

One-way wave propagation with amplitude based on pseudo-differential operators

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ABSTRACT

The one-way wave equation is widely used in seismic migration. Equipped with wave amplitudes, the migration can be provided with the reconstruction of the strength of reflectivity. We derive the one-way wave equation with geometrical amplitude by using a symmetric square root operator and a wave field normalization. The symbol of the square root operator, $\omega \sqrt{\frac{1}{c(x,z)^2} - \frac{\xi^2}{\omega^2}}$, is a function of space-time variables and frequency ω and horizontal wavenumber ξ . Only by matter of quantization it becomes an operator, and because quantization is subjected to choices it should be made explicit. If one uses a naive asymmetric quantization an extra operator term will appear in the one-way wave equation, proportional to $\partial_x c$. We propose a symmetric quantization, which maps the symbol to a symmetric square root operator. This provides geometrical amplitude without calculating the lower order term. The advantage of the symmetry argument is its general applicability to numerical methods. We apply the argument to two numerical methods. We propose a new pseudo-spectral method, and we adapt the 60 degree Padé type finite-difference method such that it becomes symmetrical at the expense of almost no extra cost. The simulations show in both cases a significant correction to the amplitude. With the symmetric square root operator the amplitudes are correct. The z -dependency of the velocity lead to another numerically unattractive operator term in the one-way wave equation. We show that a suitably chosen normalization of the wave field prevents the appearance of this term. We apply the pseudo-spectral method to the normalization and confirm by a numerical simulation that it yields the correct amplitude.

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1. Introduction

One-way wave equations allow us to separate solutions of the wave equation into down- and upward propagating waves. They are frequently used to model wave propagation in the application of depth migration [1–9]. They are also used in other fields such as underwater acoustics and integrated optics. One of the reasons to use these equations is that they provide wave field extrapolation in a certain direction [10]. Another reason to use these equations is the fact that they can be implemented cost efficiently [11].

One-way wave equations have first been used in geophysical imaging by Claerbout [12]. They were used to describe travel time and were not intended to describe wave amplitudes. In principle, this restricts the migration process to the reconstruction of the locations of the velocity heterogeneities. Roughly since 1980 the development is to also reconstruct the relative

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strength of the velocity heterogeneities and to estimate petrophysical parameters [13,14]. For the one-way wave equation to describe amplitudes it needs to be refined. One of the problems is the formulation of the *square root operator* in case the velocity is a spatial function.

The finite-difference one-way methods form a large class of one-way methods [12,15]. One attempt to tackle the amplitude problem can be found in the work of Zhang et al. [4,5]. They studied the Padé family of finite-difference one-way methods and modified it such that it provides accurate leading order WKBJ amplitudes. The Padé family of methods includes the familiar 15, 45, 60 degree equations that are reported in Claerbout's book [12].

Another important class of methods is formed by mixed domain methods. Here calculations are performed both in the lateral space, i.e. horizontal in case of downward continuation, and the lateral wavenumber domain. The fast Fourier transform is used to go forth and back. A mixed domain method can be seen as an adaptation of the phase-shift method for laterally varying media [16]. Phase shift plus interpolation (PSPI), for example, uses several reference velocities and an interpolation technique to adapt the phase-shift for laterally varying velocity [7]. Nonstationary phase shift (NSPS) uses nonstationary filter theory to make this adaptation [6]. Although these methods allow for lateral dependence, they do not preserve the wave amplitude. Among the mixed domain methods one also finds the phase-screen method and its offshoot methods like pseudo-screen and generalized screen [1,17,18]. Then the medium is considered as a series of thin slabs or diffraction 'screens', stretched out in lateral direction. It is particularly suited to model propagation through media where the raypaths do not deviate substantially from a given predominant direction.

From mathematical point of view, the one-way wave equation can be found in the rigorous framework of pseudo-differential operator theory. Stolk worked on this and investigated the damping term of the symbol [3]. He compared singularities in the mathematical sense of the wave front set and showed that singularities are described by one-way wave equations.

In this paper we investigate amplitude aspects of the one-way wave equation from theoretical and practical point of view. We identify the essential ingredients that provide the one-way wave equation with the *geometrical amplitude*, using pseudo-differential operator theory. It is comprised of an investigation of the square root operator and the *normalization operator*, which will be discussed in more detail below, and yield implementations for both. Because we focus on amplitude aspects of wave extrapolation we will show simulations of wave propagation based on one-way methods.

Although the work of Zhang et al. provided an interpretation of the square root and normalization operator through some basic ideas from the theory of pseudo-differential operators, they did not make a strict distinction between an operator and its *symbol* [19,20]. We find this aspect of the theory to be fundamental for understanding the true amplitude theory. A symbol is a function of space-time variables and their Fourier associates, e.g. $\omega \sqrt{\frac{1}{c(x)^2} - \frac{\xi^2}{\omega^2}}$, where ξ denotes the horizontal wavenumber. It can be transformed into an operator by matter of *quantization*. Because quantization is subjected to choices it should be made explicit. We will derive the one-way wave equation with amplitude description and explicitly use the theory of pseudo-differential operators. It gives insight in the equation and its modification to involve wave amplitudes.

The depth dependence of the medium leads to an extra operator term in the one-way wave equation which significantly effects the wave amplitude. It is known that by a suitably chosen normalization of the wave field, the one-way wave equation in the new variable does not contain this extra term [18,3,5]. Although numerical implementations are well-known for the square root operator [12,15,5], these are not reported for the normalization. Zhang et al., for example, used the normalization operator but lacked being explicit about its implementation. We will introduce the pseudo-spectral interpolation method, by which both the square root and the normalization operator can be implemented.

To confine the complexity, wave propagation through the earth is modeled by the heterogeneous acoustic wave equation. The heterogeneity is captured by a velocity function, $c = c(x, z)$, which is smooth by assumption. The reader might wonder how this can be applicable to seismic waves, as everybody knows that the Earth is not smooth. Some comments about this follow at the end of the introduction. The pressure $u(t, x, z)$ of an acoustic wave originating at the source $f(t, x, z)$ is governed by:

$$\left(\frac{1}{c(x, z)^2} \partial_t^2 - \partial_x^2 - \partial_z^2 \right) u(t, x, z) = f(t, x, z) \quad (1)$$

in infinite space-time, i.e. $(t, x, z) \in \mathbb{R} \times \mathbb{R}^2$. The support of the source, i.e. the set where it is nonzero, is assumed to be bounded:

$$\text{supp} f \subset [t_{s0}, t_{s1}] \times [x_{s0}, x_{s1}] \times [z_{s0}, z_{s1}].$$

Furthermore, the wave field is zero at initial time, i.e. $u(t, x, z) = 0$ for $t < t_{s0}$.

The splitting into down and up going waves relies on the assumption that the wavelength is small compared with the length scale of the heterogeneity of the medium. This means that we assume the medium velocity to vary slowly over space, and, the frequency to be high. The idea can be shown by first assuming a constant velocity. Using the Fourier transform with respect to t and x , the wave operator can be written in two factors:

$$\left(i\omega \sqrt{\frac{1}{c^2} - \frac{\xi^2}{\omega^2}} + \partial_z \right) \left(i\omega \sqrt{\frac{1}{c^2} - \frac{\xi^2}{\omega^2}} - \partial_z \right) \hat{u}(\omega, \xi, z) = 0, \quad (2)$$

with Fourier variables ω and ξ . The factors are written in arbitrary order. Restricting the solution space to $\frac{1}{c^2} - \frac{\xi^2}{\omega^2} > 0$, the kernel of each factor consists of uni-directional waves. A numerical method based on the one-way wave equation with constant velocity can be found in [21].

When $\partial_x c \neq 0$ the theory of pseudo-differential operators is used to define the square root operator properly. It is one of our goals to show how this can be done. In case $\partial_z c \neq 0$ the noncommutativity of the square root and ∂_z introduces extra terms. These terms can be removed by a suitable normalization of wave field.

We make a comprehensible derivation of the one-way wave equation and show how the square root operator has to be defined such that the equation includes the wave amplitude. The symbol of the square root operator turns out to be the sum of two terms, i.e. the principal and the subprincipal. The former provides travel time. The terms together describe travel time and the geometric amplitude.

Quantization refers to the procedure of mapping a symbol to an operator. The theory of pseudo-differential operators involves a standard quantization, which produces asymmetric operators. We introduce an alternative quantization that maps real symbols to symmetric operators and show that it maps the principal symbol of the square root to the correct operator. By correct, we mean that it properly describes the wave amplitude. The idea to use a symmetric square root is applicable to any method. We will illustrate this by two numerical methods.

We propose a new method, the pseudo-spectral interpolation method, to implement both the square root and the normalization operator. The method is closely related to some of the mixed domain methods in that it is implemented as a sum in which each term involves a multiplication and a convolution. We will verify numerically the claimed amplitude effect of the symmetric square root operator and the normalization operator by simulating wave propagation through a medium with variable velocity. These simulations also give an illustrative example of the improvements that can be expected. The results will be compared with a simulation of the full wave equation, which acts as a reference. The comparison shows a great improvement of the wave amplitude due to the symmetric square root and the normalization operator.

As said, the outcome can be applied to other one-way wave methods. We show that the 60 degree Padé type finite-difference one-way implementation can be made true amplitude by using a symmetric implementation for the square root operator. This modification entails almost no extra cost. Again, numerical simulation shows an improved wave amplitude.

The content of the remaining sections of this paper is as follows. In Section 2 we derive the one-way wave equation for smoothly varying media in the rigorous framework of pseudo-differential operator theory. The numerical implementation of our one-way wave equation is presented in Section 3, including the pseudo-spectral method to implement pseudo-differential operators. The results of the simulation and a comparison with the simulation of the full wave equation are shown in Section 4. A discussion is finally presented in Section 5.

We end this introduction by a few remarks on the application of one-way wave equations in reflection seismic imaging. This is based on the *single scattering assumption* that is generally used in seismic imaging. It involves a geometrical view of wave propagation and assumes that waves present in the data have reflected once. Multiple reflected waves are treated as noise, and to a certain degree they can be suppressed.

The single scattering data can be viewed as the result of linearization of the wave equation with respect to the coefficients, i.e. the medium velocity. Additionally, the reference velocity $c(x)$ is assumed to be smooth, while the perturbation $\delta c(x)$ is oscillatory. In practice this means that c and δc contain different wavelengths, e.g. up to 2–5 Hz for c , and starting somewhere from 5–10 Hz for the reflectivity. These values are converted to the temporal frequency domain using a typical velocity. The unperturbed wave originating from the source f_{src} is the incoming field u_{inc} . Its perturbation is the scattering field u_{sca} . They are governed by the reference and linearized PDE,

$$\frac{1}{c^2} \partial_t^2 u_{\text{inc}} - \Delta u_{\text{inc}} = f_{\text{src}}, \quad \text{and} \quad \frac{1}{c^2} \partial_t^2 u_{\text{sca}} - \Delta u_{\text{sca}} = \frac{2\delta c}{c^3} \partial_t^2 u_{\text{inc}}, \quad (3)$$

both supplemented with zero initial and appropriate boundary conditions. The data is assumed to be given by u_{sca} at measurement positions spread over the surface during some time interval.

