# A two-level iterative scheme for general sparse linear systems based on approximate skew-symmetrizers* 

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#### Abstract

We propose a two-level iterative scheme for solving general sparse linear systems. The proposed scheme consists of a sparse preconditioner that increases the skew-symmetric part and makes the main diagonal of the coefficient matrix as close to the identity as possible. The preconditioed system is then solved via a particular Minimal Residual Method for Shifted Skew-Symmetric Systems (mrs). This leads to a two-level (inner and outer) iterative scheme where the mrs has short term recurrences and satisfies an optimally condition. A preconditioner for the inner system is designed via a skew-symmetry preserving deflation strategy based on the skew-Lanczos process. We demonstrate the robustness of the proposed scheme on sparse matrices from various applications.


Key words. symmetrizer, skew-symmetrizer, Krylov subspace method, shifted skewsymmetric system, skew-Lanczos method

AMS subject classifications. 65F08, 65F10, 65F50

## 1 Introduction

We discuss the numerical solution of general linear systems

$$
\begin{equation*}
A x=b, \tag{1}
\end{equation*}
$$

where $A \in \mathbb{R}^{n \times n}$ is a general large sparse invertible matrix. If the coefficient matrix is symmetric and positive definite or symmetric and indefinite, one can use the Conjugate Gradient algorithm or the recently proposed two-level iterative scheme [22], respectively. In this paper, we propose a new robust two-level black-box scheme for solving general systems without any assumption on the symmetry or definiteness of the coefficient matrix. In contrast to most other iterative methods, where preconditioning is often used to symmetrize the system and to lower the condition number, our new approach consists of an initial step which

[^0]makes the system close to an identity plus skew-symmetric matrix that leads to an effective shifted skew-symmetric preconditioner. Both the preconditioned system and the application of the preconditioner is approached by an iterative method so that the method is a two-level (inner-outer) iterative scheme.

Our main motivation to study identity-plus-skew-symmetric preconditioners are linear systems arising in the time-discretization of dissipative Hamiltonian differential equations of the form

$$
\begin{equation*}
E \dot{z}=(J-R) z+f(t), z\left(t_{0}\right)=z_{0} \tag{2}
\end{equation*}
$$

where $\dot{z}$ denotes the derivative with respect to time, $J$ is a skew-symmetric matrix, $R$ is symmetric positive semi-definite and $E$ is the symmetric positive semi-definite Hessian of a quadratic energy functional (Hamiltonian) $\mathcal{H}(z)=\frac{1}{2} z^{T} E z$, see e.g. [2, 10, 14, 19, 25, 28, for such systems in different physical domains and applications. If one discretizes such systems in time, e.g. with the implicit Euler method, and setting $z_{k}=z\left(t_{k}\right)$ then in each time step $t_{k}$ one has to solve a linear system of the form

$$
\begin{equation*}
(E-h(J-R)) z_{k+1}=E z_{k}+h f\left(t_{k}\right) \tag{3}
\end{equation*}
$$

Similar linear systems arise also when other discretization schemes are used.
The matrix $A=E+h(R-J)$ has a positive (semi)-definite symmetric part $M=E+h R$. If $M$ is positive definite, then with a two sided preconditioning with the Cholesky factor $L$ of $M=L L^{T}$, the matrix $L^{-1} A L^{-T}$ has the form $I+\tilde{J}$, where $\tilde{J}=h L^{-1} A L^{-T}$ is skewsymmetric [5, 31]. For such systems in [5, 18, 21, 26, 31] structure exploiting Krylov subspace methods with three term recurrences were derived and analyzed. Given a general square matrix $A$, symmetrizers from right or left, respectively, are symmetric matrices, $S_{r}$ and $S_{l}$, such that $A S_{r}=S_{r}^{T} A^{T}$ and $S_{l} A=A^{T} S_{l}^{T}$. Existing algorithms to construct dense and exact symmetrizers are studied and summarized in [8]. In this paper, however, we construct twosided preconditioners so that the preconditioned systems has the form $D+\hat{J}$, where $D$ is diagonal and close to the identity and $\hat{J}$ is close to a skew-symmetric matrix (approximate shifted skew-symmetrizers (ASSS)). To this preconditioned system we then apply a two-level iterative method, where the inner iteration is a skew-symmetric Krylov subspace method. We assume that both $A$ and $S \in\left\{S_{r}, S_{l}\right\}$ are sparse and nonsymmetric, with $S$ having a user defined sparsity structure. The sparse ASSS preconditioner is obtained by first applying a nonsymmetric permutation and scaling and then solving a sparse overdetermined linear least squares (LLS) problem to obtain $S$. Similar approaches for dense symmetrizers, [8], or algorithms for improving the structural symmetry in the context of sparse direct solvers, as proposed in [23, 27], do not have the latter property.

We note that while it is possible to obtain and use either $S_{r}$ and $S_{l}$, in our experience the numerical results did not differ much as in left and right preconditioning. Therefore, in the rest of the paper we use the right variant and hereafter $S$ refers to $S_{r}$.

The paper is organized as follows. The proposed sparse approximate skew-symmetrizer is introduced in Section 2, a two-level Kyrlov subspace method based on the skew-symmetrizer is introduced in Section 3, numerical results are presented in Section 4, and the conclusions follow in Section 5 .

## 2 A sparse approximate shifted skew-symmetrizing preconditioner

Given a sparse invertible matrix $A \in \mathbb{R}^{n \times n}$, to achieve our goal of constructing a sparse approximate shifted skew-symmetrizing (ASSS) preconditioner, we first apply diagonal scalings $\left(D_{r}, D_{c}\right)$ and a row permutation $(\mathscr{P})$,

$$
\begin{equation*}
\bar{A}=\mathscr{P} D_{r} A D_{c} \tag{4}
\end{equation*}
$$

such that the diagonal entries of $\bar{A}$ have modulus one and the off-diagonal elements are of modulus less than or equal to one. Such a permutation and scaling procedure is well established in the code MC64 of the Harwell Subroutine Library (HSL) [17] and it is called the maximum product transversal with scaling. It solves a weighted bipartite matching problem and the resulting matrix $\bar{A}$ is guaranteed to contain a zero-free main diagonal if $A$ is structurally nonsingular [9. After this, we look for a sparse matrix $S$ such that

$$
\begin{equation*}
(\bar{A} S)_{i, j}=-(\bar{A} S)_{j, i}, \quad \text { for } i \neq j, \tag{5}
\end{equation*}
$$

and

$$
\begin{equation*}
(\bar{A} S)_{i, i}=1, \quad \text { for } i=1,2, \ldots, n \tag{6}
\end{equation*}
$$

where $S$ can have various sparsity structures, such as being diagonal, tri-diagonal, banded, having the sparsity of $\bar{A}$, or any structure defined by the user.

The described problem can be formulated as a sparse over-determined LLS problem, where by (5), each nonzero in the strictly upper triangular part of $|\bar{A} S|+|\bar{A} S|^{T}$ defines a constraint of the LLS problem and additional $n$ constraints are obtained via (6). Let $n z$ be the number of nonzeros in the strictly upper triangular part of $|\bar{A} S|+|\bar{A} S|^{T}$ and $n n z(S)$ be the number of nonzeros in $S$. Then the LLS problem has $n n z(S)$ unknowns and $n z+n$ equations, and if $n z+n>n n z(S)$ then the problem is overdetermined.

