this paper attains almost two orders of magnitude greater accuracy than the conventional  $O(\Delta z^2, \Delta t^2)$  FD scheme, while requiring only twice as

much CPU time. Many other numerical schemes for computing synthetics, e.g. fourth-order FD in space and second-order FD in time (Levander 1988) or pseudo-spectral in space and second-order FD in time (Fornberg 1987), have also been presented. Mizutani, Geller & Takeuchi (1997) used basically the same method that we present in this paper to derive an optimally accurate scheme that is pseudo-spectral in space and second-order FD in time.

The question which method is the best for a given problem involves not only CPU time, but also memory requirements and parallelization, and is beyond the scope of this paper. Also, optimally accurate algorithms should be derived for each type of scheme before comparisons are made.

In this paper we derive modified time-domain FD operators using the results of GT95. The modified FD operators lead to an implicit scheme; that is, the solution of a set of simultaneous linear equations is required at each time step to obtain the displacements at the next time step. To obviate this time-consuming computation, we approximate the implicit scheme by a two-part explicit ('predictor–corrector') scheme. We present results for the 1-D case in this paper. Results for 2-D and 3-D cases in Cartesian and curvilinear coordinates will be presented in future work. The derivations in this paper are not self-contained; results obtained by GT95 are in general used here without proof.

In our frequency domain calculations of synthetics we routinely include anelastic attenuation in the elastic moduli using a superposition of standard linear solids (Liu, Anderson & Kanamori 1976). For simplicity we consider a purely elastic medium in this paper. It appears possible to use an approach similar to that of Emmerich & Korn (1987) to extend our methods to the anelastic case, but we have not yet verified this.

In many FD implementations (e.g. Vireux 1986) velocity and stress are the dependent variables, and a coupled system of first-order differential equations in space and time is obtained. This system is then solved using the 'staggered grid' approach. In contrast, displacement is the only dependent variable in both the conventional and modified operators in this paper. As discussed below in Section 6, it does not appear possible to derive modified operators for staggered grid schemes.

## 2 FINITE DIFFERENCE OPERATORS

The strong form of the time-domain equation of motion for the 1-D case is as follows:

$$\rho \frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial z} \left( \mu \frac{\partial u}{\partial z} \right) = f, \quad (3)$$

where  $u$  is the displacement,  $\rho$  is the density,  $\mu$  the elastic modulus and  $f$  the external force. Following the normal FD approach, we discretize the unknown displacement  $u$ , which is a function of space and time, as follows:

$$c_{nN} = u(n\Delta z, N\Delta t). \quad (4)$$

The FD equation of motion is as follows:

$$(A_{mMnN} - K_{mMnN})c_{nN} = f_{mM}, \quad (5)$$

where  $\mathbf{A}$  is an FD operator for  $\rho(\partial^2 u / \partial t^2)$ ,  $\mathbf{K}$  is an FD operator for  $\partial / \partial z [\mu(\partial u / \partial z)]$  and  $\mathbf{f}$  is the discretized external force term. Summation over repeated indices is implied throughout this paper.

$\mathbf{A}$  and  $\mathbf{K}$  in eq. (5) are time-domain FD operators. We now compute their Fourier transforms, which are denoted by  $\mathbf{B}$  and  $\mathbf{L}$  respectively. In the frequency domain, the displacement is discretized as follows:

$$d_n = \int_{-\infty}^{\infty} \exp(-i\omega t) u(n\Delta z, t) dt. \quad (6)$$

The FD equation of motion in the frequency domain (the transform of eq. 5) is as follows:

$$(\mathbf{B}_{mn} - \mathbf{L}_{mn})d_n = f'_m. \quad (7)$$

As eq. (7) and eq. (2.1) of GT95 have essentially the same form, we can use the theory in Section 2 of GT95 to obtain formal error estimates for  $\mathbf{d}$ . The only difference is that the errors of the operators are now  $\omega$ -dependent as well as  $k$ -dependent, because of numerical dispersion in time as well as space.

## 3 OPERATORS FOR THE 1-D PROBLEM

### 3.1 Homogeneous 1-D problem

We begin by considering a homogeneous 1-D problem with a constant temporal grid interval  $\Delta t$  and a constant spatial grid interval  $\Delta z$ . In this paper the superscript <sup>0</sup> denotes the conventional operators rather than the exact operators. The conventional FD

operators  $\mathbf{A}^0$  and  $\mathbf{K}^0$  are as follows:

$$\mathbf{A}^0 = \left(\frac{\rho}{\Delta t^2}\right) \times \begin{array}{|c|cc|} \hline t + \Delta t & & 1 \\ \hline t & & -2 \\ \hline t - \Delta t & & 1 \\ \hline z - \Delta z & z & z + \Delta z \\ \hline \end{array}, \quad (8)$$

$$\mathbf{K}^0 = \left(\frac{\mu}{\Delta z^2}\right) \times \begin{array}{|c|ccc|} \hline t + \Delta t & & & \\ \hline t & 1 & -2 & 1 \\ \hline t - \Delta t & & & \\ \hline z - \Delta z & z & & z + \Delta z \\ \hline \end{array},$$

with the format

$$\mathbf{A} = \begin{array}{|c|ccc|} \hline t + \Delta t & A_{mM(m-1)(M+1)} & A_{mMm(M+1)} & A_{mM(m+1)(M+1)} \\ \hline t & A_{mM(m-1)M} & A_{mMmM} & A_{mM(m+1)M} \\ \hline t - \Delta t & A_{mM(m-1)(M-1)} & A_{mMm(M-1)} & A_{mM(m+1)(M-1)} \\ \hline z - \Delta z & z & z & z + \Delta z \\ \hline \end{array}. \quad (9)$$

Throughout this paper blank spaces in the FD stencils denote zeros.

$\mathbf{A}^0$  and  $\mathbf{K}^0$  have the numerical dispersion of normal three-point second-derivative operators. The operator error for the conventional operators is thus as follows:

$$(\delta A_{mMnN}^0 - \delta K_{mMnN}^0)c_{nN} = \frac{\Delta t^2}{12} \rho \left( \frac{\partial^4 u}{\partial t^4} \right) - \frac{\Delta z^2}{12} \mu \left( \frac{\partial^4 u}{\partial z^4} \right) \Big|_{t=t_M, z=z_m}, \quad (10)$$

where

$$\delta A_{mMnN}^0 = A_{mMnN}^0 - A_{mMnN}^{\text{exact}}, \quad (11)$$

$$\delta K_{mMnN}^0 = K_{mMnN}^0 - K_{mMnN}^{\text{exact}}. \quad (12)$$

Note that throughout this paper the error expressions are given to  $O(\Delta t^2)$  and  $O(\Delta z^2)$ , with higher-order terms omitted.

