A CLASS OF SPECTRAL TWO-LEVEL PRECONDITIONERS∗

B. CARPENTIERI†, I. S. DUFF‡, AND L. GIRAUD†

Abstract. It is well known that the convergence of Krylov methods for solving the linear system often depends to a large extent on the eigenvalue distribution. In many cases, it is observed that “removing” the smallest eigenvalues can greatly improve the convergence. Several techniques have been proposed in the past few years that attempt to tackle this problem. The proposed approaches can be split into two main families depending on whether the scheme enlarges the generated Krylov space or adaptively updates the preconditioner. In this paper, we follow the second approach and propose a class of preconditioners both for unsymmetric and for symmetric linear systems that can also be adapted for symmetric positive definite problems. We effectively solve the preconditioned system exactly in the low dimensional space associated with the smallest eigenvalues and use this to update the preconditioned residual. This update results in shifting eigenvalues from close to the origin to near to one for the new preconditioner. This is ideal when there are only a few eigenvalues near the origin while all the others are close to one because the updated preconditioned system becomes close to the identity. We illustrate the performance of our method through extensive numerical experiments on a set of general linear systems. Finally, we show the advantages of the preconditioners for solving dense linear systems arising in electromagnetism applications, which were the main motivation for this work.

Key words. adaptive preconditioning techniques, two-level preconditioners, Krylov methods, spectral correction, low-rank correction, electromagnetic scattering applications

AMS subject classifications. 65F10, 65F50, 65F15, 65R20, 65N38

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1. Introduction. The starting point for this work was the iterative solution of linear systems that arise in electromagnetism applications. In the last few years we have studied preconditioning techniques based on sparse approximate inverses and have found them to be quite effective. These preconditioners are able to cluster most of the eigenvalues close to one but still leave a few close to the origin that are difficult to remove by tuning the parameter that controls our preconditioner [1, 5, 6, 7]. This is a fairly common situation for a wide range of problems and preconditioners. We address this in a more general context in this paper, even though we present some results for the electromagnetics application in a later section. In section 2, we describe our approach and the main contribution of this paper. On the assumption that the initial preconditioner has done a good job of clustering most eigenvalues near to one with relatively few outliers near the origin, we use an explicit eigensystem computation for these small eigenvalues to effectively solve the preconditioned system in this low dimensional space. This essentially gives a combined preconditioner resulting in a preconditioned system that is close to the identity. We now discuss some background to this before discussing our approach in full detail.

It is well known that the convergence of Krylov methods for solving the linear system $Ax = b$ depends to a large degree on the eigenvalue distribution; there are
exceptions as the right-hand side might also play an important role and, even with a
good eigenvalue distribution, the convergence can be poor [2, 15]. Additionally, quite
frequently there are small eigenvalues that adversely affect the convergence. In the
symmetric positive definite (SPD) case, this can be illustrated by the bound on the rate of convergence of the conjugate gradient (CG) method given by [14], namely

\[ ||e^{(k)}||_A \leq 2 \cdot \left( \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^k ||e^{(0)}||_A, \]

where \( e^{(n)} = x^n - x^{(n)} \) denotes the error associated with the iterate at step \( k \) and
\( \kappa(A) = \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} \) denotes the condition number. From this bound, it can be seen that
increasing the size of the smallest eigenvalues might improve the convergence rate of the CG. Consequently, if the smallest eigenvalues of \( A \) could be somehow “removed,”
the convergence of the CG might be improved [17, 19, 20, 25]. Similar arguments
exist for unsymmetric systems to mitigate the bad effect of the smallest eigenvalues
on the rate of convergence of the unsymmetric Krylov solver [3, 9, 11, 22]. The main
argument is that the Krylov methods build a polynomial expansion that should be
equal to one when the argument is zero and whose roots are the eigenvalues. To get fast
convergence it is necessary to find a low order polynomial with these properties (for
example, strategies have been developed to improve the convergence of GMRES [29]).
Clearly the presence of eigenvalues close to the origin makes this difficult.

