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Two-level preconditioned Krylov subspace methods for the solution of three-dimensional heterogeneous Helmholtz problems in seismics

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Abstract

In this paper we address the solution of three-dimensional heterogeneous Helmholtz problems discretized with compact fourth-order finite difference methods with application to acoustic waveform inversion in geophysics. In this setting, the numerical simulation of wave propagation phenomena requires the approximate solution of possibly very large linear systems of equations. We propose an iterative two-grid method where the coarse grid problem is solved inexactly. A single cycle of this method is used as a variable preconditioner for a flexible Krylov subspace method. Numerical results demonstrate the usefulness of the algorithm on a realistic three-dimensional application. The proposed numerical method allows us to solve wave propagation problems with single or multiple sources even at high frequencies on a reasonable number of cores of a distributed memory cluster.

Key words. Flexible Krylov subspace methods; Helmholtz equation; Inexact preconditioning; Inhomogeneous media.

1 Introduction

Three-dimensional seismic imaging in the frequency domain requires efficient numerical methods for the approximate solution of possibly very large linear systems of equations.

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Due to the indefiniteness of the matrices, the resulting linear systems are known to be very challenging for iterative methods. Efficient preconditioners combined with Krylov subspace methods must be thus developed and in the past years several authors have proposed various numerical methods related to this challenging topic [4, 9, 13, 21]. A factorization-free two-grid preconditioner where the coarse grid problem is solved only approximately has been recently proposed and successfully applied to the second-order accurate discretization of the Helmholtz equation [12]. In this paper we extend this two-grid preconditioner to a high-order discretization of the acoustic wave equation and detail the performance of the algorithm on a a realistic three-dimensional application.

2 Acoustic full waveform inversion in the frequency domain

We briefly describe the forward problem associated with acoustic imaging [20].

2.1 Forward problem

Given a three-dimensional physical domain Ω_p, the propagation of a wave field in a heterogeneous medium can be modeled by the Helmholtz equation written in the frequency domain:

$$-\sum_{i=1}^{3} \frac{\partial^2 u}{\partial x_i^2} - \frac{(2\pi f)^2}{c^2} u \;=\; \delta(\mathbf{x}-\mathbf{x_s}), \quad \mathbf{x}=(x_1,x_2,x_3)\in\Omega_p. \tag{1}$$

The unknown u represents the pressure wavefield in the frequency domain, c the acoustic-wave velocity in ms^{-1}, which varies with position, and f the frequency in Hertz. The source term $\delta(\mathbf{x}-\mathbf{x_s})$ represents a harmonic point source located at (x_s, y_s, z_s). The wavelength λ is defined as $\lambda = \dfrac{c}{f}$. A popular approach - the Perfectly Matched Layer formulation (PML) [2, 3] - has been used in order to obtain a satisfactory near boundary solution, without many artificial reflections. Artificial boundary layers are used to absorb outgoing waves at any incidence angle as shown in [2]. We denote by Ω_{PML} the surrounding domain created by these artificial layers. This formulation leads to the following set of coupled partial differential equations with homogeneous Dirichlet boundary conditions imposed on Γ the boundary of the domain:

$$-\sum_{i=1}^{3} \frac{\partial^2 u}{\partial x_i^2} - \frac{(2\pi f)^2}{c^2} u \;=\; \delta(\mathbf{x}-\mathbf{x_s}) \quad \text{in} \quad \Omega_p, \tag{2}$$

$$-\sum_{i=1}^{3} \frac{1}{\xi_{x_i}(x_i)} \frac{\partial}{\partial x_i}\left(\frac{1}{\xi_{x_i}(x_i)} \frac{\partial u}{\partial x_i}\right) - \frac{(2\pi f)^2}{c^2} u \;=\; 0 \quad \text{in} \quad \Omega_{PML}\backslash\Gamma, \tag{3}$$

$$u \;=\; 0 \quad \text{on} \quad \Gamma, \tag{4}$$

where the ξ_{x_i} functions represent the complex-valued damping functions in each direction respectively. The set of equations (2, 3, 4) defines the forward problem related to acoustic imaging.

