Model order reduction of electromagnetic wavefields in open domains

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Summary

Reduced order models can reduce the computational burden associated with inverse scattering problems. Approximating the transfer function of the measurement setup by reduced order models allows for fast and memory efficient computation of Jacobians. Here we present several projection based model order reduction techniques to simulate electromagnetic wave propagation in unbounded domains.
We show how general wavefield principles such as reciprocity, causality, passivity, and the Schwartz reflection principle translate from the analytical to the numerical domain. Next, we introduce model order reduction techniques that preserve these structures. Projection onto polynomial, extended, and rational Krylov subspaces are discussed. The symmetry of the Maxwell equations allows for projection onto polynomial and extended Krylov subspaces without saving the basis, using short term recurrence relations. Therefore reduced order models can be obtained that are as memory efficient as time stepping algorithms.
Rational Krylov subspaces are an interpolating model order reduction technique that performs well if only a few modes contribute to the system response. In case the configuration of interest has a low conductivity and the source and receiver are situated far away from the target, long travel times need to be modelled. In this case, the approximation error of rational Krylov subspace based reduced order models can be reduced significantly by approximating the phase of the wavefield by the eikonal phase, leading to what we call phase-preconditioned Rational Krylov subspaces. We present numerical examples to highlight the advantages and disadvantages of the discussed methods.

Keywords: forward modeling, reduced order modeling, Krylov subspace method

Introduction

Reduced order models (ROM) of electromagnetic wave propagation play an important role in many areas of science and engineering. The application range spans from design optimization of an optical resonator to borehole imaging in the oil and gas industry. The goal of reduced order modeling is usually a reduction in computational load; however, one can differentiate between two types of applications, namely, applications that require a fast construction and applications where a ROM can be constructed offline and is only required to offer accurate and fast evaluation. For process control in lithography for instance one has to solve real time inverse optical problems to ensure that the fabricated structure is within the set error margins. Here one can compute a computationally expensive ROM of expected electromagnetic configurations in an offline stage, as long as evaluation of the ROM is fast.
In this contribution we discuss three types of projection based Krylov model order reduction techniques for electromagnetic problems. We show how the structure of the Maxwell equations can be used to efficiently construct ROMs, while preserving the model structure. Most applications require open domains, such that absorbing boundary conditions in the form of complex coordinate stretching (Druskin, V. and Güttel, S. and Knizhnerman, L., 2016) are incorporated. The implementation of these boundary conditions into the various ROM frameworks is discussed as well.

Problem formulation

We are interested in solving the Maxwell equations

$$-\nabla \times \mathcal{H} + \sigma \mathcal{E} + \varepsilon \partial_t \mathcal{E} = -\mathcal{J}^{\text{ext}} \tag{1}$$

$$\nabla \times \mathcal{E} + \mu \partial_t \mathcal{H} = -\mathcal{K}^{\text{ext}} \tag{2}$$

for one (or multiple) source and receiver locations. Thus we are interested in the transfer function from a source to a receiver location. After finite difference discretization on a Yee-grid we obtain the matrix equation

$$\left(\begin{bmatrix} 0 & -\mathsf{D}_\mathsf{h} \\ \mathsf{D}_\mathsf{e} & 0 \end{bmatrix} + \begin{bmatrix} \mathsf{M}_\varepsilon & 0 \\ 0 & \mathsf{M}_\mu \end{bmatrix} \partial_t + \begin{bmatrix} \mathsf{M}_\sigma & 0 \\ 0 & 0 \end{bmatrix} \right) \begin{bmatrix} \mathsf{e} \\ \mathsf{h} \end{bmatrix} = - \begin{bmatrix} \mathsf{j}^{\text{ext}} \\ \mathsf{k}^{\text{ext}} \end{bmatrix}, \tag{3}$$

with $\mathsf{D}_{\mathsf{h/e}}$ the finite difference approximations of the curl operators, $\mathsf{M}_{\varepsilon/\mu/\sigma}$ diagonal medium matrices, and e the finite difference approximation of the electric field strength $\mathcal{E}$ and so forth. Equation 3 can be written in the compact form

