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A Lanczos model-order reduction technique to efficiently simulate electromagnetic wave propagation in dispersive media

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ABSTRACT

In this paper we present a Krylov subspace model-order reduction technique for time- and frequency-domain electromagnetic wave fields in linear dispersive media. Starting point is a self-consistent first-order form of Maxwell's equations and the constitutive relation. This form is discretized on a standard staggered Yee grid, while the extension to infinity is modeled via a recently developed global complex scaling method. By applying this scaling method, the time- or frequency-domain electromagnetic wave field can be computed via a so-called stability-corrected wave function. Since this function cannot be computed directly due to the large order of the discretized Maxwell system matrix, Krylov subspace reducedorder models are constructed that approximate this wave function. We show that the system matrix exhibits a particular physics-based symmetry relation that allows us to efficiently construct the time- and frequency-domain reduced-order models via a Lanczostype reduction algorithm. The frequency-domain models allow for frequency sweeps meaning that a single model provides field approximations for all frequencies of interest and dominant field modes can easily be determined as well. Numerical experiments for two- and three-dimensional configurations illustrate the performance of the proposed reduction method.

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1. Introduction

The efficient computation of time- and frequency-domain electromagnetic wave fields in linear dispersive media is extremely important in a wide variety of applications ranging from bioelectromagnetics [10] to nano-optics [17]. To compute the complex electromagnetic wave field interactions with such materials, general solution procedures such as the Finite-Difference Time-Domain method (FDTD method, [23]) are typically used or dedicated frequency-domain solvers in which certain geometric features of the configuration of interest are exploited (as in periodic or aperiodic Fourier modal methods, see [2,28,29], for example). An advantage of an FDTD approach is that it can be applied to arbitrarily-shaped dispersive objects, but a drawback may be that it is not as efficient as a dedicated solver such as a Fourier modal method. The latter method, on the other hand, may not be as widely applicable as an FDTD method.

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In this paper we present a novel Krylov subspace model-order reduction approach, which is efficient and applicable to arbitrary three-dimensional configurations. The method is particularly effective for subwavelength resonating structures as encountered in nano-optics, for example, and both time- and frequency-domain fields can be computed simultaneously. In addition, the modes that dominate the electromagnetic field response at particular receiver locations can be determined directly at negligible additional computational costs and the method allows for so-called frequency sweeps as well, meaning that a *single* reduced-order model can be used for all frequencies within a certain frequency interval of interest even in case of dispersive frequency-dependent dielectric materials.

To fix the idea, we consider linear dielectric dispersive media for which the polarization vector is related to the electric field strength via a second-order differential equation in time. Lorentz, Drude, and Debye materials are all captured by such a constitutive relation. Furthermore, for simplicity we restrict ourselves to single pole or single pole pair dispersion models, but we stress that multiple pole models can be handled as well.

The first step of our approach consists of writing Maxwell's equations and the constitutive relation in a self-consistent first-order form. The resulting system is then discretized in space on a standard staggered Yee-grid [23], while the extension to infinity is simulated by implementing the recently developed global complex scaling method discussed in [8] and [6]. Complex scaling has already been introduced in the 1970s (see [3] and [22], for example) and can be seen as a variant of the well known Perfectly Matched Layer (PML) technique [4,5] in which the PML frequency is fixed to a frequency s_0 , say. Standard complex scaling is therefore effective only for frequencies in a neighborhood of s_0 . However, in [8] and [6] it is shown how to turn the complex scaling method into a global method that is accurate over a complete frequency band of interest with frequencies belonging to this interval that are not necessarily close to s_0 . If we now apply this global complex scaling method to simulate the extension to infinity then complex-valued step sizes within the PML are obtained and the resulting semidiscrete Maxwell system is unstable [8]. The method can therefore not be applied directly in a standard time stepping solution procedure such as FDTD and frequency-domain field approximations fail to be conjugate symmetric with respect to frequency as well. Fortunately, this situation can be resolved via the introduction of a so-called stability-corrected wave function [8]. This function corrects for the anti-stable part of the solution obtained via global scaling and produces stable, causal, and real-valued field approximations in the time-domain and conjugate-symmetric solutions in the frequencydomain. Thus global complex scaling in combination with stability correction allows us to simulate electromagnetic wave propagation in the time- and frequency-domain with a PML layer that does not explicitly depend on the frequency.

Direct evaluation of the wave function is not feasible, however, since the wave function depends on the Maxwell system matrix and the order of this matrix is simply too large. For three dimensional problems, for example, the order of this system matrix can easily run into the millions and direct evaluation is therefore practically impossible. We therefore construct timeand frequency-domain Krylov subspace reduced-order models for the stability-corrected wave function that can be evaluated directly. In particular, we show that the Maxwell system matrix exhibits a particular physics-based symmetry property that allows us to construct the reduced-order models via a three-term Lanczos-type recurrence relation. The models can therefore be computed very efficiently, since the system matrix is sparse and this matrix is only needed to form matrix–vector products in the Lanczos algorithm (see [7] for computation of matrix functions using Lanczos algorithms). With the help of the Lanczos algorithm we are also able to compute the modes that contribute the most to the response at a certain receiver location at essentially no additional costs. Furthermore, not all Lanczos vectors need to fit inside the computational memory.

For dielectric structures reduced order modeling has been shown to be efficient in model compression and reducing computation time (see [8]). Contrary to FDTD, model order reduction techniques based on the Lanczos algorithm adapt their spectrum to the spectrum of the operator as shown in [19]. In this paper, this approach is extended to dispersive materials. In general, radiation and dissipative losses enable large model-order reduction factors especially in case of a limited number of sources and receivers. Finally, the reduced-order models are expected to exhibit fast convergence for resonating subwavelength structures as encountered in nano-optics, since these configurations are typically largely oversampled and only a relatively small number of modes contribute to the overall measured signal. Our numerical experiments illustrate that the proposed solution procedure is very efficient for these types of structures, as indeed very low order approximations suffice.

This paper is organized as follows. In Section 2 we introduce a self-consistent first-order formulation for the electromagnetic field in dispersive media. The discretization of the first-order system is discussed next followed by a brief discussion on the global complex scaling method. In Section 3 we discuss the symmetry properties of the Maxwell system matrix and present our Lanczos reduction algorithm together with the time- and frequency-domain reduced-order modes. The technical details of the symmetry analysis are presented in the Appendix. Finally, in Section 4 we present a number of numerical results that illustrate the performance of the proposed solution procedure for two- and three-dimensional problems in the time- and frequency-domain and the dominant field modes for these configurations are determined as well.