As a first example of a sparsity structure, let us assume $S=\operatorname{diag}\left(s_{1,1}, \ldots, s_{n, n}\right)$, so that $n n z(S)=n$. Then, (5) and (6) are given by

$$
\begin{equation*}
\bar{a}_{i, j} s_{j, j}+\bar{a}_{j, i} s_{i, i}=0, \tag{7}
\end{equation*}
$$

and

$$
\begin{equation*}
\bar{a}_{i, i} s_{i, i}=1, \tag{8}
\end{equation*}
$$

respectively. With $s=\left[s_{1,1}, s_{2,2}, \ldots, s_{n, n}\right]^{T}$, then the resulting overdetermined system is given by

$$
\left[\begin{array}{c}
B_{u}  \tag{9}\\
B_{l}
\end{array}\right] s=\left[\begin{array}{l}
\mathbf{0} \\
\mathbf{1}
\end{array}\right]
$$

where $\mathbf{0}$ and $\mathbf{1}$ are vectors of all zeros of size $(n z+n)$ and all ones of size $n$, respectively. $B_{u}$ is a sparse matrix of size $(n z+n) \times n$, where each row has only two nonzeros, $\bar{a}_{i, j}$ and $\bar{a}_{j, i}$ in its $i$-th and $j$-th columns, respectively, while $B_{l}$ is just the diagonal of $\bar{a}_{i, i}$. So with

$$
f(s):=\left\|\left[\begin{array}{c}
B_{u} \\
B_{l}
\end{array}\right] s-\left[\begin{array}{l}
0 \\
1
\end{array}\right]\right\|_{2}^{2}
$$

the unique solution of the LLS problem is obtained by computing $\min _{s} f(s)$. The unique solution can be obtained via a direct or iterative sparse LLS solver. In order to obtain
more flexibility in the importance of the two constraints, we introduce a weighting parameter ( $\gamma>0$ ), and solve the weighted problem

$$
\begin{equation*}
f(s, \gamma)=\left\|B_{u} s\right\|_{2}^{2}+\gamma\left\|B_{l} s-\mathbf{1}\right\|_{2}^{2}=\left\|(\bar{A} S)+(\bar{A} S)^{T}\right\|_{F}^{2}+\gamma\|\mathscr{D}(\bar{A} S)-I\|_{F}^{2}, \tag{10}
\end{equation*}
$$

where $\mathscr{D}(X)$ denotes a diagonal matrix whose diagonal entries are those of $X$.
For a general sparse $S$, the LLS problem is formulated in a similar way as in the diagonal case. The set of constraints is defined for each nonzero ( $i, j$ ) in the strictly upper (or lower) triangular nonzero pattern of the matrix $|\bar{A} S|+|\bar{A} S|^{T}$ via (5), (using Matlab column notation) via

$$
\begin{equation*}
\bar{A}_{i,:} S_{:, j}+\bar{A}_{j,:} S_{:, i}=0, \tag{11}
\end{equation*}
$$

and the diagonal constraints are obtained for $i=1,2, \ldots, n$ via (6). Note that one needs to map the nonzero entries of $S$ to a vector in order to form the LLS problem and map it back to $S$ after obtaining the solution vector. This can be done using the sparse matrix storage format. In Appendix A, we present a Matlab implementation which stores the non-zeros of sparse matrices in column major order, i.e. compressed sparse column format.

## 3 A bilevel iterative scheme

Given a general sparse linear system

$$
\begin{equation*}
A x=b \tag{12}
\end{equation*}
$$

where $A \in \mathbb{R}^{n \times n}$ is nonsingular. As discussed in the introduction, many preconditioners are either applied or aim for a symmetric or symmetric positive definite system, since for these we have short recurrences in Krylov subsapce methods like the conjugate gradient method. Only very few algorithms focus on skew-symmetric or shifted skew-symmetric structure. In this section we present the theoretical basis for an algorithm that preprocesses the system such that the coefficient matrix is as close as possible to a shifted skew-symmetric matrix and then use the shifted skew-symmetric part of the matrix as preconditioner applying it as an iterative solver with short recurrences and optimality property that requires only one inner product per iteration.

Consider the splitting of the coefficient matrix into its symmetric and skew-symmetric part

$$
\begin{equation*}
A=M+J \tag{13}
\end{equation*}
$$

where $M=M^{T}$ and $J=-J^{T}$, (in applications often $J$ is even a matrix of small norm). If $M$ is positive definite then one can precondition the system by computing the Cholesky factorization $M=L L^{T}$ and solve the modified system

$$
\begin{equation*}
\left(I+L^{-1} J L^{-T}\right) L^{T} x=L^{-1} b \tag{14}
\end{equation*}
$$

where $L^{-1} J L^{-T}$ is again skew-symmetric. However, in general $M$ is not positive definite, it may be indefinite or singular. In this case we propose a black-box algorithm that employs an ASSS preconditioner. This is a two-level procedure, in which we first apply the discussed nonsymmetric row permutation and scaling to obtain a zero free diagonal with diagonal entries of modulus one and off-diagonal entries of modulus less than or equal to one. The second
step applies a sparse matrix $S$ obtained via the algorithm described in Section 2 by solving a sparse LLS problem. After ASSS preconditioning, the modified system is has the form

$$
\begin{equation*}
\widehat{A} \widehat{x}=\widehat{b} \tag{15}
\end{equation*}
$$

where $\widehat{A}=\mathscr{P}_{r} A D_{c} S, \widehat{x}=S^{-1} D_{c}^{-1} x$ and $\widehat{b}=\mathscr{P} D_{r} b$. Let $\widehat{M}=\frac{\widehat{A}+\widehat{A}^{T}}{2}$, and $\widehat{J}=\frac{\widehat{A}-\widehat{A}^{T}}{2}$ Note that due to the ASSS preconditioning, even though $\widehat{M}$ is still not guaranteed to be positive definite, it has eigenvalues clustered around 1 and typically very few negative eigenvalues. Furthermore, the skew-symmetric part, $\widehat{J}$, is more dominant now. One can now compute a Bunch-Kaufman-Parlett factorization [4, $\widehat{M}=\widehat{L} \widehat{D} \widehat{L}^{T}$ and modify the factorization to obtain

$$
\begin{equation*}
|\widehat{M}|=\widehat{L}|\widehat{D}| \widehat{L}^{T} \tag{16}
\end{equation*}
$$

where, as in [30], $|\widehat{D}|=V|\Lambda| V^{T}$ if $\widehat{D}$ has a spectral decomposition $V \Lambda V^{T}$. Then, $|\widehat{D}|$ has a Cholesky factorization $L_{|\widehat{D}|} L_{|\widehat{D}|}^{T}$, since it is positive definite. Setting $\mathcal{L}:=\widehat{L} L_{|\widehat{D}|}$, and multiplying (15) from the left with $\mathcal{L}^{-1}$ and inserting $I=\mathcal{L}^{-T} \mathcal{L}^{T}$, we obtain the system $\mathcal{A} x=\mathcal{G}$, where $\mathcal{A}=\mathcal{L}^{-1} \widehat{A} \mathcal{L}^{-T}, x=\mathcal{L}^{T} \widehat{x}$ and $\mathcal{G}=\mathcal{L}^{-1} \widehat{b}$. We note that $\mathcal{A}$ can be split as

$$
\begin{equation*}
\mathcal{A}=\underbrace{\left(L_{|\widehat{D}|}^{-1} \widehat{D} L_{|\widehat{D}|}^{-T}-I\right)}_{m_{r}}+(I+\underbrace{\mathcal{L}^{-1} \widehat{J} \mathcal{L}^{-T}}_{g}) \tag{17}
\end{equation*}
$$

where the rank of $m_{r}$ is equal to the number of negative eigenvalues of $\widehat{D}$ which is expected to be very small and $I+\mathscr{I}$ is a shifted skew-symmetric matrix. Furthermore, $m_{r}$ is symmetric and block diagonal with only a few nonzero blocks of size either $1 \times 1$ or $2 \times 2$ and is of rank $r \ll n$. The $1 \times 1$ blocks have the value -2 and the $2 \times 2$ blocks have eigenvalues $\{-2,0\}$. Due to the (almost) diagonal and low rank structure of $m_{r}$, it is simple to obtain a symmetric low-rank decomposition

$$
\begin{equation*}
m_{r}=U_{r} \Sigma_{r} U_{r}^{T} \tag{18}
\end{equation*}
$$

where $\Sigma_{r}=-2 I_{r}$, and $U_{r}$ is a sparse (with either one or two nonzero entries per column) $n \times r$ orthogonal matrix. A pseudocode for computing such low rank decomposition is presented in Figure 1 .