A typical imaging algorithm [12] involves the incoming field u_{inc} and the backpropagated receiver field, denoted by u_{bp} , which is obtained by solving a wave equation backward in time with the data as source or boundary condition. These fields are convolved in time

$$I(x, z) = \int_0^{T_{\text{acq}}} u_{\text{inc}}(t, x, z) u_{\text{bp}}(t, x, z) dt,$$

where $[0, T_{\text{acq}}]$ is the time interval for the acquisition assuming the source is set off at $t = 0$. Clearly, solving the wave equation is the most costly part of the imaging algorithm. With present-day data it is to be repeated tens of thousands of times. One-way methods constitute practical tools for modeling wave propagation through smooth media.

2. One-way wave equation

In this section we will derive the true amplitude one-way wave equation for a normalized wave field. We will present the essential steps in a self-contained way, without requiring knowledge of pseudo-differential operator theory in advance. For

the reader primarily interested in the results we point out that the one-way wave equation is in (22), the normalization in (23), and the symmetric square root operator in (19) and (8).

The approach to split the wave field followed in this section slightly differs from the factorization in (2). We will tackle the problem by writing the wave equation as a system of equations, which makes it easy to include the source. Diagonalization of the system leads to our first result, the one-way wave equation for wave propagation in the positive z -direction through a medium of which the velocity only depends on x . The decomposition relies on the square root operator. This operator will be subject of further investigation. The normalization of the wave field is used to derive the one-way wave equation for velocities that may also depend on z .

As shown in (2), the square root operator is a well-defined convolution when $\partial_x c = 0$. In case $\partial_x c \neq 0$ it becomes a non-trivial pseudo-differential operator. We will review the basic ingredients of a pseudo-differential operator, i.e. its symbol and quantization. A symbol is written as an asymptotic expansion of which the first two terms are called the principal and the subprincipal part. We apply a composition theorem to calculate the principal and subprincipal symbols of the square root operator. Referring to the standard quantization, both are to be taken into account to provide the one-way wave equation with the geometrical amplitude.

From practical point of view it is worthwhile to investigate the quantization. We introduce a symmetric quantization and formulate the symmetric square root, i.e. the operator found by symmetric quantization of the principal symbol only. We show that it provides the one-way wave equation with the geometrical amplitude too. The benefit of the symmetry argument is its applicability to other implementations. For example, the square root of the 60 degree finite-difference one-way method can be made symmetric and therefore true amplitude, as will be shown in Section 3.4.

2.1. One-way wave decomposition

The object is to derive one-way wave equations for wave propagation along or in opposite direction of the z -axis through inhomogeneous media, i.e. when $c = c(x, z)$. To start with, we write vectors $\mathbf{u} = \begin{pmatrix} u \\ \partial_z u \end{pmatrix}$ and $\mathbf{f} = \begin{pmatrix} 0 \\ f \end{pmatrix}$, operator $A = -\frac{1}{c(x, z)^2} \partial_t^2 + \partial_x^2$ and matrix operator

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ -A & 0 \end{pmatrix}.$$

The wave equation in (1) can now be rewritten as matrix differential equation:

$$\partial_z \mathbf{u}(t, x, z) = \mathbf{A} \mathbf{u}(t, x, z) - \mathbf{f}(t, x, z). \quad (4)$$

Note that it is a first-order equation with respect to ∂_z .

Suppose that operators \sqrt{A} and $A^{-\frac{1}{2}}$ exist, whose squares are A and A^{-1} , respectively. The construction of operators having approximately these properties will be discussed below. We define the following matrix operators:

$$\mathbf{V} = \begin{pmatrix} 1 & 1 \\ i\sqrt{A} & -i\sqrt{A} \end{pmatrix}, \quad \mathbf{\Lambda} = \frac{1}{2} \begin{pmatrix} 1 & -iA^{-\frac{1}{2}} \\ 1 & iA^{-\frac{1}{2}} \end{pmatrix} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} i\sqrt{A} & 0 \\ 0 & -i\sqrt{A} \end{pmatrix}.$$

The second matrix is the inverse of the first. These matrices yield an eigenvalue decomposition of matrix differential operator \mathbf{A} given by

$$\mathbf{A} = \mathbf{V} \mathbf{B} \mathbf{\Lambda}. \quad (5)$$

A change of variables is defined by $\mathbf{u} = \mathbf{V} \mathbf{v}$. The system of differential equations in (4) then transforms into

$$\mathbf{V} \partial_z \mathbf{v} = (\mathbf{A} \mathbf{V} - (\partial_z \mathbf{V})) \mathbf{v} - \mathbf{f},$$

in which the identity $\partial_z \mathbf{V} \mathbf{v} = (\partial_z \mathbf{V}) \mathbf{v} + \mathbf{V} \partial_z \mathbf{v}$ is used. Left multiplication with $\mathbf{\Lambda}$ yields

$$\partial_z \mathbf{v} = (\mathbf{B} - \mathbf{\Lambda}(\partial_z \mathbf{V})) \mathbf{v} - \mathbf{\Lambda} \mathbf{f}, \quad (6)$$

in which the decomposition (5) is used. Working out the differentiation gives

$$\mathbf{\Lambda}(\partial_z \mathbf{V}) = \frac{1}{4} A^{-1} (\partial_z A) \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

In case the medium is invariant with depth, operator term $\mathbf{\Lambda}(\partial_z \mathbf{V})$ is zero. With the sign choices for \sqrt{A} as in (2), i.e. the sign of ω , Eq. (6) then describes two decoupled one-way waves. Writing v for the second component of \mathbf{v} , the second equation describes wave propagation in the positive z -direction. The one-way wave equation for depth invariant media then is:

$$\partial_z v(t, x, z) = -i\sqrt{A} v(t, x, z) - \frac{i}{2} A^{-\frac{1}{2}} f(t, x, z), \quad (7)$$

Note that v denotes the wave field, *not the velocity*. In the following, we will review the definition of pseudo-differential operators and find explicit approximations for \sqrt{A} and $A^{-\frac{1}{2}}$. To generalize this result to depth dependent media, we will show

in the end of this section how to deal with matrix operator $\Lambda(\partial_z \mathbf{V})$. A well chosen normalization of the wave field will cancel the diagonals terms. The off-diagonals terms will shown to be negligible by a subtle argument.

2.2. Pseudo-differential operators

In case the medium is lateral invariant, i.e. $c = c(z)$, the square root of operator A can be found by using the Fourier transform with respect to t and x . It is a multiplication operator with respect to the Fourier variables and given by

$$b_0(\omega, \xi, z) = \omega \sqrt{\frac{1}{c(z)^2} - \frac{\xi^2}{\omega^2}}. \quad (8)$$

The square root is not unique due to sign choices. This form leads to uni-directional waves solutions.

When the medium laterally varies, the square root also depends on x . Although $b_0(x, \omega, \xi, z)$ is well-defined as a function, it does not define an operator yet. This function of space-time variables and Fourier associates is called symbol. It transforms into an operator by matter of quantization.

We will show that different operators can be found for one symbol. Subsequently, a short introduction of pseudo-differential operators is given, including an important theorem about composition. In this section y is an arbitrary space-time variable with η its Fourier associate. In our context one read $y = (t, x)$ and $\eta = (\omega, \xi)$. We use the following form of the Fourier transform: $(\mathcal{F}\varphi)(\eta) = \int \varphi(y) e^{-i\eta y} dy$.

Quantization refers to the procedure of mapping a function of space-time variables and their Fourier associates to an operator. Given the function $p = p(y, \eta)$, there are two obvious quantizations. These are the *left* quantization

$$\text{Op}_L(p)\varphi(y) = \frac{1}{(2\pi)^2} \int p(y, \eta) (\mathcal{F}\varphi)(\eta) e^{i\eta y} d\eta, \quad (9)$$

and the *right* quantization

$$\text{Op}_R(p)\varphi(y) = \left(\mathcal{F}^{-1} \int p(\tilde{y}, \eta) \varphi(\tilde{y}) e^{-i\eta \tilde{y}} d\tilde{y} \right)(y). \quad (10)$$

The difference becomes clear if we, for example, take $p(y, \eta) = ih(y)\eta$. Then it follows that

$$\begin{aligned} \text{Op}_L(p)\varphi(y) &= h(y) \partial_y \varphi(y) \\ \text{Op}_R(p)\varphi(y) &= \partial_y (h(y) \varphi(y)) = \text{Op}_L(p)\varphi(y) + (\partial_y h) \varphi(y). \end{aligned} \quad (11)$$

It shows that the order of multiplication with $h(y)$ and differentiation ∂_y is interchanged. The difference involves derivative $\partial_y h$, as the operators do not commute. Applying this to function b_0 , one concludes that $\text{Op}_L(b_0)$ and $\text{Op}_R(b_0)$ are different operators when the velocity depends on x .

A pseudo-differential operator is the operator found by left quantization of a symbol [20,22,19,23]. A symbol p of order $m \in \mathbb{R}$ is a smooth function of a space-time variable and its Fourier associate, say y and η , that satisfies the following technical mathematical condition. For all multi-indices α, β there exists a constant C such that

$$\left| \partial_y^\alpha \partial_\eta^\beta p(y, \eta) \right| \leq C(1 + |\eta|)^{m-|\beta|}. \quad (12)$$

This for example implies that the function $\partial_y h$ in (11) is a symbol also.

In the context of one-way wave equations it is possible to work with a smaller class, namely the *polyhomogeneous* symbols of order m . A polyhomogeneous or classical symbol can be written as an asymptotic sum

$$p(y, \eta) \sim \sum_{j=0}^{\infty} p_j(y, \eta) \quad (13)$$

of homogeneous functions $p_j(y, \eta)$. The homogeneity means that

$$p_j(y, \lambda\eta) = \lambda^{m-j} p_j(y, \eta)$$

for large η and positive λ [20,19]. The function $p_j(y, \eta)$ is thus a symbol of order $m - j$ itself and $p_0(y, \eta)$ is called the *principal* symbol. We are mainly interested in the principal symbol, which contains the greatest contribution. In some cases the sub-principal symbol, i.e. p_1 , is also considered.

