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Separation-of-variables as a preconditioner for an iterative Helmholtz solver

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Abstract

A preconditioned iterative method based on separation-of-variables for solving the Helmholtz equation in an inhomogeneous medium is tested. The preconditioner is constructed by approximating the wavenumber by a sum of two terms, one depending only on one spatial coordinate, say x, and the other depending on the remaining coordinates. The Helmholtz equation can be solved efficiently if the wavenumber has such a separable form. First, an eigenvalue-eigenvector decomposition is applied in the x-direction. With these eigenvectors, a change of variables is performed in order to obtain a set of independent systems with one dimension less than the original one. For smooth models and low frequencies, the convergence rate with this preconditioner is satisfactory. Unfortunately, it rapidly deteriorates when the roughness of the model or the frequency increases. Examples from seismic modeling are given to illustrate this behaviour. Moreover, numerical evidence is presented that suggests that the decomposition of the wavenumber in the sum of two terms cannot be improved with this approach.
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Keywords: Helmholtz equation; Preconditioner; Separation of variables; Iterative solver

1. Introduction

Wave propagation through an inhomogeneous acoustic medium with a constant density is described in the frequency domain by the Helmholtz equation

$$-\Delta u - k^2 u = f, \tag{1}$$

where u is the pressure field and f a point source term. The wavenumber $k = \omega/c$ is a function of the spatial coordinates because the velocity, c, depends on the spatial coordinates in an inhomogeneous medium.

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In practice, for instance when modeling a seismic survey, the wavenumber is such that the operator has positive and negative eigenvalues. To mimic an infinite space by a finite computational domain, absorbing boundary conditions are added. These boundary conditions make the system invertible, although it remains ill-conditioned.

To solve Eq. (1) with suitable boundary conditions, a finite-difference discretisation is applied leading to the linear system

$$\mathrm{Au} = \mathrm{f}. \tag{2}$$

The matrix A is a large but sparse matrix. The solution u is represented on a grid with between 500 and 2000 points per coordinate direction in typical seismic applications. In 2D, the system (2) can be solved by a direct method based on LU-factorisation. With the nested dissection reordering method using n points in each coordinate direction, the complexity of the LU-factorisation is $\mathrm{O}(n^3)$ and the computation of the solution has a cost of $\mathrm{O}(n^2 \log n)$, which is the optimal complexity for direct methods [5]. In 3D, a direct solver is generally too expensive. For instance, the complexity of the LU-factorisation with the nested dissection method is $\mathrm{O}(n^6)$.

To fully take into account the sparseness of A, an iterative method should therefore be applied. A preconditioner is needed to speed up the method. In the literature, the linear system (2) is often solved by an iterative preconditioned method based on Krylov spaces, for instance by the GMRES method [10]. Without being exhaustive, we mention the use of multilevel/multigrid methods [3,8], domain decomposition [7], and fast direct solvers [4,6,9] to build a preconditioner. However most of the applications in these articles are related to the exterior problem where the reflection by a given obstacle of a plane wave propagating in an homogeneous medium is studied. In [7], the system (2) is iteratively solved in a layered medium by a domain decomposition method, the preconditioner being based on a Schur-complement algorithm with fast Poisson-type preconditioners for the subdomain. The numerical example shows a fast convergence for a four-layer domain. The method seems well-suited for modeling waveguides.

Here we focus on the modeling of a seismic survey. The velocity is either a smooth model or a model consisting of a large number of inhomogeneous layers, which is unfavourable for the use of a domain decomposition approach. In seismic survey, a source is triggered at a certain position. A pressure wave propagates from the source and is reflected or refracted at discontinuities in the subsurface. The pressure field is recorded at the receiver locations. The modeling requires the computation of the wave propagation in a highly inhomogeneous medium, examples of which are given in Figs. 2 and 3. The linear system has eigenvalues with negative and positive real parts, making, for instance, the multigrid method difficult to use. This approach does not perform very well because the coarser grids must be fine enough to represent the solution. In this paper, we have decided to study an iterative solver with a preconditioner based on the separation-of-variables technique [6,9], but applied to examples where the wavenumber is not constant. This technique leads to a direct solver when the wavenumber, k, is constant. When the wavenumber is separable, meaning that it can be expressed as a sum of two terms, one depending on one coordinate, x, and the second depending on the other coordinates, the separation-of-variables would have been exact if it were not for the absorbing boundary conditions. For a general wavenumber distribution, the technique can be used as a preconditioner. The idea is to replace the wavenumber k by a separable wavenumber and use this approximation to build the preconditioner. The BIGCSTAB iterative method [11] is applied to solve the system (2).

The paper is organized as follows. First, the discretisation of the problem is described. Secondly, the separation-of-variables technique is reviewed. Thirdly, the iterative preconditioned method is outlined.

Fourthly, examples at different frequencies are considered. The method is first applied to a one-dimensional example to show the relevance of the approach when the model is separable. Then more complicated two-dimensional models are considered to study the limitations of this approach for large wavenumbers. No comparisons with other existing methods have been made, because the goal was to study the separation-of-variables in the context of seismic modeling and the results were not encouraging enough to further pursue this approach. For the same reason, no three-dimensional implementation has been carried out. Finally, numerically evidence is provided suggesting that the approach cannot easily be improved. In this paper, the general description refers to three-dimensional problems, but the examples are restricted to two space dimensions to reduce the computational requirements.

2. Setting of the problem

The propagation of the pressure field, u, in an acoustic model with constant density is assumed to obey the wave equation

$$-\Delta u(x,y,z) + \frac{1}{c^2(x,y,z)}\frac{\partial^2 u}{\partial t^2} = f(t)\delta(x,y,z), \tag{3}$$

where x, y, and z are the three spatial coordinates, c is the velocity field, and f the source function. The source is a point source.

