A NOVEL LANCZOS-TYPE PROCEDURE FOR COMPUTING EIGENELEMENTS OF MAXWELL AND HELMHOLTZ PROBLEMS

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Abstract—We introduce a novel variant of the Lanczos method for computing a few eigenvalues of sparse and/or dense non-Hermitian systems arising from the discretization of Maxwell- or Helmholtz-type operators in electromagnetics. We develop a Krylov subspace projection technique built upon short-term vector recurrences that does not require full reorthogonalization and can approximate simultaneously both left and right eigenvectors. We report on experiments for solving eigenproblems arising in the analysis of dielectric waveguides and scattering applications from PEC structures. The theoretical and numerical results reported in this study will contribute to highlight the potential and enrich the database of this technology for solving generalized eigenvalue problems in Computational Electromagnetics.

1. INTRODUCTION

In the analysis of many electromagnetism applications, one seeks eigenvalues of the algebraic set of equations arising from the discretization of Maxwell or Helmholtz-type operators. Finite element analysis of uniform waveguides filled with inhomogeneous dielectric and perfectly conducting (PEC) structures is one such example [26]. The

problem leads to a canonical sparse matrix eigensystem in the form $Qx = \gamma^2 Rx$, that yields solutions simultaneously for the propagation constant γ and the corresponding magnetic field distribution. For lossless waveguides the pertinent matrices are sparse and real, R is positive definite while Q is in general nonsymmetric, revealing possibly complex modes (see e.g., [18]). Finite difference discretizations of the Helmholtz equations for the magnetic field also lead to a nonsymmetric eigenvalue problem with special block structure where the computational task is to determine the right most eigenvalues and their corresponding eigenvectors (see details of this problem in [21] and in Section 4). Spectral information can be also incorporated in the construction of robust preconditioners for solving linear systems of equations. In the experiments reported in [5–7], we showed that updating a preconditioner with eigenvectors associated to a few small eigenvalues of the preconditioned matrix can lead to a significant reduction of the number of iterations of Krylov subspace methods in the solution of dense linear systems arising from the Method of Moments discretization of integral operators in electromagnetic scattering. Scattering analysis continues to receive much attention in electromagnetics research, see e.g., [15, 25, 30, 31, 37].

When no theoretical information is available on the spectrum of the underlying operator, one necessarily resorts to numerical methods to approximate eigenvalues and eigenvectors of interest. Several algorithms and software are developed for solving eigensystems, most of them is based on the Arnoldi or the Jacobi-Davidson method. In particular, the Implicitly Restarted Arnoldi (IRA) method has become the de facto standard for computing a few eigenpairs of general non-Hermitian matrices. It proceeds by transforming the matrix into upper Hessenberg form with the help of long vector recurrences that are orthogonalized at each step. To reduce orthogonalization costs, the procedure is restarted after a finite (typically small) number of steps with an up-to-date initial vector which is filtered from components corresponding to the undesired part of the spectrum.

In this study, we follow a different approach and explore variants of the Lanczos method for solving non-Hermitian eigensystems arising from finite element, finite difference, boundary element discretizations of wave propagation problems. The Lanczos algorithm may be computationally attractive because it is built on three-term vector recurrences that are cheap to store in memory, and it has very limited reorthogonalization cost. However, most implementations of the Lanczos methods are oriented to solve real generalized symmetric eigenvalue problems with complex Hermitian matrices and real symmetric positive-definite matrix pairs, for which it was

originally developed. Although some authors have extended the Lanczos method for solving other kinds of problems, e.g., non-Hermitian problems [2, 20], current software is less advanced and rich in functionalities compared to the Arnoldi method especially when one seeks approximate eigenvalues located in the interior of the spectrum [24]. Indeed this area of research is still open and under development.

In this paper, we present an iterative technique for solving non-Hermitian eigensystems built upon a variant of the Lanczos method, that we call the Lanczos Biconjugate A-Orthonormalization method. In a previous study we showed the remarkable efficiency of this procedure which enabled us to derive fast convergent and economical iterative linear solvers for electromagnetism applications [27]. This work is the natural extension of our earlier study to eigensystems; we develop an oblique projection techniques into suitable Krylov subspaces to compute a few eigenvalues and corresponding left/rigth eigenvectors. Key objective of the theoretical and numerical results reported in this study is to contribute to highlight the potential and enrich the database of this technology for solving generalized eigenvalue problems in Computational Electromagnetics.

The paper is structured as follows. In Section 2, we outline the Lanczos Biconjugate A-Orthonormalization procedure and some of its theoretical properties. In Section 3, we develop an eigenvalue solver from the Lanczos Biconjugate A-Orthonormalization procedure and we discuss some computational aspects as well. We report on the results of numerical experiments in Section 4. Finally, in Section 5, we draw some preliminary conclusions from this study and perspectives of future research.