To distinguish the operator P from its symbol p and simultaneously emphasize their relation, the operator will also be denoted by $p(y, D_y)$ or $\text{Op}(p) = \text{Op}_L(p)$. We have written the differential operator as $D_y = -i\partial_y$ and shall also write $D_x = -i\partial_x$ and $D_t = -i\partial_t$. By phrasing *operator symbol* or *symbol of operator*, this always refers to the standard quantization, which is left. For example, operator A is the second-order pseudo-differential operator given by

$$A = a(x, D_t, D_x, z) \quad \text{with} \quad a(x, \omega, \xi, z) = \frac{\omega^2}{c(x, z)^2} - \xi^2, \quad (14)$$

in which z is just a parameter.

An important result is that the composition of two pseudo-differential operators, $P = \text{Op}(p)$ of order m and $Q = \text{Op}(q)$ of order n , is again a pseudo-differential operator and has order $m + n$. The symbol of PQ is denoted by $p\#q$ and its asymptotic expansion can be found by a fundamental theorem of the symbolic calculus [20,19]. Because our symbols are time independent, we present this theorem with variables x and ξ :

$$p\#q(x, \xi) \sim \sum_{k=0}^{\infty} \frac{1}{k!} \partial_{\xi}^k p(x, \xi) D_x^k q(x, \xi) \sim p(x, \xi) q(x, \xi) + \partial_{\xi} p(x, \xi) D_x q(x, \xi) + r(x, \xi), \quad (15)$$

in which $r(x, \xi)$ is a symbol of order $m + n - 2$. Clearly, the principal symbol of PQ is the product of the principal symbols of P and Q . An interesting consequence is that the commutator $[P, Q]$ is a pseudo-differential operator of order $m + n - 1$.

2.3. Square root operator

The principal symbol of the square root of operator A is given by the square root of the symbol of operator A , i.e. $b_0(x, \omega, \xi, z)$ in Eq. (8) with $c = c(x, z)$, which has order 1. For the moment, we ignore the singularity, i.e. when $\frac{\omega^2}{c(x, z)^2} - \xi^2 = 0$.

The theory of one-way wave equations is based on a high frequency assumption, and the order of a term in the asymptotic expansion is an important parameter. The principal symbol b_0 determines the rays of the wave field [3]. Hence, $B_0 = \text{Op}(b_0)$ is our first candidate for the square root operator. The error $A - B_0^2$ is an operator with a first-order symbol. This follows from the application of Eq. (15).

To also describe the wave amplitudes, the subprincipal symbol b_1 is needed, as will be argued in the last subsection. Hence, we introduce $B = \text{Op}(b)$ with $b = b_0 + b_1$. The symbol $b_1(x, \omega, \xi, z)$ follows from the symbolic calculus, i.e. (15), and the observation that the error $A - B^2$ must have a zeroth-order symbol. Writing the order below each term, we get

$$\begin{aligned} (b_0 + b_1)\#(b_0 + b_1) &= \sum_{k=0}^{\infty} \frac{1}{k!} [\partial_{\xi}^k b_0 D_x^k b_0 + \partial_{\xi}^k b_0 D_x^k b_1 + \partial_{\xi}^k b_1 D_x^k b_0 + \partial_{\xi}^k b_1 D_x^k b_1] \\ &= b_0^2 + \partial_{\xi} b_0 D_x b_0 + b_0 b_1 + b_1 b_0 + r'_0, \\ &= a + \partial_{\xi} b_0 D_x b_0 + 2b_0 b_1 + r', \end{aligned}$$

in which r' is a symbol of order 0. To cancel the first-order terms, the subprincipal symbol must be

$$b_1 = -\frac{1}{2b_0} \partial_{\xi} b_0 D_x b_0 = i \frac{\xi \partial_x c}{2\omega} \left(1 - \frac{c(x, z)^2 \xi^2}{\omega^2} \right)^{-\frac{3}{2}}, \quad (16)$$

wherein the equality $\partial_{\xi} b_0 D_x b_0 = \frac{-i\omega^2 \xi \partial_x c}{a c(x, z)^3}$ is used. Observe that $-ib_1$ is real for propagated waves, which confirms its effect on the amplitude.

With principal and subprincipal parts, i.e. b_0 and b_1 , defined in (8) and (16), we have found the pseudo-differential operator $B = b(x, D_t, D_x, z)$ such that the error $B^2 - A$ is a pseudo-differential operator of order 0. It is possible to find higher order accurate square roots by repeatedly applying analogous steps. This yields a well-defined infinite asymptotic expansion $\sum_{j=0}^{\infty} b_j$. The order of the error operator $\left[\sum_{j=0}^n b_j(x, D_t, D_x, z) \right]^2 - A$ is $1 - n$ and can be taken arbitrary low [19,22,20]. This is a theoretical proposition we will not use.

2.4. Symmetric quantization

Operator $-\partial_t^2$ and multiplication with $\frac{1}{c(x, z)^2}$ are commutative positive operators. Because we restricted the domain of operator A to the propagation region, i.e. when $\frac{\omega^2}{c^2} < \frac{\omega^2}{c^2}$, A is positive symmetric. Hence, the square root of A is expected to be symmetric, i.e. $(\sqrt{A})^* = \sqrt{A}$. Neglecting regularity conditions, we use symmetry and self-adjointness interchangeably.

In fact, operator $B_0 = \text{Op}(b_0)$ is asymmetric due to the standard left quantization. We therefore define the *symmetric* quantization by

$$\text{Op}_S(p) = \frac{1}{2} [\text{Op}_L(p) + \text{Op}_R(p)]. \quad (17)$$

The right quantization is closely related to the adjoint operator, which can be expressed by $\text{Op}(p)^* = \text{Op}_R(\bar{p})$. If p is real then $\text{Op}_S(p) = \frac{1}{2} [\text{Op}(p) + \text{Op}(p)^*]$ obviously is a symmetric operator. Because b_0 is real, operator $\text{Op}_S(b_0)$ is symmetric, considering the propagation region only. The claim is that the principal and subprincipal symbols of $\text{Op}_S(b_0)$ are identical to b_0 and b_1 , respectively. Note that p and the symbol of $\text{Op}_S(p)$ are not identical.

A general theorem says that the adjoint P^* of a pseudo-differential operator $P = \text{Op}(p)$ of order m is a pseudo-differential operator of the same order. The symbol of the adjoint is denoted by p^* and its asymptotic expansion can be found by a fundamental theorem of the symbolic calculus [20,19]. Again, we present this theorem with variables x and ξ :

$$p^*(x, \xi) \sim \sum_{k=0}^{\infty} \frac{1}{k!} \partial_{\xi}^k D_x^k \bar{p}(x, \xi) \sim \bar{p}(x, \xi) + \partial_{\xi} D_x \bar{p}(x, \xi) + r(x, \xi), \quad (18)$$

in which $r(x, \xi)$ is a symbol of order $m - 2$.

By applying result (18), it can be found that

$$\text{Op}_S(b_0) = \frac{1}{2} \text{Op}(b_0 + b_0^*) = \text{Op}\left(b_0 + \frac{1}{2} \partial_{\xi} D_x b_0 + r'\right),$$

in which r' is a symbol of order -1 . By the observation that $b_0 D_x b_0 = \frac{\omega^2}{2} D_x \frac{1}{c(x, z)}$ does not depend on ξ , one concludes that

$$\partial_{\xi} D_x b_0 = -\frac{1}{b_0} \partial_{\xi} b_0 D_x b_0.$$

Looking back at (16), it can be concluded that the principal and the subprincipal symbols of $\text{Op}_S(b_0)$ are b_0 and b_1 , respectively.

To conclude with, the square root operator with symmetric quantization therefore is

$$\text{Op}_S(b_0) = \frac{1}{2} [\text{Op}_L(b_0) + \text{Op}_R(b_0)]. \quad (19)$$

The practical value of the symmetric quantization lies in the fact that it describes amplitudes without the need for lower order term b_1 . This term involves c and $\partial_x c$ and appears to be more complicated to compute than the principal part. The symmetry argument is general applicable to numerical schemes. In Section 3 we will give two examples of symmetric implementations.

2.5. Normalization

We started this section with the derivation of the one-way wave equation for inhomogeneous media. The z -dependency of the velocity gives rise to matrix operator $\Lambda(\partial_z \mathbf{V})$ in (6). The operators on the diagonal of $\Lambda(\partial_z \mathbf{V})$ will appear as extra terms in the one-way wave equation, making it less attractive from the numerical point of view. We therefore incorporate a normalization factor in the change of variables that will cancel the diagonals [3].

Matrix differential Eq. (4) is the starting point. Fractional powers of A are to be read as pseudo-differential operators with polyhomogeneous symbols. Normalization operators $A^{\frac{1}{4}}$ and $A^{-\frac{1}{4}}$ are real positive by definition.¹ We redefine matrix operators \mathbf{V} and Λ by including the normalization:

$$\mathbf{V} = A^{-\frac{1}{4}} \begin{pmatrix} 1 & 1 \\ i\sqrt{A} & -i\sqrt{A} \end{pmatrix} \quad \text{and} \quad \Lambda = \frac{1}{2} A^{\frac{1}{4}} \begin{pmatrix} 1 & -iA^{-\frac{1}{2}} \\ 1 & iA^{-\frac{1}{2}} \end{pmatrix}. \quad (20)$$

This again yields an eigenvalue decomposition of matrix operator \mathbf{A} given by $\mathbf{A} = \mathbf{V} \mathbf{B} \Lambda$. Using these matrices, the change of variables is defined by $\mathbf{u} = \mathbf{V} \mathbf{v}$. The same procedure as in the begin of this section yields the equation

$$\partial_z \mathbf{v} = (\mathbf{B} - \mathbf{E}) \mathbf{v} - \Lambda \mathbf{f}, \quad (21)$$

in which we used the definition $\mathbf{E} = \Lambda(\partial_z \mathbf{V})$. Working out the details now gives

$$\mathbf{E} = -\frac{1}{4} A^{-1} (\partial_z A) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Due to the normalization, the diagonal terms are zero.

The off-diagonal entries of matrix operator \mathbf{E} are still of concern because they couple the up and down going waves in (21). Actually, there is a subtle argument that says that these terms can be neglected. We will show this in the next subsection. Again writing v for the second component of \mathbf{v} , the one-way wave equation for propagation in the positive z -direction is

$$\partial_z v(t, x, z) = -iBv(t, x, z) + \frac{1}{2} H A^{-\frac{1}{4}} f(t, x, z), \quad (22)$$

in which B can be either $\text{Op}_L(b_0 + b_1)$ or $\text{Op}_S(b_0)$. We have used the Hilbert transform $H := -i\text{Op}(\text{sgn}(\omega))$. Assuming the first component of \mathbf{v} to be zero, i.e. no up going wave, the wave field in terms of the original variable is given by

$$u(t, x, z) = A^{-\frac{1}{4}} v(t, x, z). \quad (23)$$

Comparing (22) with (7), the factor in the source term is changed due to the normalization.