For GMRES there are essentially two different approaches for exploiting information
related to the smallest eigenvalues. The first idea is to compute a few, say \( k \),
approximate eigenvectors of \( MA \) corresponding to the \( k \) smallest eigenvalues in mag-
nitude and augment the Krylov subspace with those directions. At each restart, let
\( u_1, u_2, \ldots, u_k \) be approximate eigenvectors corresponding to the approximate eigen-
values of \( MA \) closest to the origin. The updated solution of the linear system in the next
cycle of GMRES is extracted from \( \text{Span}\{r_0, Ar_0, A^2r_0, A^3r_0, \ldots, A^{m-k-1}r_0, u_1, u_2, \ldots, u_k\} \). This approach is referred to as the augmented subspace approach (see
[4, 22, 23, 24, 27]). The approximate eigenvectors can be chosen to be Ritz vectors
from the Arnoldi process. The standard implementation of the restarted GMRES
algorithm is based on the Arnoldi process, and spectral information of \( MA \) might be
recovered during the iterations. The second idea exploits spectral information
gathered during the Arnoldi process to determine an approximation of an invariant
subspace of \( A \) associated with the eigenvalues nearest the origin, and uses this infor-
mation to construct a preconditioner or to adapt an existing one. The idea of
using exact invariant subspaces to improve the eigenvalue distribution was proposed
in [26]. Information from the invariant subspace associated with the smallest eigen-
values and its orthogonal complement are used to construct an adaptive preconditioner
in the approach proposed in [3]. This information can be obtained from the Arnoldi
decomposition of a matrix \( A \) of size \( n \) that has the form

\[ AV_m = V_m H_m + f_m e_m^T, \]

where \( V_m \in R^{n \times m}, f_m \in R^n, V_m^T V_m = I_m, V_m^T f_m = 0, \) and \( H_m \in R^{m \times m} \) is an
upper Hessenberg matrix. If the Arnoldi process is started from \( V_m e_1 = r_0/\|r_0\|, \) the
columns of \( V_m \) span the Krylov subspace \( K_m(A, r_0) \). Let the matrix \( V_k \in R^{k \times n} \) consist of
the first \( k \) columns \( v_1, v_2, \ldots, v_k \) of \( V_m \), and let the columns of the orthogonal matrix
\( W_{n-k} \) span the orthogonal complement of \( \text{Span}\{v_1, v_2, \ldots, v_k\} \). As \( W_{n-k}^T W_{n-k} = I_{n-k} \), the columns of the matrix \( [V_k W_{n-k}] \) form an orthogonal basis of \( R^n \). In [3] the
inverse of the matrix

\[ M = V_k H_k V_k^T + W_{n-k} W_{n-k}^T \]

is used as a left preconditioner. It can be expressed as

\[ M^{-1} = V_k H_k^{-1} V_k^T + W_{n-k} W_{n-k}^T. \]

At each restart, the preconditioner is updated by extracting new eigenvalues which are the smallest in magnitude. The algorithm proposed uses the recursion formulae of the implicitly restarted Arnoldi (IRA) method described in [30], and the determination of the preconditioner does not require the evaluation of any matrix-vector products with the matrix \( A \) in addition to those needed for the Arnoldi process.

Another adaptive procedure to determine a preconditioner during GMRES iterations was introduced in [11]. It is based on the same idea of estimating the invariant subspace corresponding to the smallest eigenvalues. The preconditioner is based on a deflation technique such that the linear system is solved exactly in an invariant subspace of dimension \( r \) corresponding to the smallest \( r \) eigenvalues of \( A \).

Finally, a preconditioner for GMRES based on a sequence of rank-one updates that involve the left and right smallest eigenvectors is proposed in [16]. The method is based on the idea of translating isolated eigenvalues consecutively group by group into a vicinity of one using low-rank projections of the coefficient matrix of the form

\[ \tilde{A} = A \cdot (I_n + u_1 v_1^H) \cdots (I_n + u_l v_l^H). \]

The vectors \( u_j \) and \( v_j \), \( j \in [1, l] \) are determined to ensure the numerical stability of consecutive translations of groups of isolated eigenvalues of \( \tilde{A} \). After each restart of GMRES(m), approximations to the isolated eigenvalues to be translated are computed by the Arnoldi process. The isolated eigenvalues are translated towards one, and the next cycle of GMRES(m) is applied to the transformed matrix. The effectiveness of this method relies on the assumption that most of the eigenvalues of \( A \) are clustered close to one in the complex plane.

Most of these schemes are combined with the GMRES procedure as they derive information directly from its internal Arnoldi process. In our work, we consider an additional explicit eigencomputation that is used to update the selected preconditioner. This makes the preconditioner independent of the Krylov solver used for the actual solution of the linear system. This extra cost will be overcome if the same linear system with several right-hand sides has to be solved because the number of Krylov iterations can be significantly reduced. Such a situation exists, for instance, in some applications in electromagnetism and is further discussed in section 4.