The cost of this last step is $O(r)$ arithmetic operations, since it only needs to work with a submatrix of $m_{r}$ corresponding to indices of nonzero entries. Using this factorization, we obtain $\mathcal{A}=U_{r} \Sigma_{r} U_{r}^{T}+\mathcal{S}$ where $\mathcal{S}=I+\mathscr{I}$, so that $\mathcal{A}$ is a shifted skew-symmetric matrix with a low-rank perturbation. Using the Sherman-Morrison-Woodbury formula [13, we theoretically have the exact inverse

$$
\begin{equation*}
\mathcal{A}^{-1}=\mathcal{S}^{-1}-\mathcal{S}^{-1} U_{r}\left(\Sigma_{r}^{-1}+U_{r}^{T} \mathcal{S}^{-1} U_{r}\right)^{-1} U_{r}^{T} \mathcal{S}^{-1}, \tag{19}
\end{equation*}
$$

which can be applied to the right hand side vector $\mathfrak{b}$ to obtain $x$, by solving only shifted skew-symmetric linear systems.

In practice, for large scale sparse systems, it is typically too expensive and storage intensive to compute the full $L D L^{T}$ factorization of $\widehat{M}$, instead, an incomplete factorization $\tilde{M}=$ $\tilde{L} \tilde{D} \tilde{L}^{T}$ can be utilized together with the Cholesky factorization of $|\tilde{D}|=L_{|\tilde{D}|} L_{|\tilde{D}|}^{T}$ where $\tilde{\mathcal{L}}=\tilde{L} L_{|\tilde{D}|}$. This leads to a modified system,

$$
\begin{equation*}
\tilde{L}^{-1} \widehat{A} \tilde{\mathcal{L}}^{-T} \tilde{\mathcal{L}}^{T} \widehat{x}=\tilde{\mathcal{L}}^{-1} \widehat{b} \tag{20}
\end{equation*}
$$

```
Input: \(m_{\imath} \in \mathbb{R}^{n \times n}, r\left(\right.\) rank of \(\left.m_{r}\right)\), Ind (set of indices of nonzeros of \(m_{r}\) )
\(\Sigma_{r} \leftarrow 0, U_{r} \leftarrow 0, U \leftarrow 0\)
\(i \leftarrow 1, j \leftarrow 1\)
\(m_{r}^{\prime} \leftarrow m_{r}(\) Ind, \(\operatorname{Ind})\)
while ( \(i<r\) ) do
    if \(\left(m_{r}^{\prime}(i, i+1)=0\right)\) then
        \(\Sigma_{r}(j, j) \leftarrow m_{r}^{\prime}(i, i)\)
        \(U(:, j) \leftarrow e_{i}\)
        \(i \leftarrow i+1\)
    else
        Compute the eigenpair \(\left\{\lambda_{2}, v_{2}\right\}\) of \(m_{r}^{\prime}(i: i+1, i: i+1)\)
        \(\Sigma_{r}(j, j) \leftarrow \lambda_{2}\)
        \(U(:, j) \leftarrow\left[e_{i}, e_{i+1}\right] v_{2}\)
        \(i \leftarrow i+2\)
    end if
    \(j \leftarrow j+1\)
end while
if ( \(\mathrm{i}=\mathrm{r}\) ) then
    \(\Sigma_{r}(j, j) \leftarrow m_{r}^{\prime}(i, i)\)
    \(U(:, j) \leftarrow e_{i}\)
end if
\(U_{r}(\) Ind, \(:) \leftarrow U\)
Output: \(U_{r} \in \mathbb{R}^{n \times r}, \Sigma_{r} \in \mathbb{R}^{r \times r}\)
```

Figure 1: Sparse low rank decomposition of $m_{r}=U_{r} \Sigma_{r} U_{r}^{T}$.
which then is solved iteratively using a Krylov subspace method with the preconditioner

$$
\begin{equation*}
P=\underbrace{\left(L_{|\tilde{D}|}^{-1} \tilde{D} L_{|\tilde{D}|}^{-T}-I\right)}_{\tilde{m}_{r}}+(I+\underbrace{\tilde{\mathcal{L}}^{-1} \widehat{J} \tilde{\mathcal{L}}^{-T}}_{\tilde{\mathcal{L}}}) \tag{21}
\end{equation*}
$$

or alternatively, if $r$ is zero, with a preconditioner

$$
\begin{equation*}
P=\tilde{\mathcal{S}}=I+\tilde{g} . \tag{22}
\end{equation*}
$$

One can, in principle, even apply $P^{-1}$ exactly as described earlier. However, in a practical implementation applying $\tilde{\delta}^{-1}$ via a direct solver is expensive, therefore one can apply it approximately by solving shifted skew-symmetric systems iteratively, where the coefficient matrix is $\tilde{\delta}$. This gives rise to an inner-outer iterative scheme. In addition to solving a shifted skew-symmetric system (where the coefficient matrix does not have to be formed explicitly) with a single right hand side vector, applying $P^{-1}$ requires sparse matrix-vector/vector-vector operations, solution of a dense $r \times r$ system, as well as one time cost of computing a low rank decomposition of $\tilde{m}_{r}=\tilde{U}_{r} \tilde{\Sigma}_{r} \tilde{U}_{r}^{T}$ and solving a shifted skew-symmetric system with multiple right hand side vectors. The convergence rate of the outer Krylov subspace method depends on the spectrum of the preconditioned coefficient matrix $P^{-1} \tilde{\mathcal{L}}^{-1} \widehat{A} \tilde{\mathcal{L}}^{-T}$. The incomplete factorization of $\widehat{M}$ is an approximation such that $\widehat{M}=\tilde{L} \tilde{D} \tilde{L}^{T}+E$, where $E$ is a small norm error matrix. Assuming we apply $P^{-1}$ exactly, then the preconditioned coefficient matrix is
$P^{-1} \tilde{\mathcal{L}}^{-1} \widehat{A} \tilde{\mathcal{L}}^{-T}=I+P^{-1} \tilde{\mathcal{L}}^{-1} E \tilde{\mathcal{L}}^{-T}$. Due to the sparse ASSS preconditioning step, $\widehat{M}$ is already close to identity and $\widehat{J}$ is dominant. Therefore, the norm of the perturbation of the preconditioned matrix from identity $\left(\left\|P^{-1} \tilde{\mathcal{L}}^{-1} E \tilde{\mathcal{L}}^{-T}\right\|\right)$ is expected to be small.

### 3.1 Solution of sparse shifted skew-symmetric sytems

Application of the described preconditioners involve the solution of linear systems where the coefficient matrix, $I+\tilde{\mathscr{I}}$, is shifted skew-symmetric. Specifically, we are interested in the iterative solution of such systems. While general algorithms such as Bi-Conjugate Gradient Stabilized (bicgstab) [29], Generalized Minimal Residual (gmres) [24], Quasi Minimal Residual (qmr) [12] and Transpose Free Quasi Minimal Residual (tfqmr) [11] can be used, there are some iterative solvers available for shifted skew-symmetric systems such as CGW [5, 26, 31] and the Minimal Residual Method for Shifted Skew-Symmetric Systems (mrs) [18, 21]. We use mrs , since it has a short recurrence and satisfies an optimality property. Furthermore, mrs requires only one inner product per iteration [18] which would be a great advantage if the algorithm is implemented in parallel since inner products require all to all reduction operations which create a synchronization points. In addition to shifted skew-symmetric systems with one right-hand side vector, we also need to solve such systems with multiple right-hand side vectors. As far as we know, currently, there is no "block" mrs available. Even though block Krylov methods are more amenable to breakdown, there are also ways to avoid the break down (for example, for block-CG see [20]). We instead implemented a version of the mrs algorithm based on simultaneous iterations for multiple right-hand side vectors which is given in Appendix B, In the proposed scheme, the convergence rate of mrs iterations depends on the spectrum of the shifted skew-symmetric coefficient matrix, $I+\tilde{\mathscr{I}}$. In the next subsection, we propose a technique to improve this spectrum while preserving its shifted skew-symmetry.

