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Solution of time-convolutionary Maxwell's equations using parameter-dependent Krylov subspace reduction

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ABSTRACT

We suggest a new algorithm for the solution of the time domain Maxwell equations in dispersive media. After spacial discretization we obtain a large system of time-convolution equations. Then this system is projected onto a small subspace consisting of the Laplace domain solutions for a preselected set of Laplace parameters. This approach is a generalization of the rational Krylov subspace approach for the solution of non-dispersive Maxwell's systems. We show that the projected system preserves such properties of the initial system as stability and passivity. As an example we consider the 3D quasistationary induced polarization problem with the Cole–Cole conductivity model important for geophysical oil exploration. Our numerical experiments show that the introduction of the induced polarization does not have significant effect on convergence.

1. Introduction

It was observed since 1920s [29], that electrical conductivity and dielectric permeability of rocks are frequency dependent. This phenomenon has generic name the Dispersive Media, or the Induced Polarization for the frequency-dependent conductivity, and intensively described in physical and geophysical literature [5–7,18,22,25,26,37].

The time-domain evolution of electromagnetic fields in dispersive medium is described by convolutionary Maxwell's system. There are two approaches to solving such problems. One way is time-stepping [23,24,34]. Even for the non-dispersive (a.k.a. inductive) diffusive problems this approach can be expensive due to stability limitations and slow convergence. However, the computation of convolution operator requires additional several time layers, that increases the cost compared to the non-dispersive problem. Another approach is to transform the frequency domain solution to the time domain using the discrete inverse Fourier transform [12,20]. To evaluate such integrals one needs to compute a frequency domain solution for every quadrature node that may require hundreds forward solutions for good enough accuracy. We should point out, that some improvement in this direction could be achieved by using recently developed optimized quadratures on complex plane [31].

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Krylov subspace methods (originally intended for spectral problems and linear algebraic systems) became an increasedly popular tool for the solution of parabolic equations (the matrix exponential function) in 1980s [14,16,21,28,32]. They directly project semi-discrete systems onto Krylov subspaces and can be considered as spectrally optimized explicit time-stepping methods. Such an approach (a.k.a. spectral Lanczos decomposition method) was efficiently applied to the diffusive (non-dispersive) Maxwell system in [8]. It yields faster than exponential (quadratic) convergence rate, however it is significantly affected by the problem stiffness. A more recent approach, based on so-called rational Krylov subspaces (RKS) introduced in [27], allows one to circumvent this drawback. The RKS reduction (RKSR) (a.k.a. the RKS projection) method was applied to inductive diffusive Maxwell's equations in [4,9,11,17] (see also some important results on the RKSR analysis in [3]). Similar to the implicit time-stepping and the contour integration methods the RKSR requires the solution of a number of shifted frequency domain problems, but in the latter method this number is much smaller thanks to Galerkin's optimal properties.

Due to nonlinear frequency dependence of the operator neither Krylov nor rational Krylov subspace method can be directly applied to the dispersive problems. In this work we develop a concept related in some sense to parametric model reduction [33], i.e, we project frequency domain problem onto a so-called parameter-dependent Krylov subspace (PDKS) with properly chosen parameters. We call this method the parameter-dependent Krylov subspace reduction (PDKSR). This approach is also related to so-called nonlinear Krylov subspaces, used for the computation of nonlinear spectrum [30]. For the non-dispersive case it is equivalent to the RKSR. The PDKSR is first applied in the frequency domain and then the obtained solution transformed to the time domain using numerical integration. We show that the projected problem preserves such important properties of the initial problem as stability and passivity.

As an example of application, we consider the Cole–Cole induced polarization model in conductive media (corresponding to a fractional order PDE system) arising in electromagnetic geophysical exploration. Although the conductivity is complex in this case, its high frequency asymptote is the same as for non-dispersive case. Hence for the parameter-dependent Krylov Subspace we use the real poles optimized for large-scale inductive problems in [9]. The numerical experiment shows that the introduction of the Cole–Cole dispersion qualitatively changes behavior of the solution, however it has very little effect on convergence speed of the subspace reduction.