2. THE NON-HERMITIAN LANCZOS BICONJUGATE A-ORHTONORMALIZATION METHOD

Throughout this paper we use capital letters for matrices, lower case letters for column vectors and lower case Greek letters for scalars. We denote by the symbol "*" the conjugate transpose operation and by "≡" a definition. We consider the complex n-dimensional vector space $\mathbb{C}^n$ with standard innerproduct $\langle \cdot, \cdot \rangle$ between two complex vectors $u, v \in \mathbb{C}^n$ defined as

$$\langle u, v \rangle \equiv u^* v = \sum_{i=1}^{n} \bar{u}_i v_i,$$

and associated Euclidean vector norm $\|x\| \equiv \sqrt{x^* x}$ and compatible matrix norm. We also consider the complex n-dimensional dual vector

space $(\mathbb{C}^n)^*$ of row vectors that is isomorphic to $\mathbb{C}^n$. In $(\mathbb{C}_n)^*$, we have $\langle v^*, u^* \rangle = u^* v$ and $\|x^*\| = \sqrt{x^* x}$.

Given a complex non-Hermitian matrix A and $\{v_1, w_1\}$ two vectors of unit Euclidean inner product $\langle \omega_1, Av_1 \rangle = 1$, we define Lanczos-type vectors $\{v_j, w_j\}$ and scalars $\{\delta_j, \beta_j\}$, $j = 1, 2, \ldots, m$ through the following recursions

$$\delta_{j+1} v_{j+1} = Av_j - \beta_j v_{j-1} - \alpha_j v_j, \tag{1}$$

$$\bar{\beta}_{j+1} w_{j+1} = A^* w_j - \delta_j w_{j-1} - \bar{\alpha}_j w_j, \tag{2}$$

where the scalars are chosen as

$$\alpha_j = \langle w_j, A^2 v_j \rangle \ , \ \beta_j = \langle w_{j-1}, A^2 v_j \rangle \ , \ \delta_j = \langle w_j, A^2 v_{j-1} \rangle. \tag{3}$$

This choice of the scalars guarantees that the recursions generate sequences of biconjugate A-orthonormal vectors (or briefly, A-biorthonormal vectors) $\{v_i, w_i\}$, according to the following definition

Definition 1 *Right and left Lanczos-type vectors* v_j, $j = 1, 2, \ldots, m$ *and* w_i, $i = 1, 2, \ldots, m$ *form a biconjugate A-orthonormal system in exact arithmetic, if and only if*

$$\langle \omega_i, Av_j \rangle = \delta_{i,j}, \ 1 \leq i, j \leq m. \tag{4}$$

Equations (1)–(2) can be interpreted as a two-sided Gram-Schmidt orthonormalization procedure of linear algebra. At step j, vectors v_j and w_j are multiplied by A and A^*, respectively, and then they are orthonormalized against the most recently generated Lanczos-type pairs of vectors (v_j, w_j) and (v_{j-1}, w_{j-1}). Notice that the choice (3) for the scalars β_j and δ_j is not unique; some freedom is left provided the biconjugate A-orthonormalization property (4) holds. We sketch a complete version of the Biconjugate A-Orthonormalization (BiCOR) procedure in Algorithm 1.

The matrix A is not modified by Algorithm 1 and is accessed only via matrix-vector products either by A or A^*. Compared to the Arnoldi procedure, the memory storage of the BiCOR procedure is very limited: at step j only the two most recently computed pairs of Lanczos-type vectors $\{v_k, w_k\}$, $k = j$, $j - 1$ are needed to produce $\{v_{j+1}, w_{j+1}\}$; additionally, they may be overwritten with the most recent updates. The procedure is possible to breakdown whenever γ_{j+1} vanishes while $\hat{w}_{j+1}$ and $A\hat{v}_{j+1}$ are not equal to $0 \in \mathbb{C}^n$ in line 7. In our experiments, we never observed this problem, although it is fair to mention that it may occurr in practice. In the interest of counteractions against such breakdowns, refer oneself to remedies such as so-called look-ahead strategies [19, 22, 35, 36] which can enhance stability while increasing cost modestly, or others for example [12]. But that is outside the scope of this paper and we shall not pursue that here.

Algorithm 1 The Biconjugate A-Orthonormalization Procedure (BiCOR)

1: Choose v_1, ω_1, such that $\langle \omega_1, Av_1 \rangle = 1$
2: Set $\beta_1 = \gamma_1 \equiv 0, \omega_0 = v_0 = \mathbf{0} \in \mathbb{C}^n$
3: **for** $j = 1, 2, \ldots, m$ **do**
4:     $\alpha_j = \langle \omega_j, A(Av_j) \rangle$
5:     $\hat{v}_{j+1} = Av_j - \alpha_j v_j - \beta_j v_{j-1}$
6:     $\hat{\omega}_{j+1} = A^* \omega_j - \bar{\alpha}_j \omega_j - \gamma_j \omega_{j-1}$
7:     $\gamma_{j+1} = |\langle \hat{\omega}_{j+1}, A\hat{v}_{j+1} \rangle|^{\frac{1}{2}}$
8:     $\beta_{j+1} = \dfrac{\langle \hat{\omega}_{j+1}, A\hat{v}_{j+1} \rangle}{\gamma_{j+1}}$
9:     $v_{j+1} = \dfrac{\hat{v}_{j+1}}{\gamma_{j+1}}$
10:    $\omega_{j+1} = \dfrac{\hat{\omega}_{j+1}}{\bar{\beta}_{j+1}}$
11: **end for**

The following Proposition shows that recurrences (1)–(2) produce a sequence of biconjugate A-orthonormal vectors.