### 3.2 Improving the spectrum of shifted skew-symmetric systems via deflation

One disadvantage of the mrs algorithm is that if a preconditioner is used, then the preconditioned system should be also shifted skew-symmetric which may not be easy to obtain. Therefore, we propose an alternative deflation strategy to improve the number of iterations of mrs. For a shifted skew-symmetric system,

$$
\begin{equation*}
(I+\tilde{\mathscr{G}}) z=y \tag{23}
\end{equation*}
$$

we eliminate the extreme eigenvalues of $I+\tilde{\mathscr{I}}$, by running $k$-iterations $(k \ll n)$ of the skewLanczos process on $\tilde{\mathscr{I}}$, see [16, 18, 21]. A pseudocode for this procedure is presented in Figure 2. Considering the resulting matrices

$$
S_{k}=\left[\begin{array}{cccc}
0 & \alpha_{1} & & 0  \tag{24}\\
-\alpha_{1} & \ddots & \ddots & \\
& \ddots & \ddots & \alpha_{k-1} \\
0 & & -\alpha_{k-1} & 0
\end{array}\right], \quad Q_{k}=\left[q_{1}, q_{2}, \ldots, q_{k},\right]
$$

we deflate the system in 23 by forming

$$
\begin{equation*}
\left[(I+\tilde{\mathscr{I}})-Q_{k} S_{k} Q_{k}^{T}+Q_{k} S_{k} Q_{k}^{T}\right] z=y \tag{25}
\end{equation*}
$$

```
Input: \(\tilde{\mathscr{G}} \in \mathbb{R}^{n \times n}\left(\tilde{\mathscr{g}}=-\tilde{g}^{T}\right)\) and \(k\).
Let \(q_{1}\) be an arbitrary vector \(\in \mathbb{R}^{n}\)
```

```
\(q_{1} \leftarrow q_{1} /\left\|q_{1}\right\|_{2}\)
```

$q_{1} \leftarrow q_{1} /\left\|q_{1}\right\|_{2}$
$z \leftarrow \tilde{\mathscr{I}} q_{1}$
$z \leftarrow \tilde{\mathscr{I}} q_{1}$
$\alpha_{1} \leftarrow\|z\|_{2}$
$\alpha_{1} \leftarrow\|z\|_{2}$
if $\alpha_{1} \neq 0$ then
if $\alpha_{1} \neq 0$ then
$q_{2} \leftarrow-z / \alpha_{1}$
$q_{2} \leftarrow-z / \alpha_{1}$
for $i=2$ to $k-1$ do
for $i=2$ to $k-1$ do
$z \leftarrow \tilde{\mathscr{g}} q_{i}-\alpha_{i-1} q_{i-1}$
$z \leftarrow \tilde{\mathscr{g}} q_{i}-\alpha_{i-1} q_{i-1}$
$\alpha_{i} \leftarrow\|z\|_{2}$
$\alpha_{i} \leftarrow\|z\|_{2}$
if $\alpha_{i}=0$ then
if $\alpha_{i}=0$ then
break
break
end if
end if
$q_{i+1} \leftarrow-z / \alpha_{i}$
$q_{i+1} \leftarrow-z / \alpha_{i}$
end for
end for
end if
end if
Output: $Q_{k}=\left[q_{1}, q_{2}, \ldots, q_{k}\right] \in \mathbb{R}^{n \times k}$ and $\tau=\left[\alpha_{1}, \alpha_{2}, \ldots, \alpha_{k-1}\right]^{T} \in \mathbb{R}^{k-1}$

```
Output: \(Q_{k}=\left[q_{1}, q_{2}, \ldots, q_{k}\right] \in \mathbb{R}^{n \times k}\) and \(\tau=\left[\alpha_{1}, \alpha_{2}, \ldots, \alpha_{k-1}\right]^{T} \in \mathbb{R}^{k-1}\)
```

Figure 2: Skew-Lanczos procedure
such that $Q_{k}^{T} \tilde{\mathscr{G}} Q_{k}=S_{k}$ where $Q_{k}$ is $n \times k$ with $Q_{k}^{T} Q_{k}=I$ and $S_{k}$ is a tridiagonal skewsymmetric $k \times k$ matrix. Let $\overline{\mathscr{g}}=\tilde{\mathscr{g}}-Q_{k} S_{k} Q_{k}^{T}$ which is still skew-symmetric and the largest (in modulus) eigenvalues have been set to zero. Then the system in (23) can be written as a low rank perturbation of a shifted skew-symmetric system

$$
\begin{equation*}
\left[(I+\overline{\mathscr{G}})+Q_{k} S_{k} Q_{k}^{T}\right] z=y \tag{26}
\end{equation*}
$$

which can be handled again by the Sherman-Morrison-Woodbury formula. In fact, this low rank perturbation can be combined with the low rank perturbation in (21), i.e., the preconditioner $P$ can be rewritten as

$$
P=\left[Q_{k}, \tilde{U}_{r}\right]\left[\begin{array}{ll}
S_{k} &  \tag{27}\\
& \tilde{\Sigma}_{r}
\end{array}\right]\left[\begin{array}{c}
Q_{k}^{T} \\
\tilde{U}_{r}^{T}
\end{array}\right]+\bar{\delta}
$$

where $\overline{\mathcal{S}}=I+\overline{\mathscr{g}}$. Then, the preconditioner can be applied directly as via

$$
\begin{equation*}
P^{-1}=\overline{\mathcal{S}}^{-1}-\bar{\delta}^{-1} \bar{U}_{r+k}\left(\bar{\Sigma}_{r+k}+\bar{U}_{r+k}^{T} \overline{\mathcal{S}}^{-1} \bar{U}_{r+k}\right)^{-1} \bar{U}_{r+k}^{T} \overline{\mathcal{S}}^{-1} \tag{28}
\end{equation*}
$$

where $\bar{U}_{r+k}=\left[Q_{k}, \tilde{U}_{r}\right]$ and $\bar{\Sigma}_{r+k}=\left[\begin{array}{cc}S_{k} & \\ & \tilde{\Sigma}_{r}\end{array}\right]$. Note that $P$ is the same preconditioner as in (21), except that the perturbation is of rank $r+k$ now and the shifted skew-symmetric matrix $(\bar{\delta})$ has a better spectrum, see Section 4.4 .

## 4 Numerical results

### 4.1 Implementation details for the numerical experiments

As a baseline of comparison, we implemented a robust general iterative scheme that was proposed in [3]. It uses the same permutation and scalings given in (4) followed by a symmetric
permutation. We use Reverse Cutthill-McKee (RCM) reordering since RCM reordered matrices have better robustness in subsequent applications of ILU type preconditioners [3]. After the symmetric permutation, we use ILU preconditioners with no fill-in (ilu(0)), with pivoting and threshold of $10^{-1}\left(\operatorname{ilutp}\left(10^{-1}\right)\right)$ and $10^{-2}\left(\operatorname{ilutp}\left(10^{-2}\right)\right)$ of Matlab. We call this method as mps-rcm and it is implemented in Matlab R2018a.

Our new method is also implemented in Matlab R2018a in two stages: preprocessing and iterative solution. In the preprocessing stage, we obtain the sparse ASSS preconditioner where we just need the coefficient matrix to obtain the permutation and scalings by calling HSL-MC64 via its Matlab interface. Followed by solving the LLS problem in (9), which we do directly via Matlab's backslash operation. Then, we compute an incomplete Bunch-KaufmanParlett factorization of $\widehat{M}$ via the Matlab interface of sym-ildl software package (15. We use its default parameters except we disable any further scalings. Similar to ilutp, we use $10^{-1}$ and $10^{-2}$ thresholds and allow any fill-in and similar to $i l u(0)$, we allow as many nonzeros as the original matrix per column with no threshold based dropping. We call these: $\operatorname{ildl}\left(10^{-1}\right)$, $i l d l\left(10^{-2}\right)$ and $\sim i l d l(0)$, respectively. We compute the low rank factorization in (18) and apply a few steps of the skew-Lanczos process to deflate the shifted skew-symmetric part of the coefficient matrix. Finally, we iteratively solve the shifted skew-symmetric linear system of equations that arise in (28) with multiple right hand side vectors via mrs

$$
\begin{equation*}
\bar{\delta} X=\bar{U}_{r+k} \tag{29}
\end{equation*}
$$

and form the $(r+k) \times(r+k)$ dense matrix

$$
\begin{equation*}
\bar{\Sigma}_{r+k}+\bar{U}_{r+k}^{T} \overline{\mathcal{S}}^{-1} \bar{U}_{r+k} \tag{30}
\end{equation*}
$$

explicitly. All of these preprocessing steps do not require the right hand side vector and they are done only once if a sequence of linear systems with the same coefficient matrix but with different right hand side vectors need to be solved.

