

WS13 C02

A Fast Iterative Solution of the Time-harmonic Wave Equation with MSSS-preconditioned IDR(s)

M. Baumann* (Delft University of Technology) & M.B. Van Gijzen (Delft University of Technology)

SUMMARY

For the Full Waveform Inversion in frequency-domain, the fast numerical solution of the time-harmonic wave equation is required. For large three-dimensional problems, the problem size exceeds several million of unknowns, and a short-recurrence Krylov method such as IDR(s) is used to solve linear systems of this size. Especially for high-frequency simulations, an efficient preconditioner needs to be applied in order to speed-up convergence.

In our presentation, we introduce a new preconditioner for the time-harmonic wave equation that exploits the hierarchical structure of the discretized problem. We use multilevel sequentially semiseparable (MSSS) matrix computations for the approximate inversion of the preconditioner. For large three-dimensional problems, we present a memory-efficient modification of the MSSS preconditioner that resembles the approximate solution of a sequence of two-dimensional problems. We conclude our presentation with numerical examples for the time-harmonic wave equation in both acoustic and elastic media, and in two and three spatial dimensions.

Introduction

The frequency-domain formulation of wave propagation has shown specific modeling advantages for both acoustic and elastic media. For the efficient Full Waveform Inversion, notably the waveform tomography (Virieux and Operto (2009), Plessix and Pérez Solano (2015)), a fast numerical solution of the respective *forward problem* is required. A finite element discretization of the acoustic or the elastic wave equation yields the following mathematical problem,

$$(K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}, \quad k = 1, \dots, N_\omega, \quad (1)$$

where K, M are the stiffness and mass matrix, respectively, and C incorporates Sommerfeld boundary conditions. Note that we aim to solve (1) at multiple (angular) frequencies $\{\omega_1, \dots, \omega_{N_\omega}\}$ simultaneously. The unknown vector \mathbf{x}_k consists of the Fourier-transformed displacement vector in the case of the elastic wave equation, and the pressure in the acoustic case. The right-hand side \mathbf{b} usually models a point source.

The preconditioned Induced Dimension Reduction (IDR(s)) method

For large 3D problems, the leading dimension of K, C, M exceeds several million, and short-recurrence Krylov methods are typically used to solve linear systems of that size. In our application, we use the Induced Dimension Reduction (IDR(s)) method which was introduced by Sonneveld and Van Gijzen (2008) for the iterative solution of linear systems of the form $A\mathbf{x} = \mathbf{b}$. IDR(s) has shown to outperform other short-recurrence Krylov methods such as Bi-CGSTAB (introduced by Van der Vorst (1992)) in several examples.

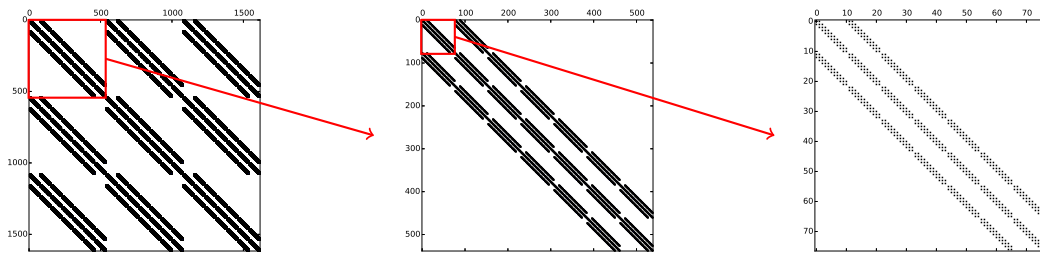


Figure 1 A `spy` plot of $\mathcal{P}(\tau)$ for a small 3D elastic problem. Appropriate zooming demonstrates the hierarchically repeating structure of the matrix when lexicographical numbering is used.

As a preconditioner for (1), we use

$$\mathcal{P}(\tau) := K + i\tau C - \tau^2 M, \quad \tau \in [\omega_{\min}, \omega_{\max}], \quad (2)$$

with *seed* frequency τ . This preconditioner has already been used by Baumann and Van Gijzen (2015) where (1) is treated as a sequence of shifted linear systems. The `spy` plot of $\mathcal{P}(\tau)$ in Figure 1 shows the hierarchical structure of the preconditioner when a Cartesian grid is used. This gives rise to the usage of multilevel sequentially semiseparable (MSSS) preconditioning technique for the efficient (approximate) inversion of $\mathcal{P}(\tau)$. In Qiu et al. (2015), the authors show that an approximate Schur decomposition $\mathcal{P}(\tau) = LSU$, with S being block-diagonal, and L, U being block bidiagonal matrices of lower and upper tridiagonal form, can be computed in linear complexity, and the usage as a preconditioner yields good results in the case of a 3D Laplace optimal control problem.

Example 1: The elastic `marmousi-2` problem

In our numerical examples, we restrict ourselves to the single-frequency case where $N_\omega = 1$, and $\tau = \omega_1$. We illustrate the performance of the preconditioner (2) using MSSS matrix computations by means of

two examples. As a two-dimensional test case, we consider the elastic *marmousi-2* problem suggested in Martin et al. (2002). The computational domain and the numerical solution at two different frequencies are shown in Figure 2.

