Efficient Computation of Electromagnetic Wave Fields on Unbounded Domains Using Stability-Corrected Wave Functions and Krylov Subspace Projection Methods

V. Druskin* R. F. Remis† M. Zaslavsky* J. T. Zimmerling†

Abstract — **We present a Krylov subspace projection framework to model electromagnetic wave propagation in unbounded domains. The extension to infinity is modeled via an optimal complex scaling method and we show that stable time-domain reduced-order models can be efficiently computed via a stability-correction procedure in conjunction with a Lanczos-type reduction algorithm. We show that dominant open resonant modes can be determined via the Lanczos algorithm and illustrate the performance of our technique through a number of numerical examples for two- and three-dimensional configurations.**

1 INTRODUCTION

In this paper we present a Krylov subspace projection framework to model electromagnetic wave propagation on unbounded domains. Krylov methods are known to exhibit fast convergence for lossy diffusion dominated problems [1] and may therefore show excellent convergence behavior for open wave propagation problems as well. Loosely speaking, the reason is that open wave field problems are inherently lossy, because infinity acts as an absorber.

To simulate the extension to infinity, the Perfectly Matched Layer (PML) technique [2] is nowadays the method of choice in local (finite-difference or finite elements) solution methods for Maxwell's equations. In this technique, the spatial coordinates are stretched inside a layer (the PML layer) that completely surrounds the computational domain of interest. Stretching of the coordinates is achieved via the introduction of so-called stretching functions in Maxwell's equations [3]. These functions are frequency dependent in general and consequently waves of all frequencies are absorbed by the PML layer without any reflection.

Within a Krylov subspace model-order reduction framework, the frequency dependence of the stretching functions leads to nonlinear eigenvalue problems in two or three spatial dimensions. This obviously hinders the efficiency of Krylov reduction methods, since nonlinear eigenproblems are much more difficult to solve than linear ones. As a solution to this problem, we can simply fix the frequency of the PML stretching functions to a frequency $\tilde{\omega}$, say. The PML technique of Berenger then turns into the so-called complex scaling method [4], [5], which was introduced already in the 1970s and has been applied in acoustics, RF MEMS simulations, and quantum mechanics, to model resonances and resonant field behavior of open systems [6] – [8].

A drawback of fixing the PML frequency is that the PML only performs well for frequencies in a neighborhood of $\tilde{\omega}$. This problem is resolved in [9], where a global complex scaling method is proposed which is optimal over an entire frequency band of interest and allows for time-domain field simulations as well (see [10] for an extension of this complex-scaling approach). More precisely, by applying optimal complex scaling in combination with a stability-correction procedure outlined in [9], stable time-domain or conjugate-symmetric frequency-domain field approximations on unbounded domains can obtained. Furthermore, the semidiscrete wave operators are essentially complex-symmetric and therefore enable us to efficiently compute time- or frequency-domain reduced-order models via a Lanczos-type three-term reduction algorithm. In Section 2, we briefly review the construction of these models and in Section 3 we illustrate the performance of our reduction method through a number of numerical examples. The conclusions are presented in Section 4 along with a brief discussion on possible extensions of the proposed model-reduction solution methodology.

2 REDUCED-ORDER MODELS

To simulate electromagnetic wave propagation on unbounded domains, we start with the first-order

*Schlumberger Doll Research, 1 Hampshire St., Cambridge, MA 02139, USA, e-mail: druskin1@slb.com, MZaslavsky@slb.com

†Circuits and Systems Group, Faculty of Electrical Engineering, Mathematics and Computer Science, Delft University of Technology, Mekelweg 4, 2628 CD, Delft, The Netherlands, email: R.F.Remis@TUDelft.NL, J.T.Zimmerling@TUDelft.NL

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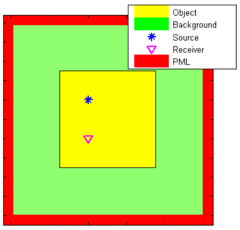

Figure 1: A square dielectric object with a relative permittivity of $\varepsilon_{\mathrm{r}} = 4$ embedded in a vacuum background domain. Both the source (asterisk) and the receiver (triangle) are located inside the object.