In the frequency domain, after a Fourier transform, this leads to the Helmholtz equation

$$-\Delta u(x,y,z) - k^2(x,y,z)u(x,y,z) = f(\omega)\delta(x,y,z), \tag{4}$$

with $k = \omega/c$ the wavenumber.

For numerical reasons, the computation are performed in a bounded domain and absorbing boundary conditions are needed where the earth model is truncated. We consider a box-shaped computational domain $[x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}] \times [z_{\min}, z_{\max}]$. First-order absorbing boundary conditions at the boundaries of the domain are:

$$\pm\frac{\partial u}{\partial n} - iku = 0, \tag{5}$$

with n representing x, y, or z, depending on the boundary.

More sophisticated boundary conditions, for instance second-order boundary conditions, can be used [1,6]. We did not implemented the second-order boundary conditions because we wanted first to test the separation-of-variables technique as a preconditioner for the Helmholtz equation in the context of seismic modeling. To investigate the usefulness of this type of preconditioner, we have decided to restrict ourselves to the first-order absorbing boundary conditions.

A finite-difference scheme is applied to solve Eq. (4) with boundary conditions (5). The domain is discretised with $M+2$ points in x, $N+2$ points in y, and $L+2$ points in z, using

$$\begin{cases} x_m = x_{\min} + m\Delta x & \forall 0 \leqslant m \leqslant M+1 \text{ with } x_{M+1} = x_{\max}, \\ y_n = y_{\min} + n\Delta y & \forall 0 \leqslant n \leqslant N+1 \text{ with } y_{N+1} = y_{\max}, \\ z_l = z_{\min} + l\Delta z & \forall 0 \leqslant l \leqslant L+1 \text{ with } z_{L+1} = z_{\max}. \end{cases} \tag{6}$$

In the interior points, the discretisation is

$$\begin{aligned}
&\frac{-u(x_{m-1}, y_n, z_l) + 2u(x_m, y_n, z_l) - u(x_{m+1}, y_n, z_l)}{\Delta x^2} \\
&\quad + \frac{-u(x_m, y_{n-1}, z_l) + 2u(x_m, y_n, z_l) - u(x_m, y_{n+1}, z_l)}{\Delta y^2} \\
&\quad + \frac{-u(x_m, y_n, z_{l-1}) + 2u(x_m, y_n, z_l) - u(x_m, y_m, z_{l+1})}{\Delta z^2} - k^2(x_n, y_m, z_l) \\
&= \delta(x_n, y_m, z_l) f(\omega),
\end{aligned} \tag{7}$$

and on the boundaries

$$\begin{cases}
u(x_0, y_n, z_l) = \dfrac{u(x_1, y_n, z_l)}{1 + ik(x_0, y_n, z_l)\Delta x} = \gamma_x^{\min}(n, l) u(x_1, y_n, z_l), \\
u(x_{M+1}, y_n, z_l) = \dfrac{u(x_M, y_n, z_l)}{1 + ik(x_{M+1}, y_n, z_l)\Delta x} = \gamma_x^{\max}(n, l) u(x_M, y_n, z_l), \\
u(x_m, y_0, z_l) = \dfrac{u(x_m, y_1, z_l)}{1 + ik(x_m, y_0, z_l)\Delta y} = \gamma_y^{\min}(m, l) u(x_m, y_1, z_l), \\
u(x_m, y_{N+1}, z_l) = \dfrac{u(x_m, y_N, z_l)}{1 + ik(x_m, y_{N+1}, z_l)\Delta y} = \gamma_y^{\max}(m, l) u(z_m, y_N, z_l), \\
u(x_m, y_n, z_0) = \dfrac{u(x_m, y_n, z_1)}{1 + ik(x_m, y_n, z_0)\Delta z} = \gamma_z^{\min}(m, n) u(x_m, y_l, z_1), \\
u(x_m, y_n, z_{L+1}) = \dfrac{u(x_m, y_n, z_L)}{1 + ik(x_m, y_n, z_{L+1})\Delta z} = \gamma_z^{\max}(m, n) u(x_m, y_l, z_L).
\end{cases} \tag{8}$$

By substituting (8) into (7), the discretisation of (4) and (5) leads to the following linear system:

$$\mathrm{Au} = \mathrm{f}, \tag{9}$$

with u and f two vectors of size MNL and A an MNL by MNL matrix.

The matrix A is a sparse matrix with only about $7MNL$ non-zero elements. A natural way to solve this system would be to apply an LU-decomposition. In 2D, this is feasible with an acceptable computational cost if the nested dissection reordering [5] is applied to reduce the fill-in. In this way, a direct solver is obtained that can be used to solve problems with about 1000 points in each coordinate direction on a workstation. In 3D, unfortunately, reordering methods are not efficient enough to avoid substantial fill-in and such direct methods are not affordable for medium-size problems. Therefore, the linear system needs to be solved by an iterative method.

3. Separation of variables

The matrix A is the sum of a matrix corresponding to the Laplacian operator with some boundary conditions and a diagonal matrix K containing the square values of the wavenumber. Except for the

boundary conditions, the separation-of-variables technique can be applied to solve the Laplacian operator. If we consider the following approximations for the absorbing boundary conditions,

$$\begin{cases} \gamma_x^{\min}(n,l) = \bar{\gamma}_x^{\min} & \text{and} \quad \gamma_x^{\max}(n,l) = \bar{\gamma}_x^{\max} \quad \forall n,l, \\ \gamma_y^{\min}(m,l) = \bar{\gamma}_y^{\min}(l) & \text{and} \quad \gamma_y^{\max}(m,l) = \bar{\gamma}_y^{\max}(l) \quad \forall m, \\ \gamma_z^{\min}(m,n) = \bar{\gamma}_z^{\min}(n) & \text{and} \quad \gamma_z^{\max}(m,n) = \bar{\gamma}_z^{\max}(n) \quad \forall m, \end{cases} \tag{10}$$