We define  $\mathbf{B}^0$ ,  $\mathbf{L}^0$ ,  $\mathbf{B}^{\text{exact}}$ ,  $\mathbf{L}^{\text{exact}}$ ,  $\delta \mathbf{B}^0$ , and  $\delta \mathbf{L}^0$  to be the Fourier transforms of  $\mathbf{A}^0$ ,  $\mathbf{K}^0$ ,  $\mathbf{A}^{\text{exact}}$ ,  $\mathbf{K}^{\text{exact}}$ ,  $\delta \mathbf{A}^0$ , and  $\delta \mathbf{K}^0$  respectively. These operators are related as follows:

$$\delta \mathbf{B}_{mn}^0 = \mathbf{B}_{mn}^0 - \mathbf{B}_{mn}^{\text{exact}}, \quad (13)$$

$$\delta \mathbf{L}_{mn}^0 = \mathbf{L}_{mn}^0 - \mathbf{L}_{mn}^{\text{exact}}. \quad (14)$$

Transforming eq. (10) into the frequency domain, we obtain

$$(\delta \mathbf{B}_{mn}^0 - \delta \mathbf{L}_{mn}^0)d_n = \frac{\omega^2 \Delta t^2}{12} \rho \omega^2 u - \frac{\Delta z^2}{12} \frac{d^2}{dz^2} \left( \mu \frac{d^2 u}{dz^2} \right) \Big|_{z=z_m}. \quad (15)$$

The quantity on the rhs of eq. (15) is the ‘basic error’ of the operators (see GT95). When the operand is an eigenfunction and the frequency approaches the corresponding eigenfrequency, the basic error given by eq. (15) will not in general equal zero. Thus the conventional operators do not in general satisfy eq. (2.20) of GT95, and are therefore not optimally accurate.

To satisfy eq. (2.20) of GT95, the basic error should be zero when  $u$  is an eigenfunction and  $\omega$  is equal to the corresponding eigenfrequency. We therefore must derive modified operators  $L_{mn}$  and  $B_{mn}$  for which, rather than eq. (15), the basic error is instead given by

$$(\delta B_{mn} - \delta L_{mn})d_n = \left( \frac{\omega^2 \Delta t^2}{12} - \frac{\Delta z^2}{12} \frac{d^2}{dz^2} \right) \left[ \rho \omega^2 u + \mu \frac{d^2 u}{dz^2} \right] \Big|_{z=z_m}. \quad (16)$$

As the quantity inside the square brackets in eq. (16) is the lhs of the exact equation of motion, it is zero for every eigenfunction when  $\omega$  is equal to the corresponding eigenfrequency, thus the basic error is zero. By taking the inverse Fourier transform, the time-domain

representation of eq. (16) is obtained:

$$\begin{aligned}
 (\delta A_{mMnN} - \delta K_{mMnN})c_{nN} &= \left\{ \rho \left[ \frac{\Delta t^2}{12} \left( \frac{\partial^4 u}{\partial t^4} \right) + \frac{\Delta z^2}{12} \left( \frac{\partial^4 u}{\partial z^2 \partial t^2} \right) \right] - \mu \left[ \frac{\Delta z^2}{12} \left( \frac{\partial^4 u}{\partial z^4} \right) + \frac{\Delta t^2}{12} \left( \frac{\partial^4 u}{\partial t^2 \partial z^2} \right) \right] \right\} \Big|_{t=t_M, z=z_m} \\
 &= \left\{ \frac{\Delta t^2}{12} \frac{\partial^2}{\partial t^2} \left[ \rho \frac{\partial^2 u}{\partial t^2} - \mu \frac{\partial^2 u}{\partial z^2} \right] + \frac{\Delta z^2}{12} \frac{\partial^2}{\partial z^2} \left[ \rho \frac{\partial^2 u}{\partial t^2} - \mu \frac{\partial^2 u}{\partial z^2} \right] \right\} \Big|_{t=t_M, z=z_m}, \quad (17)
 \end{aligned}$$

where  $\mathbf{A}$  and  $\mathbf{K}$  are the modified operators and  $\delta\mathbf{A}$  and  $\delta\mathbf{K}$  are their errors. It is easier to construct the numerical operators using the rhs of the first line of eq. (17), but the meaning of eq. (17) is more clearly shown by the second line. The latter shows clearly that the basic error of the modified operators is given by derivatives of the homogeneous equation of motion (the term in square brackets). Thus when  $u(z, t) = u_m(z) \exp(i\omega_m t)$ , where  $u_m(z)$  is the eigenfunction of a mode with eigenfrequency  $\omega_m$ , the bracketed term (and hence its derivatives) will be zero.

Omitting the details of the derivation, the modified operators that yield errors of the form of eq. (17) are as follows:

$$\mathbf{A} = \left( \frac{\rho}{\Delta t^2} \right) \times \begin{array}{c|ccc} t+\Delta t & 1/12 & 10/12 & 1/12 \\ t & -2/12 & -20/12 & -2/12 \\ t-\Delta t & 1/12 & 10/12 & 1/12 \\ \hline z-\Delta z & z & z & z+\Delta z \end{array}, \quad (18)$$

$$\mathbf{K} = \left( \frac{\mu}{\Delta z^2} \right) \times \begin{array}{c|ccc} t+\Delta t & 1/12 & -2/12 & 1/12 \\ t & 10/12 & -20/12 & 10/12 \\ t-\Delta t & 1/12 & -2/12 & 1/12 \\ \hline z-\Delta z & z & z & z+\Delta z \end{array}.$$

Note that if we sum horizontally for  $\mathbf{A}$  and sum vertically for  $\mathbf{K}$  we obtain the conventional operators in eq. (8). An intuitive explanation of eq. (18) is that we smear out the discretized second time-derivative operator in space, and smear out the discretized second spatial-derivative operator in time, so that the numerical dispersion (error of the phase velocity) of the discretized equation of motion is zero to second order in  $\Delta t^2$  and  $\Delta z^2$ .

We omit discussion of the boundary error in this paper because, as shown in Sections 2 and 3 of GT95, the boundary error does not have an important effect on the error of the numerical solution.

### 3.2 Heterogeneous 1-D problem

The conventional and modified time-domain operators for an inhomogeneous medium can be derived using the procedures given in Section 3, eqs (3.48)–(3.52), of GT95. A first-order discontinuity in elastic properties is handled by overlapping (see Fig. 3 of GT95). Details are not given here.

The explicit forms of the conventional operators  $\mathbf{A}^0$  and  $\mathbf{K}^0$  for an inhomogeneous medium are as follows:

$$\mathbf{A}^0 = \left( \frac{1}{\Delta t^2} \right) \times \begin{array}{c|ccc} t+\Delta t & \rho_m & & \\ t & -2\rho_m & & \\ t-\Delta t & \rho_m & & \\ \hline z-\Delta z & z & z & z+\Delta z \end{array}, \quad (19)$$

$$\mathbf{K}^0 = \left( \frac{1}{2\Delta z^2} \right) \times \begin{array}{c|ccc} t+\Delta t & & & \\ t & (\mu_{m-1} + \mu_m) & -(\mu_{m-1} + 2\mu_m + \mu_{m+1}) & (\mu_m + \mu_{m+1}) \\ t-\Delta t & & & \\ \hline z-\Delta z & z & z & z+\Delta z \end{array},$$

where  $\rho_m$  and  $\mu_m$  are respectively the density and rigidity at the  $m$ th node. The spatial variation of the elastic properties is assumed to be reasonably smooth. The explicit forms of the modified operators  $\mathbf{A}$  and  $\mathbf{K}$  are as follows:

$$\mathbf{A} = \left( \frac{1}{12\Delta t^2} \right) \times \begin{array}{|c|ccc|} \hline t + \Delta t & \rho_m & 10\rho_m & \rho_m \\ \hline t & -2\rho_m & -20\rho_m & -2\rho_m \\ \hline t - \Delta t & \rho_m & 10\rho_m & \rho_m \\ \hline z - \Delta z & z & z & z + \Delta z \\ \hline \end{array}, \quad (20)$$

$$\mathbf{K} = \left( \frac{1}{24\Delta z^2} \right) \times \begin{array}{|c|ccc|} \hline t + \Delta t & (\mu_{m-1} + \mu_m) & -(\mu_{m-1} + 2\mu_m + \mu_{m+1}) & (\mu_m + \mu_{m+1}) \\ \hline t & 10(\mu_{m-1} + \mu_m) & -10(\mu_{m-1} + 2\mu_m + \mu_{m+1}) & 10(\mu_m + \mu_{m+1}) \\ \hline t - \Delta t & (\mu_{m-1} + \mu_m) & -(\mu_{m-1} + 2\mu_m + \mu_{m+1}) & (\mu_m + \mu_{m+1}) \\ \hline z - \Delta z & z & z & z + \Delta z \\ \hline \end{array}.$$

The definition of  $\mathbf{A}$  in eq. (20) corresponds to  $\mathbf{T}'_{\text{right}}$  as defined in eq. (3.49) of Geller & Takeuchi (1995). We could also have defined  $\mathbf{A}$  using  $\mathbf{T}'_{\text{left}}$ , or any other linear combination  $\gamma\mathbf{T}'_{\text{right}} + (1-\gamma)\mathbf{T}'_{\text{left}}$ .

Omitting details (see GT95) the basic error for the modified operators in eq. (20) is

$$(\delta A_{mMnN} - \delta K_{mMnN})c_{nN} \approx \left\{ \frac{\Delta t^2}{12} \frac{\partial^2}{\partial t^2} \left[ \rho \frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial z} \left( \mu \frac{\partial u}{\partial z} \right) \right] + \frac{\Delta z^2}{12} \frac{\partial^2}{\partial z^2} \left[ \rho \frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial z} \left( \mu \frac{\partial u}{\partial z} \right) \right] \right\} \Big|_{t=t_M, z=z_m}. \quad (21)$$

### 3.3 Operators for boundaries

For completeness we give the operators for a left-hand boundary with a free-surface natural boundary condition. If this is an internal boundary rather than a free boundary, the operators are overlapped with those in the adjacent segment (see GT95 for details). Operators for a right-hand boundary can be readily obtained from those given below. The boundary terms for the conventional operators for a heterogeneous medium are

$$\mathbf{A}^0 = \left( \frac{1}{\Delta t^2} \right) \times \begin{array}{|c|cc|} \hline t + \Delta t & \rho_m/2 & \\ \hline t & -\rho_m & \\ \hline t - \Delta t & \rho_m/2 & \\ \hline z & z + \Delta z & \\ \hline \end{array}, \quad (22)$$

$$\mathbf{K}^0 = \left( \frac{1}{2\Delta z^2} \right) \times \begin{array}{|c|cc|} \hline t + \Delta t & & \\ \hline t & -(\mu_m + \mu_{m+1}) & (\mu_m + \mu_{m+1}) \\ \hline t - \Delta t & & \\ \hline z & z + \Delta z & \\ \hline \end{array}.$$

The modified operators for a left-hand boundary for a heterogeneous medium are

$$\mathbf{A} = \left( \frac{1}{12\Delta t^2} \right) \times \begin{array}{|c|cc|} \hline t + \Delta t & 5\rho_m & \rho_m \\ \hline t & -10\rho_m & -2\rho_m \\ \hline t - \Delta t & 5\rho_m & \rho_m \\ \hline z & z + \Delta z & \\ \hline \end{array}, \quad (23)$$

$$\mathbf{K} = \left( \frac{1}{24\Delta z^2} \right) \times \begin{array}{|c|cc|} \hline t + \Delta t & -(\mu_m + \mu_{m+1}) & (\mu_m + \mu_{m+1}) \\ \hline t & -10(\mu_m + \mu_{m+1}) & 10(\mu_m + \mu_{m+1}) \\ \hline t - \Delta t & -(\mu_m + \mu_{m+1}) & (\mu_m + \mu_{m+1}) \\ \hline z & z + \Delta z & \\ \hline \end{array}.$$

#### 4 PREDICTOR–CORRECTOR SCHEME USING THE MODIFIED OPERATORS

The modified operator ( $A_{mMnN} - K_{mMnN}$ ) given by eqs (20) and (23) has multiple non-zero elements for time  $t + \Delta t$ . If we use these modified operators in a time-marching scheme to solve eq. (5), the FD equation of motion, we obtain an implicit scheme, rather than the explicit scheme for the conventional operators in eq. (8). To obviate the need to solve a system of simultaneous linear equations at each time step, we use the modified operators in an approximate (predictor–corrector) scheme based on the first-order Born approximation. A detailed discussion of the implementation is given in the Appendix.

First we predict the wavefield at the next time step using the conventional operators  $\mathbf{A}^0$  and  $\mathbf{K}^0$  defined in eq. (8):

$$(\mathbf{A}^0 - \mathbf{K}^0)\mathbf{c}^0 = \mathbf{f}, \quad (24)$$

where  $c_{n(N+1)}^0$ , the predicted wavefield at time  $t + \Delta t$ , is obtained explicitly from eq. (24).

Next we compute  $\delta\mathbf{c}$ , the correction to the displacement at time  $t + \Delta t$ , using the first-order Born approximation. In the previous section we used  $\delta\mathbf{A}$  and  $\delta\mathbf{K}$  to denote the difference between the numerical and exact operators. However, in this and later sections we denote the difference between the conventional operators  $\mathbf{A}^0$ ,  $\mathbf{K}^0$  and the modified operators  $\mathbf{A}$ ,  $\mathbf{K}$  by  $\delta\mathbf{A}$ ,  $\delta\mathbf{K}$  respectively. To obtain the correction we thus solve

$$(\mathbf{A}^0 - \mathbf{K}^0)\delta\mathbf{c} = -(\delta\mathbf{A} - \delta\mathbf{K})\mathbf{c}^0. \quad (25)$$

As the lhs of eq. (25) uses the conventional operators, we can solve explicitly for the value of  $\delta\mathbf{c}$  at time  $t + \Delta t$ . Note that  $\delta c_{nN} = 0$  and  $\delta c_{n(N-1)} = 0$  in eq. (25).

We compute the corrected displacement  $c_{n(N+1)}$  after each time step using  $\mathbf{c}^0$  computed by eq. (24) and  $\delta\mathbf{c}$  computed by eq. (25):

$$c_{n(N+1)} = c_{n(N+1)}^0 + \delta c_{n(N+1)}. \quad (26)$$

Finally, before advancing to the next time step we redefine  $\mathbf{c}^0$ :

$$c_{n(N+1)}^0 = c_{n(N+1)}. \quad (27)$$

Note that we use the displacements given by eq. (27) as the values for  $c_{nN}^0$  and  $c_{n(N-1)}^0$  when we evaluate eq. (24) for the next time step.