2. Formulation of the problem

To fix the idea, we consider the quasistationary time-domain Maxwell system in $\mathbf{R}^3 \times \mathbf{R}$

$$\begin{aligned} \nabla \times \mathbf{H} &= \mathbf{J}_c + \mathbf{J}', \\ \nabla \times \mathbf{E} &= -\mu \tfrac{\partial \mathbf{H}}{\partial t}. \end{aligned} \tag{1}$$

Here $\mathbf{H}$ is magnetic field, $\mathbf{E}$ is electric field, $\mathbf{J}_c, \mathbf{J}'$ are conductivity and exciting (external) currents respectively; both currents are real functions of time $t \in \mathbf{R}$ and space $\mathbf{r} \in \mathbf{R}^3$ coordinates. We assume for simplicity that magnetic permeability $\mu > 0$ is constant. The quasistationary approximation (when the displacement current is neglected) is commonly assumed in deep geophysical electromagnetic exploration [6].

The conductivity current $\mathbf{J}_c$ can be expressed with the help of the generalized Ohm law in terms of electric field as follows:

$$\mathbf{J}_c = \sigma * \mathbf{E} = \int_{-\infty}^{\infty} \sigma(\tau)\mathbf{E}(t-\tau)d\tau, \tag{2}$$

where σ is an electric conductivity function of space and convolutional time τ, and

$$\sigma = 0, \quad \text{for } \tau < 0.$$

We impose the initial condition

$$\mathbf{E} = 0, \quad \mathbf{H} = 0, \quad \text{for } t < 0, \tag{3}$$

and for consistency we require that $\mathbf{J}'|_{t<0} = 0$.

Remark 1. The displacement current

$$\mathbf{J}_d = \epsilon * \frac{\partial}{\partial t}\mathbf{E} = \int_{-\infty}^{\infty} \epsilon(\tau)\frac{\partial \mathbf{E}(t-\tau)}{dt}d\tau,$$

with dispersive dielectric permittivity function ϵ can be added to the convolution system (2) without changing its structure by substituting

$$g = \sigma - \frac{d\epsilon}{d\tau}$$

instead of σ in (2), so the algorithm described below is applicable for the case of dispersive dielectric permittivity too (possibly with a different choice of optimized interpolation frequencies).

We also need the following assumptions on the temporal growth of the coefficient and $\mathbf{J}'(t, \mathbf{r})$.

Assumption 1. The Laplace transform $\tilde{\sigma}(s) = \int_0^\infty e^{-s\tau}\sigma(\tau)d\tau$ exists and is analytic in $\mathcal{C}_+ = \{s \in \mathcal{C} : \Re(s) > 0\}$. In addition, there exist $\alpha > 0$ and $\beta > 0$ such that $\beta \geqslant \Re(\tilde{\sigma}) \geqslant \alpha$ in $\mathcal{C}_+$ uniformly with respect to the spacial variable $\mathbf{r}$.

Assumption 2. For any $t \in \mathbf{R}$ the distribution $\mathbf{J}^r(t,\mathbf{r})$ is a compactly supported distribution in $\mathbf{R}^3$ and the Laplace transform $\tilde{\mathbf{J}}^r(s,\mathbf{r}) = \int_0^\infty e^{-st}\mathbf{J}^r(t,\mathbf{r})dt$ exists and is uniformly bounded with respect to $s \in \mathcal{C}_+$.

Due to Assumptions 1 and 2 we can Laplace-transform (1)–(3) to the system

$$\begin{aligned} \nabla \times \tilde{\mathbf{H}} &= \tilde{\sigma}\tilde{\mathbf{E}} + \tilde{\mathbf{J}}^r, \\ \nabla \times \tilde{\mathbf{E}} &= -s\mu\tilde{\mathbf{H}} \end{aligned} \tag{4}$$

for $s \in \mathcal{C}_+$. The solution of (4) satisfies the boundary conditions at infinity

$$\lim_{\|\mathbf{r}\|\to\infty} \tilde{\mathbf{H}} = 0, \quad \lim_{\|\mathbf{r}\|\to\infty} \tilde{\mathbf{E}} = 0.$$

Here all the variables with the tilde are functions of $\mathbf{r}$ and s. Then the time domain solution can be presented via the Fourier integral as

$$\mathbf{E}(t) = \frac{1}{2\pi i}\int_{-i\infty}^{+i\infty} e^{st}\tilde{\mathbf{E}}(s)ds \tag{5}$$

and similarly for $\mathbf{H}(t)$. Assumption 1 yields stability of the Maxwell system, and together with Assumption 2 it gives well-posedness of (1)–(3) (see Section 4).