the matrix A can be rewritten as

$$\mathrm{A} = \mathrm{A}_x \otimes \mathrm{I}_{yz} + \mathrm{I}_x \otimes \mathrm{A}_{yz} - \mathrm{K}, \tag{11}$$

with I_x the M by M identity matrix, I_{yz} the NL by NL identity matrix,

$$\begin{cases} \mathrm{A}_x(m,m) = \dfrac{2}{\Delta x^2} + \begin{cases} \bar{\gamma}_x^{\min} & \text{if } m = 1, \\ \bar{\gamma}_x^{\max} & \text{if } m = M, \\ 0 & \text{otherwise,} \end{cases} \\ \mathrm{A}_x(m+1,m) = \mathrm{A}_x(m,m+1) = -\dfrac{1}{\Delta x^2}, \end{cases} \tag{12}$$

and

$$\text{for } p = (l-1)N + n,$$

$$\begin{cases} \mathrm{A}_{yz}(p,p) = \dfrac{2}{\Delta y^2} + \dfrac{2}{\Delta z^2} + \begin{cases} \bar{\gamma}_y^{\min}(l) & \text{if } n = 1, \\ \bar{\gamma}_y^{\max}(l) & \text{if } n = N, \\ \bar{\gamma}_z^{\min}(n) & \text{if } l = 1, \\ \bar{\gamma}_z^{\max}(n) & \text{if } l = L, \\ 0 & \text{otherwise,} \end{cases} \\ \mathrm{A}_{yz}(p,p+1) = \mathrm{A}_{yz}(p+1,p) = -\dfrac{1}{\Delta y^2}, \\ \mathrm{A}_{yz}(p,p+N) = \mathrm{A}_{yz}(p+N,p) = -\dfrac{1}{\Delta z^2}. \end{cases} \tag{13}$$

Generally K prevents us from using separation-of-variables. However, the square of the wavenumber can be decomposed into

$$k^2(x,y,z) = k_x^2(x) + k_{yz}^2(y,z) + \tilde{k}^2(x,y,z), \tag{14}$$

with

$$\begin{cases} \displaystyle\int \tilde{k}^2(x,y,z)\,\mathrm{d}x = 0 \qquad \forall y,z, \\ \displaystyle\int \tilde{k}^2(x,y,z)\,\mathrm{d}y\,\mathrm{d}z = 0 \quad \forall x, \\ \displaystyle\int k_{xy}^2(y,z)\,\mathrm{d}y\,\mathrm{d}z = 0. \end{cases} \tag{15}$$

This decomposition is unique (see Appendix A).

The matrix K becomes

$$\mathrm{K} = \mathrm{K}_x \otimes \mathrm{I}_{yz} + \mathrm{I}_x \otimes \mathrm{K}_{yz} + \widetilde{\mathrm{K}}, \tag{16}$$

leading to

$$\mathrm{A} = (\mathrm{A}_x - \mathrm{K}_x) \otimes \mathrm{I}_{yz} + \mathrm{I}_x \otimes (\mathrm{A}_{yz} - \mathrm{K}_{yz}) - \widetilde{\mathrm{K}}. \tag{17}$$

The separation-of-variables technique consists of replacing the 3D problem of size MNL by M 2D problems of size NL, or in 2D, replacing a problem of size MN by M 1D problems of size N. This involves the eigenvector and eigenvalue decomposition of $\mathrm{A}_x - \mathrm{K}_x$:

$$\mathrm{W}_{\mathrm{L}}^{\mathrm{H}}(\mathrm{A}_x - \mathrm{K}_x)\mathrm{W}_{\mathrm{R}} = \Lambda, \tag{18}$$

with W_{L} the matrix of the left eigenvectors of $\mathrm{A}_x - \mathrm{K}_x$, W_{R} the matrix of the right eigenvectors ($\mathrm{W}_{\mathrm{L}}^{\mathrm{H}}\mathrm{W}_{\mathrm{R}} = \mathrm{I}_x$) and Λ the diagonal eigenvalue matrix.

Multiplying A by $\mathrm{W}_{\mathrm{L}}^{\mathrm{H}} \otimes \mathrm{I}_{yz}$ on the left and $\mathrm{W}_{\mathrm{R}} \otimes \mathrm{I}_{yz}$ on the right gives

$$\begin{aligned} \mathrm{B} &= \big(\mathrm{W}_{\mathrm{L}}^{\mathrm{H}} \otimes \mathrm{I}_{yz}\big)\mathrm{A}(\mathrm{W}_{\mathrm{R}} \otimes \mathrm{I}_{yz}) \\ &= \Lambda \otimes \mathrm{I}_{yz} + \mathrm{I}_x \otimes \mathrm{A}_{yz} - \big(\mathrm{W}_{\mathrm{L}}^{\mathrm{H}} \otimes \mathrm{I}_{yz}\big)\widetilde{\mathrm{K}}(\mathrm{W}_{\mathrm{R}} \otimes \mathrm{I}_{yz}). \end{aligned} \tag{19}$$

Let us now define the permutation matrix P such that the non-zero terms in P are

$$\mathrm{P}\big(i + (j-1)M,\, j + (i-1)NL\big) = 1, \quad 1 \leqslant i \leqslant M \text{ and } 1 \leqslant j \leqslant NL. \tag{20}$$

In this way

$$\mathrm{P}^{\mathrm{T}} B \mathrm{P} = \mathrm{D} + \widetilde{\widetilde{\mathrm{K}}}, \tag{21}$$

with D a block diagonal matrix consisting of M blocks, the block m being equal to

$$\lambda_m \mathrm{I}_{yz} + \mathrm{A}_{yz} - \mathrm{K}_{yz}, \tag{22}$$

and

$$\widetilde{\widetilde{\mathrm{K}}} = P^{\mathrm{T}}\big(\mathrm{W}_{\mathrm{L}}^{\mathrm{H}} \otimes \mathrm{I}_{yz}\big)\widetilde{\mathrm{K}}(\mathrm{W}_{\mathrm{R}} \otimes \mathrm{I}_{yz})P. \tag{23}$$