2. Basic equations

We consider an electromagnetic field in a dispersive material that is governed by the Maxwell equations

$$-\nabla \times \mathbf{H} + \partial_t \mathbf{D} = -\mathbf{J}^{\text{ext}}$$

Table 1

Parameters to obtain common dispersion models with the general second-order dispersion model. Here, τ is the characteristic relaxation time, ε_s is the static relative permittivity, ω_p is the volume plasma frequency, γ_p is the collision frequency, ω_0 is the resonant plasma frequency, and δ is the damping coefficient.

Medium	β_0	β_1	β_2	β_3
Lorentz	$\epsilon_0(\epsilon_{\rm s}-\epsilon_\infty)\omega_0^2$	ω_0^2	2δ	1
Drude	$\varepsilon_0 \omega_p^2$	0	$\gamma_{ m p}$	1
Debye	$\epsilon_0(\epsilon_s - \epsilon_\infty)$	1	τ	0
Conductivity	σ	0	1	0

and

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

where $\mathbf{D} = \varepsilon \mathbf{E} + \mathbf{P}$ with $\varepsilon = \varepsilon_0 \varepsilon_\infty$ and ε_∞ the instantaneous or high-frequency relative permittivity. The polarization vector \mathbf{P} is related to the electric field strength \mathbf{E} via the second-order constitutive relation

$$\beta_3 \partial_t^2 \mathbf{P} + \beta_2 \partial_t \mathbf{P} + \beta_1 \mathbf{P} = \beta_0 \mathbf{E},\tag{3}$$

where the β_i , i = 0, 1, 2, 3, are parameters describing the particular dispersive material of interest. For example, for a Drude material we have $\beta_0 = \varepsilon_0 \omega_p^2$, $\beta_1 = 0$, $\beta_2 = \gamma_p$, and $\beta_3 = 1$, where ω_p is the volume plasma frequency and γ_p the collision frequency. The β -coefficients of other commonly used materials are summarized in Table 1.

As a first step towards our reduced-order modeling approach, we first rewrite the second-order constitutive relation in first-order form. To this end, we introduce the auxiliary field

$$\mathbf{U} = -\partial_t \mathbf{P} \tag{4}$$

and rewrite Eq. (3) as

$$\beta_3 \partial_t \mathbf{U} + \beta_2 \mathbf{U} - \beta_1 \mathbf{P} + \beta_0 \mathbf{E} = \mathbf{0}. \tag{5}$$

Combining these last two equations with Maxwell's equations, we arrive at the first-order system

$$-\nabla \times \mathbf{H} - \mathbf{U} + \varepsilon \partial_t \mathbf{E} = -\mathbf{J}^{\text{ext}},$$
$$\mathbf{U} + \partial_t \mathbf{P} = \mathbf{0},$$
$$\beta_2 \mathbf{U} - \beta_1 \mathbf{P} + \beta_0 \mathbf{E} + \beta_3 \partial_t \mathbf{U} = \mathbf{0},$$

and

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

These equations can be written in matrix-operator form as

$$(\mathcal{D} + \mathcal{S} + \mathcal{M}\partial_t)\mathcal{F} = \mathcal{Q}',\tag{6}$$

where \mathcal{F} and \mathcal{Q} are the field and source vectors given by

$$\mathcal{F} = [E_x, E_y, E_z, P_x, P_y, P_z, U_x, U_y, U_z, H_x, H_y, H_z]^{T}$$
(7)

and

$$Q' = -[J_x^{\text{ext}}, J_y^{\text{ext}}, J_z^{\text{ext}}, 0, 0, 0, 0, 0, 0, K_x^{\text{ext}}, K_y^{\text{ext}}, K_z^{\text{ext}}]^T,$$
(8)

respectively. In this paper, we only consider external sources for which the time-dependence can be factored out (which is usually the case) and write Q' = w(t)Q, where w(t) is the source wavelet that vanishes prior to the time instant t = 0and Q is a time-independent vector. Furthermore, D is a spatial differentiation matrix containing the curl operators from Maxwell's equations and S and M are medium matrices containing the medium parameters β_i , ε , and μ . Explicitly, the differentiation matrix is given by

$$\mathcal{D} = \begin{bmatrix} 0 & 0 & 0 & -\nabla \times \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \nabla \times & 0 & 0 & 0 \end{bmatrix}$$
(9)

and the medium matrices are

$$S = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 \\ \beta_0 & -\beta_1 & \beta_2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \text{ and } \mathcal{M} = \begin{bmatrix} \varepsilon & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \beta_3 & 0 \\ 0 & 0 & 0 & \mu \end{bmatrix}.$$
 (10)

Subsequently, we discretize the above first-order Maxwell system on our domain of interest using a standard secondorder finite-difference grid (Yee grid [23]) and a complex-scaling method is used to simulate the extension to infinity [1, 3,22]. Complex-scaling has been applied extensively in computational quantum mechanics and other fields (see, for example, [13,14,16]) and can be seen as a special instance of the Perfectly Matched Layer (PML) technique as introduced by Berenger [4,5]. Specifically, the PML in a complex-scaling method is frequency *in*dependent and the extension to infinity is simulated using complex spatial step sizes. In this work we determine these step sizes using the theory of optimal grids as presented in [6] and [8] and we refer to these references for further details.