The paper is organized as follows. In the following section, we describe the proposed preconditioners and prove their shifting capabilities on diagonalizable matrices. In section 3, we illustrate the numerical efficiency of the proposed scheme on a set of unsymmetric and SPD linear systems from the Harwell-Boeing collection [10]. We devote section 4 to a particular application in electromagnetism where the same linear system has to be solved with many different right-hand sides. This situation is particularly of interest for the preconditioners we propose, as it enables us to amortize the extra eigencomputation required as it is illustrated in that section. Finally, we conclude with some remarks in section 5.
2. Two-level preconditioner via low-rank update. Many of the preconditioners proposed in the literature succeed in clustering most of the eigenvalues of the preconditioned matrix $MA$ (for left preconditioning) far from the origin. Such a distribution is highly desirable to get fast convergence of Krylov solvers. However, a few eigenvalues can be left close to zero and they potentially can significantly degrade the convergence. In order to tackle this difficulty we propose a refinement technique based on the introduction of low-rank corrections computed from spectral information associated with the smallest eigenvalues of $MA$. Roughly speaking, the proposed technique consists of solving exactly the preconditioned system in the low dimensional space spanned by the eigenvectors associated with the eigenvalues closest to the origin. This is then used to update the preconditioned residual. We first present our technique for unsymmetric linear systems and then derive a variant for symmetric and SPD matrices. For simplicity, we first consider complex linear systems. We later indicate how it can be adapted for problems in real arithmetic.

We consider the solution of the linear system

\[ Ax = b, \]

where $A$ is an $n \times n$ unsymmetric complex nonsingular matrix, and $x$ and $b$ are vectors of size $n$. The linear system is solved using a preconditioned Krylov solver, and we denote by $M_1$ the left preconditioner, meaning that we solve

\[ M_1Ax = M_1b. \]

We assume that the preconditioned matrix $M_1A$ is diagonalizable, that is,

\[ M_1A = V\Lambda V^{-1}, \]

with $\Lambda = \text{diag}(\lambda_i)$, where $|\lambda_1| \leq \cdots \leq |\lambda_n|$ are the eigenvalues and $V = (v_i)$ the associated right eigenvectors. We denote by $U = (u_i)$ the associated left eigenvectors; we then have $U^H V = \text{diag}(u_i^H v_i)$, with $u_i^H v_i \neq 0$ for all $i$ [33]. Let $V_\varepsilon$ be the set of right eigenvectors associated with the set of eigenvalues $\lambda_i$ with $|\lambda_i| \leq \varepsilon$. Similarly, we define by $U_\varepsilon$ the corresponding subset of left eigenvectors.

**Proposition 1.** Let $A_c = U_\varepsilon^H M_1 A V_\varepsilon$, $M_c = V_\varepsilon A_c^{-1} U_\varepsilon^H M_1$, and $M = M_1 + M_c$.

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

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

**Proof.** We first remark that $A_c = \text{diag}(\lambda_i u_i^H v_i)$ with $|\lambda_i| \leq \varepsilon$, and so $A_c$ is nonsingular. $A_c$ represents the projection of the matrix $M_1A$ on the space spanned by the approximate eigenvectors associated with its smallest eigenvalues.

Let $V = (V_\varepsilon, V_{\bar{\varepsilon}})$, where $V_{\bar{\varepsilon}}$ is the set of $(n-k)$ right eigenvectors associated with eigenvalues $|\lambda_i| > \varepsilon$.

Let $D_\varepsilon = \text{diag}(\bar{\lambda}_i)$ with $|\bar{\lambda}_i| \leq \varepsilon$ and $D_{\bar{\varepsilon}} = \text{diag}(\lambda_i)$ with $|\lambda_i| > \varepsilon$.

The following relations hold: $MAV_\varepsilon = V_\varepsilon(D_\varepsilon + I_k)$, where $I_k$ denotes the $(k \times k)$ identity matrix, and $MAV_{\bar{\varepsilon}} = V_{\bar{\varepsilon}}D_{\bar{\varepsilon}}$ since $U_\varepsilon^H V_{\bar{\varepsilon}} = 0$; then we have

\[ MAV = V \begin{pmatrix} D_\varepsilon + I_k & 0 \\ 0 & D_{\bar{\varepsilon}} \end{pmatrix}. \]
Proposition 2. Let $W$ be such that $\tilde{A}_c = W^H AV_\epsilon$ has full rank, $\tilde{M}_c = V_\epsilon \tilde{A}_c^{-1} W^H$, and $\tilde{M} = M_1 + \tilde{M}_c$. Then $\tilde{M}A$ is similar to a matrix whose eigenvalues are
\[
\begin{align*}
\eta_i &= \lambda_i & \text{if } |\lambda_i| > \epsilon, \\
\eta_i &= 1 + \lambda_i & \text{if } |\lambda_i| \leq \epsilon.
\end{align*}
\]

Proof. With the same notation as for Proposition 1 we have $\tilde{M}AV_\epsilon = V_\epsilon(D_\epsilon + I_k)$ and $\tilde{M}AV_\epsilon = V_\epsilon D_\epsilon + V_\epsilon C$ with $C = A_c^{-1}W^HAV_\epsilon$; then we have
\[
\tilde{M}AV = V \begin{pmatrix} D_\epsilon + I_k & C \\
0 & D_\epsilon \end{pmatrix}.
\]

For right preconditioning, that is, $AM_1y = b$, similar results hold.