After preprocessing, the linear system of equation in (15) is solved via a Krylov subspace method with the preconditioner in (27). At each iteration of the Krylov subspace method, the inverse of the preconditioner is applied as in (28). This requires the solution of a shifted skew-symmetric linear system. We use the mrs method for those shifted skew-symmetric systems.

As the outer Krylov subspace method, some alternatives are bicgstab, gmres, and tfqmr. Even though they often behave almost the same [3], gmres requires a restart parameter that defies our objective toward obtaining a black-box solver and bicgstab has erratic convergence. Alternatively, tfqmr has a smoother convergence and does not require restarting. We observe that tfqmr can stagnate, which is also noted in [32]. Therefore, as a challenge for our new approach, we use tfqmr for both our proposed scheme and mps-rcm. The stopping criterion for tfqmr is set to $10^{-5}$ and for the inner mrs iterations of the proposed scheme, we use the same stopping criterion. The right hand side is determined from the solution vector of all ones.

We note that even though we use Matlab's built-in functions as much as possible while implementing the proposed iterative scheme, mps-rcm is entirely using the built-in functions of Matlab or efficient external libraries. Therefore, no fair comparison in terms of the running times in Matlab is currently possible. An efficient and parallel implementation of the proposed scheme requires a lower level programming language such as $\mathrm{C} / \mathrm{C}++$ due to the low-level algorithmic and data structural details that need to be addressed efficiently. For
example, the proposed scheme needs efficiently accessing rows and columns of a sparse matrix. At first glance, one might tend to store the matrix both in Compressed Sparse Row and Column formats, however this approach is doubling the memory requirements. Therefore, a new storage scheme without much increase in the memory requirements is needed. Also, efficient and parallel implementation of sparse matrix-vector multiplications, where the coefficient matrix is symmetric (and shifted skew-symmetric) and parallel sparse triangular backward/forward sweeps are challenging problems. These are still active research areas by themselves [1, 6. Therefore, we leave these issues as future work and focus on the robustness of the proposed scheme in Matlab.

### 4.2 Test problems

In this subsection we give the selection criterion and describe the matrices that we use for numerical experiments. Mps-rcm makes incomplete LU based preconditioned iterative solvers very robust. Therefore, to identify the most challenging problems, we use mps-rcm to choose a highly indefinite and challenging set of 10 problems from the SuiteSparse Matrix Collection [7] in which at least one instance of $\mathrm{mps}-\mathrm{rcm}$ fails due to failure of incomplete factorization or stagnation of the Krylov subspace method. Properties of the test problems and their sparsity plots are given in Table 1 and Figure 3, respectively. All chosen problems are (numerically) non-symmetric, and only a few of them are structurally symmetric. Bp_200 and bp_600 are from a sequence of simplex basis matrices in Linear Programming. West0989 and west1505 arise in a chemical engineering plant model with seven and eleven stage column sections, respectively. Rajat19 is a circuit simulation problem. Rdb1250l, rdb32001 and rdb5000 arise in a reaction-diffusion Brusselator model. Chebyshev2 is an integration matrix using the Chebyshev method for solving fourth-order semilinear initial boundary value problems and finally, Orani678 arises in the economic modeling of Australia.

### 4.3 Effectiveness of the shifted skew-symmetrizer

The structure of the approximate skew-symmetrizer $(S)$ can be anything. We experimented with a simple diagonal $\left(S_{d}\right)$ and tridiagonal $\left(S_{t}\right)$ structures. In Table 2, the dimensions, and the number of nonzeros for the LLS problem in (9) are given. After that, we obtain a shifted skew-symmetrized matrix $(\widehat{A})$. To evaluate the effectiveness of the scaling and permutation followed by the approximate skew-symmetrizer, we use three metrics: the skew-symmetry of the off-diagonals, the distance of the main diagonal to identity, and the condition number. In Table 3, we depict these for the original matrix, for matrices after MC64 scaling and permutation, and followed by applying $S_{d}$ or $S_{t}$, which we call "Original", "MC64", "MC64+ $S_{d}$ " and "MC64+ $S_{t}$ ", respectively. As expected, for most cases MC64+ $S_{t}$ has successfully improved the skew-symmetry of the off-diagonal part compared to the original matrix. One exception is chebyshev2, which has a condition number of order $10^{15}$ and $\mathrm{MC} 64+S_{t}$ has improved both the condition number and the main diagonal. For all test problems, MC64+ $S_{t}$ has improved the main diagonal and for 8 of 10 cases, it has also improved the condition number compared to the original matrix. In all cases, $S_{t}$ improves the skew-symmetry of the off-diagonal part and the diagonal compared to $S_{d}$ except chebyshev2. The condition number becomes worse for 6 cases out of 10 using $S_{t}$. However, this is not an issue since we further precondition the system in our proposed method.

Spectra of the original, reordered, and skew-symmetrized matrices are given in Figure 4 .
$S_{t}$ (shown in red) does a better job moving the real part of most eigenvalues positive side of the real axis and clustering them around one, compared to $S_{d}$. Therefore, in the following numerical experiments we use $S_{t}$.

Table 1: Size (n), number of nonzeros (nnz), structural symmetry (Struct. S.), numerical symmetry (Num. S.) and the problem domains of the test problems.

| Matrix | n | nnz | Struct. S. | Num. S. | Problem Domain |
| :--- | ---: | ---: | :---: | :---: | :--- |
| bp_200 | 822 | 3,802 | n | n | Optimization |
| bp_600 | 822 | 4,172 | n | n | Optimization |
| west0989 | 989 | 3,518 | n | n | Chemical Process Simulation |
| rajat19 | 1,157 | 3,699 | n | n | Circuit Simulation |
| rdb12501 | 1,250 | 3,802 | y | n | Computational Fluid dynamics |
| west1505 | 1,505 | 5,414 | n | n | Chemical Process Simulation |
| cehbyshev2 | 2,053 | 18,447 | n | n | Structural |
| orani678 | 2,529 | 90,158 | n | n | Economics |
| rdb32001 | 3,200 | 18,880 | y | n | Computational Fluid Dynamics |
| rdb5000 | 5,000 | 29,600 | y | n | Computational Fluid Dynamics |

Table 2: Dimensions and number of nonzeros of the LLS problems associated with the test problems.

|  | $S_{d}$ |  |  |  | $S_{t}$ |  |  |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | :---: |
| Matrix | n | m | nnz | n | m | nnz |  |
| bp_200 | 3,722 | 822 | 3,802 | 8,131 | 2,463 | 11,404 |  |
| bp_600 | 4,007 | 822 | 4,172 | 9,604 | 2,464 | 12,514 |  |
| west0989 | 3,491 | 989 | 3,518 | 7,529 | 2,965 | 10,549 |  |
| rajat19 | 3,425 | 1,157 | 3,699 | 7,422 | 3,469 | 11,095 |  |
| rdb12501 | 4,275 | 1,250 | 7,300 | 8,570 | 3,748 | 21,892 |  |
| west1505 | 5,382 | 1,505 | 5,414 | 11,598 | 4,513 | 16,237 |  |
| chebyshev2 | 14,344 | 2,053 | 18,447 | 20,481 | 6,157 | 55,331 |  |
| orani678 | 87,358 | 2,529 | 90,158 | 112,852 | 7,585 | 270,465 |  |
| rdb32001 | 11,040 | 3,200 | 18,880 | 7,422 | 3,469 | 11,095 |  |
| rdb5000 | 17,300 | 5,000 | 29,600 | 34,645 | 14,998 | 88,792 |  |

### 4.4 Effectiveness of the deflation

In Figure 5, we present the spectrum of the original $I+\tilde{\mathscr{G}}$ (by using incomplete $L D L^{T}$ factorization of $\widehat{H}$ with zero fill in) and of the deflated shifted skew-symmetric $I+\bar{g}$ after 10 , 20 and 50 iterations of the skew-Lanczos process for all test matrices. We note that the scale of the real axis is negligible for all cases and the spectrum is purely imaginary. Even though case by case fine-tuning is possible by looking at the spectra, we observe that deflating with 20 vectors gives a meaningful balance between the number of iterations and the orthogonality between the Lanczos vectors for the test problems, since for 50 vectors the spectrum is worse and for 10 vectors it does not improve it as much as for 20 vectors. Therefore, in the following experiments, we use 20 skew-Lanczos vectors.