2.1.1 Compact fourth-order accurate discretization

Accurate solution of the forward problem (2, 3, 4) is a key ingredient in any acoustic imaging tool. Thus we consider a high-order accurate finite difference discretization of the Helmholtz problem [10] on an uniform equidistant Cartesian grid of size $n_x \times n_y \times n_z$. We denote later by h the corresponding mesh grid size, Ω_h the discrete computational domain and n_{PML} the number of points in each PML layer. A fixed value of $n_{PML} = 10$ has been considered hereafter. In [10] compact schemes based on Padé approximation (leading to a 27-point discretization stencil for three-dimensional applications) have been developed to reduce spurious dispersion, anisotropy and reflection. It has been proven that the resulting schemes have fourth-order accurate local truncation error on uniform grids and third-order in the non-uniform case. Since a stability condition has to be satisfied to correctly represent the wave propagation phenomena [6], we consider such a discretization scheme with 10 points per wavelength as in [19].

The discretization of the forward problem leads to the linear system $A_h x_h = b_h$, where $A_h \in \mathbb{C}^{n \times n}$ is a sparse complex matrix which is non Hermitian and nonsymmetric due to the PML formulation and where $x_h, b_h \in \mathbb{C}^n$ represent the discrete frequency-domain pressure field and source, respectively. Due to the large dimension of the linear system, preconditioned Krylov subspace methods are most often considered and efficient preconditioners must be then developed for such indefinite problems.

3 Two-level preconditioned Krylov subspace method

In this section we introduce the geometric two-level preconditioner that is proposed for the solution of wave propagation problems presented in Section 2.

3.1 Geometric two-level preconditioner

We first present the general framework of the preconditioner and introduce some notations for that purpose. The fine and coarse levels denoted by h and H are associated with discrete grids Ω_h and Ω_H respectively, while $\mathcal{G}(\Omega_k)$ is the set of grid functions defined on Ω_k. Due to the geophysical application where structured grids are routinely used, it seems natural to consider a geometric construction of the coarse level Ω_H. The discrete coarse grid domain Ω_H is then deduced from the discrete fine grid domain Ω_h by doubling the mesh size in each direction as classically done in geometric multigrid [17]. We select as a prolongation operator $I_H^h : \mathcal{G}(\Omega_H) \rightarrow \mathcal{G}(\Omega_h)$ trilinear interpolation and as a restriction $I_h^H : \mathcal{G}(\Omega_h) \rightarrow \mathcal{G}(\Omega_H)$ its adjoint which is often called the full weighting operator [17]. We refer the reader to [18] for a complete description of these operators in three dimensions. Finally we assume that A_H is obtained by discretization of (2, 3,

4) on Ω_H.

Algorithm 1 Geometric approximate two-level cycle applied to $A_h\ z_h = v_h$ with initial approximation z_h^0. $z_h = \mathcal{M}(v_h)$.

1: Polynomial pre-smoothing: Apply μ_1 cycles of GMRES(m_s) to $A_h\ z_h = v_h$ with initial approximation z_h^0 and symmetric Gauss-Seidel as a right preconditioner to obtain the approximation $z_h^{\mu_1}$.
2: Restrict the fine level residual: $v_H = I_h^H(v_h - A_h\ z_h^{\mu_1})$.
3: Solve approximately the coarse problem $A_H\ z_H = v_H$: Apply μ_c cycles of GMRES(m_c) to $A_H\ z_H = v_H$ with initial approximation z_H^0 and symmetric Gauss-Seidel as right preconditioner to obtain the approximation z_H.
4: Correct the fine-grid approximation: $\widetilde{z_h} = z_h^{\mu_1} + I_H^h\ z_H$.
5: Polynomial post-smoothing: Apply μ_2 cycles of GMRES(m_s) to $A_h\ z_h = v_h$ with initial approximation $\widetilde{z_h}$ and symmetric Gauss-Seidel as a right preconditioner to obtain the approximation $z_h^{\mu_2}$.

The general form of the two-level cycle to be used as a preconditioner is sketched in Algorithm 1. This cycle belongs to the class of multiplicative two-level preconditioner. The approximation at the end of the cycle z_h can be represented as $z_h = \mathcal{M}(v_h)$ where $\mathcal{M}$ is a nonlinear function. Consequently this cycle leads to a variable nonlinear preconditioner which must be combined with an outer *flexible* Krylov subspace method [16]. In this study we have selected an outer Krylov subspace method of minimum residual type namely flexible GMRES (FGMRES(m)) [14].