Assuming $\widetilde{\mathrm{K}} = 0$ and the conditions (10), the system (9) can now be solved by solving M independent systems. With the following change of variables

$$\begin{cases} \mathrm{u} = (\mathrm{W}_{\mathrm{R}} \otimes \mathrm{I}_{yz})\mathrm{P}\mathrm{v} & \big(\text{i.e., } \mathrm{v} = \mathrm{P}^{\mathrm{T}}\big(\mathrm{W}_{\mathrm{L}}^{\mathrm{H}} \otimes \mathrm{I}_{yz}\big)\mathrm{u}\big), \\ \mathrm{f} = (\mathrm{W}_{\mathrm{R}} \otimes \mathrm{I}_{yz})\mathrm{P}\mathrm{g} & \big(\text{i.e., } \mathrm{g} = \mathrm{P}^{\mathrm{T}}\big(\mathrm{W}_{\mathrm{L}}^{\mathrm{H}} \otimes \mathrm{I}_{yz}\big)\mathrm{f}\big), \end{cases} \tag{24}$$

the system becomes a block diagonal system

$$\mathrm{D}\mathrm{v} = \mathrm{g}. \tag{25}$$

Let us decompose v and g in M blocks v_m and g_m of size NL. The solution can then be obtained by solving the M systems

$$(\lambda_m \mathrm{I}_{yz} + \mathrm{A}_{yz} - \mathrm{K}_{yz})\mathrm{v}_m = \mathrm{g}_m. \tag{26}$$

These systems have one dimension less than (9). In this way, the solution of the 3D problem of size MNL is obtained by solving M 2D problems of size NL.

4. Preconditioned system

When modeling a seismic survey in a heterogeneous subsurface, k is not constant. It is therefore not possible to directly apply the separation-of-variables technique, as shown previously. Indeed, the conditions (10) and $\widetilde{\mathrm{K}} = 0$ imply that k is constant. However, k can be approximated such that the separation-of-variables technique can be used to construct a preconditioner. In this way, the system (9) is solved via an iterative preconditioner method.

The preconditioner, C, can be constructed in 3 steps:

(1) First, the wavenumber $k(x, y, z)$ is decomposed into three parts as explained in (14). This defines the matrix $\mathrm{K} = \mathrm{K}_x \otimes \mathrm{I}_{yz} + \mathrm{I}_x \otimes \mathrm{K}_{yz} + \widetilde{\mathrm{K}}$.
(2) Secondly, averaged valued at the boundaries are computed. This defines $\bar{\gamma}_x^{\min}$, $\bar{\gamma}_x^{\max}$, ... In practice, the terms $\bar{\gamma}$ are computed by summing the values of γ along each boundary and dividing by the number of points.
(3) Thirdly, the eigenvectors, W_R and W_L, and eigenvalues, Λ, of $\mathrm{A}_x - K_x$ are computed. This leads to the block diagonal matrix D.

The preconditioner is now defined by

$$\mathrm{C}^{-1} = (\mathrm{W}_\mathrm{R} \otimes \mathrm{I}_{yz})\mathrm{P}\mathrm{D}^{-1}\mathrm{P}^\mathrm{T}\big(\mathrm{W}_\mathrm{L}^\mathrm{H} \otimes \mathrm{I}_{yz}\big). \tag{27}$$

The new system that must be iteratively solved, is

$$\mathrm{C}^{-1}\mathrm{A}\mathrm{u} = \mathrm{C}^{-1}\mathrm{f}. \tag{28}$$

Here $\mathrm{C}^{-1}\mathrm{v}$ (with v a vector) is solved after the change of variables (24) as described by the system (25). We have used BICGSTAB as an iterative scheme.

5. Examples

The examples correspond to seismic modeling in heterogeneous media. We want to find the pressure field in the subsurface at a given frequency. The source is located in the middle of the domain at a depth just below the surface $z = 0$. The background velocity typically varies between 1500 m/s and 4000 m/s and the frequency between 10 Hz and 50 Hz. This means that the wavenumber, k, varies between 0.016 and 0.21 m^{-1}. To limit the required computational time, the tests are carried out on 2D problems. This means that the dimension y is not used. In this way, the matrix A_z $(= \mathrm{A}_{yz})$ in (26) is readily solved by LU-decomposition. The method to solve the full system (9) is a preconditioned BICGSTAB method [11]. The convergence is stopped when either the residual is smaller than 10^{-12} or the required number of iterations is larger than 2000. In the latter case, the algorithm is reported as non-converging.

5.1. 1D model

In this example, the velocity model varies only in z (Fig. 1), but the computation is done in the two space dimensions. The matrix A is separable except for the boundaries. In this way, C differs from A only at the boundaries. In the numerical computations in Table 1 the number of points per wavelength

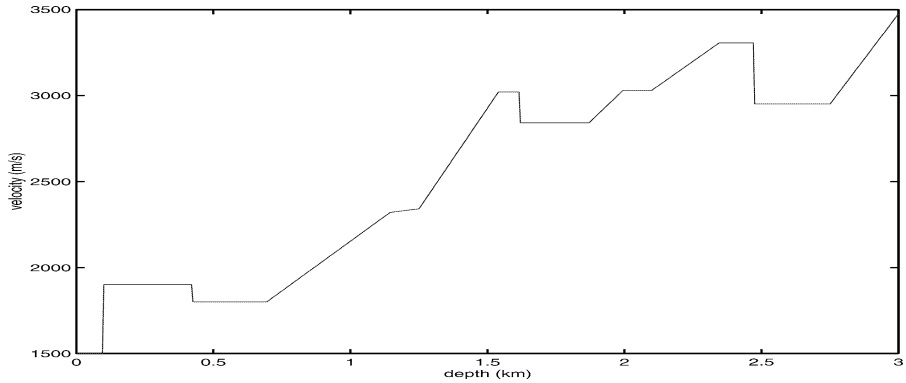

Fig. 1. A 1D velocity model.