$$(\mathsf{A} + \partial_t \mathsf{I})\mathsf{u} = \mathsf{b}, \tag{4}$$

where A is our sparse finite difference Maxwell operator that acts on the fields collected in u, which are excited by the sources in b. Equation 4 admits the formal solution and transfer function

$$\mathsf{u} = \exp(-\mathsf{A}t)\mathsf{b} \text{ and } \mathsf{f}(\mathsf{r},\mathsf{b}) = \mathsf{r}^T\mathsf{W}\exp(-\mathsf{A}t)\mathsf{b}, \tag{5}$$

respectively. With r^T the receiver vector and the diagonal matrix $\mathsf{W} = \begin{bmatrix} \mathsf{W}_\mathsf{p} & 0 \\ 0 & -\mathsf{W}_s \end{bmatrix}$ containing the volume of each primary (W_p) and secondary (W_s) finite difference voxel. From reciprocity we obtain invariance of the transfer function with respect to exchanging source and receiver vector $\mathsf{f}(\mathsf{r},\mathsf{b}) = \mathsf{f}(\mathsf{b},\mathsf{r})$, from which we obtain the symmetry relation

$$\mathsf{W}\mathsf{A} = \mathsf{A}^T\mathsf{W}. \tag{6}$$

We are mainly interested in wavefields in open domains and therefore continue our analysis in the Laplace domain with Laplace parameter s, since coordinate stretching is more easily introduced in the Laplace domain . Incorporating this technique leads to a finite difference operator A that depends on the Laplace parameter s such that Equation 4 now reads

$$(\hat{\mathsf{A}}(s) + s\mathsf{I})\hat{\mathsf{u}} = \hat{\mathsf{b}}. \tag{7}$$

The symmetry of A (Eq. 6) directly translates to the Laplace domain. Further, $\hat{\mathsf{A}}(s)$ follows the Schwartz reflection principle $\hat{\mathsf{A}}(\bar{s}) = \overline{\hat{\mathsf{A}}}(s)$, since wave fields are conjugate symmetric in the Laplace domain (here the overbar denotes conjugation).

Reduced order modelling

The finite difference system of Equation 7 can be large with millions of unknowns for real applications, such that direct solution can be cumbersome. In reduced order modeling we approximate the wavefield in a small basis, to reduce the systems of equations to be solved. Therefore, we expand the wavefield $\hat{\mathsf{u}} = \mathsf{V}\mathsf{y}$ in the basis V with expansion coefficients y. For simplicity we assume $\mathsf{V} \in \mathbb{C}^{N\times m}$ to be orthogonal in a W weighted bilinear form, with N and m the order of the full and reduced system, respectively. After imposing a Galerkin condition we obtain a relation for the expansion coefficients y as

$$(\mathsf{V}^T\mathsf{W}\hat{\mathsf{A}}(s)\mathsf{V} + s\mathsf{I})\mathsf{y} = \mathsf{V}^T\mathsf{W}\hat{\mathsf{b}}, \tag{8}$$

which is of order m, with the symmetric reduced order model $\hat{\mathsf{H}}(s) = \mathsf{V}^T\mathsf{W}\hat{\mathsf{A}}(s)\mathsf{V}$. The quality of the reduced order model is determined by the choice of approximation basis V. We discuss three popular choices in this context, namely, Polynomial, Extended, and Rational Krylov Subspaces (PKS, EKS and RKS). In PKS we build a matrix polynomial with $\hat{\mathsf{A}}$ acting on $\hat{\mathsf{b}}$. This subspace can be extended to EKS by adding inverse powers of the matrix $\hat{\mathsf{A}}$ to the basis. The RKS method builds rational functions with $\hat{\mathsf{A}}$ and shifts κ. The subspaces are defined as