¹ By setting their principal symbols to $a^{\frac{1}{4}}$ and $a^{-\frac{1}{4}}$, respectively. A consequence is that $A^{\frac{1}{4}} A^{\frac{1}{4}} = \text{Op}(\text{sgn}(\omega)) A^{\frac{1}{2}}$.

2.6. High frequency decoupling

Following a procedure based on the work of Taylor [24], we show that the off-diagonal entries of \mathbf{E} can be neglected. The argument relies on the high frequency assumption of the theory.

This assumption is made concrete by stating that the one-way wave equation is *invariant* under the transformation of dependent variables given by $\mathbf{v} \leftrightarrow (\mathbf{I} + \mathbf{K})\mathbf{v}$, in which all four entries of matrix operator \mathbf{K} are arbitrary pseudo-differential operators of order -1 . The pseudo-differential operators in Eq. (21) have polyhomogeneous symbols. Terms of their expansion that do not change under this set of transformations will be called *invariant*. A term that can be made zero is not invariant, of course.

We will show that there exists a transformation like mentioned above, such that the zeroth-order off-diagonals terms of \mathbf{E} become zero. By some knowledge in advance we define

$$\mathbf{K} = \frac{1}{8} A^{-\frac{3}{2}} (\partial_z A) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

which has operator entries of order -1 . The change of variables is defined by $\mathbf{v} = (\mathbf{I} + \mathbf{K})\tilde{\mathbf{v}}$. Inserting this into (21) and subtracting $(\partial_z \mathbf{K})\tilde{\mathbf{v}}$, yields

$$(\mathbf{I} + \mathbf{K})\partial_z \tilde{\mathbf{v}} = ((\mathbf{B} - \mathbf{E})(\mathbf{I} + \mathbf{K}) - (\partial_z \mathbf{K}))\tilde{\mathbf{v}} - \Lambda \mathbf{f}.$$

Let \mathbf{R} be a matrix pseudo-differential operator such that $\mathbf{I} - \mathbf{K} + \mathbf{R}$ is a parametrix of $\mathbf{I} + \mathbf{K}$. A parametrix is an approximate inverse in the sense that the difference between the identity and the composition of an operator with its parametrix is an operator of arbitrary low order [20,19]. It follows that the highest order of the operator entries of \mathbf{R} is -2 . By left multiplication with $\mathbf{I} - \mathbf{K} + \mathbf{R}$ we find

$$\partial_z \tilde{\mathbf{v}} = (\mathbf{I} - \mathbf{K} + \mathbf{R})((\mathbf{B} - \mathbf{E})(\mathbf{I} + \mathbf{K}) - (\partial_z \mathbf{K}))\tilde{\mathbf{v}} - (\mathbf{I} - \mathbf{K} + \mathbf{R})\Lambda \mathbf{f}.$$

The highest orders of the operator entries of the matrices in the homogeneous part of the equation are written below each term. Leaving out operator terms of order less than or equal to -1 , yields

$$\partial_z \tilde{\mathbf{v}} = (\mathbf{B} - \mathbf{E} + \mathbf{BK} - \mathbf{KB})\tilde{\mathbf{v}} - (\mathbf{I} - \mathbf{K} + \mathbf{R})\Lambda \mathbf{f}. \quad (24)$$

Neglecting the commutator $[A^{-\frac{3}{2}}(\partial_z A), A^{\frac{1}{2}}]$ because its leading order is -1 , it can be found by straight forward calculation that

$$\mathbf{BK} - \mathbf{KB} = -\frac{1}{4} A^{-1} (\partial_z A) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

This expression equals \mathbf{E} , and hence, they cancel each other in the homogeneous part of (24).

The change of variables formally shows that the zeroth-order off-diagonal terms in the homogeneous part of Eq. (21) can be neglected. The highest order terms of $\tilde{\mathbf{v}}$ and \mathbf{v} are identical, so to say. Likewise, the factor $(\mathbf{I} - \mathbf{K} + \mathbf{R})$ does not change the leading order of the source term and can be left out. Hence, the system of equations becomes decoupled:

$$\partial_z \mathbf{v} = \mathbf{B}\mathbf{v} - \Lambda \mathbf{f}. \quad (25)$$

The subprincipal part of operator \mathbf{B} describes the wave amplitudes. Therefore, the zeroth-order terms of \mathbf{B} in (25) are expected to be invariant. It is very easy to confirm this. Let K_1, \dots, K_4 be arbitrary pseudo-differential operators of order -1 and set

$$\mathbf{K} = \begin{pmatrix} K_1 & K_2 \\ K_3 & K_4 \end{pmatrix}$$

to define a formal change of variables by $\mathbf{v} \leftrightarrow (\mathbf{I} + \mathbf{K})\mathbf{v}$. By analogous steps to find (24), (25) transforms into

$$\partial_z \mathbf{v} = (\mathbf{B} + \mathbf{BK} - \mathbf{KB})\mathbf{v} - \Lambda \mathbf{f}.$$

The highest order of the operators on the diagonal of commutator $\mathbf{BK} - \mathbf{KB}$ is -1 . This shows that the first- and zeroth-order terms of \mathbf{B} are invariant. Only the principal symbols of the operator entries of \mathbf{V} and Λ are invariant. The pseudo-differential operator $A^{-\frac{1}{4}}$ in the source term of (22) can therefore be replaced by $\text{Op}(a^{-\frac{1}{4}})$.

2.7. Pseudo-differential operator on WKBJ solution

A requirement for true-amplitude one-way wave equations is that they yield the same travel time and amplitude in a WKBJ expansion as the original wave equation. Fortunately, WKBJ theory has been generalized to hyperbolic *pseudo-differential* equations. If $p(y, D_y)$ is a pseudo-differential operator of order m with polyhomogeneous symbol, then there is an asymptotic series for $p(y, D_y)\alpha(y)e^{i\tau\theta(y)}$, i.e.

$$p(y, D_y) \alpha(y) e^{i\tau\theta(y)} = \sum_{j=0}^{\infty} \beta_j(y, \tau) e^{i\tau\theta(y)}, \quad (26)$$

such that $\beta_j(y, \tau) = O(\tau^{m-j})$, assuming $\alpha(y)$ and $\theta(y)$ are C^∞ -functions. See Duistermaat's book [22], equation (4.3.3). Although a detailed treatment falls outside the scope of this paper, we note that it follows that the first two terms in (26) give exactly the required eikonal and transport equations, and therefore, the same WKBJ solution.

3. Numerical implementation

The one-way wave Eq. (22) is an ODE with respect to depth z . The right hand side involves two pseudo-differential operators, namely square root B and $\text{Op}(a^{-\frac{1}{4}})$. We introduce a method to discretize pseudo-differential operators, sufficient general that both operators can be implemented. This method uses interpolation to rephrase the dependency on the velocity such that the operator can be written as a sum of multiplications and convolutions. It will be presented in the following subsection. Other methods can be found in [6,7,25]. We solved the ODE by using the classical fourth-order Runge–Kutta scheme [26].

The (ω, ξ) -domain is split up in two regions. The inequality $\xi^2 < s^2 \omega^2$ defines the *propagation region* and $\xi^2 > s^2 \omega^2$ defines the *evanescent region*. By a *single-phase wave* we mean an uni-directional wave solution for a single (ω, ξ) -pair. Let $\phi \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ be the direction of propagation of a single-phase wave with respect to the z -axis. Then it holds that

$$\sin \phi = \frac{-\xi}{s(x, z) \omega},$$

which shows that the angle depends on the spatial coordinate. This also shows that the singularity of b_0 , i.e. when $\xi^2 = s^2 \omega^2$, coincides with horizontally propagating waves.

We are interested in propagating wave solutions. In the numerical computation, the angle of propagation is bounded. With cutoff angle ϕ_c and maximal angle ϕ_m as parameters, we introduce the angular cutoff function $\psi : [-\frac{\pi}{2}, \frac{\pi}{2}] \rightarrow [0, 1]$. If $|\phi| \leq \phi_c$ then $\psi = 1$, if $|\phi| \geq \phi_m$ then $\psi = 0$ and in between the function makes a continuously differentiable transition using a scaled version of $[0, 1] \ni v \mapsto \frac{1 - \cos(\pi v)}{2}$. Single-phase waves with $\phi \in [-\phi_c, \phi_c]$ are thus undisturbed.

3.1. Pseudo-spectral interpolation method

A pseudo-differential operator with constant coefficients, for example (8), can efficiently be implemented as an multiplication operator in the Fourier domain, using the fast Fourier transform. The integral (9) shows that, in general, the implementation of a pseudo-differential operator involves an inverse Fourier transform for each value of the space-time variable.

The numerical costs can be reduced by writing the operator as a discrete sum of multiplication and convolution operators. This idea is generally used. Bao and Symes, for example, also used this formula to implement pseudo-differential operators [27]. In terms of symbols, it is expressed as

$$p(y, \eta) \approx \sum_{k=1}^K g_k(y) h_k(\eta). \quad (27)$$

The implementation can be done termwise. The order of application of multiplication $\text{Op}(g_k)$ and convolution $\text{Op}(h_k)$ in each term is prescribed by the quantization. In left quantization the convolution comes first. The implementation of $\text{Op}_l(p)\varphi(y)$ will therefore be

$$\sum_{k=1}^K g_k(y) \mathcal{F}^{-1}(h_k(\eta) \hat{\varphi}(\eta)), \quad (28)$$

in which $\hat{\varphi} = \mathcal{F}\varphi$. This involves $1 + K$ (inverse) Fourier transforms. To implement the right quantization, one only has to interchange this order. Then $\text{Op}_r(p)\varphi(y)$ becomes

$$\mathcal{F}^{-1}\left(\sum_{k=1}^K h_k(\eta) \widehat{g_k \varphi}(\eta)\right). \quad (29)$$

The symmetric quantization (17) can therefore be implemented by using $2 + 2K$ (inverse) Fourier transforms. This is cost efficient for small K . In next paragraphs, we will discuss how to find functions g_k and h_k . Remember that we used the notation $y = (t, x)$ and $\eta = (\omega, \xi)$.

To apply this to operators B and $\text{Op}(a^{-\frac{1}{4}})$ we will use the fact that their symbols do not explicitly depend on x and z , and they do not at all depend on t . The symbols are functions of the spatially dependent velocity, which is slowly varying. To express this dependency, we will use the slowness $s(x, z) = \frac{1}{c(x, z)}$ rather than the velocity itself for a reason that will become clear.

A discrete set of slowness values is denoted by s_k with $k = 1, \dots, K$. We take the liberty of writing $g_k(s) = g_k(s(x, z))$ and the symbol of B as $b(s, \omega, \xi) = b(s(x, z), \omega, \xi)$. For each fixed s_k operator B ‘freezes’ to a convolution operator because its sym-

bol, $b(s_k, \omega, \xi)$, is independent of x . To reformulate the symbol dependency on s , we use interpolation with respect to s and approximate the symbol by an interpolant of these frozen symbols:

$$b(s, \omega, \xi) \approx \sum_{k=1}^K g_k(s) b(s_k, \omega, \xi). \quad (30)$$

This formula requires that the interpolant is a linear function of the ordinates, i.e. the frozen symbols. We used linear interpolation.