After the spatial discretization procedure with complex-scaling included, we arrive at the semidiscrete Maxwell system

$$(\mathbf{D} + \mathbf{S} + \mathbf{M}\partial_t)\mathbf{f}_{cs} = w(t)\mathbf{q},\tag{11}$$

where the subscript "cs" indicates that complex-scaling has been applied. The matrices D, S, and M are the discretized counterparts of \mathcal{D} , \mathcal{S} , and \mathcal{M} , respectively, while f_{cs} , and q are the discretized counterparts of the field and source vectors \mathcal{F} , and \mathcal{Q} . We note that D has complex entries due to the application of the complex-scaling method and the above system is therefore complex and unstable. Real-valued and stable time-domain field responses can be obtained from the above system, however, via a stability-correction procedure discussed in [8]. In particular, introducing the system matrix A as

$$\mathsf{A} = \mathsf{M}^{-1}(\mathsf{D} + \mathsf{S}),\tag{12}$$

stable field approximations can be computed as (for details see [8])

$$f(t) = w(t) * 2\eta(t) \operatorname{Re}\left[\eta(A) \exp(-At) M^{-1}q\right] \quad \text{for } t > 0,$$
(13)

where

$$\eta(z) = \begin{cases} 1 & \text{if } \operatorname{Re}(z) > 0, \\ \frac{1}{2} & \text{if } \operatorname{Re}(z) = 0, \\ 0 & \text{if } \operatorname{Re}(z) < 0 \end{cases}$$

is the Heaviside unit step function. Furthermore, by applying a one-sided Laplace transform to Eq. (13) we obtain the frequency-domain solution

$$\tilde{\mathbf{f}}(s) = \tilde{w}(s) \left[r(\mathbf{A}, s) + r(\mathbf{A}^*, s) \right] \mathbf{M}^{-1} \mathbf{q},\tag{14}$$

where the asterisk denotes complex conjugation and where we have introduced the filtered resolvent function

$$r(z,s) = \frac{\eta(z)}{z+s}.$$
(15)

Although Eqs. (13) and (14) provide us with an explicit expression for the time- and frequency-domain electromagnetic fields on our domain of interest, it cannot be evaluated directly, since the order N of the system matrix A is typically too large. For example, N may easily run into the millions for three-dimensional problems and direct evaluation of Eq. (13) or Eq. (14) is simply not feasible. However, Eqs. (13) and (14) do serve as a starting point for the Lanczos-type model-order reduction method discussed in the next section. Finally, we mention that our approach relies on an analytic model for the dielectric constant. One disadvantage of such an approach is that measured dielectric data cannot be implemented in a straightforward manner. However, if the experimental data can be fitted by an arbitrary sum of multiple Drude and Lorentz media the proposed method can still be used. Introducing auxiliary variables for every single medium leads again to a frequency independent system.

3. Symmetry and Lanczos reduction

The first-order Maxwell system matrix A exhibits a particular symmetry property that allows us to efficiently construct Lanczos-type reduced-order models for the electromagnetic field. In particular, in Appendix A it is shown that matrix A is symmetric with respect to a matrix \tilde{W} , that is, matrix A satisfies

$$\langle \mathsf{A}\mathsf{x}, \mathsf{y} \rangle_{\tilde{\mathcal{W}}} = \langle \mathsf{x}, \mathsf{A}\mathsf{y} \rangle_{\tilde{\mathcal{W}}} \quad \text{for any } \mathsf{x}, \mathsf{y} \in \mathbb{C}^N,$$
(16)

where we have introduced the bilinear form $\langle x, y \rangle_{\tilde{W}} = y^T \tilde{W} x$ for $x, y \in \mathbb{C}^N$. Furthermore, using the definition of matrix \tilde{W} (see Appendix A), we find that $\frac{1}{2} \langle f, f \rangle_{\tilde{W}}$ approximates

$$\mathcal{L} = \mathcal{L}_{\text{free}}(\mathbb{D}) + \frac{1}{2} \int_{\mathbb{D}_{\text{disp}}} \frac{\beta_1}{\beta_0} |\mathbf{P}|^2 \, \mathrm{d}V - \frac{1}{2} \int_{\mathbb{D}_{\text{disp}}} \frac{\beta_3}{\beta_0} |\partial_t \mathbf{P}|^2 \, \mathrm{d}V,$$

where \mathbb{D}_{disp} is the bounded domain containing the dispersive media, while $\mathcal{L} = \mathcal{L}_{free}(\mathbb{D})$ is the standard free-field Lagrangian given by

$$\mathcal{L}_{\text{free}}(\mathbb{D}) = \frac{1}{2} \int_{\mathbb{D}} \varepsilon |\mathbf{E}|^2 \, \mathrm{d}V - \frac{1}{2} \int_{\mathbb{D}} \mu |\mathbf{H}|^2 \, \mathrm{d}V,$$

where \mathbb{D} is the bounded domain containing the nondispersive media that are present within our computational domain of interest. If no second-order dispersive media are present in this domain then the integrals over \mathbb{D}_{disp} are absent, of course, and \mathcal{L} reduces to $\mathcal{L} = \mathcal{L}_{free}$.

The symmetry relation of Eq. (16) enables us to efficiently construct a basis for the Krylov subspace

$$\mathbb{K}_m = \operatorname{span}\{\mathsf{M}^{-1}\mathsf{q}, \mathsf{A}\mathsf{M}^{-1}\mathsf{q}, \dots, \mathsf{A}^{m-1}\mathsf{M}^{-1}\mathsf{q}\}$$

via the three-term Lanczos-type recurrence relation

$$\xi_{i+1}\mathbf{v}_{i+1} = \mathbf{A}\mathbf{v}_i - \alpha_i\mathbf{v}_i - \delta_i\delta_{i-1}^{-1}\xi_i\mathbf{v}_{i-1},$$

with $v_0 = 0$, $\delta_0 = 1$, $\xi_1 = ||M^{-1}q||$, and $v_1 = \xi_1^{-1}M^{-1}q$, and where $|| \cdot ||$ denotes the Euclidean norm [11]. The coefficients α_i and δ_i are given by $\delta_i = \langle v_i, v_i \rangle_{\bar{W}}$ and $\alpha_i = \delta_i^{-1} \langle v_i, Av_i \rangle_{\bar{W}}$ and the coefficients ξ_i follow from the normalization condition $||v_i|| = 1$, which means that in our algorithm all Lanczos vectors have a Euclidean length equal to one.

After m steps of this algorithm, we have the Lanczos decomposition

$$\mathsf{AV}_m = \mathsf{V}_m \mathsf{H}_m + \xi_{m+1} \mathsf{v}_{m+1} \mathsf{e}_m^T, \tag{17}$$

where \mathbf{e}_m is the *m*th column of the *m*-by-*m* identity matrix \mathbf{I}_m and matrix $\mathbf{V}_m = (\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_m)$ is a tall *N*-by-*m* matrix that satisfies

$$\langle \mathsf{V}_m, \mathsf{V}_m \rangle_{\widetilde{\mathsf{W}}} = \operatorname{diag}(\delta_1, \delta_2, \ldots, \delta_m).$$

Finally,

$$\mathbf{H}_m = \operatorname{tridiag}(\xi_i, \alpha_i, \delta_{i+1}\delta_i^{-1}\xi_{i+1})$$

is an *m*-by-*m* tridiagonal matrix containing the Lanczos recurrence coefficients.