Proposition 3. Let $A_c = U_c^H AM_1 V_\epsilon$, $M_c = M_1 V_\epsilon A_c^{-1} U_c^H$, and $M = M_1 + M_c$. Then $AM$ is diagonalizable and we have $AM = V \text{diag}(\eta_i)V^{-1}$ with
\[
\begin{align*}
\eta_i &= \lambda_i & \text{if } |\lambda_i| > \epsilon, \\
\eta_i &= 1 + \lambda_i & \text{if } |\lambda_i| \leq \epsilon.
\end{align*}
\]

Proposition 4. Let $W$ be such that $\tilde{A}_c = W^H AM_1 V_\epsilon$ has full rank, $\tilde{M}_c = M_1 V_\epsilon \tilde{A}_c^{-1} W^H$, and $\tilde{M} = M_1 + \tilde{M}_c$. Then $AM$ is similar to a matrix whose eigenvalues are
\[
\begin{align*}
\eta_i &= \lambda_i & \text{if } |\lambda_i| > \epsilon, \\
\eta_i &= 1 + \lambda_i & \text{if } |\lambda_i| \leq \epsilon.
\end{align*}
\]

We should point out that, if the symmetry of the preconditioner has to be preserved, an obvious choice exists. For left preconditioning, we can set $W = V_\epsilon$, but then $A_c$ may not have full rank. In the SPD case, these results extend as follows and lead to an expression that is similar to those proposed in [8, 12] for two-level preconditioners in domain decomposition.

Proposition 5. If $A$ and $M_1$ are SPD, then $M_1A$ is diagonalizable and $\tilde{A}_c = V_\epsilon^TAV_\epsilon$ is SPD. The preconditioner defined by $M = M_1 + \tilde{M}_c$, with $M_c = V_\epsilon \tilde{A}_c^{-1} V_\epsilon^T$, is SPD and $MA$ is similar to a matrix whose eigenvalues are
\[
\begin{align*}
\eta_i &= \lambda_i & \text{if } |\lambda_i| > \epsilon, \\
\eta_i &= 1 + \lambda_i & \text{if } |\lambda_i| \leq \epsilon.
\end{align*}
\]

Proof. Because the matrix $M_1$ is SPD, there exists a unique SPD matrix $M_1^{1/2}$ that is the square root of $M_1$ (see, for instance, [14]). Then the matrix $M_1A$ is similar to the matrix $M_1^{1/2}AM_1^{1/2}$ which is symmetric and consequently similar to a diagonal matrix. Therefore the matrix $M_1A$ is diagonalizable.

By construction $\tilde{A}_c$ is symmetric; let us show that it is positive definite. $V_\epsilon$ is an $n \times k$ matrix. Let $z \in \mathbb{R}^k$, $z \neq 0$.
\[
\begin{align*}
z^T \tilde{A}_c z &= z^T V_\epsilon^T AV_\epsilon z \\
&= (V_\epsilon z)^T AV_\epsilon z \\
&= ||V_\epsilon z||_A^2.
\end{align*}
\]

$V_\epsilon z \neq 0$ because $V_\epsilon$ has full rank. Then $z^T \tilde{A}_c z$ is greater than 0 because $A$ is SPD. Therefore $\tilde{A}_c$ is a SPD matrix and consequently has full rank.
Let \( x \in \mathbb{R}^n \), \( x \neq 0 \).

\[
x^T \tilde{M}_c x = x^T V_c \tilde{A}_c^{-1} V_c^T x
= (V_c^T x)^T \tilde{A}_c^{-1} V_c^T x
= ||V_c^T x||_{\tilde{A}_c^{-1}} \geq 0 \]  

as \( \tilde{A}_c \) is a SPD matrix.

Therefore \( \tilde{M}_c \) is a positive semidefinite matrix and \( \tilde{M} = M_1 + \tilde{M}_c \) is an SPD matrix because \( M_1 \) is SPD, and the results of Proposition 2 hold with \( W = V_c \).

For unsymmetric linear systems in real arithmetic some of the eigenvectors can be complex. If implemented as described so far, the preconditioner would be complex, which is not desirable because all the calculations would have to be performed in complex arithmetic. If a complex eigenvector exists, its conjugate is also an eigenvector. The drawback just described can be overcome by considering not just the eigenvectors but a real basis of the plane spanned by those two conjugate eigenvectors which are the two real vectors defined by the real part and the imaginary part of those vectors.