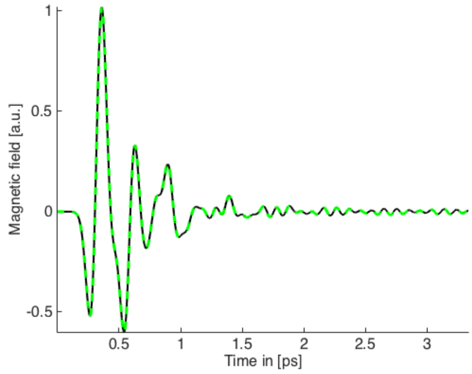

Figure 2: Magnetic field strength at the receiver location as a function of time. Solid line: response as computed by FDTD. Dashed line: reduced-order model of order 1500.

Maxwell system

$$(\mathcal{D} + \mathcal{M}\partial_t)\,\mathcal{F} = -\mathcal{Q}', \tag{1}$$

where the spatial differential operator $\mathcal{D}$ contains the curl operators in Maxwell's equations and $\mathcal{M}$ is a medium matrix containing the permittivity and permeability values of the various materials present in our domain of interest. Furthermore, the components of the electric and magnetic field strength are contained in the field vector $\mathcal{F}$, while the components of the external current densities are contained in the source vector $\mathcal{Q}'$. From this moment on, we only consider external sources for which the time dependence can be factored out, that is, we consider source vectors of the form $\mathcal{Q}' = w(t)\mathcal{Q}$, where $w(t)$ is the source wavelet that vanishes for $t < 0$ and $\mathcal{Q}$ is a time-independent vector.

Discretizing the above Maxwell system in space and applying optimal complex scaling to simulate the extension to infinity, the semidiscrete state-space system

$$(\mathsf{D} + \mathsf{M}\partial_t)\,\tilde{\mathsf{f}} = -w(t)\mathsf{q} \tag{2}$$

is obtained, where D, M, $\tilde{\mathsf{f}}$, and q denote the discrete counterparts of $\mathcal{D}$, $\mathcal{M}$, $\mathcal{F}$, and $\mathcal{Q}$, respectively. By premultiplying Eq. (2) by the inverse of the (diagonal) medium matrix, we obtain

$$(\mathsf{A} + \mathsf{I}\partial_t)\,\tilde{\mathsf{f}} = -w(t)\mathsf{M}^{-1}\mathsf{q}, \tag{3}$$

where I is the identity matrix and where we have introduced the system matrix $\mathsf{A} = \mathsf{M}^{-1}\mathsf{D}$. We note that the entries of matrix D containing the step sizes of the PML are complex-valued and matrix A is unstable (matrix A has eigenvalues with positive and negative real parts) due to the application of the complex scaling method. However, by applying the stability-correction procedure presented in [9], stable-time domain field approximations can be computed using

$$\mathsf{f}(t) = -w(t) * 2\eta(t)\mathrm{Re}\left[\eta(\mathsf{A})\exp(-\mathsf{A}t)\mathsf{M}^{-1}\mathsf{q}\right], \tag{4}$$

where the asterisk denotes convolution in time and $\eta(z)$ is the complex Heaviside unit step function ($\eta(z) = 1$ for $\mathrm{Re}(z) > 0$ and $\eta(z) = 0$ for $\mathrm{Re}(z) < 0$).