Table 1
Convergence for the 1D model with the preconditioner

Frequency (Hz)	$k_{\min}$ (m^{-1})	$k_{\max}$ (m^{-1})	Grid spacing (m)	Number of points	Number of iterations
20	0.036	0.084	5	601^2	5
30	0.056	0.13	3.33	901^2	5
40	0.072	0.17	2.5	1201^2	5
50	0.091	0.21	2	1501^2	5

Table 2
Convergence for the perturbed 1D model with the preconditioner

Frequency (Hz)	$k_{\min}$ (m^{-1})	$k_{\max}$ (m^{-1})	Grid spacing (m)	Number of points	Number of iterations
20	0.035	0.090	5	601^2	18
30	0.059	0.13	3.33	901^2	37
40	0.070	0.18	2.5	1201^2	64
50	0.088	0.22	2	1501^2	141

is kept constant and the minimum number of points per wavelength is 15. The convergence with the preconditioner based on the separation-of-variables technique is fast and appears to be independent of the frequency. The case is similar to the example presented in [6] for the scattering model where the two matrices, A and C, differ only at the boundary of the obstacle. Note that with this one-dimensional model, the method does not converge without the preconditioner.

5.2. Perturbed 1D model

The previous velocity model is perturbed by adding a lateral variation of ± 200 m/s. The matrix A is no longer separable due to the lateral variation. The convergence results are shown in Table 2. The number of iterations needed for convergence mildly increases with the frequency.

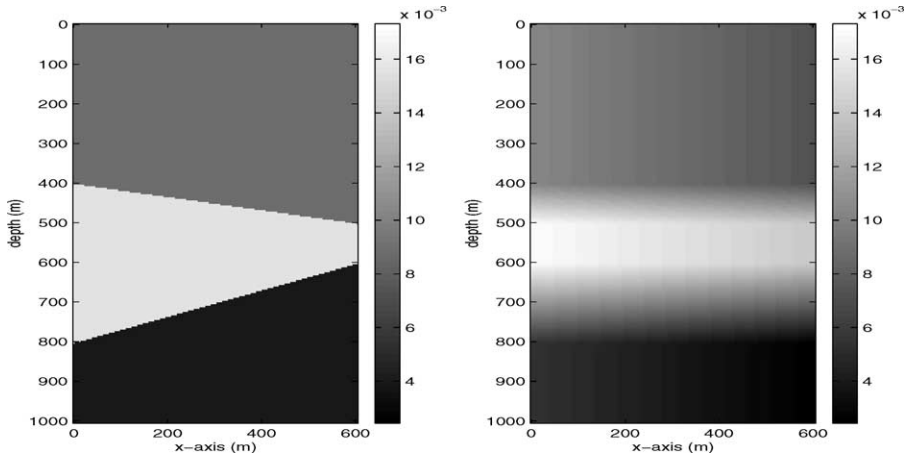

Fig. 2. On the left, the wedge model (k^2), on the right, the model used for the preconditioner ($k_x^2 + k_z^2$).

Table 3
Convergence for the wedge model with the preconditioner

Frequency (Hz)	$k_{\min}$ (m^{-1})	$k_{\max}$ (m^{-1})	Grid spacing (m)	Number of points	Number of iterations
10	0.021	0.042	4	151×251	14
10	0.021	0.042	8	76×126	14
20	0.042	0.084	4	151×251	45
30	0.063	0.126	2.6	232×386	167
40	0.084	0.17	2	301×501	830
50	0.105	0.21	1.6	376×626	> 2000

5.3. Small wedge model

The example is now a wedge model (see Fig. 2). The size of the model is 600 m in x and 1000 m in z.

Table 3 gives the convergence for different frequencies. At 10 Hz, we observe that the convergence is identical when the minimum number of points per wavelength is 37 (grid spacing 4 m) or 18 (grid spacing 8 m). The number of iterations increases rapidly when the frequency increases. At 50 Hz, the iterative method does not converge. Nevertheless, this preconditioner considerably improves the convergence rate. Without preconditioning, 2985 iterations are required at 10 Hz, whereas convergence is not reached after 2000 iterations at 20 Hz.

5.4. Marmousi model

5.4.1. Rough model

The example is a part of the Marmousi model (see Fig. 3). This model mimics a complicated subsurface geology [2]. We have taken a subset of the model. The computational model is 6 km large and 1.6 km depth. The model has many large contrasts. In the computation, the minimum number of points per wavelength is 17.

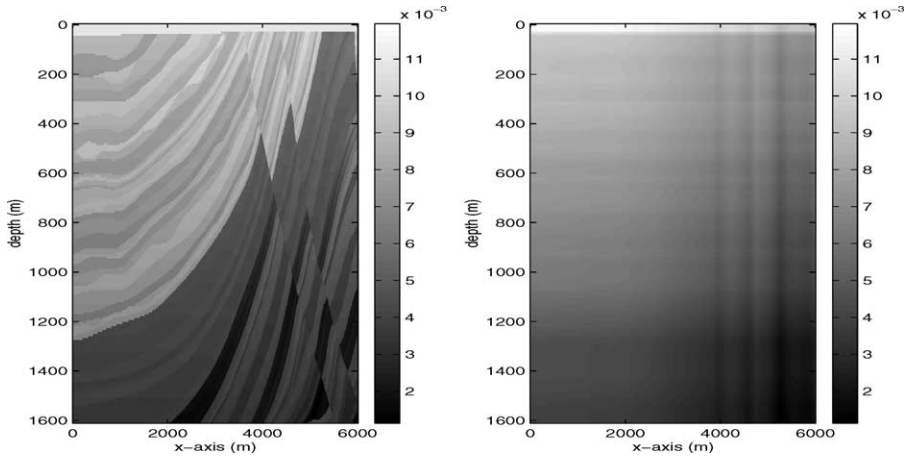

Fig. 3. On the left, the Marmousi model (k^2), on the right, the model used for the preconditioner ($k_x^2 + k_z^2$).