Proposition 1 *If Algorithm 1 proceeds m steps, then the right and left Lanczos-type vectors v_j, $j = 1, 2, \ldots, m$ and w_i, $i = 1, 2, \ldots, m$ form a biconjugate A-orthonormal system in exact arithmetic, i.e.,*

$$\langle \omega_i, Av_j \rangle = \delta_{i,j}, \quad 1 \le i, j \le m.$$

Furthermore, denote by $V_m = [v_1, v_2, \ldots, v_m]$ and $W_m = [w_1, w_2, \ldots, w_m]$ the $n \times m$ matrices and by $\underline{T_m}$ the extended tridiagonal matrix of the form

$$\underline{T_m} = \left[\begin{array}{c} T_m \\ \gamma_{m+1} e_m^* \end{array} \right], \tag{5}$$

where

$$T_m = \left[\begin{array}{cccccc} \alpha_1 & \beta_2 & & & & \\ \gamma_2 & \alpha_2 & \beta_3 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \gamma_{m-1} & \alpha_{m-1} & \beta_m \\ & & & \gamma_m & \alpha_m \end{array} \right],$$

whose entries are the coefficients generated during the algorithm implementation, and in which $\alpha_1, \ldots, \alpha_m$, $\beta_2, \ldots, \beta_m$ are complex while $\gamma_2, \ldots, \gamma_m$ positive. Then with the Biconjugate A-Orthonormalization

Procedure, the following four relations hold

$$AV_m = V_m T_m + \gamma_{m+1} v_{m+1} e_m^*, \tag{6}$$

$$A^* W_m = W_m T_m^* + \beta_{m+1} \omega_{m+1} e_m^*, \tag{7}$$

$$W_m^* A V_m = I_m, \tag{8}$$

$$W_m^* A^2 V_m = T_m. \tag{9}$$

Proof. See [28].

In exact arithmetic the biconjugate Lanczos A-orthonormalization method ideally builds up a pair of biconjugate A-orthonormal bases for the dual Krylov subspaces $K_m(A; v_1)$ and $A^* K_m(A^*; w_1)$; the vector recurrences produce a tridiagonal matrix as the result of projecting A onto the corresponding Krylov subspaces. Key relations to this study are Relations (8)–(9) which suggest to use the eigenvalues of the tridiagonal matrix T_m to approximate part of the spectrum of A by means of an oblique projection of A onto $K_m(A; v_1)$ orthogonally to $A^* K_m(A^*; w_1)$. We state this idea more clearly in the next section.

3. THE BICOR METHOD FOR EIGENSYSTEMS

We denote by $\lambda_i(A)$ the i-th eigenvalue of the complex $n \times n$ matrix A according to a given order. To each eigenvalue λ there corresponds at least one column eigenvector x and one row eigenvector y^* satisfying $Ax = x\lambda$, $y^*A = \lambda y^*$. The set $\{\lambda, x, y^*\}$ is an *eigenelement* of A. In this work, we compute a few eigenelements of A from the approximate invariant subspaces produced by Algorithm 1. We recall that the columns of a given $n \times m$ matrix Q with $m \le n$ span an invariant column-subspace of A if $AQ = QC$ for some $m \times m$ matrix C. The matrix C is uniquely determined provided the columns of Q are independent. The spectrum of C is representative of a subset of the spectrum of A as every eigenvector x of C induces an eigenvector Qx of A. In a similar way, the rows of the $m \times n$ matrix P^*, assuming they are independent, span an invariant row-subspace of A when $P^*A = DP^*$ for some uniquely determined $m \times m$ matrix D. From the chain of relations $P^*QC = P^*AQ = DP^*Q$ follows that, provided P^*Q is nonsingular, we may write $C = (P^*Q)^{-1}D(P^*Q)$ and the invariant subspaces generated by Q and P^* correspond to the same part of the spectrum of A.

The Lanczos biconjugate A-orthonormalization procedure approximates an m-dimensional invariant subspace of A by computing two $n \times m$ matrices V and W for $m < n$. The columns of V span an approximate invariant column-space of A while the rows of W^* span an approximate invariant row-space of A. Therefore, assuming that W^*V

is nonsingular we may compute a few eigenvalues of a general nonsymmetric matrix from recursions (1)–(2) by Relations (8)–(9) along the following lines

STEP 1 Run m steps of Algorithm 1, for some given $m \ll n$. Generate Lanczos-type matrices $V_m = [v_1, v_2, \ldots, v_m]$, $W_m = [w_1, w_2, \ldots, w_m]$ and the tridiagonal projection matrix T_m defined in Proposition 1.