The coefficient $\tilde{\sigma}(s)$ as a function of s can be approximated in $\mathcal{C}_+$ by an $[m/m]$ rational function of the form:

$$\sigma(s) = \sigma_\infty\left(1 + \frac{p_{m-1}^\sigma(s)}{q_m^\sigma(s)}\right), \tag{6}$$

where p_{m-1} and q_m are respectively polynomials of degree $m-1$ and m. As we mentioned before, $\tilde{\sigma} := \tilde{\sigma}(\mathbf{r},s)$, so the coefficients of p_{m-1} and q_m depend on $\mathbf{r}$. Rational approximation (6) allows us to rewrite integral equation (2) as high order ODE

$$q_m^\sigma(\partial/\partial t)\mathbf{J}_c = \sigma_\infty q_m^\sigma(\partial/\partial t)\mathbf{E} + \sigma_\infty p_{m-1}^\sigma(\partial/\partial t)\mathbf{E}, \tag{7}$$

so we obtain high order PDE problem (1), (3) and (7). Generally, thanks to Assumption 1 rational approximations (6) uniformly converge in $\mathcal{C}_+$, so integral Eq. (2) can be formally rewritten as the infinite-order ODE.

The popular Cole and Cole [5] polarization model is given by

$$\tilde{\sigma}(s) = \sigma_\infty\left(1 - \frac{\eta}{1 + (s\tau)^c}\right). \tag{8}$$

Here $\tau > 0$ is the time decay parameter, the parameter $0 \leqslant \eta < 1$ is the so-called chargeability, $0 < c \leqslant 1$ is so-called relaxation parameter. All the above parameters depend on $\mathbf{r}$. Under the assumption that η is bounded away from 1 uniformly with respect to spacial variable it is easy to observe that the Cole–Cole conductivity satisfies Assumption 1.

The Cole–Cole formula (8) allows us to rewrite the integral equation (2) as fractional order differential equation

$$\mathbf{J}_c + \tau^c D_t^c\mathbf{J}_c = \sigma_\infty(1-\eta)\mathbf{E} + \tau^c\sigma_\infty D_t^c\mathbf{E}, \tag{9}$$

where the fractional derivative $D_t^\alpha, 0 \leqslant \alpha \leqslant 1$ is a pseudo-differential operator [35] that can be defined as $D_t^\alpha f(t) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} s^\alpha e^{ist-is\tau}f(\tau)dsd\tau$ (for regular enough f), and for $\alpha = 1$ it coincides with the conventional first derivative operator (see also an equivalent definition via fractional diffusion operators [35]). So we obtain fractional order PDE problem (1), (3) and (9).

Finally, (1) and (2) can be transformed to the electric field formulation problem

$$\nabla \times \nabla \times \mathbf{E} + \mu\sigma * \frac{\partial}{\partial t}\mathbf{E} = -\mu\frac{\partial}{\partial t}\mathbf{J}^r. \tag{10}$$

After spacial discretization using a proper finite-difference (or finite-element) method with N nodes we obtain

$$Au + B * \frac{\partial}{\partial t}u = b, \quad u|_{t<0} = 0, \tag{11}$$

where $u = u(t)$ and $b = b(t)$ are N-dimensional vector-functions of $t, A = A^* \in R^{N\times N}$ is a positive-definite (on the divergence-free subspace) stiffness matrix, B is a positive-definite mass matrix with entries obtained by discretization of $\mu\sigma$ on the computational grid; * denotes convolution. For the non-dispersive case $B = B_\infty\delta(\tau)$, where B_∞ is a time-independent positive-definite diagonal matrix and δ is Dirac's delta function, we obtain the first order ODE system with symmetric positive-definite coefficients and time-dependent right hand side

$$Au + B_\infty\frac{\partial}{\partial t}u = b, \quad u|_{t<0} = 0. \tag{12}$$

Finally, assuming

$$b = \delta(t)b_0 \tag{13}$$

with a vector $b_0 \in R^N$ independent of time (corresponding to $\mathbf{J}' = \varphi(r)h(-t)$, where $h(t)$ is the Heaviside step-function), we obtain the standard initial problem for the homogeneous second order equation for $t > 0$. Obviously, this problem is reduced to computing the exponential

$$u(t) = \exp(-tA)b_0 \tag{14}$$

assuming that $B_\infty = I$.