Based on the Lanczos decomposition of Eq. (17), we can now construct the time- and frequency-domain field Lanczos model-order reduction approximations

$$f_m(t) = w(t) * 2\xi_1 \eta(t) \operatorname{Re}\left[V_m \eta(H_m) \exp(-H_m t) e_1\right]$$
(18)

and

$$\tilde{\mathbf{f}}_m(s) = \xi_1 \tilde{w}(s) \Big[\mathbf{V}_m r(\mathbf{H}_m, s) + \mathbf{V}_m^* r(\mathbf{H}_m^*, s) \Big] \mathbf{e}_1.$$
(19)

These models can be evaluated very efficiently, since only matrix functions of the small *m*-by-*m* matrix H_m need to be evaluated. Our Lanczos reduction approach allows for frequency sweeps as well, meaning that a single model provides field approximations in dispersive media on a complete frequency interval of interest. Furthermore, we note that if field responses are required at certain specified receiver locations then only the *rows* of the Lanczos matrix V_m that correspond to these receiver locations need to be kept in memory to evaluate the reduced-order models. Specifically, assume the field needs to be computed at N_r distinct receiver locations in space. Now given an $N_r \times N$ dimensional receiver matrix R we define $Q_m = R^T V_m$ to obtain the solution at the receiver locations as

$$\mathbf{f}_m(t) = \mathbf{w}(t) * 2\xi_1 \eta(t) \operatorname{Re}\left[\mathbf{Q}_m \eta(\mathbf{H}_m) \exp(-\mathbf{H}_m t) \mathbf{e}_1\right]$$
(20)

and

$$\tilde{\mathsf{f}}_m(s) = \xi_1 \tilde{w}(s) \Big[\mathsf{Q}_m r(\mathsf{H}_m, s) + \mathsf{Q}_m^* r(\mathsf{H}_m^*, s) \Big] \mathsf{e}_1.$$
⁽²¹⁾

Only the $N_r \times m$ matrix Q_m needs to be stored.

Finally, we mention that it is possible to give a general error bound for polynomial Krylov methods (see, for example, [15]), but such a bound is usually not tight and leads to a gross overestimation of the required number of iterations. In practice, we therefore check the difference between two constructed models approximately every 500 iterations and terminate the algorithm as soon as their difference falls below a specified threshold.



Fig. 1. A golden box embedded in vacuum. The side length of the box is 50 nm and a Drude model with medium parameters $\varepsilon_{\infty} = 1$, $\omega_p = 13.8 \cdot 10^{15} \text{ s}^{-1}$, and $\gamma_p = 1.075 \cdot 10^{14} \text{ s}^{-1}$ is used as a constitutive relation. The star and triangle indicate the source and receiver location, respectively. The domain of interest is surrounded by a PML (red area) to simulate the extension to infinity. The PML is realized using the optimal complex-scaling method [6,8]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

4. Numerical results

In this section we present several numerical experiments that illustrate the performance of our proposed reduction technique. In our first experiment, we consider H-polarized fields in a two-dimensional configuration that is invariant in the *z*-direction. The configuration consists of a square golden box that is embedded in vacuum (see Fig. 1). The side length of the box is 50 nm and a Drude model with medium parameters $\varepsilon_{\infty} = 1$, $\omega_p = 13.8 \cdot 10^{15} \text{ s}^{-1}$, and $\gamma_p = 1.075 \cdot 10^{14} \text{ s}^{-1}$ [17] is used as a constitutive relation. The box is illuminated by electromagnetic waves that are generated by a line source (star in Fig. 1) and we are interested in the magnetic field response at the receiver location (triangle in Fig. 1). The source wavelet is a derivative of a time-shifted Gaussian (Ricker wavelet) with a peak frequency that corresponds to a wavelength $\lambda_{\text{peak}} = 350 \text{ nm}$ in vacuum. The configuration is discretized on a uniform grid with a step size of $\delta = 1 \text{ nm}$ and after incorporating the complex-scaling method, a discretized Maxwell system of approximately 47000 unknowns is obtained. We subsequently apply the Lanczos algorithm to construct the reduced-order models for the magnetic field strength at the receiver location. As a reference simulation, an ADE-FDTD scheme [23] is used that captures the electromagnetic response of a medium with Drude relaxation. The convergence of the time-domain reduced-order model towards the ADE-FDTD response is shown in Fig. 2. From this figure, we observe that early times are approximated first as can be expected from a polynomial Krylov method. In addition, the oscillations in the field response are quickly captured (already by a reduced-order model of order m = 2500, see Fig. 2 – top), but the amplitude is correct for early times only. Increasing the order to m = 4500(Fig. 2 – middle) clearly leads to an improved response. The reduced-order model starts to align itself with the FDTD result on the entire time interval of interest and there is only a mismatch in amplitude after approximately t > 6 fs. Increasing the number of iterations even further to m = 6500 (Fig. 2 – bottom), the reduced-order model response completely coincides the FDTD result on the time interval of interest. The indicated convergence behavior is typical for polynomial Krylov reduced-order wave field models. Early times are approximated first and field oscillations are captured quickly. Furthermore, the accuracy of the model improves as the order of the model is increased and usually arrival times are approximated first after which the amplitude of the signal is corrected. Finally, we remark that other validation results for resonant modes and time- and frequency-domain wave fields in dispersive and nondispersive media can be found in [27,26,8], and [9].