STEP 2 Seek approximate eigenpairs of A of the form (λ, u) with $\lambda \in \mathbb{C}$ and $u \in \mathcal{K}_m = K_m(A; v_1)$ imposing the Petrov-Galerkin condition

$$\langle Au - \lambda u, z \rangle = 0 \quad \forall z \in \mathcal{L}_m \equiv A^* K_m(A^*; w_1). \qquad (10)$$

The mth dimensional space $\mathcal{K}_m$ is referred to as the subspace of approximants or search subspace and the mth dimensional space $\mathcal{L}_m$ as the constraints subspace. Expanding u in terms of the basis V_m we have

$$u = V_m y,$$

and Eq. (10) becomes in matrix form

$$(A^* W_m)^* (AV_m y - \lambda V_m y) = 0.$$

By substitution and computation with Eqs. (8)–(9), the problem can be written in equivalent form as

$$\text{find } \lambda \in \mathbb{C}, \ y \neq 0 \text{ such that } T_m y - \lambda y = 0. \qquad (11)$$

At this stage, we have to compute eigenpairs (λ, y) of the reduced tridiagonal matrix T_m. To each (λ, y), there correspond a *right Ritz vector* $V_m y$ and a *left Ritz vector* $W_m y$ of A.

STEP 3 Accept $\{\lambda, V_m y, W_m y\}$ as approximate eigenelement of A if the corresponding residual norms are small enough, i.e.,

$$\|AV_m y - \lambda V_m y\| \leq tol, \quad \|A^* W_m y - \lambda W_m y\| \leq tol$$

for some user-defined tolerance tol. Otherwise, enlarge the Krylov subspace and repeat the process again.

In finite precision arithmetic, the sequence of vectors $\{v_j, w_j\}$ generated by Algorithm 1 does not mantain the biconjugate A-orthonormalization property. Complete reorthogonalization at step j of the latest computed vector $\{v_j, w_j\}$ against all previously computed vectors $\{v_i, w_i\}$ for $i = 1, \ldots, j - 1$ is possible by adding the following two loops after line 10 in Algorithm 1:

$$\begin{aligned}
v_j &= v_j - \overline{(v_j^* A^* w_i)} v_i, \quad i = 1, \ldots, j - 1, \\
w_j &= w_j - \overline{(w_j^* A v_i)} w_i \quad i = 1, \ldots, j - 1.
\end{aligned} \qquad (12)$$

This extra cost may quickly become a bottleneck of the procedure especially for large matrices. With no reorthogonalization, although the projection of A is not optimal it can still yield useful information on the spectrum of A. In fact, for sufficiently large m the eigenvalues of A appear amongst the eigenvalues of T_m. An explanation of this phenomenon was suggested for the symmetric case [9]. However, there is clear evidence that it is also valid for nonsymmetric recurrences such as Relations (1)–(2). One problem due to the loss of A-biorthonormalization is that some eigenvalues of T_m may not approximate well any eigenvalue of A and we need to define an identification test to distinguish "converged" from "spurious" eigenvalues in the spectrum of T_m. In STEP 3, we use the residual estimates to classify "good" and "bad" eigenvalues. The reasoning behind this strategy is based on the following results of the theory of backward error analysis for eigenproblems of diagonalizable matrices [29, 40].

Theorem 1 *Let A and two unit vectors x and z with $x^*z \neq 0$ be given. For any scalar μ define two corresponding residual vectors*

$$r \equiv Ax - \mu x, \quad s \equiv A^*z - \mu z.$$

Define the subset of perturbation matrices

$$\mathcal{E} = \{E \mid (A - E)\, x = \mu x, \ (A^* - E^*)\, z = \mu z\}$$

Then

$$\min_{\mathcal{E}} \|E\| = \max \{\|r\|, \|s\|\}. \tag{13}$$

Proof. See [29].

We aim at computing eigenelements that are correct approximations to those of perturbed matrices $B = A - E$ where E is small. Unless $\max \{\|r\|, \|s\|\}$ is satisfactorily small, an eigenvalue λ of T_m should not be used as approximate eigenvalue of A. From the matrix form of the Lanczos recursions (6)–(7), it turns out that the closest matrix to A with eigenelement $(\lambda, V_m y, W_m y)$ is $B - E$ for an E satisfying

$$\|E\| = \max \left\{ \frac{|\beta_{m+1} y(m)| \, \|v_{m+1}\|}{\|V_m y\|}, \frac{|\beta_{m+1} y(m)| \, \|w_{m+1}\|}{\|W_m y\|} \right\}. \tag{14}$$

Direct measure of the accuracy of the computed eigenvalue approximation may be established by the relation

$$|\mu - \lambda| \leq cond(\mu) \, \|E\| + \mathcal{O}\left(\|E\|^2\right) \tag{15}$$

where the conditioning of the eigenvalue μ is defined as

$$cond(\mu) = \|x\| \, \|z\| \, / \, |x^*z|, \tag{16}$$

and x and z denote the right and left eigenvectors of A corresponding to μ. In Eq. (14), it is possible to avoid the computation of the right eigenvectors of T_m by resorting to a symmetric formulation of recurrences (1)–(2). For any irreducible tridiagonal matrix there exists a diagonal similarity transformation which maps it into a complex symmetric tridiagonal matrix, for which an expression of the corresponding right eigenvector may be derived [10]. Besides immediate availability of the right eigenvectors, computing eigenelements of symmetric tridiagonal Lanczos-type matrices may be also advantageous for symmetrization of error propagation, better control of round-off errors and a priori balancing. However, this computational aspect is out of the scope of this paper and we will not pursue it further in this study.