Table 4
Convergence for the Marmousi model with the preconditioner

Frequency (Hz)	$k_{\min}$ (m^{-1})	$k_{\max}$ (m^{-1})	Grid spacing (m)	Number of points	Number of iterations
1	0.0013	0.0042	8	751×201	3
10	0.013	0.042	8	751×201	114
20	0.026	0.084	4	1501×401	648
30	0.042	0.126	3	2001×534	>2000

Table 5
Convergence for the smooth Marmousi model with the preconditioner

Frequency (Hz)	$k_{\min}$ (m^{-1})	$k_{\max}$ (m^{-1})	Grid spacing (m)	Number of points	Number of iterations
1	0.0013	0.0042	8	751×201	3
10	0.013	0.042	8	751×201	38
20	0.026	0.084	4	1501×401	118
30	0.042	0.126	3	2001×534	>2000

Table 4 shows the convergence of the method. Around 30 Hz, the method does not converge: after 2000 iterations, the residual norm is still oscillating around the initial value without any substantial decrease. Convergence is difficult to obtain due to the large contrasts and the roughness of the model.

5.4.2. Smooth model

A far smoother model is now used in order to study the influence of the roughness of the model. As shown in Fig. 4, the difference between k^2 and $k_x^2 + k_z^2$ is reduced but still is not small.

Table 5 shows that the convergence is faster in a smooth background. However, at 30 Hz, the method fails to converge.

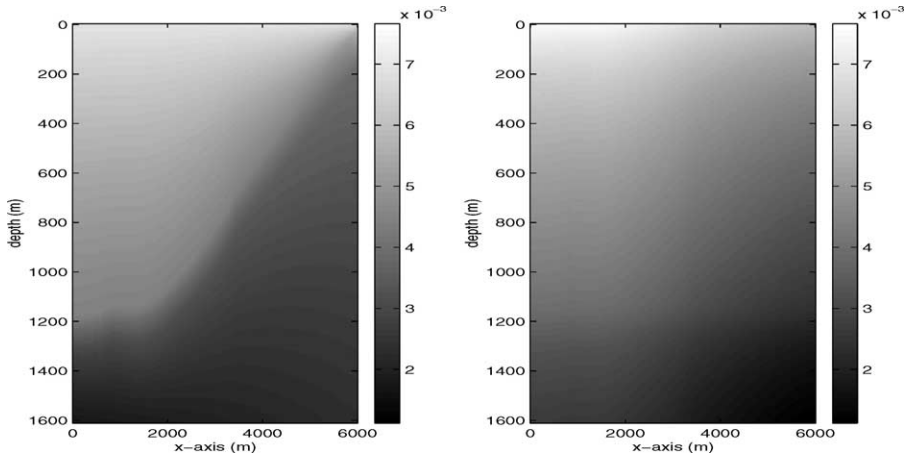

Fig. 4. On the left, a highly smoothed version of the Marmousi model (k^2), on the right, the model used for the preconditioner ($k_x^2 + k_z^2$).

6. An improved preconditioner?

One likely reason for the non-convergence of the method is that large phase shifts exist between the solution in the original model and the solution of the approximated model used in the preconditioner. This explains why the convergence is more difficult in a rough model than in a smooth model and why the efficiency of this preconditioner decreases at higher frequencies. The question we would like to address here is: would it be possible to improve the preconditioning, namely to remove the condition $\widetilde{\widetilde{\mathrm{K}}} = \widetilde{\mathrm{K}} = 0$?

In fact, the above formulation can be slightly generalised. If we assume that $\widetilde{\widetilde{\mathrm{K}}}$ can be approximate by a block diagonal matrix, with $\widetilde{\widetilde{\mathrm{K}}}_m$ the diagonal block m, the M systems (26) become

$$\bigl(\lambda_m \mathrm{I}_{yz} + \mathrm{A}_{yz} - \mathrm{K}_{yz} - \widetilde{\widetilde{\mathrm{K}}}_m\bigr)\mathrm{v}_m = \mathrm{g}_m. \tag{29}$$

Therefore, the problem is still split into M independent problems. To keep the same computational time for the preconditioner, an idea would be to impose that $\widetilde{\widetilde{\mathrm{K}}}_m$ has the same shape as A_{yz}. But can $\widetilde{\widetilde{\mathrm{K}}}$ be approximated by a non-zero block diagonal matrix?

The matrix

$$\widetilde{\mathrm{K}}' = \bigl(\mathrm{W}_{\mathrm{L}}^{\mathrm{H}} \otimes \mathrm{I}_{yz}\bigr)\widetilde{\mathrm{K}}(\mathrm{W}_{\mathrm{R}} \otimes \mathrm{I}_{yz})$$

is a block diagonal matrix with each block having a size NL, because $\widetilde{\mathrm{K}}$ is a diagonal matrix. The permutation P permutes the diagonals through all the blocks, see Eq. (23). The matrix $\widetilde{\widetilde{\mathrm{K}}} = P^{\mathrm{T}}\widetilde{\mathrm{K}}'P$ is block diagonal only if $\widetilde{\mathrm{K}}'$ is diagonal. In that case, $\widetilde{\widetilde{\mathrm{K}}}$ is diagonal. In practice, $\widetilde{\mathrm{K}}'$ is usually not diagonal (see Figs. 5 and 6). But if $\widetilde{\mathrm{K}}'$ would be diagonally dominant, we might replace it by its main diagonal and therefore approximate $\widetilde{\widetilde{\mathrm{K}}}$ by a block diagonal matrix, which could perhaps improve the convergence rate.