In Fig. 3 we show all stable eigenvalues or Lanczos poles (crosses) of the reduced tridiagonal matrix H_m of order m = 6500 in the complex λ -plane ($\lambda = 2\pi c_0/\omega$). The star in this figure indicates the wavelength that corresponds to the peak frequency of the source ($\lambda_{peak} = 350$ nm). Clearly, many eigenvalues are clustered near the origin and the Lanczos poles or resonances that contribute the most to the field response can easily be distinguished from this figure. These eigenvalues are located close to the real axis and can be identified as plasmonic resonances with a high quality factor. Having identified these resonances with our Lanczos algorithm, we can also compute the corresponding resonance fields. The magnitude of the magnetic field and the real part of the *x*-component of the electric field of a number of these resonant fields are shown in Fig. 4. These modes can be computed without storing the complete basis by doubling the computation time. Specifically, assume the eigenvalue decomposition $H_m = SAS^{-1}$ of the reduced tridiagonal matrix is at hand after running the Lanczos algorithm. Now the expansion coefficients of the Krylov basis that approximate the *i*th eigenvalue are given by the *i*th column of S. Thus we can rerun the Lanczos algorithm and construct the approximate eigenvector without saving the basis as the expansion coefficients are known. Usually a few vectors will actually fit into memory, such that the resonances of interest can be computed at once in the second run. The accuracy of the resonances can be determined using Eq. (17) (see [12]).



Fig. 2. Reduced-order models of order m = 2500 (top), m = 4500 (middle), and m = 6500 (bottom) for the magnetic field strength at the receiver location in Fig. 1 (dashed line). The solid line signifies the magnetic field response as computed by ADE-FDTD.

It can be seen that the resonance fields are strongly localized and confined to the boundary of the box, which is typical for plasmonic fields. Moreover, due to the dispersive character of gold the number of field oscillations increases as the magnitude of the wavelength increases (increase in the magnitude of the permittivity at lower frequencies). We also observe that E_x is continuous across the tangential boundary and exhibits a jump with change of sign across the normal boundary, as expected for a material with a negative dielectric function.

To illustrate that the proposed reduced-order technique can handle large-scale wave field problems, we compute frequency-domain responses of a three-dimensional silver nano antenna that is excited by an electric dipole (see Fig. 5). The antenna has a cuboid shape, a height of 100 nm, and a width and length of 32 nm. A Drude model is chosen to describe the dispersion of silver with medium parameters $\omega_p = 13.7 \cdot 10^{15} \text{ s}^{-1}$, $\gamma_p = 5.139 \cdot 10^{14} \text{ s}^{-1}$, and $\epsilon_{\infty} = 1$ as given in [25]. The electric dipole is located 10 nm above the center of the upper *yz*-plane of antenna and is oriented in the *x*-direction. The dipole is modeled as an external electric-current density $J_x^{\text{ext}} = i\omega p \delta(\mathbf{r} - \mathbf{r}_s)$, where *p* is the magnitude of the dipole moment and \mathbf{r}_s is the position vector of the dipole and both the antenna and the dipole are embedded in a homogeneous nondispersive background medium with a relative permittivity of $\varepsilon_r = 2.25$. We use nine receivers to measure



Fig. 3. Stable eigenvalues of the reduced tridiagonal matrix H_{6500} in the complex λ -plane (crosses). The star indicates the wavelength that corresponds to the peak frequency of the source.

the electromagnetic field response in the vicinity of the nano antenna on a 700 to 1200 nm wavelength interval. Specifically, the nine receivers are all located on a line that runs through the dipole location (see Fig. 5). The dipole is located at the center of the line and the receivers are symmetrically distributed on the line such that the location of receiver number 5 coincides with the dipole location. Configurations such as the one depicted in Fig. 5 are extensively studied in the field of nano optics and find their application in coherent plasmon generation and the modification of the spontaneous decay rate of quantum emitters, for example [17,21].

To obtain the field responses at the receiver locations, we discretize the first-order Maxwell system on a uniform Yee grid with a spatial step size of 2 nm and incorporate the optimal scaling method to simulate the extension to infinity. The resulting order of the discretized first-order Maxwell system is approximately nine million. Direct evaluation of the stability-corrected frequency-domain wave function is obviously not practical and we therefore construct the reduced-order model of Eq. (19) to approximate the electromagnetic field responses at the receiver locations on the wavelength interval of interest. We stress that a *single* reduced-order model provides field approximation for all wavelengths (frequencies) of interest. The order of the final model is determined by constructing reduced-order models every 500 iterations. As soon as the relative global error between two successively constructed models falls below a user specified tolerance (10^{-3} in our experiments) we terminate the iteration process and accept the final model as an accurate approximation of the electromagnetic field response on the complete wavelength interval of interest. In our Matlab implementation, the construction of the final model takes about one hour on an Intel i5-3470 CPU @ 3.2 GHz under 64-bit Windows 7, while the evaluation of the model on our wavelength interval of interest takes less than one second for one thousand uniformly sampled wavelength values (so-called wavelength or frequency sweep).

In Fig. 6 we show the reduced-order model for the *x*-component of the electric field strength at all receiver locations and on our wavelength interval of interest. The responses measured to the left and to the right of the dipole coincide as they should, of course, since the measurement setup and configuration are symmetric with respect to the dipole location. We also observe that the electric field exhibits resonant behavior for a wavelength of about 820 nm, which is due to the dispersive nature of the silver nano antenna. Finally, we note that the largest peak in the imaginary part of the *x*-component of the electric field strength is measured at receiver 5, which coincides with the dipole location. This implies that the spontaneous decay rate of a quantum emitter can be significantly increased if such an emitter is placed at the electric dipole location.

Comparing the order of the converged reduced-order models in our two examples, we observe that the reduction factor for the three-dimensional nano antenna configuration is much larger than the reduction factor for the two-dimensional golden box problem. Apart from the obvious difference that these two problems are solved in different domains (the box problem in the time-domain, the antenna problem in the frequency-domain) and in different spatial dimensions (2D vs 3D) this difference can be explained by the number of resonances that contribute to the measured field responses. For the nano antenna example, this number is much smaller than the number of contributing resonances for the golden box problem. Specifically, in Fig. 7 all stable Lanczos poles (stable eigenvalues of matrix H_m) are plotted (crosses) along with the wavelength interval of interest. From this spectral plot we can identify which resonances contribute to the measured signals. For the source-receiver setup considered here, only a small number of poles essentially contribute to the measured signals with the most contributing pole located at $\lambda = 828 - 39i$ nm (see Fig. 7). These contributing poles need to be found by the Lanczos algorithm, of course, and it apparently takes our Lanczos algorithm 4500 iterations to find the contributing poles that accurately describe the field responses on the wavelength interval of interest at all nine receiver locations. Compared with the order of the unreduced system (approximately nine million), the reduced-order model is



Fig. 4. Magnitude of H_z (left) and real part of E_x (right) for resonant fields corresponding to the complex wavelengths $\lambda = 231 - 1i$ nm (top), $\lambda = 162 - 1i$ nm (middle), and $\lambda = 166 - 1i$ nm (bottom).

approximately 2000 times smaller clearly demonstrating that significant order reduction can be achieved for dispersive resonating structures.