Assumptions 1 and 2 allow us to obtain the Laplace transform of (11) in $\mathcal{C}_+$ in the form

$$\widetilde{A}(s)\tilde{u}(s) = \tilde{b}(s), \tag{15}$$

where

$$\widetilde{A}(s) = A + s\widetilde{B}(s) \tag{16}$$

is a complex symmetric $N \times N$ matrix value function, $\tilde{u}(s), \tilde{b}(s)$ are vector functions in $\mathcal{C}^N$.

Due to dependence of $\tilde{\sigma}$ on $\mathbf{r}$ matrices $\widetilde{A}(s)$ for different values of s may not commute, otherwise the problem can be solved using the conventional Krylov subspace approximation, as it was done for a convolutionary (fractional diffusion) PDE in [19].

The time domain solution can be computed using the Fourier integral

$$u(t) = \frac{1}{2\pi i}\int_{-i\infty}^{+i\infty} e^{st}\tilde{A}(s)^{-1}\tilde{b}(s)ds. \tag{17}$$

Our main application arises from geophysical deep hydrocarbon exploration, in which case A can be a large ill-conditioned matrix. This problem is of multiscale nature and may require the solution for positive time intervals $[t_{\min}, t_{\max}]$ with large ratio $t_{\max}/t_{\min}$. Evaluation of (17) using quadrature formulas directly may require evaluations of $\tilde{A}(s)^{-1}\tilde{b}(s)$ for significant number of s's even using efficient specialized quadratures [31], that may be computationally very expensive.

3. Parameter-dependent Krylov subspace reduction

As it was already mentioned in the previous section, the convolutionary Maxwell's system can be considered as an infinite-order differential equation. In principle, this problem can be transformed to a first order system with infinite number of unknowns [or $(m+1)N$ unknowns for (7)] and then solved using a structure preserving Krylov subspace projection method of [13]. Here we suggest an approach allowing to avoid such increase of dimensionality.

We choose $n (n \leqslant N)$ distinct complex parameters (frequencies) s_j symmetrically with respect to the real axis, such that they are not in the nonlinear spectrum of $\tilde{A}(s)$. Let us assume that the solutions of (15) for these frequencies are linearly independent, i.e., they span subspace

$$U_n = \ \mathrm{span}\{\widetilde{A}(s_1)^{-1}\tilde{b}(s_1), \widetilde{A}(s_2)^{-1}\tilde{b}(s_2), \ldots, \widetilde{A}(s_n)^{-1}\tilde{b}(s_n)\}. \tag{18}$$

Generally, it is similar to the subspaces generated in the parametric model reduction, hence the name: parameter-dependent Krylov subspace reduction (PDKSR). For $s \in \mathbf{R}$ both $\tilde{A}(s)$ and $\tilde{b}(s)$ are real, so $\tilde{u}(s) = \bar{u}(\bar{s})$, i.e., there is no need to compute the solution for the conjugate s_j. If $\tilde{b}$ is independent on s, then U_n is related to the Nonlinear Krylov Subspace introduced for solving nonlinear eigenproblems [30]. In addition, if $\widetilde{A}(s)$ is a linear polynomial of s, then U_n becomes the rational Krylov subspace and the PDKSR will be equivalent to the rational Krylov subspace reduction described in [9].

Remark 2. Our choice of parameters s_j is given by the solution of the Zolotarev problem (see Appendix A) and they are well separated. But we can imagine the case when several s_j are very close to each other. In this case one should use (possibly high order) derivatives of $\widetilde{A}(s)^{-1}\tilde{b}(s)$ with respect to s for constructing U_n. But this problem is out of the scope of the current paper.

Let $G^n = \{g_1, \ldots, g_n\} \in R^{N\times n}$ be the matrix of an orthogonal basis on U_n. Then the approximate solution of (15) is obtained by projection to the PDKS as

$$\tilde{u}^n(s) = G^n V^n(s)^{-1}(G^n)^T\tilde{b}(s), \tag{19}$$

where

$$V^n(s) = (G^n)^T\widetilde{A}(s)G^n.$$

Obviously, any subspace reduction becomes efficient if $n \ll N$.

