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Model Reduction Approaches for Solution of Wave Equations for Multiple Frequencies

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SUMMARY

We have developed a novel approach for solving multi-frequency frequency domain wave equation. The approach is based on efficient Krylov subspace approximants and projection-based model reduction techniques. We have considered polynomial Krylov and extended Krylov subspaces for approximating the solution given by stability-corrected resolvent. Our numerical examples indicate that polynomial Krylov subspace allows to obtain solution for the whole a priori given frequency range at the cost of solution for minimal frequency (for that frequency range) obtained using unpreconditioned BiCGStab solver. Extended Krylov subspace has been shown to improve the convergence by providing more uniform rate for the whole frequency range.

Introduction

Developing fast and robust forward-modeling methods for frequency-domain wave problems is not only a significant topic by itself, it is also of great importance for full wave inversion. When solutions for multiple frequencies are required, conventional workflow consists of solving discretized frequency-domain problems for each frequency separately. Typically, however, discretization grids for 3D problems consist of up to a billion nodes and even with state-of-the-art preconditioners such a workflow results in rather computationally intensive tasks.

Model reduction is a well-established tool, allowing us to efficiently obtain solutions in the time- or frequency-domains by projecting the large-scale dynamical system on a small Krylov or rational Krylov subspace. For lossy diffusion dominated problems, for example, model reduction has been shown to provide significant speed ups (see Zaslavsky et al. (2011)). For seismic exploration, we note that problems involving lossless media in unbounded domains effectively behave as lossy ones since infinity can be viewed as an absorber of outgoing waves. In fact, two of the authors showed that these problems, polynomial Krylov subspace (PKS) model reduction outperforms the finite-difference time-domain method on large time intervals (see Druskin and Remis (2013)).

In this paper we extend the PKS approach and use extended Krylov subspaces (EKS) for reduced-order model construction (Druskin and Knizhnerman (1998)). An EKS is generated by the system matrix and its inverse and reduced-order models taken from such a space usually converge much faster than PKS reduced-order models especially if a wide frequency range containing small frequencies is of interest. To compute the models in an efficient manner, we use a modified version of the EKS algorithm proposed by Jagels and Reichel (2009). Specifically, we generate a complex-orthogonal basis of the EKS via short-term recurrences by exploiting the complex-symmetric structure of the system matrix.

Problem formulation

Consider the multidimensional Helmholtz equation

$$Au + \omega^2 u = b. \quad (1)$$

In this equation, A is a self-adjoint nonnegative partial differential equation operator on an unbounded domain that has an absolutely continuous spectrum. We note that via a proper change of variables, all frequency-domain acoustic and elastic field equations can be written in a form as given by Eq. (1). We now discretize (1) using a second-order grid in the interior of the computational domain and use a PML for domain truncation. As a result, we obtain a matrix $\tilde{A}_N \approx A$, where $\tilde{A}_N \in \mathcal{C}^{N \times N}$ is complex symmetric. In practice, the order of this matrix can be up to billion or even more.

When the computational domain is truncated using a conventional time-domain perfectly matched layers (PML) formulation (Berenger (1994)), operator \tilde{A}_N becomes frequency-dependent. Indeed, that is sufficient for traditional preconditioned solvers that treat each frequency one by one. In our approach, however, we intend to reuse the same operator for multi-frequency computations. We therefore follow Druskin and Remis (2013) and Druskin et al (2013) and apply a *fixed-frequency* PML with *optimal* discrete stretching allowing low cost error control for a prescribed frequency interval.

It is tempting to substitute straightforwardly the approximate operator \tilde{A}_N in (1) and take the solution $u_N(\omega) = (\tilde{A}_N + \omega^2 I)^{-1} b_N$ as an approximation to u . Here, we note that it is our goal to solve Eq. (1) for multiple frequencies employing a fixed-frequency PML such that it is still possible to transform the frequency-domain solution back to the time-domain. However, using the non-Hermitian matrix \tilde{A}_N

instead of its exact Hermitian counterpart A , qualitatively changes the behavior of the solution on the complex plane. In particular, the symmetry relation $u(\omega) = \overline{u(-\omega)}$ breaks for the approximate solution and the time-domain transform of $u_N(\omega)$ is unstable. Fortunately, it is shown in Druskin and Remis (2013) that we can correct for these defects by using the stabilized approximation to Eq. (1) in the form

$$\tilde{u}_N(\omega) = -\frac{1}{2} \left[B_N^{-1} (B_N + i\omega I)^{-1} + \overline{B}_N^{-1} (\overline{B}_N + i\omega I)^{-1} \right] b_N, \quad B_N = (-\tilde{A}_N)^{1/2} \quad (2)$$

Model reduction and Krylov subspace methods

With the stability-corrected field approximations available, we can now construct reduced-order models based on EKS in the usual way. Specifically, the models are drawn from the Krylov subspace

$$\mathcal{K}_{m_1, m_2} = \text{span}\{\tilde{A}_N^{-m_1+1} b_N, \dots, \tilde{A}_N^{-1} b_N, b_N, \tilde{A}_N b_N, \dots, \tilde{A}_N^{m_2-1} b_N\}.$$