5. Conclusions

In this paper we have presented a Lanczos model-order reduction technique for the efficient computation of time- and frequency-domain electromagnetic wave fields in second-order dispersive media. We have combined Maxwell's equations and the dispersion relation into a first-order system and we subsequently discretized our domain of interest on a standard Yee grid. To implement the extension to infinity, we have made use of the recently developed global complex-scaling method presented in [6] and [8], where it is also shown that stable time-domain or conjugate symmetric frequency-domain field approximations can be computed via so-called stability-corrected wave functions. Direct evaluation of these functions is not feasible, however, since the order of the spatially discretized first-order system is simply to large. We therefore approximate these wave functions by elements from a standard polynomial Krylov subspace. We have shown that for dispersive media the first-order Maxwell system exhibits a particular physics-based symmetry relation and exploited this symmetry relation to efficiently construct a basis of the Krylov subspace via a Lanczos-type three-term recurrence relation. The Lanczos algorithm provides us with a so-called Lanczos decomposition that allows us to construct time- or frequency-domain reduced-order models for the electromagnetic wave field that approximate the stability-corrected wave functions on a desired time or frequency interval. In the frequency-domain, the models allow for so-called frequency (or wavelength) sweeps meaning that a *single* model provides field approximations on a complete frequency interval of interest. Our numerical ex-



Fig. 5. A three-dimensional silver nano antenna embedded in a nondispersive homogeneous background medium. The antenna has a height of 100 nm and a width and length of 32 nm and is excited by an x-directed electric dipole located 10 nm above the antenna. A Drude model with medium parameters $\omega_p = 13.7 \cdot 10^{15} \text{ s}^{-1}$, $\gamma_p = 5.139 \cdot 10^{14} \text{ s}^{-1}$, and $\epsilon_{\infty} = 1$ is used as a constitutive relation for silver and both the antenna and the dipole are embedded in a nondispersive homogeneous background medium with a relative permittivity of $\varepsilon_r = 2.25$. The arrow indicates the location of the dipole, while the blue triangles indicate the location of the receivers. The location of receiver 5 coincides with the dipole location.

periments for two- and three-dimensional configurations show that significant reduction is possible especially for dispersive resonating nanostructures. The main reasons for these large reduction factors is that subwavelength structures are heavily oversampled and only a relative small number of resonances contribute to the measured field response. We have shown that for a given nanoscale structure, these resonances can be identified using our Lanczos algorithm. The number of Lanczos iterations should be large enough, however, to capture the most contributing resonances in the configuration. These results indicate that even though significant reduction factors can already be achieved using polynomial Lanczos reduction, a further order reduction may be realized by constructing reduced-order models based on rational Krylov subspaces [20]. Parameter dependent rational Krylov subspaces have already been applied successfully for diffusive electromagnetic fields in [24] and future work will focus on extending these rational subspace techniques to hyperbolic wave field problems in dispersive media.

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Appendix A. Symmetry properties of the system matrix

In this appendix we discuss the symmetry of the system matrix A that is exploited in our Lanczos-type reduction algorithm. We first consider instantaneously reacting materials and subsequently discuss the dispersive case.

We discretize the first-order field equations on a staggered Yee grid [23] using primary and dual nodes in each Cartesian direction. For example, the primary and dual nodes in the *y*-direction are defined as

$$\Omega_{y}^{p} = \{ y_{q} \in \mathbb{R}, q = 0, 1, \dots, N_{y} + 1, y_{q} > y_{q-1} \},$$
(A.1)

and

$$\Omega_{y}^{d} = \{ \hat{y}_{q} \in \mathbb{R}, q = 1, \dots, N_{y} + 1, \, \hat{y}_{q+1} > \hat{y}_{q} \}, \tag{A.2}$$



Fig. 6. The x-component of the electric field strength at the receiver locations 1-9 on the wavelength interval of interest.



Fig. 7. Stable eigenvalues of H_{4500} in the complex λ -plane. The most contributing eigenvalue is located at $\lambda = 828 - 39i$ nm.

respectively, with corresponding step sizes given by

$$\delta_{y,q} = y_q - y_{q-1}, \quad q = 1, \dots, N_y + 1 \quad \text{and} \quad \hat{\delta}_{y,q} = \hat{y}_{q+1} - \hat{y}_q, \quad q = 1, \dots, N_y.$$
 (A.3)

Dual step sizes carry a hat, while primary step sizes do not. Grid nodes in the *x*- and *z*-direction are introduced in a similar manner with N_x dual step sizes in the *x*-direction and N_z dual step sizes in the *z*-direction.

On a Yee grid, differentiation in each Cartesian direction can conveniently be described in terms of bidiagonal differentiation matrices. In particular, if the introduce the $(N_{\gamma} + 1)$ -by- $(N_{\gamma} + 1)$ diagonal matrix of primary step sizes

$$W_{y} = \text{diag}(\delta_{y;1}, \delta_{y;2}, \dots, \delta_{y;N_{y}+1})$$
(A.4)

and the N_y -by- $(N_y + 1)$ bidiagonal matrix bidiag $_{N_y}(-1, 1)$ with -1 on the diagonal and +1 on the first upper diagonal, then differentiation of field quantities defined on primary grid nodes in the *y*-direction is carried out by the differentiation matrix

$$Y = -W_{v}^{-1} \text{bidiag}_{N_{v}} (-1, 1)^{T}.$$
(A.5)

In a similar manner we can define a differentiation matrix that acts on field quantities defined on the dual nodes. Introducing the N_y -by- N_y diagonal step size matrix

$$\hat{\mathsf{W}}_{y} = \operatorname{diag}(\hat{\delta}_{y;1}, \hat{\delta}_{y;2}, \dots, \hat{\delta}_{y;N_{y}}),\tag{A.6}$$

the difference matrix

. . .

$$\hat{\mathbf{Y}} = \hat{\mathbf{W}}_{\nu}^{-1} \text{bidiag}_{N_{\nu}}(-1, 1) \tag{A.7}$$

computes two-point finite-differences of field quantities defined on dual nodes in the *y*-direction. Moreover, both differentiation matrices are related to each other via the obvious symmetry relation

$$\hat{\mathbf{Y}}^T \hat{\mathbf{W}}_y = -\mathbf{W}_y \mathbf{Y}. \tag{A.8}$$

Differentiation matrices X, \hat{X} , Z, and \hat{Z} in the x- and z-direction are defined in an analogous manner.