$\delta\mathbf{A}$  and  $\delta\mathbf{K}$  are obtained by taking the difference of eqs (20) and (19):

$$\delta\mathbf{A} = \left(\frac{1}{12\Delta t^2}\right) \times \begin{array}{c|ccc} t + \Delta t & \rho_m & -2\rho_m & \rho_m \\ t & -2\rho_m & 4\rho_m & -2\rho_m \\ t - \Delta t & \rho_m & -2\rho_m & \rho_m \\ \hline z - \Delta z & z & z & z + \Delta z \end{array}, \quad (28)$$

$$\delta\mathbf{K} = \left(\frac{1}{24\Delta z^2}\right) \times \begin{array}{c|ccc} t + \Delta t & (\mu_{m-1} + \mu_m) & -(\mu_{m-1} + 2\mu_m + \mu_{m+1}) & (\mu_m + \mu_{m+1}) \\ t & -2(\mu_{m-1} + \mu_m) & 2(\mu_{m-1} + 2\mu_m + \mu_{m+1}) & -2(\mu_m + \mu_{m+1}) \\ t - \Delta t & (\mu_{m-1} + \mu_m) & -(\mu_{m-1} + 2\mu_m + \mu_{m+1}) & (\mu_m + \mu_{m+1}) \\ \hline z - \Delta z & z & z & z + \Delta z \end{array}. \quad (29)$$

$\delta\mathbf{A}$  and  $\delta\mathbf{K}$  for the boundary elements are obtained by differencing eqs (23) and (22).

#### 5 STABILITY AND ACCURACY

##### 5.1 Stability

It is well known that the time step,  $\Delta t$ , must be less than or equal to the Courant limit,  $\Delta t_{\text{courant}}$ , in order to obtain stable solutions using the conventional operators. In this section we show that the Courant stability limits for the conventional and modified operators are equal for a homogeneous medium.

The stability condition for both modified and conventional operators is the condition that there cannot be any exponentially growing modes in the FD equation of motion (eq. 5). To derive the stability condition we solve a generalized eigenvalue problem (e.g. Section 7.7 of Golub & Van Loan 1989). We begin by formulating the stability condition for the conventional operators. We consider harmonic solutions of eq. (5) with spatial dependence  $\mathbf{c}$  and temporal dependence  $\exp(i\omega t)$ . We substitute this solution into eq. (5) to

obtain the following:6.5pt

$$\mathbf{H}\mathbf{c} = \frac{2}{\Delta t^2} (1 - \cos \omega \Delta t) \mathbf{T}\mathbf{c}, \quad (30)$$

where  $\mathbf{T}$  and  $\mathbf{H}$  are the spatially dependent parts of  $\mathbf{A}$  and  $-\mathbf{K}$ .  $\mathbf{T}$  and  $\mathbf{H}$  for a homogeneous medium are as follows:

$$\mathbf{H} = \frac{\mu}{\Delta z^2} \begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix}, \quad \mathbf{T} = \rho \begin{bmatrix} 1/2 & & & & & \\ & 1 & & & & \\ & & \ddots & & & \\ & & & 1 & & \\ & & & & & 1/2 \end{bmatrix}. \quad (31)$$

We define eigenvalues  $\lambda_n$  and eigenvectors  $\mathbf{c}_n$  (Note that in this section  $n$  refers to the eigenvector and eigenvalue rather than to a particular node.) for  $\mathbf{T}$  and  $\mathbf{H}$  as follows:

$$\mathbf{H}\mathbf{c}_n = \lambda_n \mathbf{T}\mathbf{c}_n, \quad (32)$$

where  $0 \leq \lambda_0 < \lambda_1 < \dots < \lambda_{\max}$ . Comparing eqs (30) and (32) we get

$$\frac{2}{\Delta t^2} (1 - \cos \omega \Delta t) = \lambda_n \quad (33)$$

or

$$\cos \omega \Delta t = 1 - \frac{\Delta t^2}{2} \lambda_n. \quad (34)$$

Since  $\lambda_n$  is real and  $\lambda_n \geq 0$  for all  $n$ , the requirement for real roots is

$$\cos \omega \Delta t \geq -1. \quad (35)$$

The most severe constraint is imposed by  $\lambda_n = \lambda_{\max}$ . Combining eqs (34) and (35), we thus require

$$1 - \frac{\Delta t^2}{2} \lambda_{\max} \geq -1 \quad (36)$$

or

$$\Delta t^2 \leq \frac{4}{\lambda_{\max}}. \quad (37)$$

The eigenvectors of eq. (32) for the matrices for a homogeneous medium (eq. 31) are

$$\mathbf{c}_n = \begin{pmatrix} \cos 0 \\ \cos(n\pi)/N \\ \cos(2n\pi)/N \\ \vdots \\ \cos((N-1)n\pi)/N \\ \cos(n\pi) \end{pmatrix}, \quad (38)$$

where  $N$  is the number of grid intervals. The corresponding eigenvalues are given by

$$\lambda_n = \frac{2[1 - \cos(n\pi)/N]\beta^2}{\Delta z^2}, \quad n = 0, \dots, N, \quad (39)$$

where  $\beta = \sqrt{\mu/\rho}$  is the wave velocity. We thus see from eqs (39) and (37) that

$$\lambda_{\max} = 4\beta^2/\Delta z^2. \quad (40)$$

From eqs (37) and (40) the stability condition is

$$\Delta t \leq \Delta t_{\text{courant}}, \quad (41)$$

where

$$\Delta t_{\text{courant}} = \frac{\Delta z}{\beta}. \quad (42)$$

Thus the Courant stability condition holds rigorously for the conventional operators in a 1-D homogeneous medium with free boundaries.

We now consider the stability condition for the modified operators for a homogeneous medium. The spatial operator  $\mathbf{T}$  corresponding to the modified operator  $\mathbf{A}$  is given by

$$\mathbf{T}' = \rho \begin{bmatrix} 5/12 & 1/12 & & & \\ 1/12 & 10/12 & 1/12 & & \\ & & \ddots & \ddots & \ddots \\ & & & 1/12 & 10/12 & 1/12 \\ & & & & 1/12 & 5/12 \end{bmatrix}. \quad (43)$$

The generalized eigenvalue problem for  $\mathbf{H}$  and  $\mathbf{T}'$  is given by

$$\mathbf{H}\mathbf{c}_n = \lambda'_n \mathbf{T}'\mathbf{c}_n, \quad (44)$$

where  $\mathbf{c}_n$  is given by eq. (38). We use the generalized eigenvalue problem for  $\mathbf{T}'$  and  $\mathbf{T}$  as an intermediate result:

$$\mathbf{T}'\mathbf{c}_n = \gamma_n \mathbf{T}\mathbf{c}_n, \quad (45)$$

where

$$\gamma_n = \left( \frac{5}{6} + \frac{1}{6} \cos \frac{n\pi}{N} \right) \quad (46)$$

and  $\mathbf{c}_n$  is given by eq. (38). Using eqs (39) and (44)–(46), we have

$$\lambda'_n = \frac{\lambda_n}{\gamma_n} = \frac{2[1 - \cos(n\pi/N)]\beta^2/\Delta z^2}{[5 + \cos(n\pi/N)]/6}. \quad (47)$$