We note that the PKS $\mathcal{K}_m = \text{span}\{b_N, \tilde{A}_N b_N, \dots, \tilde{A}_N^{m-1} b_N\}$ corresponds to \mathcal{K}_{1, m_2} and PKS reduced-order models with application to stability-corrected solutions were investigated in Druskin and Remis (2013). The advantage of such a PKS model-order reduction approach is that its computational costs are essentially the same as the costs of m_2 steps of the explicit finite-difference time-domain method or m_2 steps of the unpreconditioned bi-CG method for the single frequency Helmholtz equation. However, the reduced-order models taken from the PKS may not provide us with the fastest convergence if wide frequency ranges with small enough frequencies are of interest. For such problems, we therefore resort to an EKS reduced-order modeling approach. An EKS can be seen as a special case of a rational Krylov subspace with one expansion point at zero and one at infinity. The action of \tilde{A}_N^{-1} on a vector is required to generate a basis for such a space. This essentially amounts to solving a Poisson-type equation for which efficient solution techniques are available. Computing matrix-vector products with the inverse of the system matrix is generally still more expensive than computing matrix-vector products with the system matrix itself, however, and from a computational point of view we therefore prefer to deal with EKS \mathcal{K}_{m_1, m_2} with $m_1 < m_2$. In addition, the basis vectors should be constructed via short-term recurrence relations, since storage of all basis vectors is generally not practical for large-scale applications. In Jagels and Reichel (2009), the authors developed such an EKS algorithm in which the orthogonal bases

$$V_{k(i+1)} = [v_0, v_1, \dots, v_i, v_{-1}, \dots, v_{-k+1}, \dots, v_{ik}]$$

for the sequence of subspaces $\mathcal{K}_{1, i+1} \subset \mathcal{K}_{2, 2i+1} \subset \dots \subset \mathcal{K}_{k, ki+1}$ are indeed generated via short term recurrences. Here, i is an integer that allows us to optimize the accuracy and computational costs. In this paper, we modify this algorithm and generate complex-orthogonal basis vectors of the EKS by exploiting the complex-symmetric structure of matrix \tilde{A}_N . Denote $d = k(i+1)$ and let $V_d \in \mathbb{C}^{N \times d}$ be matrix with columns being the generated basis vectors. Then all iterations can be summarized into the equation

$$\tilde{A}_N V_d = V_d H_d + z_d e_d^T,$$

where $z_d = h_{d+1, d} v_{-k} + h_{d+2, d} v_{ik+1}$ and h_{ij} is the (i, j) entry of matrix H_d . Furthermore, matrix H_d is a pentadiagonal matrix that satisfies $D_d H_d = V_d^T \tilde{A}_N V_d$, where D_d is diagonal matrix with entries $\delta_0, \delta_1, \dots, \delta_i, \delta_{-1}, \dots, \delta_{-k+1}, \dots, \delta_{ik}$. The entries of matrix H_d can easily be obtained in explicit form from the pentadiagonal matrix given in Jagels and Reichel (2009). The frequency-domain EKS reduced-order model is given by

$$\tilde{u}_d(\omega) = -\frac{1}{2} \delta_0 \left[V_d B_d^{-1} (B_d + i\omega I_d)^{-1} + \overline{V}_d \overline{B}_d^{-1} (\overline{B}_d + i\omega I_d)^{-1} \right] e_1, \quad (3)$$

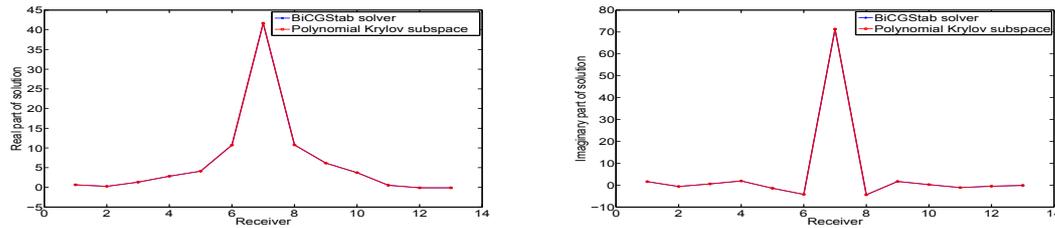


Figure 1 SEG/EAGE Salt model. Real and imaginary parts of the solution for a frequency of 7.5 Hz computed using the BiCGStab and PKS solvers with 1,600 matrix-vector multiplications and 1,800 iterations, respectively. The solutions are almost indistinguishable.

where $B_d = \left(-D_d^{1/2} H_d D_d^{-1/2}\right)^{1/2}$, $I_d \in \mathbb{R}^{d \times d}$ is the identity matrix, and e_1 is its first column. With the help of our modified EKS algorithm, we now have reduced the computation of functions of a very large finite-difference matrix \tilde{A}_N to the action of functions of a much smaller five-diagonal matrix $-D_d^{1/2} H_d D_d^{-1/2}$ times a “skinny” matrix V_d . Once both of these matrices have been computed, simulation of the frequency domain curve can be done rather cheaply.