### 4.5 Iterative solution of general sparse linear systems

In the following numerical experiments we use the proposed method as described earlier. For the proposed method the number of Lanczos vectors is set to 20 . Compared to the nondeflated version of the proposed method, the number of mrs iterations are $30.8 \%$ better on average when the inner system is deflated with 20 Lanczos vectors for the test problems. We have also experimented with the skew-Lanczos method with full reorthogonalization for 20 Lanczos vectors and the improvement in the number of iterations is negligible for the test problems. Since it is used just as a preconditioner, we believe that in general it may not be necessary to fully or partially reorthgonalize in the skew-Lanczos process. Therefore, we only report the proposed method with deflation using 20 Lanczos vectors without any reorthogonalization.

In Table 4, the ranks of $\tilde{m}_{r}$ for various incomplete factorizations, as well as the percentages of the rank with respect to the matrix dimension are given. For the set of test problems the largest one is 56 , which is only $3.7 \%$ of the matrix dimension. They are roughly invariant for incomplete factorization for all problems except $r d b l 1250 l$. For the cases when the rank is zero, we use the preconditioner in (22), otherwise we use the preconditioner in (21). We have also experimented with the preconditioner in 22 for problems where the rank is not zero but relatively small. However, the number of iterations has increased significantly even for the case where rank is equal to one ( $r d b l 3200 l$ with $i l d l\left(10^{-2}\right)$ ). We have tried to solve the LLS problem with the regularization parameters $\gamma=0.1,1$ and 10 . Since $\gamma=0.1$ and 10 are worse in terms of the number of iterations, we only report the results with $\gamma=1$.

In Table 5, the number of tfqmr iterations for the proposed method and $\mathrm{mps}-\mathrm{rcm}$ are given. For the proposed method, we also give the average number of inner iterations in parenthesis. As seen in the table, for all test problems and regardless of the choice of the dropping tolerance, the proposed method succeeds. On the other hand, mps-rcm fails for $80 \%$, $90 \%$, and $20 \%$ of problems using ilu(0), ilutp $\left(10^{-1}\right)$, and ilutp $\left(10^{-2}\right)$, respectively. For $i l u(0)$ the majority of the failures are due to tfqmr stagnating. While for $\operatorname{ilutp}\left(10^{-1}\right)$ it happens because of a zero pivot encountered during factorization. As expected, when the dropping tolerance decreases to $10^{-2}$ the failures also decrease since the incomplete factorization is more like a direct solver. Hence, mps-rcm becomes more robust. When it does not fail, the required number of $t f q m r$ iterations for $m p s-r c m$ is quite low except for $r d b 5000$. The proposed method, on the other hand, is robust regardless of the quality of the incomplete factorization for the test problems. There are no failures during the incomplete factorization and no failures of the iterative scheme. The required number of tfqmr iterations improve as a more accurate incomplete factorization is used. The number of iterations if $\operatorname{ildl}\left(10^{-2}\right)$ is used are comparable to those obtained by mps-rcm with ilutp $\left(10^{-2}\right)$. Except, for two cases ( $r d b 3200 l$ and $r d b 5000$ ) for which the proposed method is significantly better and for two other cases (orani678 and $r d b 1250 l$ ) for which $\mathrm{mps}-\mathrm{rcm}$ is significantly better. For the proposed method the number of average inner mrs iterations is not dependent on the choice of the incomplete factorization for all test problems except for $r d b 1250 l$; in this case, it is almost halved when $\operatorname{ildl}\left(10^{-1}\right)$ is used compared to $\sim \operatorname{ildl}(0)$ and $\operatorname{ildl}\left(10^{-2}\right)$. We believe this is due to the fact that for the same matrix using $i l d l\left(10^{-1}\right)$, the rank of $\tilde{m}_{r}$ is 1 which is much smaller than those of $\sim \operatorname{ildl}(0)$ and $\operatorname{ildl}\left(10^{-1}\right), 36$ and 26 , respectively.

## 5 Conclusions

A robust two-level iterative scheme is presented for solving general sparse linear system of equations. The robustness of the scheme is shown on challenging matrices that arise in various problems which are obtained from the SuiteSparse Matrix Collection. While it requires some additional preprocessing steps, the results presented in this paper indicate that the proposed scheme significantly improves the robustness of iterative methods for general sparse linear systems compared to existing methods. This result is irrespective of the quality of the incomplete factorization, even for a challenging set of test problems. The proposed scheme requires some additional memory, but this is shown to be kept within a small percentage of the problem size. We believe with the introduction of the proposed scheme, iterative solvers will become much more viable alternatives for solving problems in chemical engineering, optimizations, economics, etc. Its efficient parallel implementation requires addressing some algorithmic challenges which we leave as future work.

## References

[1] C. Alappat, A. Basermann, A. R. Bishop, H. Fehske, G. Hager, O. Schenk, J. Thies, and G. Wellein, A recursive algebraic coloring technique for hardwareefficient symmetric sparse matrix-vector multiplication, ACM Transactions on Parallel Computing (TOPC), 7 (2020), pp. 1-37.
[2] C. Beattie, V. Mehrmann, H. Xu, and H. Zwart, Port-Hamiltonian descriptor systems, Math. Control Signals Systems, 30:17 (2018), p. Appeared electronically. https://doi.org/10.1007/s00498-018-0223-3.
[3] M. Benzi, J. C. Haws, and M. Tuma, Preconditioning highly indefinite and nonsymmetric matrices, SIAM Journal on Scientific Computing, 22 (2000), pp. 1333-1353.
[4] J. R. Bunch, L. Kaufman, and B. N. Parlett, Decomposition of a symmetric matrix, Numerische Mathematik, 27 (1976), pp. 95-109.
[5] P. Concus and G. H. Golub, A generalized conjugate gradient method for nonsymmetric systems of linear equations, in Computing Methods in Applied sciences and Engineering, Springer, 1976, pp. 56-65.
[6] і̇. ÇuĞu and M. Manguoğbu, A parallel multithreaded sparse triangular linear system solver, Computers \& Mathematics with Applications, 80 (2020), pp. 371-385.
[7] T. A. Davis and Y. Hu, The university of florida sparse matrix collection, ACM Transactions on Mathematical Software (TOMS), 38 (2011), pp. 1-25.
[8] F. Dopico and F. Uhlig, Computing matrix symmetrizers, part 2: New methods using eigendata and linear means; a comparison, Linear Algebra and its Applications, 504 (2016), pp. 590-622.
[9] I. S. Duff and J. Koster, On algorithms for permuting large entries to the diagonal of a sparse matrix, SIAM Journal on Matrix Analysis and Applications, 22 (2001), pp. 973996.
[10] H. Egger, Structure preserving approximation of dissipative evolution problems, Numerische Mathematik, 143 (2019), pp. 85-106.
[11] R. W. Freund, A transpose-free quasi-minimal residual algorithm for non-hermitian linear systems, SIAM Journal on Scientific Computing, 14 (1993), pp. 470-482.
[12] R. W. Freund and N. M. Nachtigal, QMR: a quasi-minimal residual method for non-hermitian linear systems, Numerische Mathematik, 60 (1991), pp. 315-339.
[13] G. H. Golub and C. F. Van Loan, Matrix Computations, The Johns Hopkins University Press, Baltimore, MD, 3rd ed., 1996.
[14] N. Gräbner, V. Mehrmann, S. Quraishi, C. Schröder, and U. von Wagner, Numerical methods for parametric model reduction in the simulation of disc brake squeal, Z. Angew. Math. Mech., 96 (2016), pp. 1388-1405.
[15] C. Greif, S. He, and P. Liu, Sym-ildl: Incomplete ldlt factorization of symmetric indefinite and skew-symmetric matrices, ACM Transactions on Mathematical Software (TOMS), 44 (2017), pp. 1-21.
[16] C. Greif and J. M. Varah, Iterative solution of skew-symmetric linear systems, SIAM Journal on Matrix Analysis and Applications, 31 (2009), pp. 584-601.
[17] HSL, A collection of fortran codes for large scale scientific computation., See http: //www.hsl.rl.ac.uk, (2007).
[18] R. Idema and C. Vuik, A minimal residual method for shifted skew-symmetric systems, Tech. Report REPORT 07-09, Delft University of Technology, 2007.
[19] B. Jacob and H. Zwart, Linear port-Hamiltonian systems on infinite-dimensional spaces, Operator Theory: Advances and Applications, 223, Birkhäuser/Springer Basel AG, Basel CH, 2012.
[20] H. Ji And Y. Li, A breakdown-free block conjugate gradient method, BIT Numerical Mathematics, 57 (2017), pp. 379-403.
[21] E. Jiang, Algorithm for solving shifted skew-symmetric linear system, Frontiers of Mathematics in China, 2 (2007), pp. 227-242.
[22] M. Manguoglu and V. Mehrmann, A robust iterative scheme for symmetric indefinite systems, SIAM Journal on Scientific Computing, 41 (2019), pp. A1733-A1752.
[23] R. Portase and B. UÇar, On matrix symmetrization and sparse direct solvers, Research Report RR-8977, Inria - Research Centre Grenoble - Rhône-Alpes, Nov. 2016, https://hal.inria.fr/hal-01398951.
[24] Y. SaAd and M. H. Schultz, GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM Journal on Scientific and Statistical Computing, 7 (1986), pp. 856-869.
[25] A. J. v. Schaft, Port-Hamiltonian differential-algebraic systems, in Surveys in Differential-Algebraic Equations I, Springer, 2013, pp. 173-226.
[26] D. B. Szyld and O. B. Widlund, Variational analysis of some conjugate gradient methods, East-West Journal of Numerical Mathematics, 1 (1993), pp. 51-74.
[27] B. UÇar, Heurisstics for a matrix symmetrization problem, in Parallel Processing and Applied Mathematics, R. Wyrzykowski, J. Dongarra, K. Karczewski, and J. Wasniewski, eds., Berlin, Heidelberg, 2008, Springer Berlin Heidelberg, p. 718727.
[28] A. J. van der Schaft and D. Jeltsema, Port-Hamiltonian systems theory: An introductory overview, Foundations and Trends in Systems and Control, 1 (2014), pp. 173-378.
[29] H. A. Van der Vorst, Bi-CGSTAB: A fast and smoothly converging variant of bi-cg for the solution of nonsymmetric linear systems, SIAM Journal on Scientific and Statistical Computing, 13 (1992), pp. 631-644.
[30] E. Vecharynski and A. V. Knyazev, Absolute value preconditioning for symmetric indefinite linear systems, SIAM Journal on Scientific Computing, 35 (2013), pp. A696A718.
[31] O. Widlund, A Lanczos method for a class of nonsymmetric systems of linear equations, SIAM Journal on Numerical Analysis, 15 (1978), pp. 801-812.
[32] J. Zhang, Preconditioned Krylov subspace methods for solving nonsymmetric matrices from cfd applications, Computer methods in Applied Mechanics and Engineering, 189 (2000), pp. 825-840.