As the weight functions g_k do not depend on ω and ξ , their definition can best be explained by thinking of ω and ξ being fixed. Let $\Pi_j(s)$ be the first-order polynomial in s through the points $\{(s_i, b(s_i, \omega, \xi))\}_{i=j, j+1}$ with $j \in \{1, \dots, k-1\}$. The weight functions are such that the interpolant, i.e. the right hand side of (30), equals $\Pi_j(s)$ if $s_j \leq s \leq s_{j+1}$. This means that for an arbitrary value of the slowness, the interpolant is a weighted sum of the frozen symbols at the two neighboring discrete slowness values.

Various other interpolation methods can be used also like Hermite interpolation, Taylor series extrapolation and spline. Besides linear interpolation we tried piecewise Lagrange interpolation with cubical polynomials [26]. Let $\Pi_j(s)$ be the unique cubic polynomial in s through the points $\{(s_i, b(s_i, \omega, \xi))\}_{i=j, \dots, j+3}$ with $j \in \{1, \dots, k-3\}$. Then the weight functions are such that the interpolant equals $\Pi_j(s)$ if $s_{j+1} \leq s \leq s_{j+2}$. No improvement was found in the simulation.

3.2. Symmetric square root and normalization

We will apply the pseudo-spectral interpolation method to implement the symmetric square root operator (19). To avoid spurious oscillations in the neighborhood of the singularity, we regularize the principal symbol (8) by multiplying s^2 with $1 - i\epsilon(1 - \psi)$, using the angular cutoff function ψ . Here we use $\phi_c = 60^\circ$ and $\phi_m = 75^\circ$. Subsequently writing the slowness in front, this yields

$$b_{0,\epsilon}(s, \omega, \xi) = s\omega \sqrt{1 - \frac{\xi^2}{s^2\omega^2} - i\epsilon(1 - \psi)}. \quad (31)$$

The constant $\epsilon = 0.04$ is an empirically optimized parameter. Waves with propagation angle larger then the cutoff angle will thus be damped out. To conclude with, the square root operator is given by the symmetric quantization of the symbol:

$$\sum_{k=1}^K g_k(s(x, z)) b_{0,\epsilon}(s_k, \omega, \xi). \quad (32)$$

Note that the angular cutoff function inside $b_{0,\epsilon}(s_k, \omega, \xi)$ uses s_k to determine the angle.

For low values of ξ , the principal symbol (8) approaches a linear function with respect to the slowness and a hyperbola with respect to the velocity. Using the slowness in the interpolation, instead of the velocity, the error is expected to be lower. Because the slowness is slowly varying the number K can be kept low. The set of slowness values, i.e. $\{s_k\}_{k=1, \dots, K}$, are chosen on a logarithmic grid with increment factor $\gamma = 1.08$. For the same K , a logarithmic grid yields a smaller discretization error in (32) then a linear grid.

Fig. 1 shows the symbol of the square root (32) in a dimensionless form. When $s = s_k$ for some k , the discretization error is absent. In that case the deviation of (32) from the single square root, i.e. $v \rightarrow \sqrt{1 - v^2}$ [15], is caused by the regularization only. To visualize the worse case scenario, a large set of curves is shown.

Once the one-way wave equation is solved, the solution is transformed to the original variable by the pseudo-differential equation $u(t, x, z) = \text{Op}(a^{-\frac{1}{4}})v(t, x, z)$. This is implemented by the pseudo-spectral method too. Using the angular cutoff function ψ with $\phi_c = 50^\circ$ and $\phi_m = 90^\circ$ for regularization, the symbol of the operator becomes

$$\sum_{k=1}^K g_k(s(x, z)) \psi(s_k^2 \omega^2 - \xi^2)^{-\frac{1}{4}}. \quad (33)$$

The angular cutoff function uses s_k to determine the angle. It suppresses single-phase waves with propagation angle greater then ϕ_c and evanescent waves. The weight functions $g_k(s)$ are the same as in (30), since they are determined by the set $\{s_k\}_{k=1, \dots, K}$. In accordance with the left quantization, the convolution is applied first. Fig. 2 shows the symbol of the normalization operator (33) in the same way as for the square root.

3.3. Absorbing boundaries and stability

The domain of computation is bounded in the x -coordinate. Due to the discrete Fourier transform it becomes periodic. To suppress the periodicity, absorbing boundaries are obtained by two damping layers with thickness X_d . This is implemented by cutoff function $\chi_d : [-X_d, X + X_d] \rightarrow [0, 1]$. For $x \in [0, X]$ we set $\chi_d(x) = 1$. On $[-X_d, 0]$ and on $[X, X + X_d]$ the function makes a

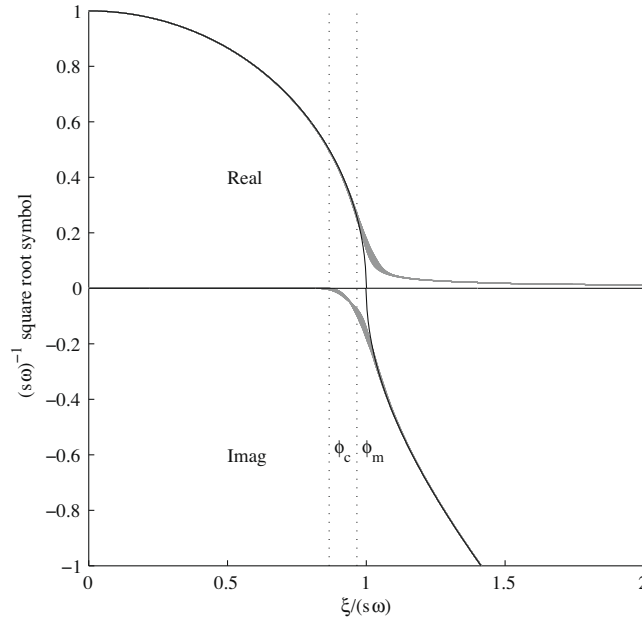


Fig. 1. Real and imaginary part of the square root symbol (32) with $\phi_c = 60^\circ$, $\phi_m = 75^\circ$, $\gamma = 1.08$ and $\epsilon = 0.04$. The graph shows 50 curves, each for a specific slowness s that is randomly chosen between 2×10^{-4} and 7×10^{-4} s/m.

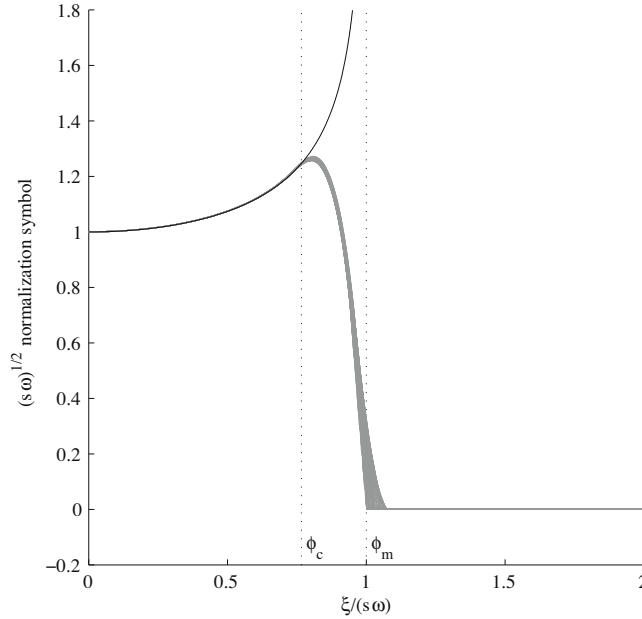


Fig. 2. Real part of the normalization symbol (33) with $\phi_c = 50^\circ$, $\phi_m = 90^\circ$ and $\gamma = 1.08$. The graph shows 50 curves, each for a specific slowness s that is randomly chosen between 2×10^{-4} and 7×10^{-4} s/m.

continuously differentiable transition using a scaled version of $[0, 1] \ni v \mapsto \frac{1 - \cos(\pi v)}{2}$. The damping will be applied simultaneously with solving the ODE. Because the damping should not depend on step size Δz , we apply the root

$$\chi_d(x)^{\frac{\Delta z}{2}} \quad (34)$$

as multiplication operator on the solution after each depth step of the ODE solver. Here, Z_d is the length scale of the damping, measured along the z -axis. This comprises a well-defined, i.e. Δz -independent, damping in the z -direction. For having comprehensible definitions for X_d and Z_d , we relate them to the maximal occurring wavelength λ_{\max} and the maximal propagation angle ϕ_m . We used the empirical lower bounds: $Z_d \geq \lambda_{\max}$ and $X_d \geq Z_d \tan \phi_m$ with $\phi_m = 75^\circ$.

Large negative eigenvalues give rise to stiffness problems [28,29]. We approximate the eigenvalues of operator $-iB$ by its principal symbol $-ib_0$, using (8). With Δz the step size of the z -grid, the dimensionless number $-ib_0\Delta z$ must be in the stability domain of the ODE solver. Using the fourth-order Runge–Kutta scheme, this yields the restrictive condition $\xi_{\max}\Delta z \leq 2.7853$. In our simulations holds $\xi_{\max}\Delta z = 3.1416$. Because we are interested in propagated waves, the stability problems are avoided by smoothly chopping off the negative real values of the square root symbol. Only the real part of $-ib_0$ that negatively exceeds a threshold value is modified. For the threshold we took $-\frac{\omega_{\max}}{\epsilon_{\min}} = -0.1571$.

3.4. Symmetric finite-difference one-way

One-way wave equations can be made true amplitude by using a symmetric square root operator and the wave field normalization specified in (23). In this section we will show how to construct a symmetric finite-difference one-way scheme in 2-D by giving an example. The modification concerns the order of application of multiplication operators and differentiation. The extra numerical cost is therefore small. We present a symmetric implementation of the 60 degree equation [12,15]. Other approximations can be treated similarly.

The square root symbol is written as $\frac{\omega}{c}\sqrt{1-s^2}$ with operator symbol $s = \frac{c\epsilon}{\omega}$. This usage of letter s is restricted to this subsection. Elsewhere it refers to the slowness. To get a symmetric operator, we propose the following quantization. Split the factor $\frac{1}{c}$ into two by defining multiplication operator $M = c(x, z)^{-\frac{1}{2}}$. The square root operator is now written as the composition ωMSM , in which operator S is a symmetric quantization of the symbol $\sqrt{1-s^2}$, or an approximation of this symbol. Note that factors ω can be manipulated easily, as the calculation is done in the frequency domain.