Direct evaluation of Eq. (4) is not feasible, however, since the order n of the system matrix A is too large especially for three-dimensional problems. Fortunately, matrix A satisfies the symmetry relation

$$\langle \mathsf{Ax}, \mathsf{y}\rangle = \langle \mathsf{x}, \mathsf{Ay}\rangle \quad \text{for all } \mathsf{x}, \mathsf{y} \in \mathbb{C}^n, \tag{5}$$

where $\langle\cdot,\cdot\rangle$ is a bilinear form given by $\langle \mathsf{x}, \mathsf{y}\rangle = \mathsf{y}^T\mathsf{W}\mathsf{M}\mathsf{x}$ and W is a step size matrix containing the step sizes of the spatial grid. The free-field Lagrangian $\mathcal{L}_{\mathrm{free}}$ is induced by this bilinear form [11], that is, $\frac{1}{2}\langle \mathsf{f}, \mathsf{f}\rangle$ approximates

$$\mathcal{L}_{\mathrm{free}} = \frac{1}{2}\int_{\mathbf{x}\in\mathbb{D}} \varepsilon|\mathbf{E}|^2\,\mathrm{d}V - \frac{1}{2}\int_{\mathbf{x}\in\mathbb{D}} \mu|\mathbf{H}|^2\,\mathrm{d}V, \tag{6}$$

where $\mathbb{D}$ is our computational domain of interest.

By exploiting the symmetry relation of Eq. (5), we can generate reduced-order models for the electromagnetic field via a three-term Lanczos-type reduction algorithm [9]. This algorithm generates a basis of the Krylov subspace

$$\mathbb{K}_m = \mathrm{span}\{\mathsf{M}^{-1}\mathsf{q}, \mathsf{A}\mathsf{M}^{-1}\mathsf{q}, ..., \mathsf{A}^{m-1}\mathsf{M}^{-1}\mathsf{q}\} \tag{7}$$

and after $m \ll n$ iterations we have the summarizing equation

$$\mathsf{A}\mathsf{V}_m = \mathsf{V}_m\mathsf{H}_m + \mathsf{r}_m\mathsf{e}_m^T, \tag{8}$$

where the n-by-m matrix V_m has the m Lanczos basis vectors v_i as its columns, H_m is a tridiagonal m-by-m matrix containing the Lanczos recurrence coefficients, r_m is a residual vector, and e_m

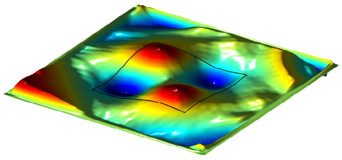

Figure 3: Magnetic field strength of a 2π open resonant mode in and around the square dielectric object of Figure 1.

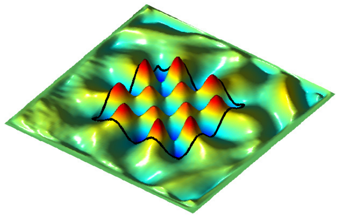

Figure 4: Magnetic field strength of a 5π open resonant mode in and around the square dielectric object of Figure 1.

is the mth column of the m-by-m identity matrix. We note that in our implementation of the Lanczos algorithm, all basis vectors have unit 2-norm ($\|\mathsf{v}_i\| = 1$) and are "orthogonal" with respect to the bilinear form introduced above.

Based on the Lanczos decomposition of Eq. (8), we can now construct the reduced-order models

$$\mathsf{f}_m(t) = -w(t) * 2n_\mathrm{s}\eta(t)\mathrm{Re}\left[\mathsf{V}_m \eta(\mathsf{H}_m)\exp(-\mathsf{H}_m t)\mathsf{e}_1\right], \tag{9}$$

where $n_\mathrm{s} = \|\mathsf{M}^{-1}\mathsf{q}\|$. To compute these models, only matrix functions of matrix H_m need to be evaluated. The order of this matrix is much smaller than the order of the system matrix A and matrix H_m is tridiagonal as well. Finally, we remark that dominant open resonant modes can also be extracted from the Lanczos decomposition of Eq. (8) as will be illustrated in Section 3.