We use the following algorithm to construct G^n. Let us first assume that all s_j are real (as in our numerical experiments, see Section 5). We choose g_1 to be the normalized $\widetilde{A}(s_1)^{-1}\tilde{b}(s_1)$. If we constructed already G^{n-1}, then compute

$$r_n = \widetilde{A}(s_n)^{-1}\left[\tilde{b}(s_n) - \widetilde{A}(s_n)G^{n-1}V^n(s)^{-1}(G^{n-1})^T\tilde{b}(s_n)\right]. \tag{20}$$

Then we obtain g_n via the Gram-Schmidt process by orthogonalizing r_n to G^{n-1}. In the case of complex s_j we consider only one s_j from every conjugate pair and do the Gram–Schmidt process consequently to $\Re r_j$ and $\Im r_j$ to avoid complex vectors in the basis. Sometimes this process requires up to three re-orthogonalizations to achieve orthogonality of the computer (double) precision level. However, as we shall see, even in spite of the orhogonality of basis vectors, the algorithm loses approximately half of significant digits, more precisely has a convergence plateau on the level of the square root of the roundoff error.

Finally we obtain the time-domain approximate solution $u^n(t)$ via Fourier integral

$$u^n(t) = \frac{1}{2\pi i}\int_{-i\infty}^{+i\infty} e^{st}G^nV^n(s)^{-1}(G^n)^T\tilde{b}(s)ds, \tag{21}$$

that is computed using optimized contour deformations and quadratures developed in [31].

Remark 3. To compute $u^n(t)$, all n basis vectors of U_n need to be stored in memory. That might be problematic for 3D large-scale problems. Thanks to efficient choice of s_j, we need to store at most 60 real solutions for accuracy 10^{-8} on the entire time interval in our numerical examples (see Section 5).

4. Stability, passivity and interpolation properties of the parameter-dependent Krylov subspace reduction

Two essential properties associated with linear time-invariant dynamical systems are stability and passivity. A system is stable, i.e., the solution is uniformly bounded in time, if it does not have spectral points in $\mathcal{C}_+$. The second question is whether or not the system is passive, i.e., capable to generate energy without any external source [2,13]. Obviously, a passive system is always stable. Let us define the nonlinear numerical range of $\widetilde{A}(z)$ according to [15] as

$$W(\widetilde{A}) = \{z \in \mathcal{C} : v^H\widetilde{A}(z)v = 0\}$$

for some nontrivial $v \in \mathcal{C}^N$, here ^{H} means Hermitian conjugate. For any $w \in \mathcal{C}^n$ it follows $w^HV_nw = v^HAv$ with $v = G_nw$ (from the definition of V_n), so

$$W(V_n) \subset W(\widetilde{A}).$$

Therefore both $u(t)$ and $u^n(t)$ are passive, if

$$W(\widetilde{A}) \subset \mathcal{C}_-. \tag{22}$$

It is easy to see, that Assumption 1 is sufficient for validity of (22). In fact, entries of matrix operator $\widetilde{B}$ in (16) are the nodal values (or cell averages) of $\tilde{\sigma}$ (with factor $\mu > 0$) satisfying Assumption 1, so $\widetilde{B} \succ 0$ for $s \in \mathcal{C}_+$. From that and positive-definiteness of A we obtain that

$$\Re\left(\frac{1}{s}\widetilde{A}(s)\right) = \frac{\Re(s)}{|s|^2}A + \Re(\tilde{B}) \succ 0, \quad \text{for } s \in \mathcal{C}_+,$$

that yields (22). Let us now further restrict points s_i placing them in $\mathcal{C}_+$. By construction $\tilde{u}^n(s)$ is the Galerkin approximation of $\tilde{u}(s)$ on the subspace of $\tilde{u}(s_j)$, $j = 1,\ldots,n$. We obtain the interpolation property of the approximate solution

$$\tilde{u}(s_j) = \tilde{u}^n(s_j), \quad j = 1,\ldots,n$$

thanks to the uniqueness of the Galerkin solution for $s \in \mathcal{C}_+$ following from (22).