## A Shifted skew-symmetrizer matlab code

```
function S = skew_symmetrize_sparse_right(A,n,gamma, S)
% Find S such that off-diaognals of AS are skew-symmetric
% and the diagonal of AS is as close to the identity as possible.
%
% Input
% A: square (nxn), sparse input matrix
% n: size of A
% gamma: a positive regularization parameter
% S: a sparsity pattern of the S matrix
% Output
% S: the given sparsity structure such that AS is as
% shifted skew-symetrix as possible
%
% compute the sparsity structure of AS
AA}=\operatorname{spones}(\textrm{A})*\operatorname{spones}(\textrm{S})
% sparsity structure of the strictly upper triangular part
% each nonzero defines one equality in the LLS problem
U = triu(AA+AA',1);
% number of equations of the LLS for the symmetry requirement only
neq = nnz(U);
% and their indices
[I,J]= find(U);
% extract the indices of unknowns in column major order
II = find(S);
```

```
% number of unknowns
nu = length(II);
% place "the compressed" indices in the corresponding nonzero entries
S(II) = [1:nu];
% Allocate the LLS coeffcient matrix
B= sparse(neq+n,nu);
% for each nonzero: (AS)ij
for i=1:neq
    % Our equality is:
    % (AS)ij+(AS)ji=0
    % first we need to determine those indices of nonzeros that contribute to the equality
    ASij = spones(A(I (i ),:))'.* spones(S(:,J(i)));
    ASji = spones(A(J(i),:))'.*spones(S(:, I (i)));
    INDij=find (ASij);
    B(i,S(INDij,J(i))) = A(I(i),INDij);
    INDji=find(ASji);
    B(i,S(INDji,I(i)))=A(J(i),INDji);
end
% additional constraints to obtain ones on the main diagonal
for i=1:n
    ASii = spones(A(i,:))'.* spones(S(:, i ));
    INDii=find(ASii);
    B(i+neq,S(INDii, i ) ) = sqrt(gamma)*A(i, INDii);
end
% set the right hand side vector
v}=[zeros(neq,1); sqrt(gamma)*ones(n,1)]
% Solve the sparse LLS problem
x = B\v;
% map solution back to S matrix
S(II) = x;
return
```

Shifted skew-symmetric iterative solver for multiple right hand side vectors based on simultaneous mrs iterations

```
function [x, its, res, relres_hist] = mrs(alpha,S,b,maxit,tol)
%solves linear systems (alpha*I+S)x=b
% where b and x are of size nxnrhs
% Input
% alpha : a scalar
% S : a sparse skew-symmetrix matrix
% b : the right hand side vector
% maxit : maximum number of iteratations
% tol : stopping tolerance
% Output
% x : solution vector
% its: number of iterations
% res : number of iterat
% relres_hist: relative residual history
[n,nrhs] = size(b)
x = zeros(n, nrhs);
r = b;
```

```
for j =1:nrhs
    r0(j) = norm(r (:, j ), 2);
    relres_hist (j) = [r0(j)/r0(j)];
    s(j)=r0(j);
    q(:, j) = r (:, j)/s(j );
    beta(j) = 0;
    theta1(j) = alpha;
    c_old(j) = 1;
    s_old(j) = 0;
    delta(j) = 0;
    delta_old(j) = 0;
end
q_old = zeros(n, nrhs);
p_old = zeros(n, nrhs);
p_old2 = zeros(n, nrhs);
for i=1:maxit
    q_new }=\textrm{S}*\textrm{q}+\textrm{q_old}*\operatorname{diag}(\mathrm{ beta );
    q_old = q;
    for j=1:nrhs
        beta(j) = norm(q_new (:, j ), 2);
        if (beta(j) ~}=0)q(:,j)= q_new (:, j)/beta(j); en
    end
    theta = sqrt(theta1.*theta1 + beta.* beta);
    c_k = theta1./ theta;
    s_k = beta./ theta;
    delta = -s_old.* beta;
    theta1= c_old.*theta;
    p = (q_old - p_old 2*diag(delta_old ))* diag (1./ theta);
    x = x + p*diag(s)*diag(c_k);
    s = -s.*s_k;
    relres_hist = [relres_hist; abs(s)./r0];
    if (max(abs(s)./r0)<tol)
            its= i
            for j = 1:nrhs
            res(j) = norm(b(:, j)-alpha*x(:,j)-S*x(:,j), 2);
            end
            relres = res./r0;
            break;
    end
    p_old2 = p_old;
    p_old = p;
    s_old = s_k;
    c_old = c_k;
    delta_old = delta;
end
```



Figure 3: Sparsity structures of the test matrices.


Figure 4: Spectrum of the original matrix, after applying MC64 and shifted skewsymmetrizers.