Polynomial smoothers based on the GMRES Krylov subspace method [15] have been selected for both pre- and post-smoothing phases as in [8]. The main originality of this cycle is to consider an approximate solution z_H of the indefinite coarse level problem $A_H\ z_H = v_H$. As far as we know this feature has been analysed algebraically by Notay [11] in the framework of symmetric positive definite systems. In [11] it has been proven that the coarse level solution in a standard two-level cycle is not required to be accurate to obtain an efficient cycle to be used as a solver or as a preconditioner. In the framework of indefinite Helmholtz problems with homogeneous velocity field solving only approximately the coarse level problem has been analysed by Local Fourier Analysis and Robust Fourier Analysis in [12] for second-order accurate discretization schemes. Theoretical developments supported by numerical experiments have notably shown that the approximate solution of the coarse level problem may also lead to an efficient preconditioner. We report the reader to [12, Section 3.4] for a complete description of this analysis on three-dimensional model problems. In Section 4 numerical experiments will demonstrate that such a strategy is also efficient when solving realistic heterogeneous problems with high-order discretization schemes.

4 Numerical performance on a large three-dimensional model

We investigate the performance of the two-grid preconditioner combined with Flexible GMRES(m) for the solution of (2, 3, 4) on a realistic heterogeneous velocity model.

4.1 Settings

In the two-grid cycle (Algorithm 1) we consider the case of two iterations of symmetric Gauss-Seidel preconditioned GMRES as a smoother ($m_s = 2$, $\mu_1 = 1$ and $\mu_2 = 1$), a restart parameter equal to $m_c = 5$ for the preconditioned GMRES method to be used on the coarse level, a maximal number of coarse cycles equal to $\mu_c = 20$ and zero initial guesses ($z_h^0 = 0, z_H^0 = 0$). We consider a moderate value for the restart parameter of the outer Krylov subspace method ($m = 5$) as in [12]. In the numerical experiments the unit source is located at $(x_s/h, y_s/h, z_s/h) = (n_x/2, n_y/2, n_{PML}+1)$. A zero initial guess is chosen and the iterative method is stopped when the Euclidean norm of the residual normalized by the Euclidean norm of the right-hand side satisfies the following relation:

$$\frac{||b_h - A_h x_h||_2}{||b_h||_2} \leq 10^{-5}. \tag{5}$$

The numerical results have been obtained on Jade, a SGI Altix ICE 8200 cluster located at CINES[1] (each node of Jade is equipped with 2 Intel Quad-Core X5560 processors) using a Fortran 90 implementation with MPI in single precision arithmetic. Physical memory on a given node (8 cores) of Jade is limited to 34 GB. This code was compiled by the Intel compiler suite with the best optimization options and linked with the Intel vendor BLAS and LAPACK subroutines.

4.2 The SEG/EAGE Salt dome model: forward problem

The SEG/EAGE Salt dome model [1] is a velocity field containing a salt dome in a sedimentary embankment. It is defined in a parallelepiped domain of size $13.5 \times 13.5 \times 4\ km^3$. The minimum value of the velocity is 1500 $m.s^{-1}$ and its maximum value is 4481 $m.s^{-1}$ respectively. This testcase is considered as challenging due to both the occurrence of a geometrically complex structure (salt dome) and the large dimensions of the computational domain.

4.2.1 Weak scalability analysis

We analyze now the weak scalability of the algorithm and thus consider different problems with increasing frequencies on a growing number of cores so that the local problem size is only slightly changing. Numerical experiments are reported in Table 1. In the homogeneous case, when the frequency is multiplied by a factor of 2, a ratio of 8 between

[1] http://www.cines.fr

the size of two consecutive grids should be considered to obtain a fixed local problem size. Nevertheless due to the fixed number of points taken in the PML layer that is chosen independently of the frequency and due to the heterogeneous nature of the velocity field, the number of unknowns on two consecutive grids is found to be multiplied by a factor greater than 8 in practice. These factors are indicated in the "Ratio" column in Table 1.