We now consider harmonic solutions of eq. (5) for a homogeneous medium. We obtain

$$\left( \frac{5}{6} + \frac{1}{6} \cos \omega\Delta t \right) \mathbf{H}\mathbf{c}_n = \frac{2}{\Delta t^2} (1 - \cos \omega\Delta t) \mathbf{T}'\mathbf{c}_n. \quad (48)$$

Comparing eqs (44) and (48), we have

$$\lambda'_n = \frac{2(1 - \cos \omega\Delta t)}{\Delta t^2(5 + 6 \cos \omega\Delta t)/6}. \quad (49)$$

Solving for  $\cos \omega\Delta t$ , we obtain

$$\cos \omega\Delta t = \frac{2 - 5\lambda'_n \Delta t^2 / 6}{2 + \lambda'_n \Delta t^2 / 6}. \quad (50)$$

We require  $|\cos \omega\Delta t| \leq 1$  for all values of  $\lambda'_n$ . The most severe constraint is imposed by  $\lambda'_{\text{max}}$ . From eq. (47) we have

$$\lambda'_{\text{max}} = \frac{6\beta^2}{\Delta z^2}. \quad (51)$$

Substituting eq. (51) into eq. (50) we have

$$\cos \omega\Delta t = \frac{2 - 5\beta^2 \Delta t^2 / \Delta z^2}{2 + \beta^2 \Delta t^2 / \Delta z^2}. \quad (52)$$

As the condition for stability is  $|\cos \omega\Delta t| \leq -1$ , we obtain from eq. (52)

$$\Delta t \leq \frac{\Delta z}{\beta}. \quad (53)$$

Thus both the modified and conventional operators must satisfy the same stability condition.

$\lambda_{\max}$  can be determined for heterogeneous media by numerically finding the maximum eigenvalue of eq. (32) using the Sturm sequence property (Peters & Wilkinson 1969). We can then obtain the stability condition for the inhomogeneous case following the same procedures. In general, the stability condition for an inhomogeneous medium is

$$\Delta t \leq \left( \frac{\Delta z}{\beta} \right)_{\min} (1 + \epsilon) \quad (54)$$

for both conventional and modified operators, where  $\epsilon$  is a finite but relatively small number whose amplitude and sign depend on the exact nature of the problem. We omit further details.

## 5.2 Accuracy

The analytic eigenvalues for a homogeneous 1-D medium are the squares of the eigenfrequencies,

$$\lambda_n^{\text{exact}} = \left( \frac{n\pi\beta}{L} \right)^2, \quad (55)$$

where  $L = N\Delta z$  is the length of the medium. If we expand  $\cos(n\pi/N)$  in a Taylor series, we obtain the following from eqs (39) and (47) respectively:

$$\lambda_n = \lambda_n^{\text{exact}} \left[ 1 - \frac{n^2\pi^2}{12N^2} + O\left(\left(\frac{n\pi}{N}\right)^4\right) \right], \quad (56)$$

$$\lambda'_n = \lambda_n^{\text{exact}} \left[ 1 + O\left(\left(\frac{n\pi}{N}\right)^4\right) \right]. \quad (57)$$

Note that  $n\pi/N = k\Delta z$ , where  $k$  is the wavenumber. Thus we see that the eigenfrequencies for the modified operators have an error of  $O(k^4\Delta z^4)$ , while the eigenfrequencies for the conventional operators have an error of  $O(k^2\Delta z^2)$ . This is an expected result, because, as discussed by GT95, setting the basic error of the modified operators to zero is equivalent to requiring the error of the eigenfrequencies of the modified operators to be zero to  $O(\Delta z^2)$ , excepting possible minor  $O(\Delta z^2)$  boundary errors.

## 6 STAGGERED GRID APPROACHES

For the 1-D problem in a homogeneous medium the first-order staggered grid approach of Vireux (1986) consists of solving the two following coupled first-order equations:

$$\frac{\partial \sigma}{\partial t} = \mu \frac{\partial v}{\partial z}, \quad (58)$$

$$\rho \frac{\partial v}{\partial t} - \frac{\partial \sigma}{\partial z} = -f, \quad (59)$$

where  $\sigma$  is stress and  $v$  is velocity. Eq. (58) is approximated by the finite difference scheme

$$\frac{\sigma(z, t + \Delta t/2) - \sigma(z, t - \Delta t/2)}{\Delta t} = \mu \frac{v(z + \Delta z/2, t) - v(z - \Delta z/2, t)}{\Delta z}. \quad (60)$$

A Taylor series expansion of eq. (58) yields (neglecting higher-order terms)

$$\frac{\partial \sigma}{\partial t} + \frac{\Delta t^2}{24} \frac{\partial^2}{\partial t^2} \left( \frac{\partial \sigma}{\partial t} \right) = \mu \left[ \frac{\partial v}{\partial z} + \frac{\Delta z^2}{24} \frac{\partial^2}{\partial z^2} \left( \frac{\partial v}{\partial z} \right) \right]. \quad (61)$$

However, to satisfy the general criterion for optimally accurate operators (GT95) we want modified operators that will instead yield the Taylor series:

$$\frac{\partial \sigma}{\partial t} + \frac{\Delta t^2}{24} \frac{\partial^2}{\partial t^2} \left( \frac{\partial \sigma}{\partial t} - \mu \frac{\partial v}{\partial z} \right) = \mu \frac{\partial v}{\partial z} + \frac{\Delta z^2}{24} \frac{\partial^2}{\partial z^2} \left( \mu \frac{\partial v}{\partial z} - \frac{\partial \sigma}{\partial t} \right). \quad (62)$$

It is easy to derive formally operators that have the error required by eq. (62):

$$P\sigma = \frac{1}{\Delta t} \times \begin{array}{|c|c|c|c|} \hline t + \Delta t/2 & 1/12 & 10/12 & 1/12 \\ \hline t - \Delta t/2 & -1/12 & -10/12 & -1/12 \\ \hline z - \Delta z & z & z + \Delta z & \\ \hline \end{array}, \quad (63)$$

$$Qv = \frac{\mu}{\Delta z} \times \begin{array}{|c|c|c|} \hline t + \Delta t & -1/12 & 1/12 \\ \hline t & -10/12 & 10/12 \\ \hline t - \Delta t & -1/12 & 1/12 \\ \hline z - \Delta z/2 & z + \Delta z/2 & \\ \hline \end{array},$$

where the modified scheme for eq. (58) is

$$P\sigma = Qv. \quad (64)$$

Unfortunately, the modified operator  $Q$  requires knowledge of  $v(z, t + \Delta t)$ , which we do not yet have, in order to determine  $\sigma(z, t + \Delta t/2)$ , based on knowledge of  $v(z \pm \Delta z/2, t)$  and  $\sigma(z, t - \Delta t/2)$ . Thus the modified operators formally exist (as given by eq. 63) but their use would lead to an apparently intractable implicit scheme.

Luo & Schuster (1990) present an approach they call the ‘parsimonious staggered grid differencing scheme’. Their starting point is a conventional staggered grid scheme, but they rearrange the equations to eliminate stress as a dependent variable. This rearrangement essentially consists of integrating the discretized strong form of the equation of motion by parts to obtain the discretized weak form of the equation of motion. (See Geller & Ohminato 1994 for a general discussion of the weak form and strong form.) Luo & Schuster’s (1990) derivation seems unnecessarily complicated as the same result (essentially equivalent to the conventional scheme in this paper) could have been directly obtained from the weak form of the equation of motion.