5. Solution of the induced polarization problem with the Cole–Cole conductivity model

We consider the three-dimensional problem of so-called control source electromagnetic exploration with the diffusive Cole–Cole conductivity model (1), (3) and (9) and the "step-off" excitation mode given by $\mathbf{J}' = h(-t)\mathbf{b_0}(\mathbf{r})$ ($h(t)$ is the Heaviside step-function). This problem is becoming increasingly important for electromagnetic hydrocarbon exploration [6, etc.]. Its multiscale nature requires the computation for time intervals including very small and large diffusion times, i.e., effectively we need good accuracy in the sense

$$\delta^n_{L_2[0,\infty]} = \sqrt{\int_0^\infty \|u^n(t) - u(t)\|^2\, dt}.$$

The problem of optimal choice of a subspace U_n, i.e., the choice of interpolation nodes $s_j, j = 1,\ldots,n$ for accurate solution, was rigorously solved for the non-dispersive diffusive case (12) in [9]. The Plancherel identity yields

$$\delta^n_{L_2[0,\infty]} \equiv \frac{1}{2\pi}\sqrt{\int_{-i\infty}^{i\infty} \|\tilde{u}^n(s) - \tilde{u}(s)\|^2\, ds},$$

i.e. the optimization problem is reduced to the frequency domain. The latter can be reduced to the third Zolotarev problem in extended complex plane, that yields an optimal solution (in the Cauchy–Hadamard sense) with *real* s_i given in terms of elliptic integrals (see Appendix A). The Zolotarev interpolating frequencies yield the following Cauchy–Hadamard error bound

$$\overline{\lim_{n\to\infty}} \sqrt[n]{\delta^n_{L_2[0,\infty]}} \lesssim e^{-\frac{\pi^2}{2\log(4\kappa)}}, \tag{23}$$

where κ is the condition number of the matrix pencil (A, B_∞). As one can see, logarithmic dependence of (23) on the condition number makes such choice of interpolating points efficient for large scale problems and rather weakly sensitive to the errors in a priori spectral estimates. The real solution is another advantage of using the Zolotarev theory, because that greatly simplifies handling of linear systems for interpolating frequencies.

The conductivity given by the Cole–Cole model has high frequency limit σ_∞, i.e., Eqs. (10) and (12) has the same leading terms, if the elements of diagonal matrix B_∞ are obtained using the discretization of $\mu\sigma_\infty$ on the same computational grid. So, it is reasonable to assume that the interpolation points chosen for (12) are also good for (10). As we shall see, our numerical experiments confirm this assumption, however a more rigorous analysis is needed.

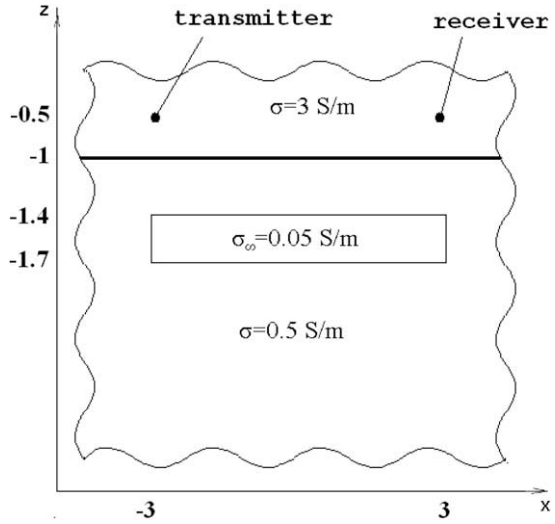

Fig. 1. Medium for 3D test.