We consider a range of frequencies from $2.5Hz$ to $40Hz$ in this study. We note that the largest frequency case ($f = 40Hz$) requires to solve an indefinite linear system with more than 15 billion of unknowns. In Table 1 we report the number of preconditioner applications (Pr), the corresponding computational times in seconds (T) and the maximal requested memory in GB (M). We remark that when the frequency is multiplied by a factor of two, the number of preconditioner applications is also multiplied by a factor close to two for small to mid frequencies. This behaviour has been reported by various authors [4, 9, 13] who obtained a similar behaviour on heterogeneous problems defined on smaller computational domains although. However in the case of large frequencies, the number of preconditioner applications tends to grow considerably. A similar behaviour has been reported on both homogeneous and heterogeneous problems for second-order accurate schemes in [12]. We note however that this increase in preconditioner applications is found to be less pronounced in the case of the high-order discretization scheme considered here (e.g., 227 preconditioner applications are required at $f = 20$ Hz for the second-order discretization scheme). Finally we note that the maximal requested memory is growing linearly with the problem size. This notably reflects the fact that the numerical method does not rely on any numerical factorization of sparse matrices either at the fine or at the coarse level.

SEG/EAGE Salt dome - Weak scaling								
h (m)	f (Hz)	Grid	Ratio	Cores	Partition	T (s)	Pr	M (GB)
60	2.5	$225 \times 225 \times 71$	1.00	1	$1 \times 1 \times 1$	171	10	1.35
30	5	$451 \times 451 \times 143$	8.1	8	$2 \times 2 \times 2$	385	18	10.9
15	10	$903 \times 903 \times 287$	65.1	64	$4 \times 4 \times 4$	989	43	87.8
7.5	20	$1807 \times 1807 \times 575$	522.3	512	$8 \times 8 \times 8$	2710	112	704.2
3.75	40	$3615 \times 3615 \times 1151$	4184.7	4096	$16 \times 16 \times 16$	7984	293	5641.8

Table 1: Two-grid preconditioned Flexible GMRES(5) for the solution of the Helmholtz equation for the SEG/EAGE Salt dome model with mesh grid size h such that $h = \min_{(x,y,z)\in\Omega_h} c(x,y,z)/(10\,f)$. The parameter T denotes the total computational time in seconds, Pr the number of preconditioner applications and M the requested memory in GB.

4.2.2 Strong scalability analysis

We propose to analyze now the strong scalability property of the numerical method. Thus we fix the global problem size to approximately 246 millions of unknowns (i.e. a grid of size $927 \times 927 \times 287$ corresponding to a frequency of $10 Hz$ is used) and we consider a growing number of cores. Whatever the number of cores the same physical problem is thus solved. Numerical results are shown in Table 2. The number of preconditioner applications (Pr) is found to be nearly constant. The slight differences in terms of preconditioner applications can be explained by the local nature of the symmetric Gauss-Seidel method used as a preconditioner in both smoothing and coarse phases. To further analyze the behaviour of the method we provide a scaled speed-up factor (τ) as an indication of the scalability of the algorithm: the code is said to perfectly scale when τ is equal to 1. Taking as reference values for T_{ref} and P_{ref} the computational time and number of cores corresponding to the first numerical experiment (first row of Tables 2), it appears that the numerical method enjoys good strong scalability properties up to 1024 cores. This is a very satisfactory behaviour on such a realistic application.

SEG/EAGE Salt dome - Strong scaling								
h (m)	f (Hz)	Grid	Cores	Partition	T (s)	Pr	τ	M (GB)
15	10	$927 \times 927 \times 287$	32	$4 \times 4 \times 2$	1969	43	1.00	91.2
15	10	$927 \times 927 \times 287$	64	$4 \times 4 \times 4$	1009	43	0.97	92.5
15	10	$927 \times 927 \times 287$	128	$8 \times 4 \times 4$	524	43	0.94	93.2
15	10	$927 \times 927 \times 287$	256	$8 \times 8 \times 4$	282	44	0.87	94.1
15	10	$927 \times 927 \times 287$	512	$8 \times 8 \times 8$	156	44	0.79	96.6
15	10	$927 \times 927 \times 287$	1024	$16 \times 8 \times 8$	90	44	0.68	98.2
15	10	$927 \times 927 \times 287$	2048	$16 \times 16 \times 8$	52	44	0.60	99.9