Numerical experiments

First, we have considered the 3D SEG/EAGE Salt model and benchmarked our solver against an independently developed unpreconditioned BiCGStab algorithm that is a competitive conventional iterative Helmholtz solver (see Pan et al (2012) for details). Here, we took the case $m_1 = 1$ which corresponds to PKS. Fig. 1 shows excellent agreement between two approaches. Then we note that the PKS approach requires one matrix-vector multiplication per iteration, while BiCGStab needs two. Since this part constitutes the most computationally intensive part of the iteration process, it makes sense to compare the performance of these two methods in terms of matrix-vector multiplications rather than in terms of iterations. We have plotted the convergence rates of BiCGStab against the PKS model-order reduction method on Fig. 2 (left). Clearly, for this single frequency problem, both rates are rather close. We note that both approaches converge faster for higher frequencies and convergence slows down for lower frequencies. Indeed, Fig. 2 (right) shows how the reduced-order modeling method converges for different frequencies in the range from 2.5 Hz to 7.5 Hz. However, the principal difference between the PKS method and BiCGStab is that the former approach obtains solutions for the whole given frequency range at the convergence cost of BiCGStab for the lowest (from that range) frequency. Next, we consider what adding negative powers gives us in terms of performance. In Fig. 3 (left), we have plotted a number of convergence curves (with respect to increasing k) for approximants obtained using EKS $\mathcal{H}_{k,ki+1}$ for different values of fixed i ($i = \infty$ corresponds to PKS) and on a frequency range running from 2.5 Hz to 7.5 Hz. As is clear from this figure, adding negative powers ($i < \infty$) visibly improves the convergence of the Krylov subspace method. Indeed, while PKS converges faster for higher frequencies, EKS improves convergence for smaller frequencies and, consequently, convergence is more uniform on the entire frequency range. To confirm that point, in Fig. 3 (right), we have plotted convergence curves for the EKS method on a frequency range with expanded lower part. As one can observe, PKS significantly slows down while EKS performs as efficient as for a narrower frequency range.

Conclusions

We have developed a powerful model-order reduction tool for solving large-scale multi-frequency wave problems. The PKS method allows obtaining solutions for a whole range of frequencies at the cost of

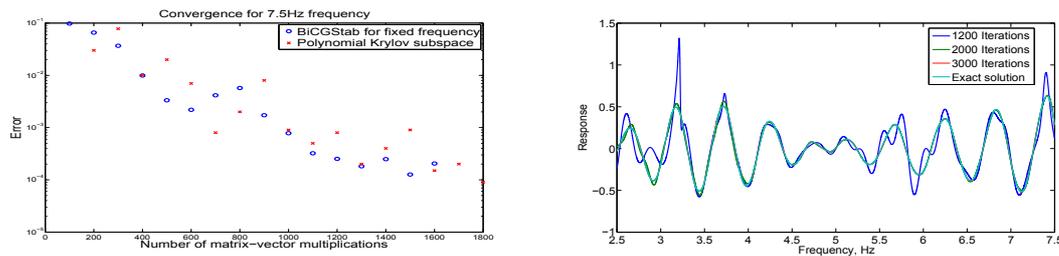


Figure 2 SEG/EAGE Salt model. Convergence rates of BiCGStab and PKS at a fixed frequency of 7.5 Hz (left) and convergence behavior of PKS for a frequency range running from 2.5 Hz to 7.5 Hz (right).

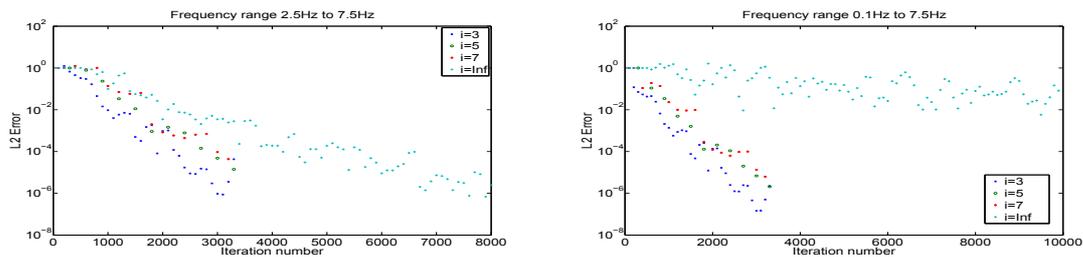


Figure 3 SEG/EAGE Salt model. Convergence of EKS for different values of i and for frequencies ranging from 2.5 Hz to 7.5 Hz (left) and from 0.1 Hz to 7.5 Hz (right).

solving a single-frequency problem with the BiCGStab solver. Moreover, EKS model-order reduction significantly outperform polynomial reduced-order modeling when solutions for small frequencies are required. We also note that the EKS approach can be applied to wave problems in the time-domain. Furthermore, our approach is not limited to second-order schemes in the interior. In fact, since the optimal discrete PML has spectral accuracy (see Druskin and Remis (2013); Druskin et al (2013)), it would be preferable to use optimal grids (Asvadurov et al (2000)) or spectral methods for interior part.

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