A practical procedure built on the non-Hermitian Lanczos biconjugate A-orthonormalization procedure for eigensystems is summarized in Algorithm 2. For brevity, we refer to it as BiCOR-EIG. We stress that we do not perform complete reorthogonalization of the sequence of vectors; we reorthogonalize the sequence only locally, i.e., by adding the following two loops after line 10 in Algorithm 1:

$$
\begin{aligned}
v_j &= v_j - \overline{(v_j^* A^* w_i)} v_i, \quad i = j-3, \ldots, j-1, \\
w_j &= w_j - \overline{(w_j^* A v_i)} w_i \quad i = j-3, \ldots, j-1.
\end{aligned}
\tag{17}
$$

Algorithm 2 The Biconjugate A-Orthonormalization Procedure for Eigenvalues (BiCOR-EIG)

1: Run m steps of Algorithm 1.
2: Compute the eigenvalues of T_m.
3: Compute the eigenvectors corresponding to each eigenvalue of T_m.
4: Check convergence for right Ritz vectors using Eq. (14).
5: If convergence is not achieved, enlarge m and repeat the procedure.

3.1. Combining BiCOR-EIG with Shift-invert and Implicit Restart Techniques

One problem with Arnoldi/Lanczos-type algorithms is that convergence to eigenvalues located in the interior of the spectrum may be rather slow; their computation typically requires approximate invariant subspaces of large size. One possibility to speed-up convergence is to incorporate a shift-invert mechanism in Algorithm 2. Assuming that the problem is to compute the k eigenvalues closest to a shift θ, we apply the procedure to the matrix $B = (A - \theta I)^{-1}$. Extremal

eigenvalues of B are the eigenvalues of A closest to the shift θ. The closer θ to an eigenvalue of A, the faster the convergence. Matrix B is never explicitly formed; an LU factorization of B is computed and used each time we need to apply B. Clearly, one can use iterative solvers to compute with B avoiding a costly factorization, see, e.g., [39]. Another possible strategy may be to run Algorithm 2 on A to compute a layer of extremal eigenvalues and then to deflate the converged eigenvalues from the spectrum of A. The next run will attempt to approximate the extremal eigenvalues of the deflated matrix which is a layer of interior eigenvalues of A. The procedure should be repeated until the desired part of the spectrum is well approximated. We mention by the way that there is a growing research effort to compute interior eigenvalues from the so called harmonic Ritz values, see, e.g., [33, 34]. However, in the numerical experiments reported in study we limit ourselves to apply shift-invert whenever necessary.

The BiCOR-EIG procedure can be run iteratively by starting with a modified initial vector v_1 at each step. At the end of each iteration, a linear combination of the right Ritz vectors corresponding to the desired part of the spectrum, say the k eigenvalues satisfying a user-defined criterion, is selected as new up-to-date initial vector v_1. Components of v_1 in the direction of the unwanted eigenvalues are filtered by performing $m - k$ implicitly shifted QR steps on T_m (the unwanted eigenvalues are chosen as shifts), similarly to the IRA method. Then the procedure is restarted. The results of this computational step is to compress the original $m \times m$ factorization — Eq. (6) — into a $k \times k$ factorization of A.

4. NUMERICAL EXPERIMENTS

In this section, we illustrate the numerical behavior of the BiCOR-EIG algorithm applied to solving eigensystems arising from the discretization of Maxwell/Helmholtz-type operators in the analysis of waveguides. The waveguide problem arises in many different contexts in electromagnetics, see e.g., [8, 14, 23, 32, 38, 41] for some recent studies. The model problems are extracted from the testbed collection described in [1]; it was proposed with the primary purpose of testing numerical algorithms for solving difficult non-Hermitian eigenvalue problems in real applications. Experiments are carried out in MATLAB 7.7.0 on a PC equipped with an Intel(R) Core(TM)2 Duo CPU P8700 running at 2.53 GHz and with 4 GB of RAM.

The first test case arises in the analysis of dielectric channel waveguides. Finite difference discretization of the Helmholtz equations for the magnetic field H leads to a nonsymmetric generalized eigenvalue

problem of the form

$$
\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \begin{pmatrix} H_x \\ H_y \end{pmatrix} = \beta^2 \begin{pmatrix} B_{11} & \\ & B_{22} \end{pmatrix} \begin{pmatrix} H_x \\ H_y \end{pmatrix}
$$