Table 2: Two-grid preconditioned Flexible GMRES(5) for the solution of the Helmholtz equation for the SEG/EAGE Salt dome model with mesh grid size h such that $h = \min_{(x,y,z)\in\Omega_h} c(x,y,z)/(10\, f)$. The parameter T denotes the total computational time in seconds, Pr the number of preconditioner applications and M the requested memory in GB. $\tau = \frac{T_{ref}}{T} / \frac{P}{P_{ref}}$ is a scaled speed-up factor where T, P denote the elapsed time and corresponding number of cores on a given experiment respectively.

4.2.3 Multiple right-hand side problems

The solution of multiple right-hand side problems is also an important issue in acoustic imaging corresponding to the occurrence of multiple sources in the computational domain. Thus we analyze the performance of the two-grid preconditioner combined with a block flexible Krylov subspace method for the solution of heterogeneous Helmholtz problems with p right-hand sides. The block flexible Krylov subspace method (BFGMRESD(m) proposed in [5, Algorithm 3]) allows variable preconditioner and relies on the idea of block size reduction to derive an efficient method in terms of computational operations. At each restart of the block flexible Krylov subspace method it detects linear combinations of linear systems that have approximately converged to effectively reduce the current number of linear systems to consider during convergence. The number of linear systems considered along convergence is thus always non-increasing. In [5] numerical experiments with a second-order accurate discretization scheme have been reported showing the efficiency of this new method on an application related to seismics. Here we consider the case of high-order discretization schemes and investigate the performance of the outer preconditioned block Krylov subspace method with respect to the number of right-hand sides at a given frequency ($5\ Hz$). Table 3 reports both the number of preconditioner applications on a *single* vector and corresponding computational times versus the number of right-hand sides p and number of cores for the standard block flexible GMRES(m) proposed in [7] and BFGMRESD(m) respectively. The maximal number of right-hand sides is 256 on 1024 cores. Using the block size reduction in the block flexible Krylov subspace method allows us to decrease the number of linear systems considered along the convergence. This leads to a significant decrease of the computational times (a reduction of about 55% is indeed obtained for $p = 256$ or $p = 1024$). This is a rather satisfactory result on this practical application.

SEG/EAGE Salt dome - *Grid* : $479 \times 463 \times 143$, $f = 5\ Hz$								
(p, Cores)	$(4, 16)$		$(16, 64)$		$(64, 256)$		$(256, 1024)$	
Method	Pr	T (s)	Pr	T (s)	Pr	T (s)	Pr	T (s)
BFGMRES(5)	76	902	304	970	1216	1094	4864	1522
BFGMRESD(5)	50	600	150	464	535	483	2102	681

Table 3: Two-grid preconditioned Block Flexible GMRES methods (with or without deflation) for the solution of the Helmholtz equation for the SEG/EAGE Salt dome model with mesh grid size h such that $h = \min_{(x,y,z)\in\Omega_h} c(x, y, z)/(10\, f)$. Case of multiple right-hand side problems (p denotes the number of right-hand sides considered and Cores the number of cores). The parameter T denotes the total computational time in seconds and Pr the number of preconditioner applications on a single vector.

5 Conclusions

The solution of heterogeneous Helmholtz problems is recognized as of high interest in many application fields. In this paper we have focused on a specific three-dimensional application in seismics related to acoustic wave propagation problems in the subsoil. The numerical simulation of such phenomena requires the approximate solution of possibly very large indefinite linear systems of equations. We have proposed an iterative two-grid method where the coarse grid problem is solved only approximately. A cycle of this method is used as a variable preconditioner for a flexible Krylov subspace method.

Numerical experiments on small to high frequency problems have shown the efficiency of such a preconditioner applied to a high-order discretization of the acoustic wave equation on structured grids. Problems with multiple right-hand sides have also been addressed and the reported numerical experiments show a satisfactory behaviour of the numerical method on a given realistic three-dimensional problem. The proposed numerical method allowed us to solve wave propagation problems even at high frequency on a reasonable number of cores of a distributed memory computing platform.

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