$$\begin{aligned}
\mathcal{K}^m_{\mathrm{PKS}} &= \operatorname{span}\left\{\hat{\mathsf{b}}, \hat{\mathsf{A}}\hat{\mathsf{b}}, \ldots, \hat{\mathsf{A}}^m\hat{\mathsf{b}}\right\}, \\
\mathcal{K}^{n_\mathrm{n},n_\mathrm{p}}_{\mathrm{EKS}} &= \operatorname{span}\left\{\hat{\mathsf{A}}^{-n_\mathrm{n}}\hat{\mathsf{b}}, \ldots, \hat{\mathsf{b}}, \ldots, \hat{\mathsf{A}}^{n_\mathrm{p}}\hat{\mathsf{b}}\right\}, \\
\mathcal{K}^m_{\mathrm{RKS}}(\kappa) &= \operatorname{span}\left\{(\hat{\mathsf{A}}(\kappa_1) + \kappa_1\mathsf{I})^{-1}\hat{\mathsf{b}}, \ldots,\right. \\
&\qquad \left.(\hat{\mathsf{A}}(\kappa_m) + \kappa_m\mathsf{I})^{-1}\hat{\mathsf{b}}\right\}.
\end{aligned} \tag{9}$$

Adding a vector to a PKS is computationally cheap and just requires one matrix vector multiplication; however, adding a vector to an RKS is computationally expensive, as one has to numerically solve the Maxwell equations for singe frequency points in κ. Depending on the investigated configuration, this cost difference can be balanced by the RKS superior approximation qualities, leading to accurate reduced order models with small subspaces. In fact to obtain a reasonable approximation with PKS and EKS often requires a model order m that makes storing the basis V infeasible. Furthermore, V would be frequency dependent with a frequency dependent PML. To resolve these issues for EKS and PKS we fix the PML frequency and use short term recurrence relations to compute the reduced order model $\hat{\mathsf{H}}(s)$ without storing the basis.

Fixed frequency PML

Recent developments in near-optimal PMLs allow for frequency independent PMLs that are matched over a spectral inveral (Druskin, V. and Güttel, S. and Knizhnerman, L., 2016). Fixing the PML frequency at $s = s^\mathrm{f}$ and using the notation $\hat{\mathsf{A}}^\mathrm{f} = \hat{\mathsf{A}}(s^\mathrm{f})$ we obtain

$$(\hat{\mathsf{A}}^\mathrm{f} + s\mathsf{I})\hat{\mathsf{u}} = \hat{\mathsf{b}}, \tag{10}$$

which violates the Schwarz reflection principle as $\hat{\mathsf{u}}(\bar{s}) \neq \overline{\hat{\mathsf{u}}}(s)$ and makes Equation 10 unstable as $\hat{\mathsf{A}}^\mathrm{f}$ has eigenvalues with a negative real part. However, stable field approximations can be obtained by computing stability-corrected (Druskin, Remis, & Zaslavsky, 2014; Druskin & Remis, 2013) transfer functions via

$$\mathsf{f}(\mathsf{r},\mathsf{b}) = 2\eta(t)\mathsf{r}^T\mathsf{W}\,\mathrm{Re}(\eta(\hat{\mathsf{A}}^\mathrm{f})\exp(-\hat{\mathsf{A}}^\mathrm{f}t)\mathsf{b}), \tag{11}$$

which also upholds the Schwartz reflection principle in the Laplace domain since

$$\begin{aligned}\hat{\mathsf{f}}(\mathsf{r},\mathsf{b}) =& \mathsf{r}^T\mathsf{W}\eta(\hat{\mathsf{A}}^{\mathrm{f}})(\hat{\mathsf{A}}^{\mathrm{f}}+s\mathsf{I})^{-1}\mathsf{b}+\\ & \mathsf{r}^T\mathsf{W}\eta(\overline{\hat{\mathsf{A}}^{\mathrm{f}}})(\overline{\hat{\mathsf{A}}^{\mathrm{f}}}+s\mathsf{I})^{-1}\mathsf{b}.\end{aligned} \quad (12)$$

Here $\eta(z)$ is the Heaviside step function acting on the real part of its argument, such that $\eta(\hat{\mathsf{A}}^{\mathrm{f}})$ is a projector onto the stable part of our finite difference matrix. Reduced order models of the upper transfer functions using EKS and PKS can be computed efficiently without storing the basis V, since $\hat{\mathsf{A}}^{\mathrm{f}}$ is J-symmetric (see 6). Using PKS, a tridiagonal H can be computed via the modified Lanczos algorithm (Freund & Nachtigal, 1995) and a pentadiagonal H can be computed when EKS are used as approximation basis (Jagels & Reichel, 2011). The short recursion relations together with the fact that only the bilinear form $\mathsf{r}^T\mathsf{W}f(\hat{\mathsf{A}}^{\mathrm{f}})\mathsf{b}$ is needed rather than the whole field approximation allows for the computation of the transfer function without storing the basis. Generally, EKS performs well if low frequencies need to be approximated. Essentially, one has to solve three Poisson equations to compute an iteration with a negative power of A.