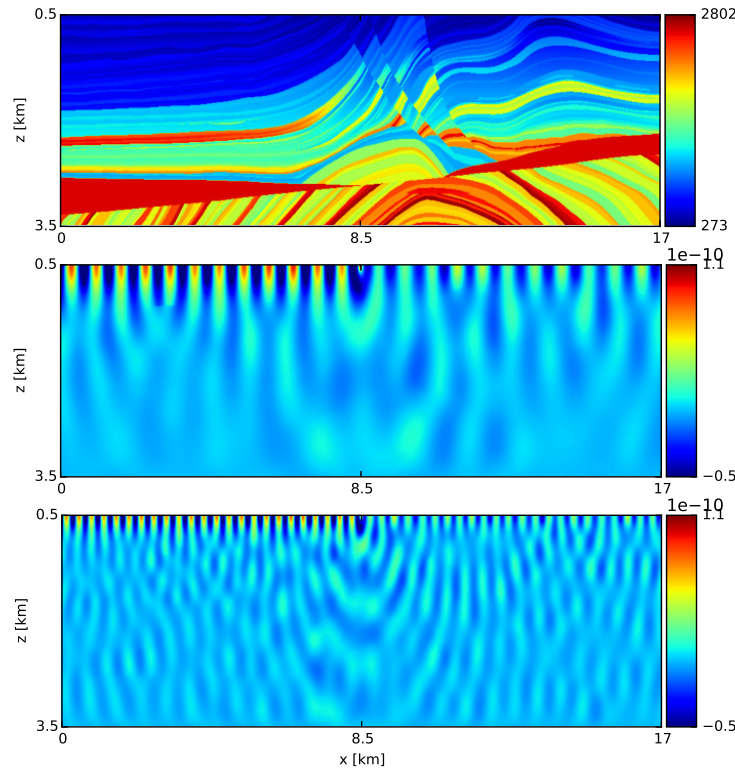


Figure 2 Speed of S-waves (top), and real part of the z -component of the displacement vector in frequency-domain at $f = 2$ Hz (middle) and $f = 4$ Hz (bottom) for the *marmousi-2* model, cf. Martin et al. (2002) for a complete parameter set.

We perform numerical tests on the *marmousi-2* problem at different grid sizes h in order to illustrate the performance of the preconditioner (2) when MSSS matrix computations are used. We note that in the single-frequency case, the preconditioner has the same form as the original problem. In order to apply MSSS matrix operations in linear computational complexity, it is required to limit the rank of off-diagonal blocks using model order reduction techniques, cf. Qiu et al. (2015). In Table 1 we show that an inexact application of the MSSS preconditioner leads to a convergence of the outer Krylov method within very few iterations. Moreover, we see in the third column of Table 1 that the MSSS operations grow linearly with the number of degrees of freedom (dofs) when the discretization size is divided by two.

Table 1 Numerical experiments for the *marmousi-2* problem at $f = 4$ Hz with residual tolerance 10^{-9} and off-diagonal rank truncated at $r_{\max} = 10$.

h	# dofs	MSSS decomposition	IDR($s = 4$)	Bi-CGSTAB
40m	64,752	3.64 sec	0.45 sec (9 iter.)	0.40 sec (8 iter.)
20m	257,002	23.12 sec	3.01 sec (10 iter.)	3.25 sec (11 iter.)
10m	1,024,002	89.94 sec	17.04 sec (15 iter.)	17.84 sec (16 iter.)

In a second experiment we simultaneously increase problem size and wave frequency. The results in Table 2 show that the number of Krylov iterations can be controlled at a constant level when the maximum off-diagonal rank r_{\max} of the MSSS computations is slightly increased. By comparing both experiments we note that the time for the MSSS decomposition does not differ a lot when different off-diagonal ranks are chosen.

Table 2 Numerical experiments for the *marmousi-2* problem when the frequency is increased.

f	h	r_{max}	MSSS decomposition	IDR($s = 4$)	Bi-CGSTAB
1 Hz	40m	3	2.44 sec	1.94 sec (41 iter.)	2.14 sec (43 iter.)
2 Hz	20m	5	19.63 sec	10.91 sec (38 iter.)	12.43 sec (44 iter.)
4 Hz	10m	8	82.04 sec	40.72 sec (37 iter.)	44.32 sec (41 iter.)

Example 2: A three-dimensional acoustic wedge problem

As a second example, we consider an extension of the acoustic wedge problem presented in Plessix and Mulder (2004) to a three-dimensional domain $\Omega = [0, 600m] \times [0, 600m] \times [0, 1000m]$. The domain models three layers of different physical properties with parameter $c(x, y, z) = \{2000, 1500, 3000\}m/s$, as shown in Figure 3.