## 7 NUMERICAL EXAMPLES

In this section we present numerical examples to show the effectiveness of the modified operators. Some subtle points arise because, as we show below, the error for solutions computed using the conventional operators strongly depends on  $\Delta t/\Delta z$ , as the error terms for  $\Delta t$  and  $\Delta z$  have opposite signs. First we consider the basic error of the solutions obtained using the conventional operators for a homogeneous medium. The normal modes satisfy the equation of motion, eq. (3), for  $f=0$ . We therefore have, in the frequency domain,

$$\rho\omega_p^2 u_p + \mu \frac{d^2 u_p}{dz^2} = 0, \quad (65)$$

where  $u_p$  is the eigenfunction of the  $p$ th mode and  $\omega_p$  is the corresponding eigenfrequency. From eq. (15) the basic error for the conventional operators can be written as follows in the frequency domain:

$$(\delta B_{mn} - \delta L_{mn})d_n = \frac{\omega_p^2 \Delta t^2}{12} \rho\omega_p^2 u_p + \frac{k_p^2 \Delta z^2}{12} \mu \frac{d^2 u_p}{dz^2} \Big|_{z=z_m}, \quad (66)$$

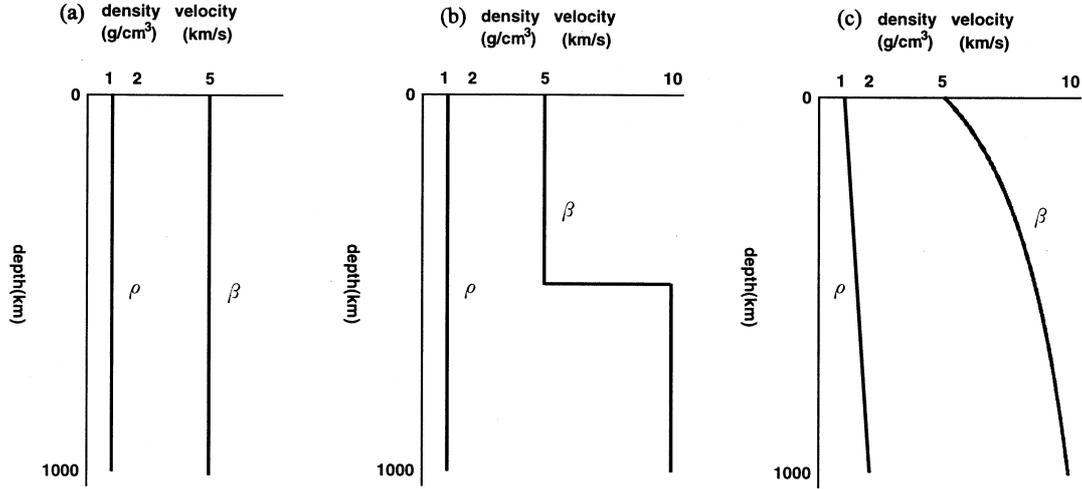
where  $k_p$  is the wavenumber of the mode and

$$\omega_p^2 = \beta^2 k_p^2, \quad (67)$$

where  $\beta^2 = \mu/\rho$ . Using eqs (65) and (67) in eq. (66), we obtain

$$\begin{aligned} (\delta B_{mn} - \delta L_{mn})d_n &= \mu \frac{d^2 u_p}{dz^2} \left[ \frac{k_p^2 \beta^2}{12} \left( \frac{\Delta z^2}{\beta^2} - \Delta t^2 \right) \right] \\ &= \mu \frac{d^2 u_p}{dz^2} \left[ \frac{k_p^2 \beta^2}{12} (\Delta t_{\text{courant}}^2 - \Delta t^2) \right]. \end{aligned} \quad (68)$$

Eq. (68) shows that the accuracy of the synthetics computed using the conventional operators for a given value of  $\Delta z$  depends strongly on the choice of  $\Delta t$ . At the Courant limit,  $\Delta t_{\text{courant}} = \Delta z/\beta$ , the rhs of eq. (68) is zero. Thus at the Courant limit the conventional operators for a homogeneous medium satisfy the general criterion for optimally accurate operators.



**Figure 1.** (a,b) Density and velocity structure used in the numerical examples for Fig. 2. (c) Density and velocity structure used in the numerical example for Fig. 3.

We now consider the conventional operators for an inhomogeneous medium. It can be shown that the conventional operators approximately satisfy the general criterion for optimally accurate operators when

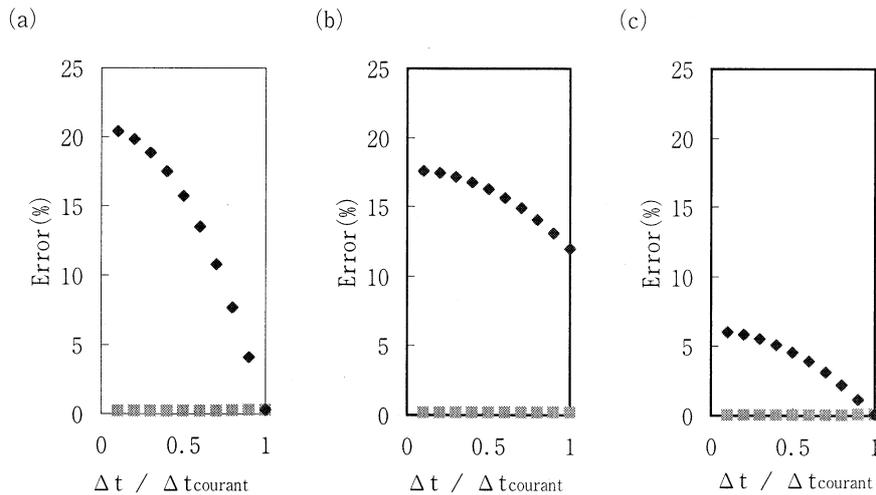
$$\frac{\omega^2 \Delta t^2}{12} \approx \frac{k_m^2 ((\Delta z_{m-1} + \Delta z_m)/2)^2}{12} \quad (69)$$

for all grid points  $m$ , where  $k_m$  is the wavenumber at  $z = z_m$  and  $\Delta z_m$  is the grid interval between the  $m$ th and  $(m+1)$ th grid points. On the other hand, the Courant condition for an inhomogeneous medium is

$$\Delta t \leq (1 + \epsilon) \frac{(\Delta z_{m-1} + \Delta z_m)/2}{\beta_m}, \quad (70)$$

for all  $m$ , where  $\beta_m$  is the wave velocity at  $z = z_m$ . To obtain accurate synthetics, both eqs (69) and (70) must be satisfied. This can be achieved only if variable grid spacing is chosen so that the number of nodes per wavelength is approximately constant everywhere, and  $\Delta t$  is chosen to be slightly less than the Courant limit.

We now present numerical examples. First, we study the accuracy as a function of the time step normalized by the Courant limit. We consider a homogeneous medium (Fig. 1a) and a two-layered medium (Fig. 1b). We calculate synthetics with a duration of 750 s.