Finally, we mention that we can use an additional scaling in the low-rank update so that the \( k \) smallest eigenvalues are not just shifted by one, but rather are all transformed to one, with multiplicity equal to \( k \). This feature is obtained by using:

\[
M_c = V_c (I - D_c) \tilde{A}_c^{-1} U_c^H M_1 \quad \text{in Proposition 1}
\]

and:

\[
M_c = V_c (I - D_c) \tilde{A}_c^{-1} W U_c^H \quad \text{in Proposition 2}.
\]

Similar transformations can be applied to get the same property for right preconditioning. In addition, we mention that these later formulations enable us to move to one any set of eigenvalues lying in any particular region of the spectrum; if for some particular applications some eigenvalues different from the smallest ones perturb the convergence, they can be removed using the same technique. In our numerical experiments we focus on removing only the effect of the smallest eigenvalues. In that case, we observe that the use of these formulations does not affect the numerical behavior of the method from that of the simpler formulations. Because it makes the expression of the preconditioner slightly more complicated, we do not develop this variant further.

3. Numerical experiments. In order to illustrate the efficiency of the preconditioners, we first present numerical experiments on general linear systems that are either unsymmetric or symmetric indefinite. Then we consider SPD linear systems to assess the effectiveness of the preconditioners on those problems as well. For all the numerical experiments reported in this section, the preconditioner \( M_1 \) is constructed using incomplete factorizations; these are \( ILU(t) \) [28], incomplete \( LU \) factorization using \( t \) as the threshold in the dropping strategy for nonsymmetric matrices, and \( IC(t) \), incomplete Cholesky factorization [21] with \( t \) as the threshold, for SPD matrices. All the experiments have been performed in Matlab using left preconditioners. Because we compare different (left) preconditioners we choose as stopping criterion the reduction of the normalized unpreconditioned residual by \( 10^{-6} \), so that the stopping criterion is independent of the preconditioner. Even though this quantity might be a by-product of the Krylov solver we explicitly compute the true unpreconditioned residual at each iteration. The initial guess is the zero vector. In all the tables, the symbol “-” means that convergence is not obtained after 1000 iterations. The eigenvectors are computed using the Matlab function \( \text{eigs} \) that calls ARPACK [18].

We note that, in section 4, we also provide numerical experiments conducted using a Fortran implementation of the preconditioner. We then illustrate, on one example coming from an application in electromagnetism, that the extra cost due to the eigendecomputation can be quickly overcome if a few linear systems have to be solved with different right-hand sides.
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3.1. Non-Hermitian linear systems. In Table 1 we display the list of test problems from the Harwell-Boeing collection that we have considered for the experiments on general matrices.

In Table 2, we show the number of iterations required by restarted GMRES and BiCGStab [32] varying the dimension of the low-rank correction in the range 1 to 10. The choice of the threshold for ILU has been set to illustrate the behavior generally observed when the spectrum of the preconditioned system has only a few eigenvalues close to the origin, that is, when the preconditioner is already effective.
Table 3

Number of iterations varying the dimension of the low-rank update with $W = V_\epsilon$.

<table>
<thead>
<tr>
<th>Matrix</th>
<th>$t$</th>
<th>Solver</th>
<th>Dimension of the small dimensional correction space</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOR131</td>
<td>$4 \cdot 10^{-2}$</td>
<td>GMRES(5)</td>
<td>51 36 33 34 30 31 25 26 27 24 25</td>
</tr>
<tr>
<td></td>
<td></td>
<td>BiCGStab</td>
<td>19 14 13 13 11 10 9 9 9 9 9</td>
</tr>
<tr>
<td>ORSIRR1</td>
<td>$5 \cdot 10^{-2}$</td>
<td>GMRES(30)</td>
<td>50 49 44 40 37 35 34 30 29 27 27</td>
</tr>
<tr>
<td></td>
<td></td>
<td>BiCGStab</td>
<td>28 28 24 24 21 22 20 18 18 17 16</td>
</tr>
<tr>
<td>GRR1107</td>
<td>$1 \cdot 10^{-2}$</td>
<td>GMRES(40)</td>
<td>- 80 40 36 35 33 32 28 28 26 26</td>
</tr>
<tr>
<td></td>
<td></td>
<td>BiCGStab</td>
<td>100 79 87 74 84 82 56 47 65 67 40</td>
</tr>
<tr>
<td>YOUNG2C</td>
<td>$7 \cdot 10^{-2}$</td>
<td>GMRES(30)</td>
<td>- 292 257 261 193 173 173 169 165 168 166</td>
</tr>
<tr>
<td></td>
<td></td>
<td>BiCGStab</td>
<td>76 59 55 52 46 44 40 45 47 48 48</td>
</tr>
</tbody>
</table>