A.1. Instantaneously reacting media

Discretizing the first-order Maxwell system on a standard Yee grid and arranging the unknowns in lexicographical order, we arrive at the state-space representation

$$(\mathsf{D} + \mathsf{S} + \mathsf{M}\partial_t) \mathbf{f} = \mathsf{q}'. \tag{A.9}$$

The order of this system is denoted by N and it is typically very large for real-world 3D problems (millions or even a billion of unknowns is not uncommon).

In the above representation, the spatial differentiation matrix is given by

$$\mathsf{D} = \begin{bmatrix} \mathsf{0} & \mathsf{D}_{\mathsf{h}} \\ \mathsf{D}_{\mathsf{e}} & \mathsf{0} \end{bmatrix},\tag{A.10}$$

with

$$\mathsf{D}_{\mathsf{h}} = \begin{bmatrix} \mathsf{0} & \hat{\mathsf{Z}} \otimes \mathsf{I}_{N_{y}} \otimes \mathsf{I}_{N_{x+1}} & -\mathsf{I}_{N_{z}} \otimes \hat{\mathsf{Y}} \otimes \mathsf{I}_{N_{x+1}} \\ -\hat{\mathsf{Z}} \otimes \mathsf{I}_{N_{y+1}} \otimes \mathsf{I}_{N_{x}} & \mathsf{0} & \mathsf{I}_{N_{z}} \otimes \mathsf{I}_{N_{y+1}} \otimes \hat{\mathsf{X}} \\ \mathsf{I}_{N_{z}+1} \otimes \hat{\mathsf{Y}} \otimes \mathsf{I}_{N_{x}} & -\mathsf{I}_{N_{z}+1} \otimes \mathsf{I}_{N_{y}} \otimes \hat{\mathsf{X}} & \mathsf{0} \end{bmatrix}$$
(A.11)

and

$$\mathsf{D}_{\mathsf{e}} = \begin{bmatrix} \mathsf{0} & -\mathsf{Z} \otimes \mathsf{I}_{N_{y}+1} \otimes \mathsf{I}_{N_{x}} & \mathsf{I}_{N_{z}+1} \otimes \mathsf{Y} \otimes \mathsf{I}_{N_{x}} \\ \mathsf{Z} \otimes \mathsf{I}_{N_{y}} \otimes \mathsf{I}_{N_{x}+1} & \mathsf{0} & -\mathsf{I}_{N_{z}+1} \otimes \mathsf{I}_{N_{y}} \otimes \mathsf{X} \\ -\mathsf{I}_{N_{z}} \otimes \mathsf{Y} \otimes \mathsf{I}_{N_{x}+1} & \mathsf{I}_{N_{z}} \otimes \mathsf{I}_{N_{y}+1} \otimes \mathsf{X} & \mathsf{0} \end{bmatrix},$$
(A.12)

and \otimes is the Kronecker (tensor) product. Furthermore, the medium matrix S is given by

$$\mathbf{S} = \begin{bmatrix} \mathbf{M}_{\sigma} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix},\tag{A.13}$$

where M_{σ} is a diagonal semi-positive definite matrix with (averaged) conductivity values on its diagonal. The medium matrix M is given by

$$\mathsf{M} = \begin{bmatrix} \mathsf{M}_{\varepsilon} & \mathsf{0} \\ \mathsf{0} & \mathsf{M}_{\mu} \end{bmatrix} \tag{A.14}$$

and both M_{ε} and M_{μ} are diagonal and positive definite medium matrices with averaged permittivity and permeability values on their diagonal. The field vector is of the form

$$f = [e_x^T, e_y^T, e_z^T, h_x^T, h_y^T, h_z^T]^T,$$
(A.15)

where all field quantities are stored in lexicographical order in the corresponding field vectors e_i and h_i , i = x, y, z. Finally, the finite-difference approximations of the external sources are stored in the source vector

$$q' = -[j_x^{ext;T}, j_y^{ext;T}, j_z^{ext;T}, k_x^{ext;T}, k_y^{ext;T}]^T.$$
(A.16)

Premultiplying Eq. (A.9) by the inverse of the medium matrix M, we arrive at

$$(\mathsf{A} + \mathsf{I}\partial_t) \mathsf{f} = \mathsf{M}^{-1} \mathsf{q}', \tag{A.17}$$

where we have introduced the system matrix as

$$A = M^{-1}(D + S).$$
(A.18)

This is the system matrix for instantaneously reacting materials.

A.1.1. Symmetry relations

To discuss the symmetry properties satisfied by the system matrix, we first introduce the diagonal step size matrices

$$W_{e} = \begin{bmatrix} \hat{W}_{z} \otimes \hat{W}_{y} \otimes W_{x} & 0 & 0\\ 0 & \hat{W}_{z} \otimes W_{y} \otimes \hat{W}_{x} & 0\\ 0 & 0 & W_{z} \otimes \hat{W}_{y} \otimes \hat{W}_{x} \end{bmatrix},$$
(A.19)

and

$$W_{h} = \begin{bmatrix} W_{z} \otimes W_{y} \otimes \hat{W}_{x} & 0 & 0 \\ 0 & W_{z} \otimes \hat{W}_{y} \otimes W_{x} & 0 \\ 0 & 0 & \hat{W}_{z} \otimes W_{y} \otimes W_{x} \end{bmatrix}.$$
(A.20)

Using the symmetry relation of Eq. (A.8) (and the corresponding relations in the *x*- and *z*-directions), it is now easily verified that

$$\mathsf{D}_{\mathsf{h}}^{T}\mathsf{W}_{\mathsf{e}} = -\mathsf{W}_{\mathsf{h}}\mathsf{D}_{\mathsf{e}} \quad \text{and} \quad \mathsf{D}_{\mathsf{e}}^{T}\mathsf{W}_{\mathsf{h}} = -\mathsf{W}_{\mathsf{e}}\mathsf{D}_{\mathsf{h}}. \tag{A.21}$$

Furthermore, with

$$W = \begin{pmatrix} W_e & 0\\ 0 & -W_h \end{pmatrix}$$
(A.22)

we also have

$$\mathsf{D}^T\mathsf{W} = \mathsf{W}\mathsf{D},\tag{A.23}$$

which leads to the symmetry property

$$A^{T}\tilde{W} = \tilde{W}A \quad \text{with} \quad \tilde{W} = MW = WM = \tilde{W}^{T}. \tag{A.24}$$

This symmetry property is related to reciprocity as shown in [18].