where C_{11} and C_{22} are five- or tri-diagonal matrices, C_{12} and C_{21} are tridiagonal matrices, and B_{11} and B_{22} are nonsingular diagonal matrices. Since B is diagonal, the generalized eigenvalue problem is reduced to a standard eigenvalue problem $Ax = x\lambda$ where $A = B^{-1}C$. The computational task is to determine the right most eigenvalues and their corresponding eigenvectors. This eigensystem is reported to present a challenge to existing numerical methods [13, 21]. In our experiments we select two matrices, DWA512 and DW2048, of size respectively 512×512 and 2048×2048. On the matrix DWA512, an approximate invariant subspace of dimension $m = 100$ without full reorthogonalization enables us to compute 18 eigenvalues to a residual accuracy of 10^{-11}. In Figure 1, we see the pictorial convergence of the 6 right-most eigenvalues, and in Figure 2, the convergence of 10 eigenvalues on the opposite part of the spectrum. On our system, Algorithm 1 takes $0.3\,\mathrm{s}$ to generate the relevant approximate invariant space. For simple comparison, the MATLAB command eigs which interfaces the ARPACK routines implementing the IRA method computes the 6 right-most eigenvalues at approximately the same level of accuracy in $0.24\,\mathrm{s}$ and the 10 left-most eigenvalues in $0.3\,\mathrm{s}$. For $m = 200$, the computation takes $0.6\,\mathrm{s}$ and enables us to locate accurately 27 right-most eigenvalues (see Figure 3). More eigenvalues
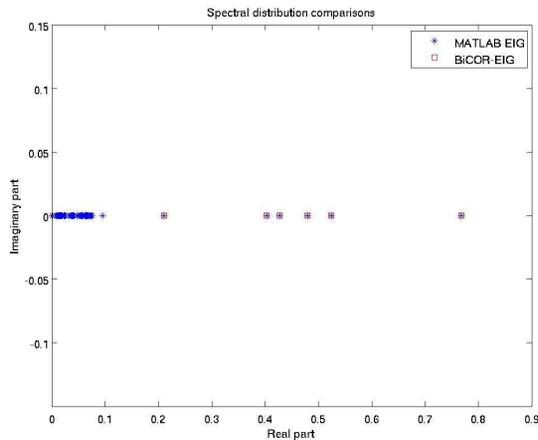

Figure 1. Experiments on the DWA512 problem using $m = 100$. The subset of the spectrum corresponds to the right-most eigenvalues.
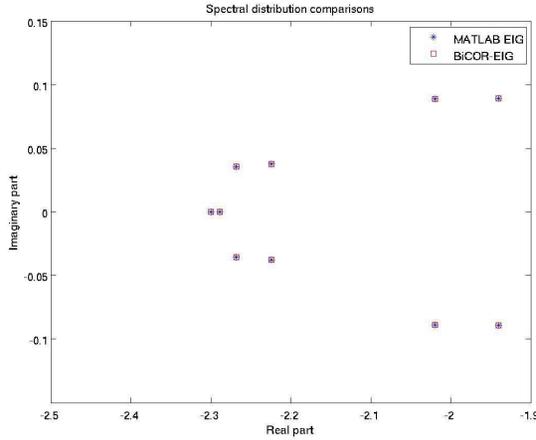
Figure 2. Experiments on the DWA512 problem using $m = 100$. The subset of the spectrum corresponds to the left-most eigenvalues.
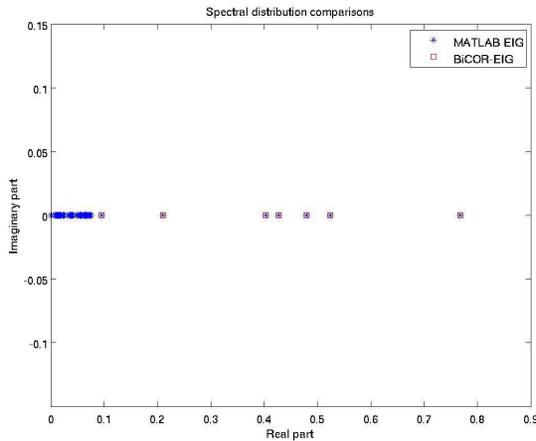

Figure 3. Experiments on the DWA512 problem using $m = 200$.

of T_m converge to the true eigenvalues of A when m is increased. The same trend is observed for larger problems as well, e.g., for the DW2048 matrix; with $m = 300$, 4 righ-most and 19 left-most eigenvalues are approximated to a tolerance of 10^{-10}. Also, more eigenvalues converge by using approximate invariant subspaces of larger dimension.

A different eigenvalue problem is derived from using the edge element method to model dispersive waveguide structures, e.g., for

solving the waveguide problem of conductors with finite conductivity and cross section in a lossy dielectric media. It is a complex symmetric eigensystem $Ax = \lambda Bx$ where both A and B are complex symmetric non-Hermitian and have the following block form

$$\begin{pmatrix} A_{11} & 0 \\ 0 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}.$$

The computational task is to find the eigenvalues with the smallest positive real parts. We select the matrix problem DWG961b of size 961×961 which has a subblock A_{11} of dimension 705×705 and is banded. On this problem, the BiCOR-EIG algorithm converges first to the eigenvalues with largest imaginary part which is an undesired part of the spectrum (see Figure 4). However, with shift-invert technique using $\theta = 0$ and $m = 100$ we are able to locate correctly the subset of the spectrum very close to 0 as shown in Figure 5. For simple comparison, the MATLAB command eigs does not compute the desired subset of the eigenvalues of A (those with largest real part located close to zero) after 300 iterations.