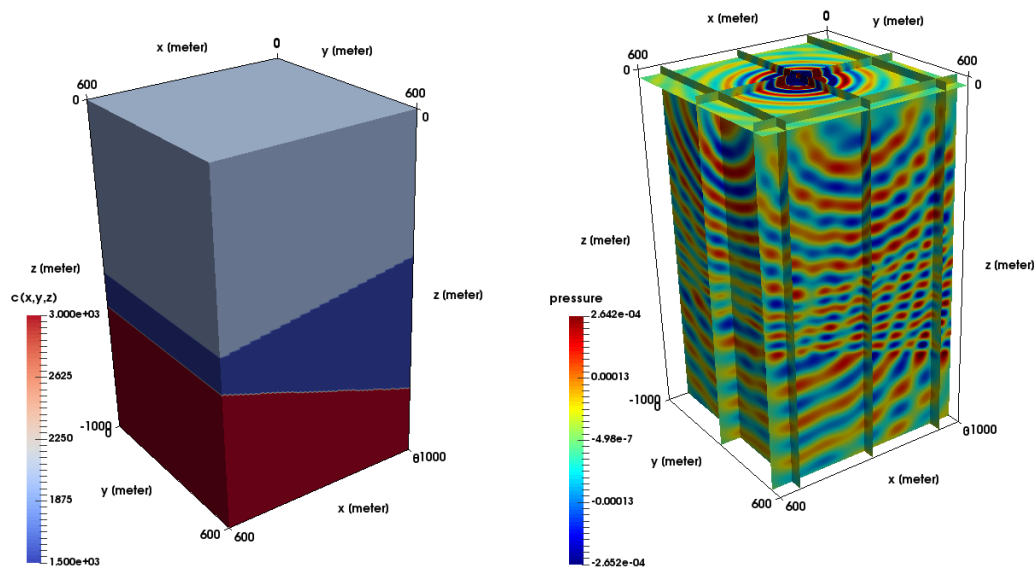


Figure 3 Underlying sound velocity profile (left) and numerical solution at $f = 32$ Hz (right) for the three-dimensional acoustic wedge problem using a grid size of $h = 5m$.

The application of the MSSS preconditioner in 3D differs from the two-dimensional case: In order to design a memory-efficient MSSS algorithm, we simplify the block *LSU* decomposition of (2) such that the Schur complements that appear in the matrix S only consist of diagonal blocks of the original preconditioner $\mathcal{P}(\tau)$. This approach limits the increase in rank of the MSSS structure, and can be interpreted as solving the 3D case as a sequence of two-dimensional problems.

Table 3 Numerical experiments for the 3D wedge problem at $f = 4$ Hz with residual tolerance 10^{-9} .

h	# dofs	MSSS decomposition	IDR($s = 4$)	Bi-CGSTAB
20m	49,011	0.77 sec	4.69 sec (73 iter.)	7.92 sec (122 iter.)
10m	375,821	6.70 sec	79.20 sec (139 iter.)	156.51 sec (273 iter.)
5m	2,942,841	57.24 sec	1511.91 sec (287 iter.)	3198.13 sec (614 iter.)

We present numerical experiments for the three-dimensional wedge problem in Table 3. Clearly, we see that the MSSS decomposition scales linearly with the problem size and that the previously described simplifications lead to a worse preconditioner in terms of number of Krylov iterations. By comparing the last two columns we note that IDR(4) outperforms Bi-CGSTAB by a factor of ~ 2 when the same MSSS preconditioner is used. IDR(s) requires the storage of $3s + 4$ vectors compared to 7 vectors in Bi-CGSTAB which is small for the default value $s = 4$, cf. Sonneveld and Van Gijzen (2008).

Extension to multiple frequencies and multiple right-hand sides

In order to deal with multiple frequencies (and multiple right-hand sides), we suggest to re-formulate problem (1) to,

$$\mathcal{A}(\mathbf{X}) \equiv \mathbf{K}\mathbf{X} + i\mathbf{C}\mathbf{X}\Sigma - \mathbf{M}\mathbf{X}\Sigma^2 = \mathbf{B}, \quad (3)$$

where $\Sigma := \text{diag}(\omega_1, \dots, \omega_{N_\omega})$, and with a block right-hand side $\mathbf{B} := [\mathbf{b}, \dots, \mathbf{b}]$ that allows to include multiple sources. The unknown in (3) is the matrix of all solutions to (1), $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_{N_\omega}]$, and a short-hand notation of the matrix equation (3) is, thus, given by $\mathcal{A}(\mathbf{X}) = \mathbf{B}$. Most recently, Astudillo and Van Gijzen (2015) extended IDR(s) to solve linear matrix equations.

Conclusions and future work

We demonstrate the performance of IDR(s) with an MSSS preconditioner for time-harmonic wave problems in acoustic and elastic media. First numerical experiments have shown that problems in two and three spatial dimensions of the order of million unknowns can be solved efficiently, and linear computational complexity is observed for the MSSS matrix operations. The dependence of the suggested preconditioner (2) on the considered frequency will be elaborated in future work. This is of particular importance when multiple frequencies in the sense of (3) are solved simultaneously.

For a more detailed description of the IDR(s) algorithm preconditioned with an MSSS preconditioner, we refer to our recent technical report Astudillo et al. (2016).

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