A.2. Dispersive media

Loosely speaking, the main difference in setting up the semidiscrete Maxwell system for dispersive media is the presence of the polarization vectors **P** and **U** in the field equations. These vectors are only active at points where a dispersive material is present. From a storage point of view, it is therefore advantageous to only keep the finite-difference approximations of **P** and **U** at these points in memory. Since the polarization is related to the electric field strength and electric field strength approximations are defined over the total computational domain, we need to introduce support matrices to implement the local dispersion relations. To this end, we define selection or logical projection matrices, which select the relevant electric field strength components from the total electric field vector. For example, if I_y^{sup} is the support matrix of a dispersive material in the *y*-direction and e_y contains all finite-difference approximations of the *y*-component of the electric field strength, then the vector $I_y^{sup}e_y$ contains only those *y*-components of E_y located within the dispersive material. An illustration of how the support matrix is constructed is shown in Fig. 8.

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Fig. 8. Construction of a support matrix. Grid points y_2 and y_3 are within the dispersive medium and thus $y_2, y_3 \in \Omega^{sup}$. The rows of I^{sup} are the basis vectors of Ω^{sup} expressed in the basis vectors of Ω^{DOI} .

Using this definition of the support matrices, the constitutive relation of Eq. (3) relating the electric and polarization fields to each other can be implemented in a straightforward manner. For example, for the *y*-component of Eq. (3) we have

$$B_{3,y}\partial_t u_y + B_{2,y}u_y - B_{1,y}p_y + B_{0,y}l_y^{sup}e_y = 0,$$
(A.25)

where the matrices $B_{\{0,1,2,3\},y}$ are diagonal matrices with (averaged) medium values $\beta_{\{0,1,2,3\}}$ on their diagonal.

Using the Yee grid introduced earlier, approximating the partial derivatives by two-point finite-difference formulas, and arranging the unknowns in lexicographical order, we now again arrive at the state-space representation

$$(\mathsf{D} + \mathsf{S} + \mathsf{M}\partial_t) \mathsf{f} = \mathsf{q}'. \tag{A.27}$$

In this equation, the spatial differentiation matrix is given by

$$D = \begin{bmatrix} 0 & 0 & 0 & D_h \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ D_e & 0 & 0 & 0 \end{bmatrix},$$
(A.28)

where D_h and D_e are given by Eqs. (A.11) and (A.12), respectively.

Furthermore, matrix S is given by

$$S = \begin{bmatrix} 0 & 0 & -I^{sup;T} & 0 \\ 0 & 0 & I & 0 \\ B_0 |^{sup} & -B_1 & B_2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$
 (A.29)

where $B_{\{0,1,2\}}$ are diagonal matrices only defined on the support of the dispersive media. In addition, I^{sup} is the total support matrix and the medium matrix M is given by

$$\mathbf{M} = \begin{bmatrix} \mathbf{M}_{\varepsilon} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{B}_{3} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{M}_{\mu} \end{bmatrix},$$
(A.30)

where B_3 is again a dispersion matrix and both M_{ε} and M_{μ} are diagonal and positive definite medium matrices with averaged permittivity and permeability values on their diagonal. The field vector is now of the form

$$\mathbf{f} = [\mathbf{e}_{x}^{T}, \mathbf{e}_{y}^{T}, \mathbf{e}_{z}^{T}, \mathbf{p}_{x}^{T}, \mathbf{p}_{y}^{T}, \mathbf{p}_{z}^{T}, \mathbf{u}_{x}^{T}, \mathbf{u}_{y}^{T}, \mathbf{u}_{z}^{T}, \mathbf{h}_{x}^{T}, \mathbf{h}_{y}^{T}, \mathbf{h}_{z}^{T}]^{T},$$
(A.31)

where all field quantities are stored in lexicographical order in the corresponding field vectors e_i , p_i , u_i , and h_i , i = x, y, z. Finally, the finite-difference approximations of the external sources are stored in the source vector

$$\mathbf{q}' = -[\mathbf{j}_x^{\text{ext};T}, \mathbf{j}_y^{\text{ext};T}, \mathbf{j}_z^{\text{ext};T}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{k}_x^{\text{ext};T}, \mathbf{k}_y^{\text{ext};T}, \mathbf{k}_z^{\text{ext};T}]^T.$$
(A.32)

A.2.1. Symmetry relations

The system matrix for media exhibiting relaxation is given by

$$A = M^{-1}(D + S).$$
(A.33)

To discuss its symmetry properties, we introduce the matrix

$$W = \begin{bmatrix} W_e & 0 & 0 & 0 \\ 0 & W_p & 0 & 0 \\ 0 & 0 & -W_u & 0 \\ 0 & 0 & 0 & -W_h \end{bmatrix}$$
(A.34)

and W_e and W_h as defined in Eqs. (A.19) and (A.20). Furthermore, W_u and W_p are given by

$$W_u = B_0^{-1} I^{sup} W_e I^{sup;T}$$
 and $W_p = B_1 W_u = B_1 B_0^{-1} I^{sup} W_e I^{sup;T}$. (A.35)

It is now easily verified that the system matrix satisfies the symmetry relation

$$A^T \tilde{W} = \tilde{W} A$$
 with $\tilde{W} = MW = WM = \tilde{W}^T$, (A.36)

which is similar in form to the symmetry relation for instantaneously reacting media. Equation (A.36) can be exploited in a Lanczos-type algorithm to efficiently construct a basis of a Krylov subspace generated by the system matrix A.

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