Fig. 2. Convergence history varying the dimension of the low-rank correction for GRE1107 and $ILU(1 \cdot 10^{-2})$.

in clustering most of the eigenvalues. In Figure 1, we display the spectrum of the preconditioned matrices using only $ILU(t)$. For the experiments shown in Table 2, we use the formulation described in Proposition 1, that is, $W^H = U_1^HM_1$. Similar results are displayed in Table 3 using the formulation described in Proposition 2, that is, with $W = V_\epsilon$. In this latter case, the cost for the eigencomputation to set up the update is halved because only right eigenvectors need to be computed. As expected, it can be seen that, for these two choices of $W^H$, the numerical trends are the same; that is, the larger the rank of the correction the faster the convergence. However, the decrease is not always monotonic with the dimension of the rank correction. This behavior is observed both for GMRES and BiCGStab.

As can be seen, a correction of rank-ten enables us to half the number of iterations in most of the cases. In general, a very small dimension correction (i.e., one or two) improves the convergence of the Krylov solver significantly. In some cases, it even enables convergence that was otherwise not obtained. This situation is illustrated in Figure 2 where we display the convergence history of GMRES(30) on the Grenoble test problem, GRE1107. Without correction the residual stagnates (as well as with a correction of dimension one or two) and the convergence is obtained only for a correction of dimension larger than three. Even though this aspect is discussed later, we can already observe the link that exists between the dimension of the update and the size of the restart of GMRES since GMRES(40) converges with a rank-one update (see Table 2) while GMRES(30) does not (see Figure 2). This linear system has very small eigenvalues that are fairly isolated and cannot be captured with a small restart. Once the smallest is removed by the preconditioner, GMRES(40) succeeds in capturing the next one and then converges, while GMRES(30) still does not. This
latter converges only once the three smallest are removed by the preconditioner.

To illustrate that the proposed updates should be used to improve an already effective preconditioner, we report in Table 4 the number of iterations when the threshold of \( ILU(t) \) is relaxed making the original preconditioner less and less efficient. We see that, in that case, the update significantly improves the convergence up to a certain level above which it has less effect or no more effect at all. That corresponds to the situation where there are many eigenvalues close to zero and shifting a few of them does not further affect the convergence. In particular, using the low-rank correction on the unpreconditioned system, that is, only shifting few among many small eigenvalues, does not enable the solver to converge.

As shown by the numerical experiments, removing the effect of small eigenvalues in the preconditioned matrix can have a beneficial effect on the convergence. This observed behavior has a nice consequence for restarted GMRES. That is, if the small eigenvalues are removed, the restart value for GMRES might no longer be critical and the convergence should not be affected much by the choice of the restart parameter. A similar observation is also reported in the framework of deflated GMRES in [24]. We can see this in Figure 3 where we show, for different choices of the restart parameter, the number of GMRES iterations as a function of the dimension of the low-rank correction. It can be seen that the number of iterations with all the restarts tend to behave as full-GMRES as the dimension of the update increases.

### 3.2. SPD linear systems.

In this section we illustrate, on the set of SPD matrices listed in Table 5, the SPD variant of the update presented in Proposition 5, where \( M_1 \) is \( IC(t) \).
We observe a similar improvement for SPD linear systems to what was seen in the previous section. This is illustrated in Table 6, where we show the number of CG iterations as we vary the dimension of the positive semidefinite update. A significant reduction in the iteration counts can be observed with a moderate dimension of the low-rank update.

### 3.3. Sensitivity to the accuracy of the eigencomputation.

As mentioned earlier, the eigenvalue calculation is performed in a preprocessing phase using ARPACK on the preconditioned matrix. When a set of isolated eigenvalues close to zero are computed, the backward error associated with the smallest ones is always the best. Even if we relax the stopping criterion, the smallest are still well computed. In order to investigate the sensitivity of the eigencomputation accuracy on the low-rank update improvement we would like to have a similar backward error on each eigenpair and to vary it. To do this, we compute the eigenpairs of a slightly perturbed matrix, \( (M_1A + E) \), with \( \frac{||E||}{||M_1A||} = \eta \), and we use these eigenvectors to build our preconditioners and compute the backward error of these eigenvectors as if they were eigenvectors of \( M_1A \). By varying \( \eta \), we can monitor the level of the backward error associated with each eigenvalue that then becomes comparable for each eigenvector.