Finite-difference methods rely on a rational approximation of $\sqrt{1-s^2}$ in terms of s^2 . The 60 degree approximation is

$$\sqrt{1-s^2} \approx \frac{1-s^2+\frac{1}{8}s^4}{1-\frac{1}{2}s^2} = 1 - \frac{1}{4}s^2 - \frac{\frac{1}{4}s^2}{1-\frac{1}{2}s^2}. \quad (35)$$

Because it is a rational function of s^2 with constant coefficients, we only have to map s^2 into a symmetric operator. An obvious choice is to interpret s^2 as operator $Q = -\frac{1}{\omega^2}\partial_x c(x, z)^2 \partial_x$. The operator is to be interpreted asymptotically, i.e. for large ω , and because numerator and denominator commute, the quotient in approximation (35) is well-defined.

Application of our proposal yields the one-way wave equation in symmetric form:

$$\partial_z u = i\omega M \left(-1 + \frac{1}{4}Q + \frac{\frac{1}{4}Q}{1-\frac{1}{2}Q} \right) M u \quad (36)$$

We will explain how to calculate $u(z + \Delta z)$ from $u(z)$. The one-way wave equation involves three operator terms, dividing the implementation into three sub steps. Each operator term is calculated separately, using operator splitting.

The second and third terms are implemented with a slightly modified Crank–Nicolson method that can be framed in the following scheme with temporary variables \tilde{u} , N and D :

$$\partial_z \tilde{u} = M \frac{N}{D} M \tilde{u}(z) \quad \rightarrow \quad \frac{\tilde{u}(z + \Delta z) - \tilde{u}(z)}{\Delta z} = M \frac{N}{D} M \frac{\tilde{u}(z + \Delta z) + \tilde{u}(z)}{2}. \quad (37)$$

Operator $M \frac{N}{D} M$ is, unlike Crank–Nicolson, evaluated at intermediate grid point $z + \frac{1}{2}\Delta z$. Due to the fact that the velocity is slowly varying, the associated discretization error is negligible. The lateral discretization is done with a central difference. This will be shown in a moment. Rewriting discretization formula (37) and left multiplying with DM^{-1} yield the result:

$$\left(DM^{-1} - \frac{1}{2}\Delta z NM \right) \tilde{u}(z + \Delta z) = \left(DM^{-1} + \frac{1}{2}\Delta z NM \right) \tilde{u}(z). \quad (38)$$

We first apply this to the third operator of the one-way wave equation in (36), i.e. with $N = i\omega \frac{1}{4}Q$ and $D = 1 - \frac{1}{2}Q$. The first intermediate result u_1 is found by solving:

$$\left(\left[1 - \frac{1}{2}Q \right] M^{-1} - \frac{1}{8}\Delta z i\omega Q M \right) u_1 = \left(\left[1 - \frac{1}{2}Q \right] M^{-1} + \frac{1}{8}\Delta z i\omega Q M \right) u(z). \quad (39)$$

Then the second operator is to be calculated. We set $N = i\omega \frac{1}{4}Q$ and $D = 1$. The second intermediate result u_2 is given by:

$$\left(M^{-1} - \frac{1}{8}\Delta z i\omega Q M \right) u_2 = \left(M^{-1} + \frac{1}{8}\Delta z i\omega Q M \right) u_1. \quad (40)$$

The final step is the calculation of the first operator, which gives a phase shift. The result is our numerical approximation of $u(z + \Delta z)$:

$$u(z + \Delta z) = e^{-i\frac{\omega}{c}\Delta z} u_2, \quad (41)$$

in which the velocity c is conformably evaluated at $z + \frac{1}{2}\Delta z$.

We used the central difference formula to discretize M and Q laterally. As the calculation is done in the frequency domain, we may equally discuss how to implement $-\omega^2 Q = \partial_x c(x, z)^2 \partial_x$. By the numerical scheme in (37) the velocity is evaluated at $z + \frac{1}{2} \Delta z$, so we omit the depth argument now. Written in temporary variable \tilde{u} , the discrete form of $\partial_x c(x)^2 \partial_x \tilde{u}(x)$ is

$$\frac{c(x + \frac{1}{2} \Delta x)^2 [\tilde{u}(x + \Delta x) - \tilde{u}(x)] - c(x - \frac{1}{2} \Delta x)^2 [\tilde{u}(x) - \tilde{u}(x - \Delta x)]}{\Delta x^2}. \quad (42)$$

The value of the velocity at an intermediate grid point is approximated by the average of the values at the two closest grid points, i.e. $c(x + \frac{1}{2} \Delta x)^2 \approx \frac{1}{2} [c(x)^2 + c(x + \Delta x)^2]$. Because c is smooth the error is small.

Together with (42) the numerical formulae in (39) and (40) are tridiagonal linear systems that are solved successively. The exponential in (41) then gives the wave field at next depth. The system is closed with homogeneous Dirichlet boundary conditions at $x = -X_d$ and $x = X_d$. The effect of these hard walls is abolished by the absorbing boundaries discussed above.

It is interesting to make a comparison with the work of Zhang et al. in [4,5]. They interpreted s^2 as the asymmetric operator $-\frac{1}{\omega^2} (c \partial_x)^2$, see [4] Appendix A. However, they did not split the $\frac{1}{c}$ multiplication in two, but kept it on the left side. Careful examination reveals that their square root operator equals ωMSM if we interpret s^2 as $-\frac{1}{\omega^2} c^{\frac{1}{2}} \partial_x c \partial_x c^{\frac{1}{2}}$, which is an symmetric alternative. Their true-amplitude scheme can hence be derived from our symmetrization procedure.

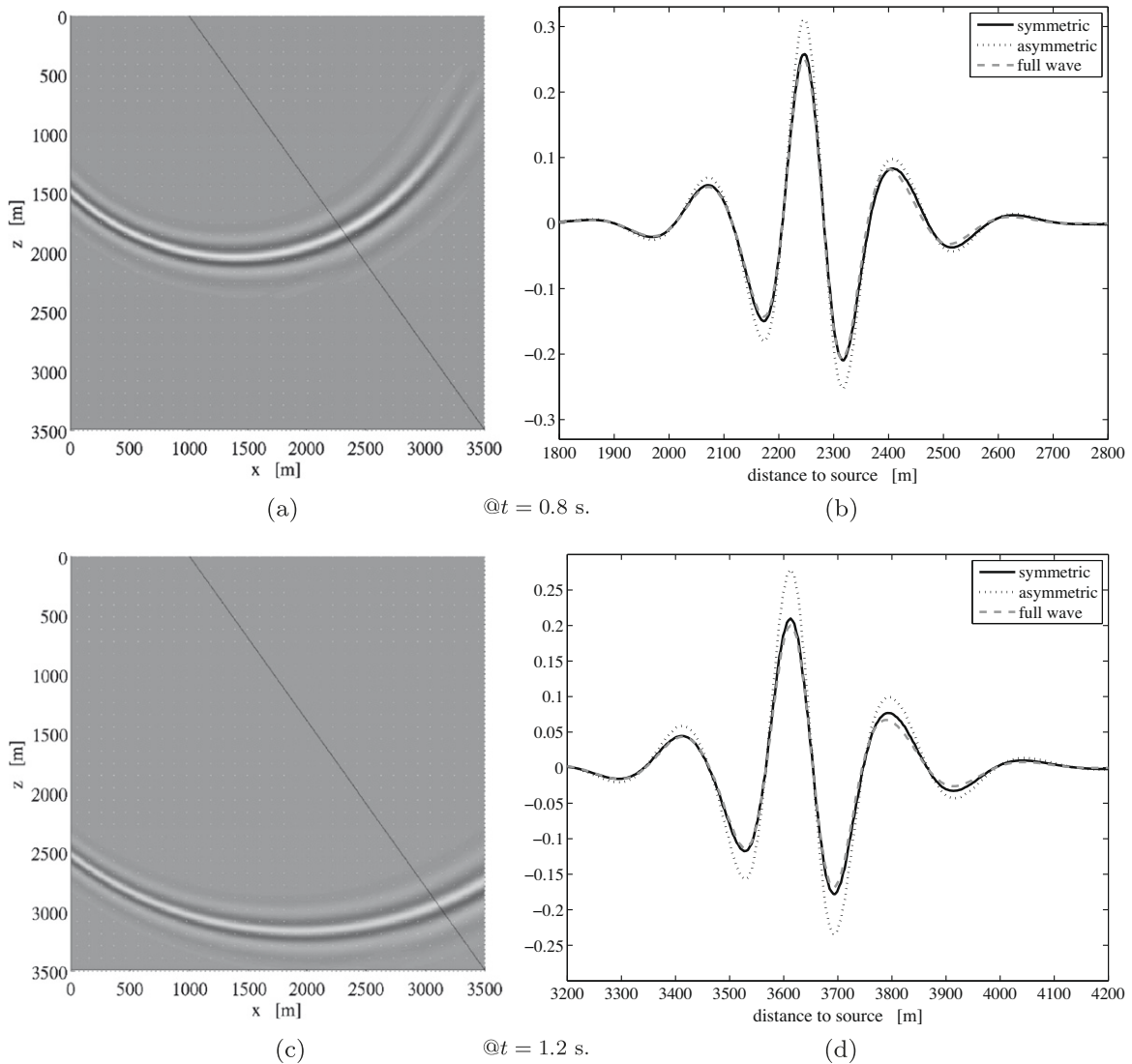


Fig. 3. (a) & (c): snapshots of wave field $v(t, x, z)$ simulated with pseudo-spectral method. The black line indicates where the cross-section is taken. (b) & (d): cross-section of snapshot. Solid line: symmetric square root. Dotted line: asymmetric square root. Dashed line: full wave equation. The velocity is $c = 2000 + 0.5x$.

The symmetric implementation will be used in wave propagation simulations. We make a comparison with an asymmetric implementation of the 60 degree equation. In the asymmetric variant we write coefficients on the left of derivatives, replacing formulae (39) and (40) with

$$\left(1 + \frac{1}{2} \frac{c^2}{\omega^2} \partial_x^2 + \frac{1}{8} \Delta z i \frac{c}{\omega} \partial_x^2\right) u_1 = \left(1 + \frac{1}{2} \frac{c^2}{\omega^2} \partial_x^2 - \frac{1}{8} \Delta z i \frac{c}{\omega} \partial_x^2\right) u(z) \quad (43)$$

and

$$\left(1 + \frac{1}{8} \Delta z i \frac{c}{\omega} \partial_x^2\right) u_2 = \left(1 - \frac{1}{8} \Delta z i \frac{c}{\omega} \partial_x^2\right) u_1. \quad (44)$$

The lateral operators are straight forward discretized with the central difference method.