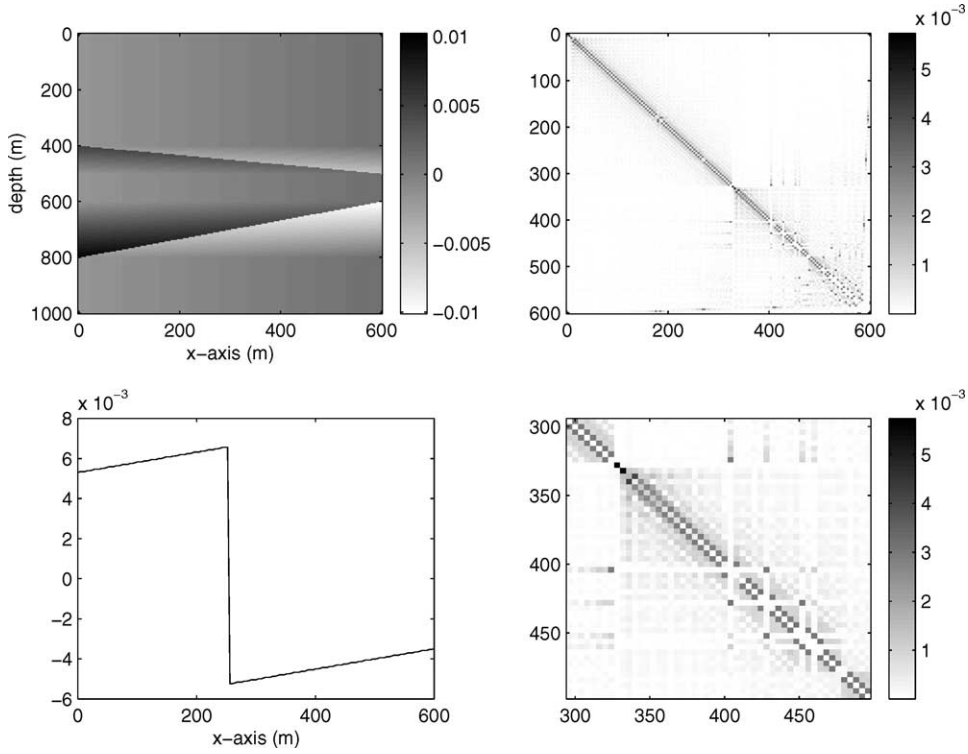

Fig. 5. On the top left the difference $k^2 - (k_x^2 + k_z^2)$ for the wedge model, on the top right the block diagonal nr. 180 of $\widetilde{\mathrm{K}}'$, on the bottom left, the slice of $k^2 - (k_x^2 + k_z^2)$, corresponding to the line 180, and on the bottom right an enlargement of the block diagonal 180.

Let us therefore study the structure of $\widetilde{\mathrm{K}}'$. We begin with a simple case. Assume that $k_x = 0$, implying that the matrix A_x corresponds to the discretisation of the Poisson equation. In that case, an eigenvector, w, satisfies $\mathrm{w}(i) = \mathrm{w}(M - i)$. Also, $q = k^2 - k_z^2$ obeys $\int q \, \mathrm{d}x = 0$ (see (14) and (15)). If we assume that $\mathrm{q}(i) = -\mathrm{q}(M - i)$, then the diagonal term is equal to

$$\sum_{i=1}^{M} \mathrm{q}(i)\big|\mathrm{w}(i)\big|^2 = \sum_{i=1}^{M/2} \mathrm{q}(i)\big|\mathrm{w}(i)\big|^2 + \sum_{i=1}^{M/2} \mathrm{q}(M - i)\big|\mathrm{w}(M - i)\big|^2 = 0.$$

This means that $\widetilde{\mathrm{K}}'$ is not a diagonally dominant matrix. Numerically a similar behavior is observed for the two examples of the previous section. Figs. 5 and 6 show some blocks of $\widetilde{\mathrm{K}}'$ for the wedge model and the Marmousi model. In both cases, the matrix $\widetilde{\mathrm{K}}'$ seems to have an almost band-limited structure. However, the terms on the diagonal are almost zero. The larger terms are on the off-diagonals, as shown in the right plots of Figs. 5 and 6. This means that $\widetilde{\mathrm{K}}'$ is not a diagonally dominant matrix and therefore $\widetilde{\widetilde{\mathrm{K}}}$ cannot be successfully approximated by a block diagonal matrix.