Rational Krylov Subspaces

Contrary to EKS and PKS the rational Krylov method has no problem in handling frequency dependent finite difference matrices as the subspace is spanned by single frequency solutions to the problem. The quality of an RKS-ROM is dependent on the choice of so-called shifts or interpolation points κ which are the Laplace frequencies whose Maxwell solutions span the RKS. We would like the reduced order model to preserve the symmetry, passivity and Schwartz reflection principle of the full order model, to honor the underlying physics. To this end, the interpolation points κ need to be closed under conjugation, such that the RKS itself is closed under conjugation and contains solutions $\mathsf{u}(\kappa_j)$ and $\mathsf{u}(\overline{\kappa_j}) = \overline{\mathsf{u}(\kappa_j)}$. This can be achieved by a choosing the real structure preserving Rational Krylov subspace (spRKS) subspace

$$\begin{aligned}\mathcal{K}^{2m}_{\mathrm{spRKS}} = \mathrm{span}\,\{&\mathrm{Re}\ \hat{\mathsf{u}}(\kappa_1), \mathrm{Im}\ \hat{\mathsf{u}}(\kappa_1), \ldots,\\ &\mathrm{Re}\ \hat{\mathsf{u}}(\kappa_m), \mathrm{Im}\ \hat{\mathsf{u}}(\kappa_m)\}\,.\end{aligned} \quad (13)$$

Now let $\mathsf{V} \in \mathbb{R}^{N\times 2m}$ span this subspace, then the reduced order wavefield $\hat{\mathsf{u}}_m$ can be obtained as

$$\hat{\mathsf{u}}_m = \mathsf{V}(\mathsf{V}^T\mathsf{W}\hat{\mathsf{A}}(s)\mathsf{V} + s\mathsf{V}^T\mathsf{W}\mathsf{V})^{-1}\mathsf{V}^T\mathsf{W}\hat{\mathsf{b}}. \quad (14)$$

Phase preconditioning

The described model order reduction technique yields fast convergence in small subspaces when only a few modes of the system contribute to the response. For highly conductive media, the method exhibits fast convergence as well and in the limiting case of electromagnetic diffusion, RKS show excellent convergence properties, and optimal shifts κ are known (Knizhnerman, Druskin, & Zaslavsky, 2009). For applications in explorational geophysics with little or no losses present and long travel times between source, target and receiver the frequency domain transfer function becomes very oscillatory since a delay in the time domain turns into a complex exponent in the Laplace domain. An interpolatory method like RKS should at least have two points per wavelength of the largest travel time modelled, which leads to prohibitively large RKS. However, this sampling requirement can be lowered by approximating the phase term of the wavefield by the eikonal phase term $\exp(s\mathcal{T}^{\mathrm{eik}})$, where $\mathcal{T}^{\mathrm{eik}}$ is the eikonal travel time obtained from the eikonal equation $|\nabla\mathcal{T}^{\mathrm{eik}}|^2 = \varepsilon\mu$ (Druskin, Remis, Zaslavsky, & Zimmerling, submitted). Thus, at each interpolation point the wavefield $\hat{\mathsf{u}}$ can be split into an incoming and outgoing wave amplitude $\mathsf{c}^{\mathrm{in/out}}$ and phase term

$$\hat{\mathsf{u}}(\kappa_i) = \exp(-\kappa_i\mathsf{T})\mathsf{c}^{\mathrm{out}}(\kappa_i) + \exp(\kappa_i\mathsf{T})\mathsf{c}^{\mathrm{in}}(\kappa_i), \quad (15)$$

using one-way wave equations. Now a phase preconditioned Rational Krylov subspace can be built by multiplying the amplitudes $\mathsf{c}^{\mathrm{in/out}}$ with the eikonal phase at every frequency where the ROM is evaluated. Thus we obtain a field approximation $\hat{\mathsf{u}}_m(s)$ of the form