Table 3: The effect of MC64 and the shifted skew symmetrizer. In the table Skew-symmetry, Diagonal and Cond denote $\left\|\left(X-X^{T}\right) / 2\right\|_{F} /\|X-\mathscr{D}(X)\|_{F},\|D(X)-I\|_{F}$ and the condition number of $X$, respectively and rounded to one decimal place where $X$ is either the original matrix, after applying MC64, MC64 followed by $S_{d}$ or MC64 followed by $S_{t}$ in which $S_{d}$ and $S_{t}$ are diagonal and tridiagonal shifted skew-symetrizers, respectively.

| Matrix |  | Original | MC64 | $\mathrm{MC} 64+S_{d}$ | $\mathrm{MC} 64+S_{t}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| bp_200 | Skew-symmetry | $70.7 \%$ | $71 \%$ | $70.7 \%$ | $86.2 \%$ |
|  | Diagonal | 28.7 | 35.8 | 12.2 | 11.6 |
|  | Cond | $6.4 \times 10^{6}$ | $4.0 \times 10^{2}$ | $4.8 \times 10^{2}$ | $1.0 \times 10^{4}$ |
| bp_600 | Skew-symmetry | $70.7 \%$ | $70.7 \%$ | $71.3 \%$ | $74.8 \%$ |
|  | Diagonal | 28.7 | 36.6 | 13.2 | 12.7 |
|  | Cond | $1.5 \times 10^{6}$ | $3.2 \times 10^{2}$ | $3.5 \times 10^{2}$ | $7.8 \times 10^{3}$ |
| west0989 | Skew-symmetry | $70.7 \%$ | $70.7 \%$ | $70.7 \%$ | $100 \%$ |
|  | Diagonal | $2.3 \times 10^{4}$ | 28.8 | 13.4 | 12.6 |
|  | Cond | $9.9 \times 10^{11}$ | $6.7 \times 10^{3}$ | $8.3 \times 10^{3}$ | $9.3 \times 10^{5}$ |
| rajat19 | Skew-symmetry | $28.4 \%$ | $67.1 \%$ | $68.1 \%$ | $83.4 \%$ |
|  | Diagonal | 33.9 | 29.5 | 11.9 | 9.8 |
|  | Cond | $1.1 \times 10^{10}$ | $2.3 \times 10^{10}$ | $1.1 \times 10^{11}$ | $5.7 \times 10^{10}$ |
| rdb12501 | Skew-symmetry | $49 \%$ | $56.2 \%$ | $55.4 \%$ | $97.9 \%$ |
|  | Diagonal | 690.8 | 70.7 | 17.2 | 9.8 |
|  | Cond | $4.7 \times 10^{2}$ | $4.9 \times 10^{2}$ | $3.6 \times 10^{2}$ | $3.1 \times 10^{2}$ |
| west1505 | Skew-symmetry | $70.7 \%$ | $70.7 \%$ | $70.7 \%$ | $100 \%$ |
|  | Diagonal | $2.3 \times 10^{4}$ | 35.9 | 16.6 | 15.7 |
|  | Cond | $1.6 \times 10^{12}$ | $8.8 \times 10^{3}$ | $1.1 \times 10^{4}$ | $1.2 \times 10^{6}$ |
| chebyshev2 | Skew-symmetry | $70.7 \%$ | $11.8 \%$ | $7.6 \%$ | $37.4 \%$ |
|  | Diagonal | 898.5 | 3.5 | 21.9 | 21.9 |
|  | Cond | $5.5 \times 10^{15}$ | $8.6 \times 10^{9}$ | $2.9 \times 10^{10}$ | $1.5 \times 10^{10}$ |
| orani678 | Skew-symmetry | $70.7 \%$ | $70.8 \%$ | $70.6 \%$ | $100 \%$ |
|  | Diagonal | 53.5 | 97.5 | 15.2 | 15.1 |
|  | Cond | $9.6 \times 10^{3}$ | $7.5 \times 10^{3}$ | $1.2 \times 10^{4}$ | $6.4 \times 10^{6}$ |
| rdb5000 | Skew-symmetry | $21.9 \%$ | $27.9 \%$ | $27.1 \%$ | $99.7 \%$ |
|  | Diagonal | $2.5 \times 10^{3}$ | 113.1 | 20.6 | 12 |
|  | Cond | $1.1 \times 10^{3}$ | $9 \times 10^{2}$ | $8.2 \times 10^{2}$ | $7.3 \times 10^{2}$ |
|  | Skew-symmetry | $14.4 \%$ | $18.3 \%$ | $17.9 \%$ | $99.9 \%$ |
|  | Diagonal | $4.8 \times 10^{3}$ | 141.4 | 24.6 | 14.1 |
|  | Cond | $4.4 \times 10^{3}$ | $3 \times 10^{3}$ | $2.8 \times 10^{3}$ | $3.6 \times 10^{3}$ |
|  |  |  |  |  |  |

Table 4: Rank of $\tilde{m}_{r}$ and its percentage with respect to the matrix dimension $\left(\frac{r}{n} \times 100\right)$ rounded to one decimal place in parenthesis.

| Matrix | $\sim \operatorname{ildl}(0)$ | ildl $\left(10^{-1}\right)$ | $i l d l\left(10^{-2}\right)$ |
| :--- | :--- | :--- | :--- |
| bp_200 | $33(4 \%)$ | $32(3.8 \%)$ | $32(3.8 \%)$ |
| bp_600 | $48(5.8 \%)$ | $46(5.6 \%)$ | $45(5.5 \%)$ |
| west0989 | $35(3.5 \%)$ | $32(3.2 \%)$ | $35(3.5 \%)$ |
| rajat19 | $38(3.3 \%)$ | $38(3.3 \%)$ | $38(3.3 \%)$ |
| rdb12501 | $36(2.9 \%)$ | $1(0.1 \%)$ | $26(2.1 \%)$ |
| west1505 | $54(3.6 \%)$ | $55(3.7 \%)$ | $56(3.7 \%)$ |
| chebyshev2 | $5(2 \%)$ | $7(0.3 \%)$ | $7(0.3 \%)$ |
| orani678 | $19(0.8 \%)$ | $26(1 \%)$ | $28(1.1 \%)$ |
| rdb3200l | $0(0 \%)$ | $0(0 \%)$ | $1(0 \%)$ |
| rdb5000 | $0(0 \%)$ | $0(0 \%)$ | $0(0 \%)$ |

Table 5: Number of tfqmr iterations. The average number of inner mrs iterations for the proposed method rounded to one decimal place is given in parenthesis. $*$ : tfqmr stagnated, $\dagger$ : tfqmr reached the maximum number of iterations $(2,000)$ without reaching the required relative residual, $\ddagger$ : zero pivot is encountered during factorization.

|  | Proposed method |  |  | mps-rcm |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Matrix | $\sim \operatorname{ildl}(0)$ | $i l d l\left(10^{-1}\right)$ | $\operatorname{ildl}\left(10^{-2}\right)$ | $\operatorname{ilu}(0)$ | $\operatorname{ilutp}\left(10^{-1}\right)$ | ilutp $\left(10^{-2}\right)$ |
| bp_200 | $26(53.6)$ | $88(54.4)$ | $3(55.8)$ | $\dagger$ | $\ddagger$ | 2 |
| bp_600 | $15(65.7)$ | $33(66.6)$ | $4(67)$ | $\dagger$ | $\ddagger$ | 2 |
| west0989 | $74(134.6)$ | $45(106.9)$ | $3(105.5)$ | $*$ | 20 | 1 |
| rajat19 | $10(35.6)$ | $46(35.8)$ | $17(35.2)$ | $\ddagger$ | $\ddagger$ | $\ddagger$ |
| rdb12501 | $90(66.7)$ | $10(37.1)$ | $49(71.8)$ | $*$ | $\ddagger$ | 10 |
| west1505 | $57(162.9)$ | $75(166.9)$ | $1(163)$ | $\dagger$ | $\ddagger$ | 1 |
| chebyshev2 | $10(15.9)$ | $15(12)$ | $14(15.6)$ | 1 | $\ddagger$ | $\ddagger$ |
| orani678 | $15(229.3)$ | $13(235.9)$ | $12(249)$ | 15 | $\ddagger$ | 4 |
| rdb32001 | $9(63.6)$ | $15(61)$ | $3(69.1)$ | $*$ | $\ddagger$ | 20 |
| rdb5000 | $8(100.6)$ | $16(101.5)$ | $6(100.9)$ | $*$ | $\dagger$ | 129 |



Figure 5: Spectrum of the original skew-symmetric matrix and after deflation.


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