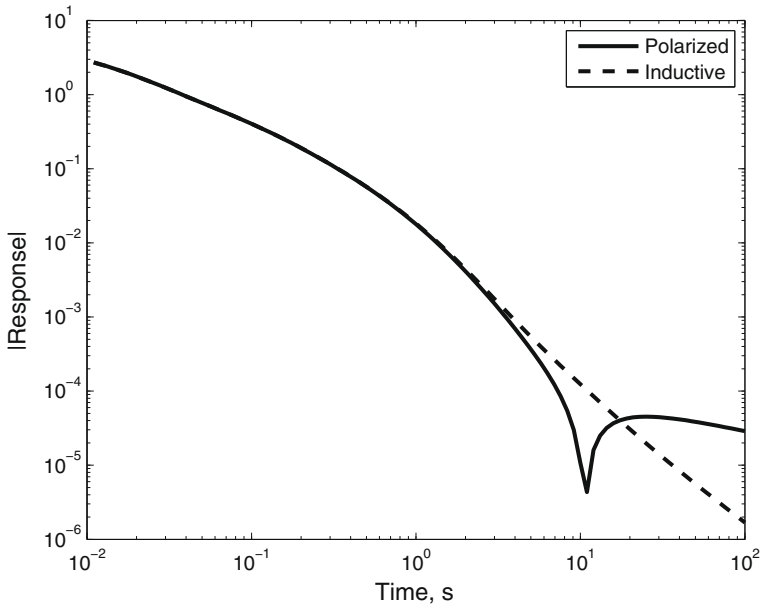

Fig. 2. Electric response at transmitter position for both non-dispersive (inductive) and dispersive (polarized) problems.

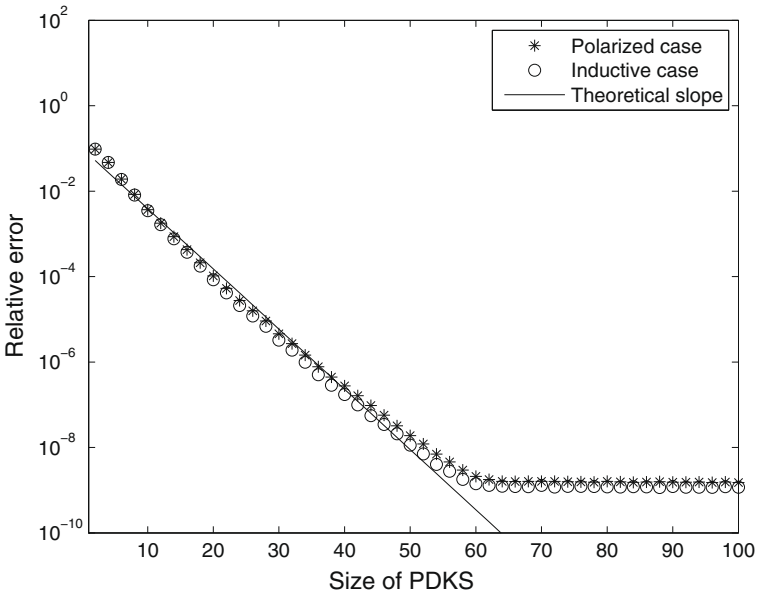

Fig. 3. Convergence for non-dispersive (inductive) and dispersive (polarized) problems. Both show the same rate.

Consider the three-dimensional problem in the medium consisting of one finite body of size $6 \times 4 \times 0.3$ km^3 embedded into two non-polarized layers (see its median vertical slice in Fig. 1). In the first case the body is non-polarized with $\eta = 0$ and for the second case it is described by the Cole–Cole model with $\eta = 0.5, c = 0.5, \tau = 1$ s. To construct G_n, we used the preconditioned conjugate gradient algorithm of [36] for the solution of (15). Typically, solution of linear systems constitute about 95% of the computational time, the rest is due to orthogonalization. In Fig. 2 we plotted the responses for the case when the receiver and the transmitter coincide (see Fig. 1) (both vertical electric dipoles). The curves almost coincide for $t \ll \tau$, but for larger t the non-normality of the operator for the polarized problem manifests itself by non-monotonic behavior and sign reversal.

The convergence graphs are plotted in Fig. 3. For the both cases we used the same spatial discretization with $N = 3 \cdot 10^5$ and $\kappa \approx 1.3 \times 10^8$ (estimated via the Gershgorin theorem). The both cases show similar convergence behavior with the linear rate very well approximated by the theoretical estimate (23).

The computations were performed with the double precision, however the both curves have plateaus on the level of the single precision. That indicates presence of cancelation effects in (20). Our experiments with the rational Arnoldi algorithm of [27] applied to the induction problem showed no loss of accuracy. Unfortunately, that algorithm in the present form is limited only to the RKS, i.e., the non-dispersive problems.