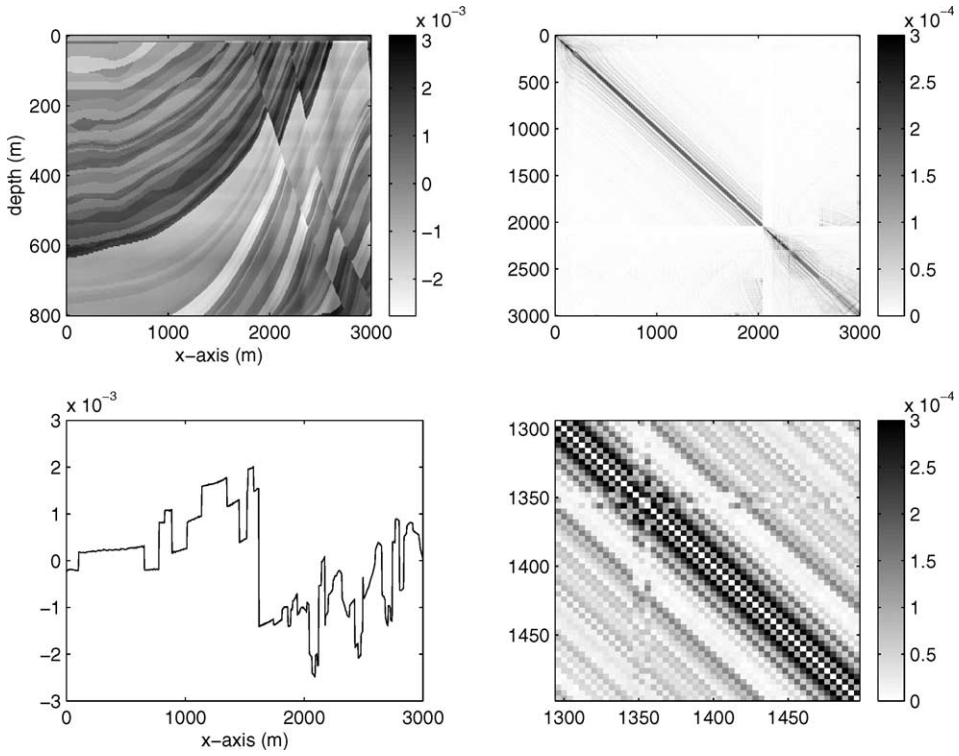

Fig. 6. On the top left the difference $k^2 - (k_x^2 + k_z^2)$ for the Marmousi model, on the top right the block diagonal 100 of $\widetilde{\mathrm{K}}'$, on the bottom left, the slice of $k^2 - (k_x^2 + k_z^2)$, corresponding to the line 100, and on the bottom right an enlargement of the block diagonal 100.

These result suggest that it is unlikely to find a $\widetilde{\widetilde{\mathrm{K}}}_m \neq 0$ that can improve the convergence rate of the iterative method based on the separation-of-variables technique.

7. Conclusion

When modeling the wave propagation in a 3D inhomogeneous media in the frequency domain, an iterative method needs to be used. The efficiency of this iterative solver of the Helmholtz equation depends on the preconditioner. A preconditioner based on separation-of-variables has been implemented. The convergence rate depends on the frequency and on the roughness of the velocity model. When the wavenumber varies only in one dimension (i.e., with one-dimensional models), this preconditioner is efficient. Only a few iterations are needed to obtain convergence of the iterative scheme. For smooth models and low frequencies, the convergence rate is satisfactory. However, for complex models, the method is not good enough when the frequency increases. Moreover, numerically examples suggest that it is not possible to find a better decomposition of the wavenumber that would improve the convergence rate of this approach.

Appendix A

In this appendix, we explain how to decompose a function $f(x, y, z)$ into

$$\begin{cases} f(x,y,z) = f_1(x) + f_2(y,z) + f_3(x,y,z), \\ \displaystyle\int_0^1\int_0^1 f_3(x,y,z)\,\mathrm{d}y\,\mathrm{d}z = 0, \quad \forall x, \\ \displaystyle\int_0^1 f_3(x,y,z)\,\mathrm{d}x = 0, \qquad \forall y, z. \end{cases} \tag{A.1}$$

Let f be a function in $[0,1]^3$. We define

$$\begin{cases} \displaystyle f_0 = \int_0^1\int_0^1\int_0^1 f(x,y,z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z, \\ \displaystyle f_1(x) = \int_0^1\int_0^1 f(x,y,z)\,\mathrm{d}y\,\mathrm{d}z, \\ \displaystyle f_2(y,z) = \int_0^1 f(x,y,z)\,\mathrm{d}x, \\ f_3(x,y,z) = f(x,y,z) + f_0 - f_1(x) - f_2(y,z). \end{cases} \tag{A.2}$$

Then f_3 verifies

$$\begin{cases} \displaystyle\int_0^1\int_0^1 f_3(x,y,z)\,\mathrm{d}y\,\mathrm{d}z = 0, \quad \forall x, \\ \displaystyle\int_0^1 f_3(x,y,z)\,\mathrm{d}x = 0, \qquad \forall y, z \end{cases} \tag{A.3}$$

and we have

$$f(x,y,z) = f_1(x) + \big(f_2(y,z) - f_0\big) + f_3(x,y,z). \tag{A.4}$$

Suppose now that

$$f(x,y,z) = f_1(x) + f_2(y,z) + f_3(x,y,z) = g_1(x) + g_2(y,z) + g_3(x,y,z), \tag{A.5}$$

with

$$\begin{cases} \displaystyle\int_0^1 f_3(x,y,z)\,\mathrm{d}x = \int_0^1 g_3(x,y,z)\,\mathrm{d}x = 0, \qquad \forall y, z, \\ \displaystyle\int_0^1\int_0^1 f_3(x,y,z)\,\mathrm{d}y\,\mathrm{d}z = \int_0^1\int_0^1 g_3(x,y,z)\,\mathrm{d}y\,\mathrm{d}z = 0, \quad \forall x. \end{cases} \tag{A.6}$$

By integrating over x, we obtain

$$g_2(y,z) = f_2(y,z) + \int_0^1 \big(f_1(x) - g_1(x)\big)\,\mathrm{d}x, \tag{A.7}$$

and by integrating over y and z, we obtain

$$g_1(x) = f_1(x) + \int_0^1\int_0^1 \big(f_2(y,z) - g_2(y,z)\big)\,\mathrm{d}y\,\mathrm{d}z. \tag{A.8}$$

Therefore, we have

$$\begin{cases} g_1(x) = f_1(x) + C, \\ g_2(y,z) = f_2(y,z) - C, \\ g_3(x,y,z) = f_3(x,y,z), \\ C = \displaystyle\int_0^1\int_0^1 \big(f_2(y,z) - g_2(y,z)\big)\,\mathrm{d}y\,\mathrm{d}z. \end{cases} \tag{A.9}$$

Therefore the decomposition is unique up to a constant. We then can impose

$$\int_0^1\int_0^1 f_2(y,z) = 0. \tag{A.10}$$

If f is defined on $D=[x_1,x_2]\times[y_1,y_2]\times[z_1,z_2]$, we first apply a change a variable from D to $[0,1]^3$ and then apply the previous decomposition.

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