In Table 7, we give the number of iterations of the Krylov solvers when varying the backward error of the computed eigenvectors. As we have one backward error per eigenvector, we give the average of them in the table. It can be seen that, in general, there is no need for very high accuracy in the computation of the eigenvectors. However, if some of the eigenvectors are ill-conditioned, even a small backward error might imply a large forward error and lead us to make a correction in the wrong space. Such a behavior can be observed on the GRE1107 matrix.

### 4. A case study in electromagnetism applications.

In recent years, there has been a significant amount of work on the simulation of electromagnetic wave propagation phenomena, addressing various topics ranging from radar cross section to electromagnetic compatibility, to absorbing materials, and to antenna design. To address these problems the Maxwell equations are often solved in the frequency domain leading to singular integral equations of the first kind. The discretization by the boundary element method results in linear systems with dense complex matrices that are challenging to solve. The solution of these linear systems using iterative Krylov methods has recently become feasible thanks to a combination of the fast multipole
Table 7

<table>
<thead>
<tr>
<th>Backward error</th>
<th>Dimension of the small dimensional correction space</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
</tr>
<tr>
<td>( \approx 1 \times 10^{-15} )</td>
<td>(-)</td>
</tr>
<tr>
<td>( \approx 1 \times 10^{-10} )</td>
<td>(-)</td>
</tr>
<tr>
<td>( \approx 2 \times 10^{-8} )</td>
<td>(-)</td>
</tr>
<tr>
<td>( \approx 1 \times 10^{-4} )</td>
<td>(-)</td>
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</tbody>
</table>

<table>
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<tr>
<th>Backward error</th>
<th>Dimension of the small dimensional correction space</th>
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</thead>
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<td>86</td>
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<tr>
<td>( \approx 3 \times 10^{-10} )</td>
<td>86</td>
</tr>
<tr>
<td>( \approx 5 \times 10^{-6} )</td>
<td>86</td>
</tr>
<tr>
<td>( \approx 2 \times 10^{-3} )</td>
<td>86</td>
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<td>( \approx 5 \times 10^{-4} )</td>
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<th>Dimension of the small dimensional correction space</th>
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<td>( \approx 2 \times 10^{-4} )</td>
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<tr>
<td>( \approx 1 \times 10^{-3} )</td>
<td>78</td>
</tr>
<tr>
<td>( \approx 2 \times 10^{-3} )</td>
<td>78</td>
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</table>

Fig. 4. Eigenvalue distribution for the coefficient matrix preconditioned by the Frobenius-norm minimization method on the satellite problem.

The Frobenius-norm minimization preconditioner succeeds in clustering most of the eigenvalues far from the origin. This can be observed in Figure 4, where we see a big cluster near one in the spectrum of the preconditioned matrix. This matrix is associated with a satellite that is particularly challenging to solve. The corresponding mesh, discretized with 1701 degrees of freedom, is displayed in Figure 5.
The construction of the Frobenius-norm minimization preconditioner is inherently local. Each degree of freedom in the approximate inverse is coupled to only a very few neighbors, and this compact support does not allow an exchange of global information. When the exact inverse is globally coupled, the lack of global information may have a severe impact on the quality of the preconditioner. Although the discrete Green’s function in electromagnetic applications exhibits a rapid decay, the exact inverse is dense and thus has global support. In that context, the use of the two-level spectral preconditioners seems appropriate. In addition, in such electromagnetism applications the same linear system has to be solved with many right-hand sides when lighting an object with the same wave frequency but different incident angles. Depending on the object and the simulation, the number of right-hand sides can vary from a few to a few thousand. This situation is particularly suitable as the eigencomputation required to set up the correction can be compensated by the saving in iteration counts over the multiple right-hand sides.

All the numerical experiments are performed using a Fortran implementation in double precision complex arithmetic on a SGI Origin 2000. In these experiments, we consider low-rank updates of dimension up to 20, different Krylov solvers, and we use left preconditioning. For this test problem, we perform experiments with two levels of accuracy in the GMRES solution to gain more insight into the robustness of our method. In that section, we show the qualitative numerical behavior of our method on one test example that is representative of the general trend in electromagnetic applications [5]. In Figure 6, we show the number of iterations required by GMRES(10) to reduce the normwise backward error to $10^{-8}$ and $10^{-5}$ for increasing dimension of the update. The numerical results show that the introduction of the low-rank updates can remarkably enhance the robustness of the approximate inverse. The plateau in Figure 6 that can be observed before a significant jump corresponds to a cluster of eigenvalues. When the eigenvalues within the cluster are shifted, a quick speedup of convergence is observed. By selecting up to 10 eigenpairs the number of iterations decreases by more than a factor of two on most of the experiments reported. The gain is more relevant in absolute value when high accuracy is required for the approximate solution but remains almost constant in relative gain. As already observed on the other examples in the previous section, the preconditioning updates enable fast convergence of GMRES with a low restart within a tolerance of $10^{-8}$, whereas no convergence was obtained in 1500 iterations without updates. However, a substantial
improvement in the convergence is observed also when low accuracy is required. In the most effective case, by selecting 10 corrections, the number of GMRES iterations needed to achieve convergence of $10^{-5}$ using low restarts reduces by more than a factor of two. If more eigenvectors are selected, generally no substantial improvement is observed.