4. Numerical results

As was theoretically shown in Section 2, the one-way wave equation describes uni-directional waves with correct amplitude if the symmetric square root operator $\text{Op}_s(b_0)$ is used and the normalization of the wave field $u = A^{-\frac{1}{4}}v$. We numerically

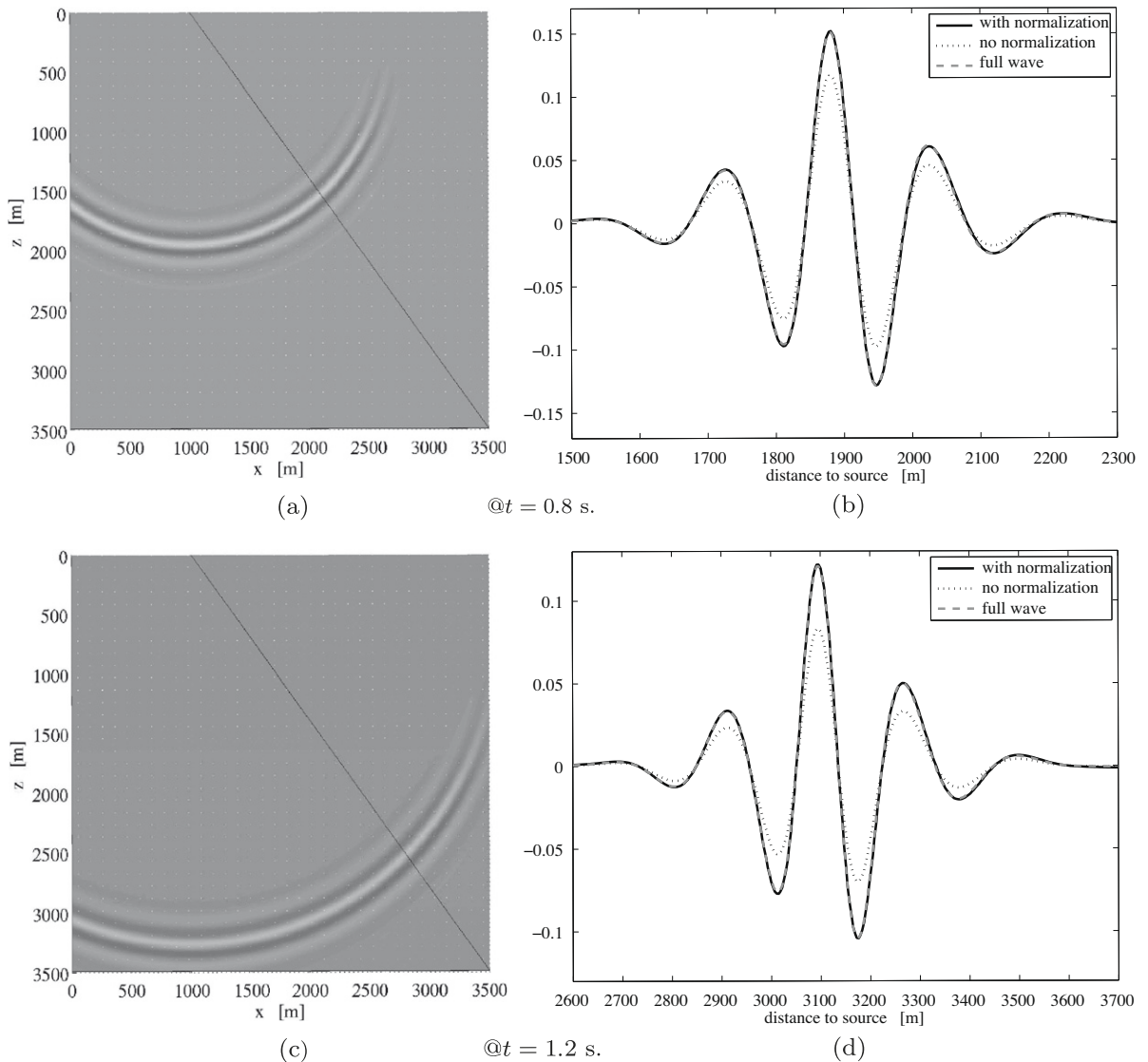


Fig. 4. (a) & (c): snapshots of wave field $v(t, x, z)$ simulated with pseudo-spectral method. The black line indicates where the cross-section is taken. (b) & (d): cross-section of snapshot. Solid line: with normalization. Dotted line: without normalization. Dashed line: full wave equation. The velocity is $c = 2000 + 0.5z$.

verify this by simulating wave propagation through media with linearly varying velocity. We first use the implementation of the pseudo-spectral method, both with symmetric and asymmetric square root and compare the results. A similar experiment is done with and without normalization, using, respectively, (7) and (22). We subsequently repeat the first simulations, now using the finite-difference one-way scheme to implement the symmetric and asymmetric square root operator. The solution of the full wave equation act as a reference. It is implemented by a finite-difference time domain solver. Finally, a simulation with a more complex velocity function is done.

The source term in our model is an approximated delta function given by

$$f(t, x, z) = \delta(t - t_s) \frac{1}{2\pi\sigma^2} e^{-\frac{1}{2} \frac{(x-x_s)^2 + (z-z_s)^2}{\sigma^2}}.$$

This source is used in all simulations. It is located at $(t_s, x_s, z_s) = (0s, 1000m, 0m)$ in time and space. The radius of the circular shaped cross-section at half height is $\sigma\sqrt{2\ln 2}$ with $\sigma = 25m$. To regularize the intrinsic singularity with respect to time, a convolution operator is used to cancel high and low frequencies. The frequency band 20–30 Hz is undisturbed. From 20 to 10 Hz and from 30 to 50 Hz the source is gradually suppressed to zero.

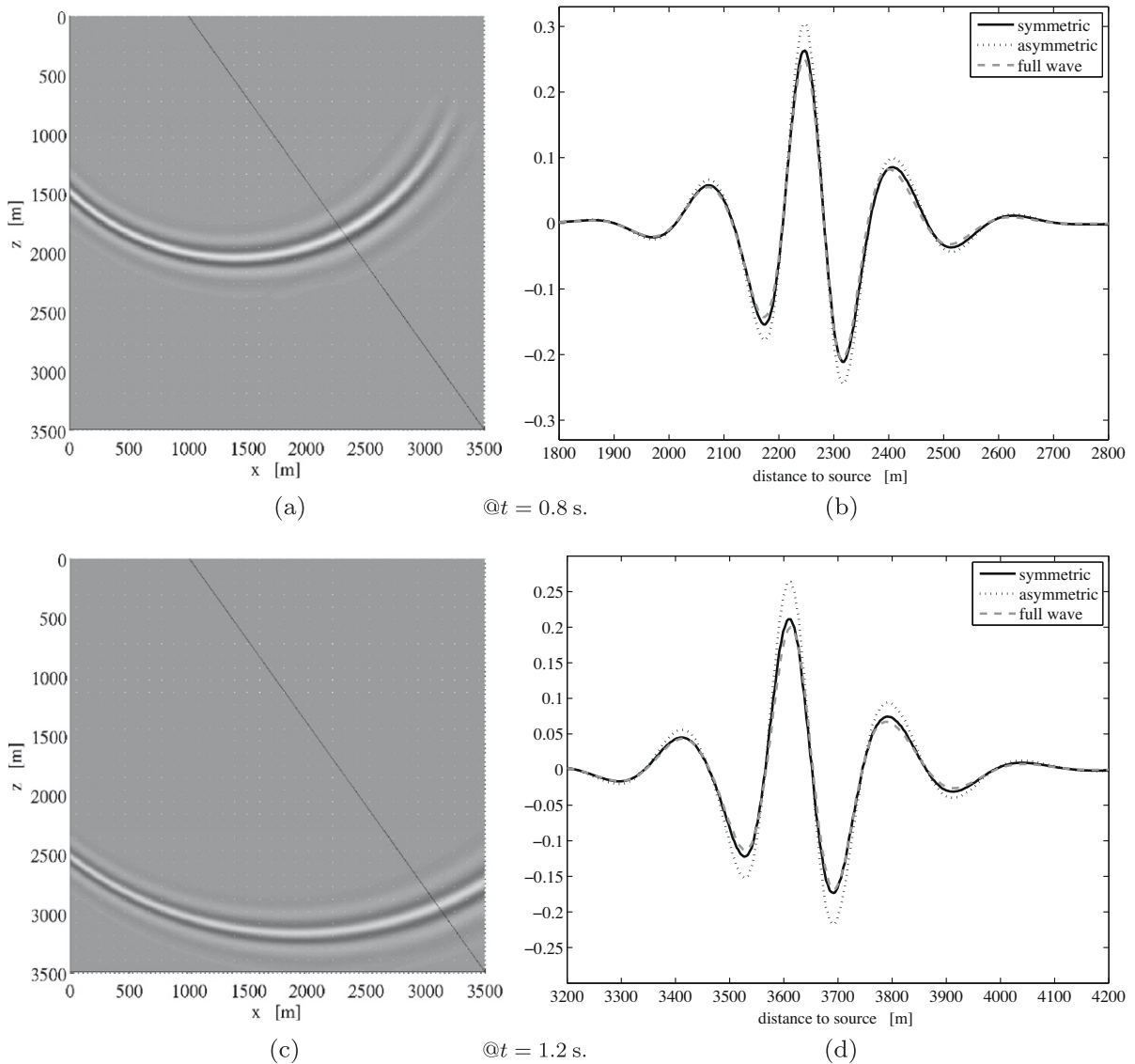


Fig. 5. (a) & (c): snapshots of wave field $v(t, x, z)$ simulated with finite-difference one-way as depth stepper. The black line indicates where the cross-section is taken. (b) & (d): cross-section of snapshot. Solid line: symmetric implementation square root. Dotted line: asymmetric square root. Dashed line: full wave equation. The velocity is $c = 2000 + 0.5x$.

As was mentioned before, operator $\text{Op}(a^{-\frac{1}{4}})$ is also involved in the source term of the one-way wave Eq. (22). The source we used in the modeling has a small support in x and z . In the implementation of the operator we therefore approximate the slowness by a constant, i.e. the average value within the support.

The effect of the symmetric square root is verified in a simulation with the lateral varying velocity function $c = 2000 + 0.5x$. Fig. 3(a) and (c) show snapshots of the simulated wave field $v(t, x, z)$ at times $t = 0.8$ and 1.2 s. These are simulated with the one-way wave equation and the symmetric square root operator, i.e. Eq. (22) with (19). The straight black lines indicate where a cross-section is taken.

Fig. 3(b) and (d) show the cross-section of the snapshot as function of the distance to the source, zoomed in on the wave front. Besides the cross-section plotted with a solid line, it also shows the analogous curves from other numerical simulations. The dotted line is calculated with the one-way wave equation and the asymmetric square root operator, i.e. $B_0 = \text{Op}(b_0)$. The dashed line is from a simulation of the full wave equation. With respect to the full wave simulation at $t = 1.2$ s, the amplitude from the asymmetric implementation is 39% larger. With the symmetric implementation this is reduced to 5%.