The third set of eigenvalue problems that we consider in this study is made kindly available by Prof. Rolf Schuhmann at University of Paderborn. It arises from three different discretizations of a hollow waveguide with a dielectric inset (quarter size of the cross section) with relative permittivity $\epsilon = 4$. The data matrix is nonsymmetric, with a mixture of real and complex eigenmodes [3]. We consider problem dimensions $n = 2764, 11524, 47044$, corresponding to grid sizes 50×30,
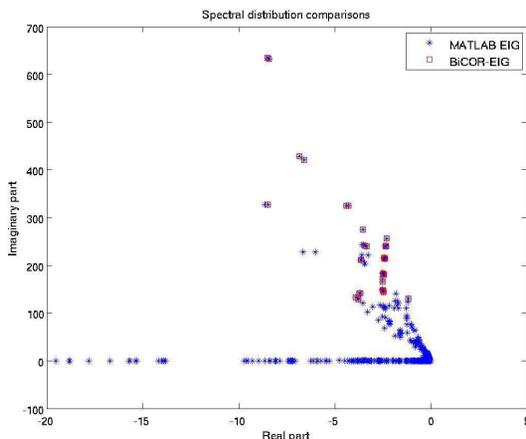

Figure 4. Experiments on the DWG961b problem using $m = 300$. The whole spectrum is shown.
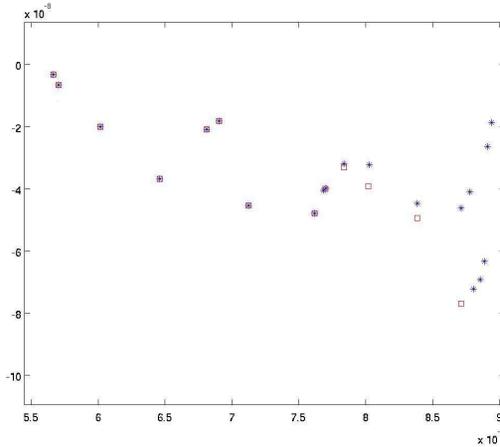
Figure 5. Experiments on the DWG961b problem using $m = 200$. The subset of the spectrum corresponds to eigenvalues with the smallest positive real parts.

100×60, and 200×120, respectively. The three matrices are named accordingly as $A2764$, $A11524$, $A47044$. The computational task is to compute the eigenvalues with smallest real part, which is negative. In Figures 6–8, we show the pictorial convergence that we observe for the three problems. On the $A2764$ problem, the Lanczos procedure using $m = 400$ approximates the two eigenvalues with smallest real part with twelve digits of accuracy, the third smallest eigenvalue with eleven digits, the fourth with ten significant places and the fifth with nine. For the largest matrices, we analyse the pictorial convergence for increasing dimension m of the search space. On the $A11524$ problem, using a projection space of size $m = 500$ the two eigenvalues with smallest real part computed by the Lanczos procedure stabilize at twelve digits of accuracy. The third smallest converges at nine digits, the fourth at seven and the fifth at five; increasing the size of the projection space, we may compute more eigenvalues. Finally, on the $A47044$ problem using $m = 1000$ the two eigenvalues with smallest real part stabilize at twelve significant places. The third smallest converges at eight places (only at four using $m = 500$), the fourth at five digits, and the fifth at four digits.

Finally, we illustrate an application to electromagnetics scattering, for solving dense complex non-Hermitian linear systems $Ax = b$ which arise from the Method of Moments discretization of the Maxwell's equations expressed in an integral formulation. For similar studies, see e.g., [11, 16, 17]. Denoting by M_1 the left preconditioner matrix,

we solve the preconditioned system $M_1 A x = M_1 b$ and we assume that the matrix $M_1 A$ is diagonalisable, that is $M_1 A = V \Lambda V^{-1}$, with $\Lambda = \mathrm{diag}(\lambda_i)$, where $|\lambda_1| \leq \ldots \leq |\lambda_n|$ are the eigenvalues and $V = (v_i)$ (resp. $U = (u_i)$) are the associated right (resp. left) eigenvectors. Let
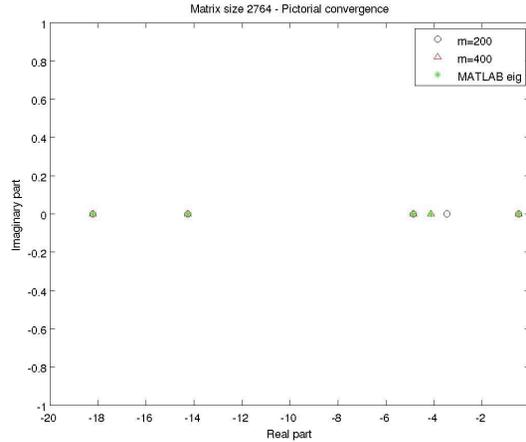