Similarly to experiments reported in section 3.1, we show, in Table 8, the number of iterations with two different choices for $W$. As expected, and already observed, with these two choices of $W^H$ the numerical trends are the same; that is, the larger the rank of the correction the faster the convergence.

In Table 9, we show the number of matrix-vector products required by the ARPACK implementation of the IRA method to compute the smallest approximate eigenvalues and the associated approximate right eigenvectors (note that we do not need the invert mode). We remark that the matrix-vector products do not include those required for the iterative solution. Although the computation can be expensive, the cost can be amortized if the preconditioner is reused to solve linear systems with the same coefficient matrix and several right-hand sides. In the third column of this table we show the number of amortization vectors relative to GMRES(10) and a tolerance of $10^{-5}$, that is, the number of right-hand sides that have to be considered to amortize the extra cost for the eigencomputation. The localization of a few eigenvalues within a cluster may be more expensive than the computation of a full group of small eigenvalues. It can be seen that, for that example, the number of amortization vectors is reasonably small, especially compared to real electromagnetic calculations where linear systems with the same coefficient matrix and up to thousands of right-hand sides are often solved.

In Figure 7 we display the number of iterations of SQMR [13] (QMR version for symmetric matrices with symmetric preconditioner). These experiments show that convergence of SQMR also benefits from the low-rank update. We also notice the remarkable robustness of this Krylov solver on electromagnetic applications; it clearly outperforms GMRES with large restart.

5. Concluding remarks. In this work, we consider a low-rank correction scheme that is particularly suited to improve a given preconditioner that leaves only few eigen-
Table 8

Number of iterations required by GMRES(10) preconditioned by a Frobenius-norm minimization method updated with spectral corrections to reduce the normwise backward error by $10^{-8}$ for increasing number of corrections on the satellite. Different choices are considered for the operator $W^H$.

<table>
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<tr>
<th>Dimension of low-rank update</th>
<th>Choice for the operator $W^H$</th>
<th>$W^H = U_M^H M_1$</th>
<th>$W = V_\epsilon$</th>
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<td>260</td>
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<td>20</td>
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Table 9

Number of matrix-vector products required by ARPACK to compute approximate eigenvalues nearest 0 and the corresponding right eigenvectors.

<table>
<thead>
<tr>
<th>Dimension of low-rank update</th>
<th># ARPACK Mat-vec</th>
<th># Amortization rhs</th>
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<tbody>
<tr>
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<td>-</td>
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<tr>
<td>2</td>
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</tr>
<tr>
<td>20</td>
<td>300</td>
<td>4</td>
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</table>
values close to zero. The update of the preconditioner is beneficial to many Krylov solvers but requires an a priori eigencomputation that might be performed without too high an accuracy. Because the technique is used in combination with a first preconditioner that already succeeds in clustering most of the eigenvalues close to one leaving only few isolated eigenvalues close to the origin, ARPACK in forward mode is an efficient approach to compute the associated eigenvectors. In that context, another advantage is that ARPACK computes with a better accuracy than the smallest eigenpairs. These are the most important to compute accurately as they often play an important role in the convergence of the Krylov solvers. This extra calculation can be amortized if several linear systems with the same coefficient matrix but different right-hand sides have to be solved. We indicate that, on real life problems arising in electromagnetism applications, this extra cost can be fairly quickly overcome. As an empiric criterion for the selection of the dimension of the low-rank correction we can indicate that removing all the eigenvalues that are small and isolated (sometimes in a small cluster) is an effective approach. For instance, in the electromagnetic application, removing the few eigenvalues of magnitude less than $10^{-3}$ was enough to speed up the convergence on all our test examples [5]. Finally, when the Krylov solver is GMRES, we suggest that the techniques described in [3] can be applied. This consists of recovering the eigenvectors from the Arnoldi process embedded in the GMRES iterations and then updating the preconditioner at each GMRES restart.

Acknowledgments. We would like to thank Serge Gratton for his fruitful and stimulating discussions during the development of this work as well as the anonymous referees for their constructive comments.

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