6. Conclusions

We developed a new algorithm for solution of diffusion Maxwell's system in dispersive media (a.k.a. induced polarization). The algorithm is based on the parameter-dependent Krylov subspace reduction (PDKSR) with proper choice of subspace parameters. The latter is based on the rational Krylov subspace algorithm for the conventional (non-dispersive) diffusion problem [9]. Our numerical results for the 3D problem show the same convergence rate for dispersive and non-dispersive models (both coinciding with the theoretical optimal bound for the non-dispersive case).

The parameter-dependent Krylov subspace reduction can be extended to other convolutionary problems, such as electromagnetic and elastic wave propagation in dispersive media.

A detailed theoretical analysis of the new algorithm is in press [10].

Appendix A. Choice of s_i and the third Zolotarev problem

Here we give short summary of results obtained in [9,17] for the shift optimization for the classical diffusion (a.k.a. inductive) problem. The optimal choice of s_i for this case can be reduced to the minimization problem

$$\hat{\sigma}_n = \min_{s_1,\ldots,s_n} \max_{s\in[\lambda_{\min},\lambda_{\max}]} |h(-s)/h(s)|, \tag{A.1}$$

where

$$h(s) = \prod_{j=1}^{n}(s + s_j).$$

Here $\lambda_{\min}$ and $\lambda_{\max}$ are the minimum and the maximum eigenvalues of matrix pencil $(A; B_\infty)$. This is the Zolotarev problem, which is known to have solution with real values of parameters s_j expressed in terms of elliptic integrals. Let K and K' (see [1, Chapter 17]) be respectively the principal

$$K(\varkappa) = \int_0^1 \frac{dt}{\sqrt{(1-t^2)(1-\varkappa^2 t^2)}}$$

and complementary

$$K'(\varkappa) = K\left(\sqrt{1-\varkappa^2}\right)$$

complete elliptic integrals of modulus $\varkappa, 0 < \varkappa < 1$,

$$\mu = \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^2 \quad \text{and} \quad \kappa = \frac{\lambda_{\max}}{\lambda_{\min}}.$$

We shall also need the Jacobi elliptic function

$$\mathrm{dn}(v, \varkappa) = \sqrt{1 - \varkappa^2 \mathrm{sn}(v, \varkappa)^2},$$

where sn is another elliptic function defined by

$$\mathrm{sn}(v, \varkappa) = \sin\psi, \qquad v = \int_0^{\psi} \frac{d\zeta}{\sqrt{1 - \varkappa^2 \sin^2\zeta}}$$

(see [1, Chapter 16]). In this case the solution of (A.1) is given by

$$s_j = \lambda_{\max}\ \mathrm{dn}\left(\frac{2(n-j)+1}{2n} K'(\tfrac{1}{\kappa}), \sqrt{1-\frac{1}{\kappa^2}}\right) \tag{A.2}$$

for $j = 1, \ldots, n$.

Remark 4. In practice we do not know $\lambda_{\min}$ and $\lambda_{\max}$ exactly, but have just their estimates. Different estimates might affect the location of optimal points, but according to (23) it has just slight impact on the convergence rate.

Points s_j fill $[\lambda_{\min}; \lambda_{\max}]$, and for large κ/n they are close to a geometric progression. The points yield the following (optimal in the Cauchy–Hadamard sense) error bound

$$\overline{\lim_{n\to\infty}} \sqrt[n]{\delta^n_{L_2[0,\infty]}} \leqslant \exp\left[-\frac{\pi}{4}\cdot\frac{K'(\mu)}{K(\mu)}\right]. \tag{A.3}$$

For $\kappa \to \infty$ the right hand side part of (A.3) can be simplified: using asymptotic expansions (see [1])

$$\mu = 1 - \frac{4}{\sqrt{\kappa}} + o\left(\frac{1}{\sqrt{\kappa}}\right), \quad K(\mu) = \frac{1}{2}\log\left(2\sqrt{\kappa}\right) + o(1), \quad K'(\mu) = \frac{\pi}{2} + o(1),$$

we obtain

$$\exp\left[-\frac{\pi}{4}\cdot\frac{K'(\mu)}{K(\mu)}\right] = e^{-\frac{\pi^2}{2\log(4\kappa)}} + o(1).$$

This yields (23).

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