$$\begin{aligned}\hat{\mathsf{u}}_m(s) =& \sum_{i=1}^{m} a_i \exp(-s\mathsf{T})\mathsf{c}^{\mathrm{out}}(\kappa_i) + \ldots\\ & \sum_{j=1}^{m} b_j \exp(s\mathsf{T})\mathsf{c}^{\mathrm{in}}(\kappa_j)\end{aligned} \quad (16)$$

where the expansion coefficients a_i, b_i can be found from a Galerkin condition. Now the first arrival times are factored out and corrected analytically, such that low order field approximations can be obtained.

Results

To show the approximation qualities of the introduced ROMs we consider a configuration arising in exploration with a ground penetrating radar (GPR). We investigate a lossy subsurface with a box shaped anomaly in a frequency band between 50 MHz and 2.4 GHz. The simulated configuration is shown in Figure 1, where the exact medium parameters are provided in the caption. A current source directed in the z-direction is used for excitation and the z-component of the electrical field is measured at the ground-air interface. Finite-difference discretization with a second-order accurate operator and 8 points per wavelength at 2.4 GHz leads to a first order Maxwell system with $N = 62 \cdot 10^3$ unknowns. Using this full operator, we compute the transfer function for this configuration using an FDFD method as comparison solution for our reduced order models. This comparison solution is shown alongside the responses of the PKS, EKS and RKS reduced order models in Figure 2. The order of the reduced order models was increased until the reduced order models and the comparison solution essentially overlap.

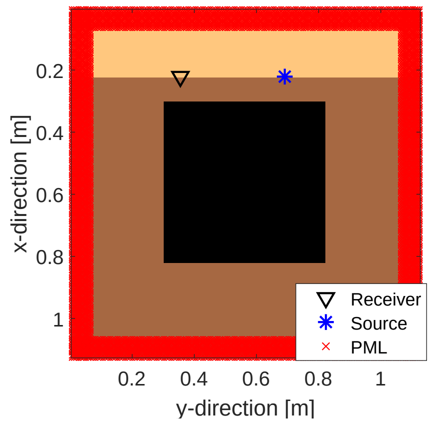

Figure 1: Simulated GPR configuration, with a $(\varepsilon_{\mathrm{r}} = 4, \sigma = 10^{-2}\,\mathrm{S/m})$ anomaly embedded in a $(\varepsilon_{\mathrm{r}} = 1, \sigma = 5 \cdot 10^{-4}\,\mathrm{S/m})$ surface layer, with dry air $\varepsilon_{\mathrm{r}} = 1, \sigma = 0$ on top.

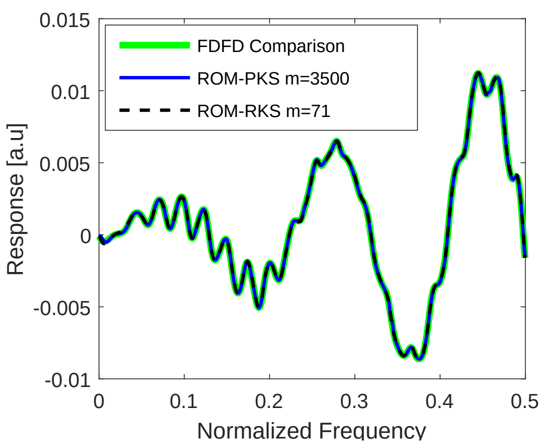

Figure 2: Imaginary part of the transfer function over the frequency interval of interest. A FDFD method is compared to two different ROMs.

For the RKS method we choose equidistant shifts on the imaginary axis between 50 MHz and 2.4 GHz. The RKS method leads to the smallest model with $m = 71$; however, a single iteration is much more expensive than a PKS iteration. The PKS method needs $m = 3500$ iterations until convergence, where one iteration is as expensive as an FDTD step.

Conclusion

We presented several reduced order modeling techniques for the Maxwell equations targeted at but not limited to applications in geophysics. RKS generally yields the smallest models; however, for some applications and configurations the low cost of a single iteration of PKS or EKS outweighs this advantage. Furthermore, generating a RKS demands more memory as we have to save the basis.

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