**Figure 2.** Error of the waveforms obtained by the conventional (black diamonds) and modified (grey squares) operators. The time step is normalized by the Courant stability limit. (a) Errors for a homogeneous medium with a homogeneous grid. (b) Errors for a two-layered medium with a homogeneous grid. (c) errors for a two-layered medium with an inhomogeneous grid chosen so that the number of nodes per wavelength is constant throughout the medium. The dependence of the errors for the conventional operators for (a) and (c) matches the  $(\Delta t_{\text{courant}}^2 - \Delta t^2)$  dependence predicted by eq. (68).

**Table 1.** CPU time required on Super-SPARC (60 MHz, 1 CPU) and error for conventional and modified operators.

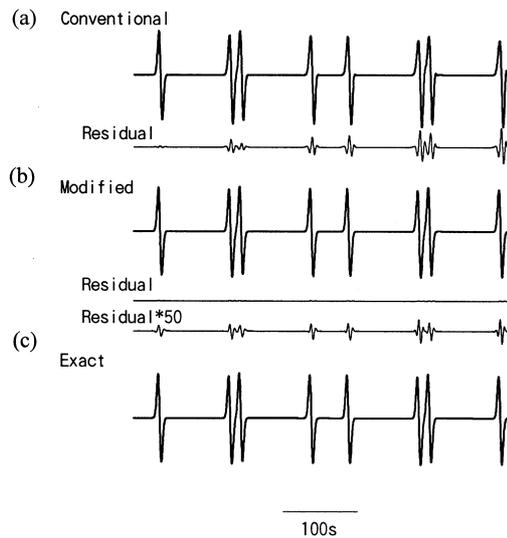
	CPU time			Convent.	Error	
	Convent.	Mod	Ratio		Mod	Ratio
500 grids 5000 steps	1 s	2 s	<b>0.5</b>	22%	0.32%	<b>69</b>
1000 grids 10000 steps	5 s	10 s	<b>0.5</b>	5.6%	0.054%	<b>104</b>
10000 grids 100000 steps	455 s	921 s	<b>0.49</b>			

The source is a single force with a Ricker wavelet time history whose central frequency is 10 s. The source is at  $z=500$  km and the receiver is at  $z=300$  km. For the homogeneous medium we use a spatial grid with  $\Delta z=1$  km. For the two-layered medium we use two spatial grids: (1) a homogeneous grid with  $\Delta z=1$  km, and (2) an inhomogeneous grid with  $\Delta z=0.5$  km in the upper layer and  $\Delta z=1$  km in the lower layer. The latter grid has a constant number of nodes per wavelength.

Fig. 2 shows the error of the synthetics obtained using the conventional (black diamonds) and modified (grey squares) operators. Fig. 2(a) shows the error (rms residual) for the homogeneous medium (Fig. 1a) with a homogeneous grid. Fig. 2(b) shows the error for the two-layered medium (Fig. 1b) with a homogeneous grid. Fig. 2(c) shows the error for the two-layered medium (Fig. 1b) with an inhomogeneous grid (chosen so that  $\beta\Delta z=\text{constant}$ ). The error for all of the cases considered in this paper is computed using the numerical solution for an extremely fine grid as the reference solution.

As theoretically predicted, the error for the conventional operators is much worse in general than that for the modified operators, but approaches that for the modified operators if and only if  $\Delta t$  is close to the Courant limit everywhere in the medium. Note that the errors for the conventional operators in both Figs 2(a) and (c) show the  $(\Delta t_{\text{courant}}^2 - \Delta t^2)$  dependence predicted by eq. (68). On the other hand, the error of the solutions obtained using the modified operators is essentially uniform regardless of the choice of  $\Delta t$  and spatial grid.

The reader might conclude that the conventional operators with a spatially varying grid interval chosen to give an essentially constant number of nodes per wavelength and a time step close to the Courant limit are sufficient for accurate computation of synthetics, but in general this is not the case. For 2-D or 3-D problems waves propagate in various directions, and both  $P$  and  $S$  waves exist. No spatial grid for the conventional operators will yield optimally accurate solutions for such problems. On the other hand, the modified operators will yield optimally accurate solutions in general. Fig. 2(b) (uniform gridding for a heterogeneous medium) is thus probably most representative of the advantage of the modified operators for real problems. Explicit results for 2-D and 3-D cases will be presented in future papers.



**Figure 3.** Comparison of waveforms obtained by the modified and conventional schemes. (a) Waveforms (top) obtained by the conventional scheme and (second trace) their residuals relative to the (almost exact) reference solution (rms error=22 per cent). (b) Waveforms (top) obtained using the modified operators, (second trace) residuals relative to the reference solution (rms error=0.32 per cent), and (third trace) residual magnified by a factor of 50. (c) Waveforms for (almost exact) reference solution.

**Table 2.** Computed values of  $\epsilon$  (defined in eq. 54).

	Conventional	Modified
500 grids	0.0027	0.0030
1000 grids	0.0017	0.0019

We now compare the error and the CPU time for solutions obtained using the modified and conventional operators for the heterogeneous medium shown in Fig. 1(c). The results are shown in Table 1. The length of the medium is 1000 km as shown in Fig. 1(c), and the length of the time series is 500 s for each case. We use homogeneous temporal and spatial gridding. Thus, for example for the case of 500 nodes and 5000 time steps,  $\Delta z = 2$  km and  $\Delta t = 0.1$  s. For each case the ratio of the spatial and temporal grid intervals is  $\Delta t/\Delta z = 0.05$  s km<sup>-1</sup>, whereas the Courant condition is roughly  $\Delta t/\Delta z \leq 0.01$  s km<sup>-1</sup>. Thus  $\Delta t/\Delta t_{\text{courant}} \approx 0.5$ .

As shown in the Appendix, the modified operators require twice the number of floating point multiplications and three times the number of floating point additions. As multiplication operations require more CPU time than addition operations, the theoretically predicted CPU time for the new method is about twice that of the conventional method. The actual CPU times (Table 1) follow this prediction. On the other hand the new method yields waveforms that are about 60–100 times more accurate than the conventional method. Fig. 3 shows a comparison of the accuracy of the waveforms for the case of 500 nodes and 5000 time steps. As expected based on the results in Section 2 of GT95, the modified operators yield accurate phase velocities, whereas the conventional operators cause large frequency-dependent phase errors. We can see that the modified operators are especially effective for later phases for this reason. The improvement factor is 69 for this time-series, but would be larger for longer time-series.

Fig. 3 raises an important general point. A visual comparison of the synthetic for the conventional operator (a) and the reference solution (c) might lead to the erroneous conclusion that there was ‘good agreement’, because all of the expected arrivals are present at about the right arrival times. But, as shown by the residual (the second trace of a), the rms residual is actually 22 per cent. The large rms error is due to the error in phase in the synthetics for the conventional operators. The human eye is unfortunately not well suited to evaluating such phase errors. Thus a quantitative evaluation of the rms error is an essential step in the evaluation of any method for computing synthetic seismograms.

In summary, the modified operators require about twice the CPU time, but reduce the error by a factor of about 60–100 for reasonable choices of  $\Delta t$  and  $\Delta z$ . This means that by using the modified operators either (1) the required CPU time can be reduced by a factor of about 40 to obtain waveforms with the same accuracy, or (2) the error can be reduced by a factor of about 40 if the CPU time is kept constant.