The effect of the normalization is verified in simulations with velocity function $c = 2000 + 0.5z$. Fig. 4(a) and (c) show snapshots of the simulated wave field $v(t, x, z)$ at times $t = 0.8$ and 1.2 s. These are simulated with the one-way wave equation with normalization (22). Again, straight black lines indicate cross-sections.

Fig. 4(b) and (d) show the cross-section of the snapshot as function of the distance to the source, analogous to the previous figure. Besides the cross-section plotted with a solid line, it also shows other numerical results. The dotted line is calculated with the one-way wave equation without normalization, i.e. Eq. (7). In both cases, the symmetric square root operator (19) is used. The dashed line is again from a simulation of the full wave equation. Again compared with the full wave simulation at $t = 1.2$ s, the amplitude from the implementation without normalization is 31% smaller. With normalization, the amplitude is 1% larger with respect to the full wave simulation. The cross-section graphs coincide almost completely.

We derived a symmetric and an asymmetric version of the 60 degree finite-difference equation. With these, we simulated wave propagation with velocity function $c = 2000 + 0.5x$. The normalization operator is still implemented by the pseudo-spectral method. Fig. 5(a) and (c) show snapshots of the simulated wave field $v(t, x, z)$ at times $t = 0.8$ and 1.2 s. Fig. 5(b) and (d) show cross-sections of several simulations. The dotted line is calculated with the asymmetric square root, the solid line with the symmetric one. The dashed line is from the full wave simulation. With respect to the full wave simulation at $t = 1.2$ s, the amplitude from the asymmetric implementation is 32% larger. With the symmetric implementation this is again reduced to 5%.

Our last simulation has a more complex velocity function, consisting of a circular smooth blob of increased velocity superimposed on a velocity that linearly increases with depth, see Fig. 6. We compare the pseudo-spectral method with the finite-difference implementation of the full wave equation. Fig. 7 shows the wave fields $v(t, x, z)$ at times $t = 0.9$ s and $t = 1.3$ s for both methods and the cross-sections on the indicated diagonal line. The solid black line represents the one-way wave, the dashed gray the full wave. One clearly notices the absence of wide angle wave propagation in the one-way wave simulation. This is of course a consequence of using a one-way method. Apart from this the similarity is quite good, although some small differences remain as can be seen in the bottom graphs of Fig. 7.

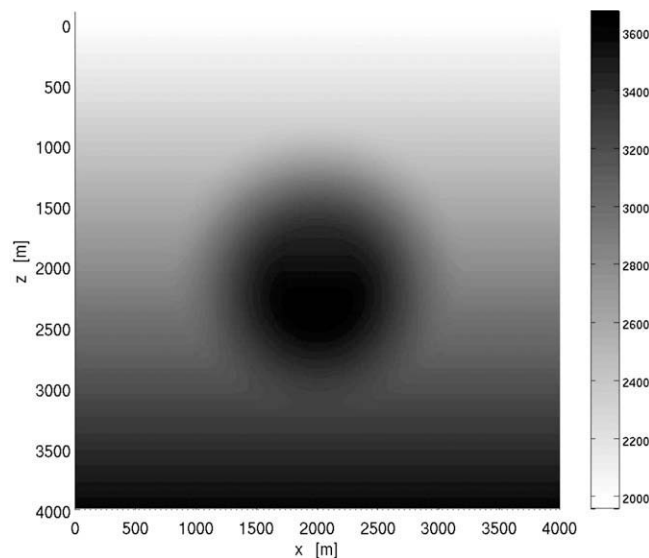
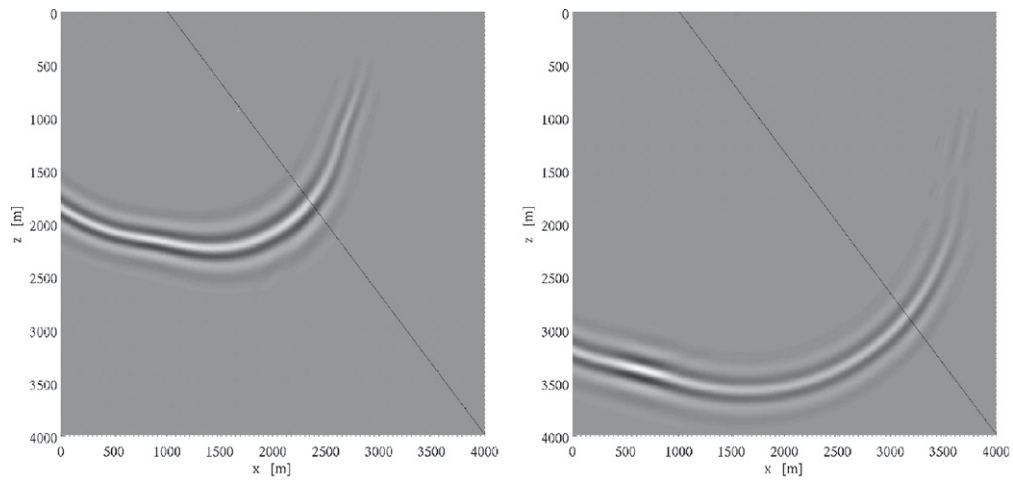
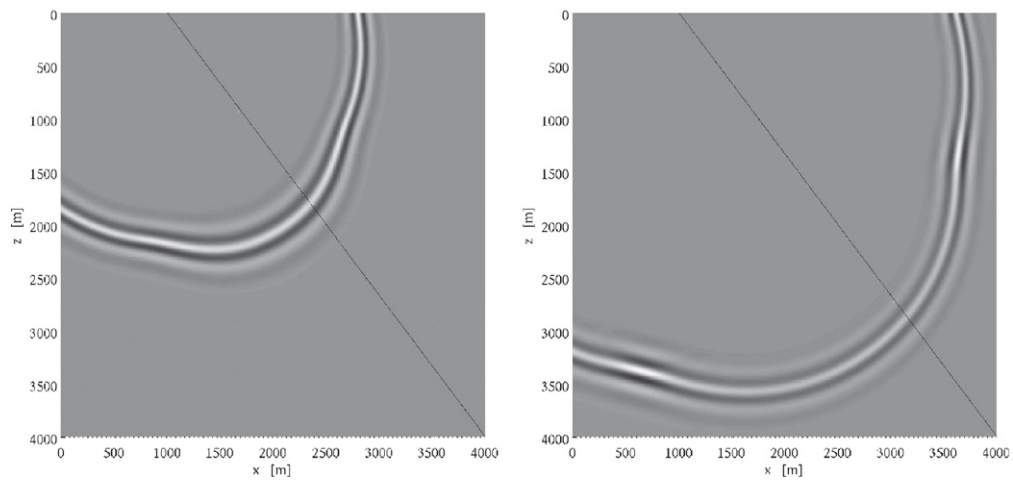


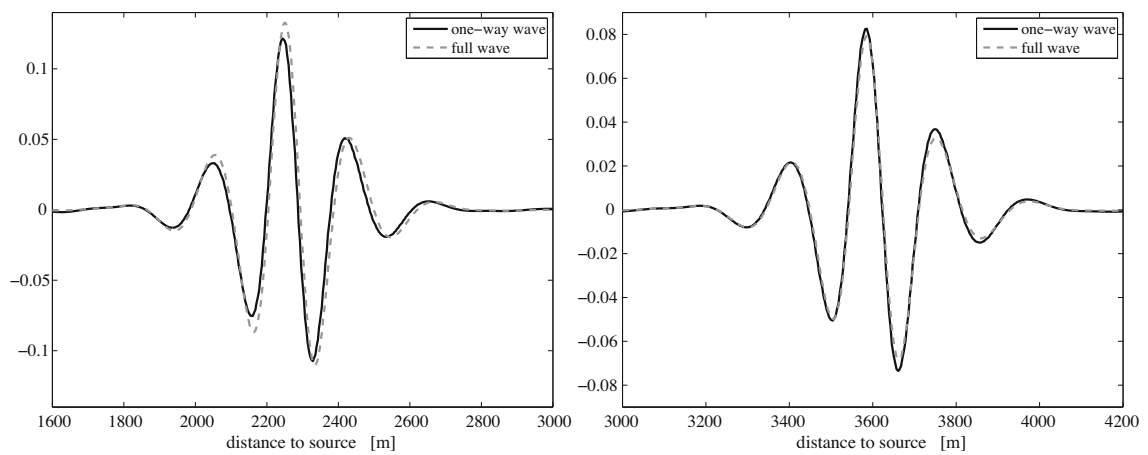
Fig. 6. Velocity model $c = c(x, z)$ in m/s.



Pseudo-spectral method on one-way wave equation (22).



Finite-difference solver on full wave equation.



Cross sections of both.

Fig. 7. Snapshots of simulated wave field $v(t, x, z)$. Left column: at $t = 0.9$ s. Right column: at $t = 1.3$ s. The black line in the first four graphs indicates where the cross-section is taken. The velocity is given in Fig. 6.

5. Discussion

The above examples show that the symmetrization of the square root operator and the normalization of the wave field together yield a one-way wave method with correct amplitudes. The theoretical basis is that symmetrization and normalization, respectively, remove the following two correction terms from the equation:

$$-ib_1 = \frac{\xi \partial_x c}{2\omega} \left(1 - \frac{c(x, z)^2 \xi^2}{\omega^2} \right)^{-\frac{3}{2}} \quad (45)$$

correcting the asymmetric square root, and

$$-\frac{1}{4}A^{-1}(\partial_z A) = \frac{\partial_z c}{2c} \left(1 - \frac{c(x, z)^2 \xi^2}{\omega^2} \right)^{-1} \quad (46)$$

changing the amplitude in depth dependent media. As an alternative we could have calculated these terms explicitly.

The factor $(\cos \phi)^{-3}$ in correction term (45) has a strong singularity making it difficult to implement. The symmetry argument on the other hand, can easily be applied in numerical schemes by properly choosing the order of multiplications and derivatives. And the symmetrization of the finite-difference one-way method leads to almost no extra cost. The implementation of correction term (46) has the same objection, and because it is to be applied at every depth step, this gives an accumulation of errors. The normalization operator on the other hand, has the advantage that it is to be applied only at source and at depths where output is written, not in every depth step.

We did not make a detailed analysis of the computational cost of the pseudo-spectral interpolation method. For depth stepping it appears to be expensive due to the relatively small step size taken in the explicit Runge–Kutta solver. It clearly approximates the pseudo-differential operator and has the advantage to be applicable for both the square root and the normalization operator. Further study could be valuable, for example to find a fast implementation of the normalization.

We found that the normalization and the angular cutoff are sensitive to details of the implementation, for example the choice of cutoff angle ϕ_c . Poor parameter choices may lead to artifacts. A better understanding could be an interesting motivation for further study.

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