Figure 6. Pictorial convergence of the eigenvalues with smallest real part computed by the Lanczos procedure for different size of the projection space for problem A2764.
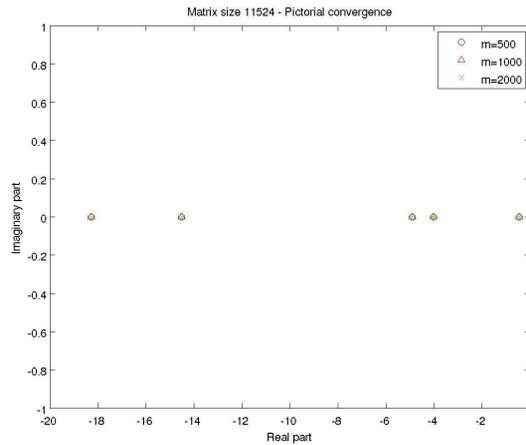

Figure 7. Pictorial convergence of the eigenvalues with smallest real part computed by the Lanczos procedure for different size of the projection space for problem A11524.
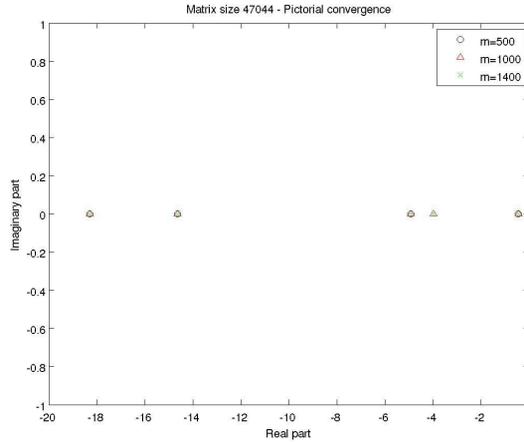
Figure 8. Pictorial convergence of the eigenvalues with smallest real part computed by the Lanczos procedure for different size of the projection space for problem A47044.

V_ε be the set of right eigenvectors associated with the set of eigenvalues λ_i with $|\lambda_i| \leq \varepsilon$ and U_ε the corresponding subset of left eigenvectors. The following result shows that it is possible to enhance the spectral distribution of the coefficient matrix by means of low-rank matrix updates for the preconditioner M_1. The preconditioning updates are made up of eigenvectors corresponding to the smallest eigenvalues of $M_1 A$. This in turn results in faster convergence of iterative Krylov methods.

Theorem 1   *Let*

$$A_c = U_\varepsilon^H M_1 A V_\varepsilon,$$

the projection of the matrix $M_1 A$ on the coarse space defined by the approximate eigenvectors associated with its smallest eigenvalues.

$$M_c = V_\varepsilon A_c^{-1} U_\varepsilon^H M_1$$

and

$$M = M_1 + M_c.$$

   Then MA is diagonalisable and we have $MA = V\mathrm{diag}(\eta_i)V^{-1}$ with

$$\begin{cases} \eta_i = \lambda_i & \text{if} \quad |\lambda_i| > \varepsilon, \\ \eta_i = 1 + \lambda_i & \text{if} \quad |\lambda_i| \leq \varepsilon. \end{cases}$$

For right preconditioning, that is $AM_1 y = b$, similar results hold.

Proof. The proof is presented in [6].

On a sphere illuminated at 190 MHz and discretized with $n = 2430$ grid points (approximately ten discretization points per wavelength), applying the spectral updates on top of the left preconditioned system $M_1 A y = b$, where M_1 is a sparse approximate inverse preconditioner, accelerates remarkably the iterative solution; GMRES(30) converges in 374 iterations without preconditioner, in 87 iterations with only M_1, in 66 iterations using 4 additional eigenvectors and 43 using 8 eigenvectors. From a numerical point of view we observe that the larger the coarse space, the better the preconditioner. Furthermore, the gain is larger if restarted GMRES is considered than if full GMRES is used as solver. In [4], the authors employ such techniques to solve the Almond test problem which is an official test case for the JINA 2002 Conference (12th Int. Workshop on Antenna design, Nice 2002) describing a realistic scattering application. The geometry has size 22 wavelengths and is illuminated at 2.6 GHz and discretized with 104793 points. Using 50 eigenvectors and a sparse approximate inverse as preconditioner M_1, GMRES(10) converges in 1867 iterations while no convergence is achieved in +3000 iterations only with M_1. The number of iterations of unrestarted GMRES decreases from 229 to 13; not only the number of iterations is significantly reduced but also the solution time, from 13 m to 6 m.

5. CONCLUDING REMARKS

We have presented a novel computational technique that is suitable to compute a subset of the spectrum of sparse and/or dense matrices arising from the discretization of Maxwell and Helmholtz-type operators. We determine eigenvalues from approximate invariant subspaces generated by a variant of the Lanczos method for non-Hermitian matrices called the Lanczos Biconjugate A-Orthonormalization procedure. The algorithm is cheap in memory because it is based on three-term vector recurrences, it enables to compute simultaneously both left and right eigenvectors and their corresponding eigenvalues, and does not require full orthogonalization which may be computationally expensive. Combined with polynomial filtering and shift-invert techniques, the method can approximate any subset of the spectrum of interest in applications. Reported experiments show the favourable convergence properties to the true eigenvalues of Maxwell/Helmholtz-type operators in practical applications. We believe that these results may contribute to highlight the potential and enrich the database of this technology. Perspectives of future research include exploring deflation techniques and deriving

convergence results for inexact inverse iterations applied to the BiCOR-EIG algorithm with shift-invert.

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