Finally, we present an eigenvalue calculation. We numerically solve the eigenvalue problems defined by eqs (32) and (45) for the inhomogeneous structure in Fig. 1(c). The computed values of  $\epsilon$  as defined in eq. (54) are shown in Table 2. We thus confirm that the stability condition given by eq. (54) is correct for both the modified and conventional operators. As a further check, we conducted calculations for values of  $\Delta t$  slightly greater and slightly less than  $\left(\frac{\Delta z}{\beta}\right)_{\min} (1 + \epsilon)$ . We confirmed that stable solutions were obtained for a heterogeneous medium for  $\left(\frac{\Delta z}{\beta}\right)_{\min} \leq \Delta t \leq \left(\frac{\Delta z}{\beta}\right)_{\min} (1 + \epsilon)$ , but that exponential instability occurred when  $\Delta t > \left(\frac{\Delta z}{\beta}\right)_{\min} (1 + \epsilon)$ . Numerical experiments (not presented here) for optimally accurate schemes for other problems (e.g. 2-D *P-SV*) have shown that  $|\epsilon|$  is small, but that its sign is sometimes negative.

## 8 DISCUSSION

The error of FD or other numerical schemes has generally been evaluated by considering the numerical dispersion (error of phase velocities) as a function of the number of grid points per wavelength (e.g. Alford, Kelly & Boore 1974). It is frequently assumed that the errors due to spatial and temporal discretization can be considered separately (see e.g. Fig. 4 of Fornberg 1987), but this is not the case. The key point of this paper is that the net error of the synthetics due to the combined effects of temporal and spatial discretization must be considered as a single quantity. This error can be minimized by tuning the operators so that the errors due to spatial and temporal discretization come as close as possible to cancelling each other.

Second-order (in space and time) FD schemes have been deemed inferior both to FD schemes which are fourth order in space and second order in time and to schemes which are pseudo-spectral in space and second order in time (e.g. Fornberg 1987). This evaluation seems correct for conventional second-order FD schemes. However, modified second-order FD schemes of the type presented in this paper may be preferable for many applications.

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## APPENDIX A: IMPLEMENTATION OF ALGORITHMS

We give the explicit form and required floating point operation counts for the conventional and modified operators for the general inhomogeneous problem. For simplicity, we consider homogeneous gridding (constant  $\Delta t$  and  $\Delta z$ ). A first-order discontinuity in elastic properties or spatial grid interval is handled by overlapping (see Fig. 3 of GT95).

## A1 Conventional operators

The explicit scheme for the 1-D heterogeneous problem using the conventional operators (eqs 19 and 24) is as follows:

$$\begin{aligned}
 c_n^{N+1} = & -c_n^{N-1} \\
 & + \left( \frac{\mu_{n-1} + \mu_n}{2\rho_n} \frac{\Delta t^2}{\Delta z^2} \right) c_{n-1}^{N-1} \\
 & + \left( 2 - \frac{\mu_{n-1} + 2\mu_n + \mu_{n+1}}{2\rho_n} \frac{\Delta t^2}{\Delta z^2} \right) c_n^N \\
 & + \left( \frac{\mu_n + \mu_{n+1}}{2\rho_n} \frac{\Delta t^2}{\Delta z^2} \right) c_{n+1}^N \\
 & + \left( \frac{\Delta t^2}{\rho_n} F_n^N \right), \tag{A1}
 \end{aligned}$$

where  $c_n^N$  and  $F_n^N$  are the displacement and the body force at  $z = n\Delta z$  and  $t = N\Delta t$  respectively, and  $\rho_n$  and  $\mu_n$  are the density and rigidity at  $z = n\Delta z$  respectively.  $c_n^{N+1}$  is the unknown displacement at  $t + \Delta t$  to be determined; the other quantities in eq. (A1) are all known. Note that we write  $c_n^N$  in this Appendix, whereas we used  $c_{nN}$  in the body of the paper. The coefficients in parentheses in eq. (A1) are computed once for each node  $n$  and stored. As we can use convolution for more complex sources, it is sufficient to compute a Green's function for a delta-function source time history for a point source;  $F_n^N$  is thus zero except for  $N = 0$ , and for some particular value of  $n$ . Thus the required floating operation counts for the conventional operators are as follows (neglecting the source term in the following discussion) for computing the new displacement at one node for one time step:

$$\boxed{3 \text{ MULS, } 3 \text{ ADDS}}.$$

## A2 Modified operators

The modified operators in eq. (20) are used in a predictor–corrector scheme. The explicit algorithm for the predictor step is given in eq. (A1). Note that we drop the superscript  $0$  used in eqs (24)–(26). The explicit discretized equation for the correction step (eq. 25) is

as follows (note that  $\delta c_n^N = \delta c_n^{N-1} = 0$ ):

$$\begin{aligned} \delta c_n^{N+1} = & \left( -\frac{1}{12} + \frac{1}{24} \frac{\mu_{n-1} + \mu_n}{\rho_n} \frac{\Delta t^2}{\Delta z^2} \right) [c_{n-1}^{N+1} - 2c_{n-1}^N + c_{n-1}^{N-1}] \\ & + \left( \frac{1}{6} - \frac{1}{24} \frac{\mu_{n-1} + 2\mu_n + \mu_{n+1}}{\rho_n} \frac{\Delta t^2}{\Delta z^2} \right) [c_n^{N+1} - 2c_n^N + c_n^{N-1}] \\ & + \left( -\frac{1}{12} + \frac{1}{24} \frac{\mu_n + \mu_{n+1}}{\rho_n} \frac{\Delta t^2}{\Delta z^2} \right) [c_{n+1}^{N+1} - 2c_{n+1}^N + c_{n+1}^{N-1}]. \end{aligned} \quad (\text{A2})$$

The coefficients in parentheses in eq. (A2) can be computed once for each node and stored. Furthermore, the first two bracketed terms in eq. (A2) will have been previously computed in the loops for adjacent nodes (the  $n-2$  and  $n-1$ th nodes) and can be reused. Only the last bracketed term need be computed at this point. As  $2c_{n+1}^N$  can be computed by addition ( $c_{n+1}^N + c_{n+1}^N$ ), we count this as an addition operation, rather than a multiplication. Thus the operation count for the corrector scheme is three multiplications and five additions.

Finally, after computing  $\delta c_n^{N+1}$  for all nodes, and before proceeding to the next time step, we combine eqs (A2) and (A1) to get the net displacement:

$$c_n^{N+1} \leftarrow c_n^{N+1} + \delta c_n^{N+1}, \quad (\text{A3})$$

where we use  $\leftarrow$  to denote a replacement rather than a mathematical equality.

Combining the three multiplications and three additions for the predictor scheme (eq. A1), three multiplications and five additions for the corrector scheme (eq. A2) and one addition for the update (eq. A3), the total operation count for the new predictor–corrector method is as follows:

$$\boxed{6 \text{ MULS, } 9 \text{ ADDS}}.$$

Thus the operation count for the new scheme is about double that of the conventional scheme. A slight further optimization could be made by evaluating  $A+A$  using specialized software for incrementing the exponent of a floating point number, or by bit shifting.