3 NUMERICAL RESULTS

As a first example, we consider H-polarized fields in a two-dimensional configuration that is invariant in the z-direction. The configuration consists of a square dielectric object with a relative permittivity of $\varepsilon_\mathrm{r} = 4$ and the object is embedded in a vacuum background domain. Furthermore, the side length of the square is 50 μm and both the source (asterisk) and the receiver (triangle) are located inside the object (see Figure 1). The source wavelet is a derivative of a Gaussian and its spectrum has a maximum at a wavelength $\lambda_\mathrm{peak} = 94$ μm in vacuum. After discretizing this configuration in space, a semidiscrete Maxwell system is obtained with about 37000 time-dependent unknowns.

In Figure 2 we show the magnetic field response at the receiver location. The solid line signifies the response as computed by FDTD, while the dashed line is the magnetic field reduced-order model of order 1500. We observe that this reduced-order model essentially overlaps with the FDTD result on the time interval of interest and its order is about 24.5 times smaller than the order of the original unreduced system.

Using the Lanczos decomposition of Eq. (8), we can also determine the open resonant modes that are excited by the external source. In Figures 3 and 4 we show the magnetic field component of two of these modes. Both modes have converged and contribute to the time-domain signal shown in Figure 2. Other higher order modes can be determined as well, of course, but their retrieval may require a larger number of Lanczos iterations.

As a second example, we compute dominant resonant modes for the three-dimensional configuration shown in Figure 5. This configuration consists of an electric dipole located in the vicinity of a dielectric box with side lengths equal to 50 μm. The relative permittivity of the box is set to $\varepsilon_\mathrm{r} = 4$ and the box is again embedded in vacuum. After discretizing this configuration in space, the resulting semidiscrete Maxwell system has an order of about 8.4 million. Using the Lanczos algorithm, we can now compute the dominant resonant modes that are excited by the dipole. Figure 6 shows the imaginary part of the x-component of the electric field strength of one of these modes and was obtained from the Lanczos algorithm after 10000 iterations. Clearly, the mode shows a 5π resonant field pattern in the y- and z-directions and only a fundamental resonance pattern in the x-direction, which is the direction in which the electric dipole is oriented.

4 CONCLUSIONS

In this paper we have presented a Krylov subspace reduction method to simulate electromagnetic wave propagation on unbounded domains. To simulate the extension to infinity, we have implemented an optimal complex scaling method and stable time-domain field approximations have been computed via a stability-correction procedure in conjunction with a Lanczos-type reduction algorithm. The algorithm allows for the efficient computation of electromagnetic wave fields and dominant resonant modes that are excited by the external source can be determined as well.

In this paper we have restricted ourselves to instantaneously reacting media, but our reduction

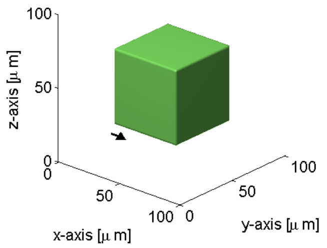

Figure 5: A square dielectric box with a relative permittivity of $\varepsilon_{\mathrm{r}} = 4$ embedded in a vacuum background domain. The side length of the box is 50 μm and an x-directed electric dipole is located in the xz-plane in the vicinity of the box.

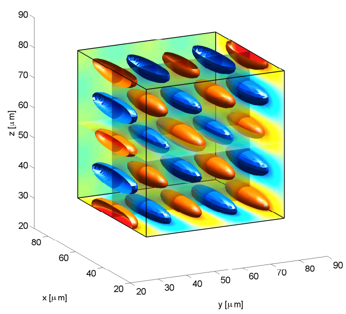

Figure 6: Imaginary part of the x-component of the electric field strength of an open resonant mode as excited by an x-directed dipole located in the xz-plane just outside a three-dimensional box with a relative permittivity of $\varepsilon_{\mathrm{r}} = 4$.

approach can be extended to dispersive media as well [12]. Furthermore, since the stability-corrected wave function is a nonentire function of the Maxwell system matrix, we expect that rational Krylov methods may converge much faster than standard Krylov methods [13], since the wave function is then approximated by a rational function instead of a polynomial as in a standard Krylov method. Future work will therefore focus on developing effective rational Krylov methods for wave propagation problems on unbounded domains.

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