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Limited memory preconditioners for symmetric indefinite problems with application to structural mechanics

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SUMMARY

This paper presents a class of limited memory preconditioners (LMP) for solving linear systems of equations with symmetric indefinite matrices and multiple right-hand sides. These preconditioners based on limited memory quasi-Newton formulas require a small number k of linearly independent vectors and may be used to improve an existing first-level preconditioner. The contributions of the paper are threefold. First, we derive a formula to characterize the spectrum of the preconditioned operator. A spectral analysis of the preconditioned matrix shows that the eigenvalues are all real and that the LMP class is able to cluster at least k eigenvalues at 1. Secondly, we show that the eigenvalues of the preconditioned matrix enjoy interlacing properties with respect to the eigenvalues of the original matrix provided that the k linearly independent vectors have been prior projected onto the invariant subspaces associated with the eigenvalues of the original matrix in the open right and left half-plane, respectively. Third, we focus on theoretical properties of the Ritz-LMP variant, where Ritz information is used to determine the k vectors. Finally, we illustrate the numerical behaviour of the Ritz limited memory preconditioners on realistic applications in structural mechanics that require the solution of sequences of large-scale symmetric saddle-point systems. Numerical experiments show the relevance of the proposed preconditioner leading to a significant decrease in terms of computational operations when solving such sequences of linear systems. A saving of up to 43% in terms of computational effort is obtained on one of these applications.

KEY WORDS: limited memory; linear systems; preconditioners; Ritz vectors; symmetric indefinite matrices

1. INTRODUCTION

The numerical solution of sequences of linear algebraic systems is frequently required in many applications in computational science and engineering. For small to medium-scale problems, algorithms related to (sparse or dense) direct methods based on Gaussian elimination are usually employed. When the coefficient matrix is fixed, these methods are especially relevant because the factorization can be performed once for all and reused all along the sequence. In the general case where both the left-hand and right-hand sides are changing, it is known that preconditioned Krylov subspace methods are the method of choice for large-scale problems. Indeed, the operators in subsequent linear systems have most often similar spectral properties. Hence, a first possible approach to design efficient numerical methods is to extract information generated during the solution of a given linear system to improve the convergence rate of the Krylov subspace method during the subsequent

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solutions. Deflated and augmented Krylov subspaces [1–4] or Krylov subspace methods with recycling [5–8] have been proposed in this setting. We refer the reader to [9–12] for a comprehensive theoretical overview on these methods and to references therein for a summary of applications, where the relevance of these methods has been shown. An alternative consists in exploiting information generated during the solution of a given linear system to improve a preconditioner when solving the next linear system in the sequence. This is the main subject that we want to address in this paper.

When the coefficient matrices in the sequence are symmetric positive definite, Morales and Nocedal [13] have proposed a preconditioner which has the form of a limited memory quasi-Newton matrix [14]. This automatic preconditioner generated using information from the conjugate gradient method only [15, 16] does not require explicit knowledge of the coefficient matrix and is therefore suitable for problems where only products of the matrix times a vector can be computed, as in data assimilation. In [13], Morales and Nocedal have then used the conjugate gradient method in combination with this preconditioner to solve the original symmetric positive definite linear systems arising in the sequence. The effectiveness of this approach has been tested within a Hessian-free Newton method for optimization and by solving certain linear systems arising in finite element models. We note that this contribution extends earlier attempts in this direction; see, for example, [17, 18]. More recently, Gratton, Sartenaer, and Tshimanga [19] have concentrated on the case where a first preconditioner (called first-level preconditioner hereafter), able to cluster most eigenvalues at 1 with relatively few outliers, is already available. In order to improve the efficiency of this first-level preconditioner, they have analyzed a class of second-level preconditioners, called the limited memory preconditioners (LMP), aiming at capturing directions (in a low-dimensional subspace) which have been left out by the first-level preconditioner and are slowing down the convergence of the conjugate gradient method. These preconditioners require a small number k of linearly independent vectors and can be seen as a block variant of the BFGS updating formula for quadratic problems [20, 21]. A spectral analysis of the preconditioned matrix has shown that the LMP class is able to cluster at least k eigenvalues at 1 and that the eigenvalues of the preconditioned matrix enjoy interlacing properties with respect to the eigenvalues of the original matrix. The efficiency of the preconditioner has been shown on a real-life application in data assimilation [19, 22].

When the coefficient matrices in the sequence are symmetric indefinite, the approaches existing in the literature are either based on recycling Krylov subspace methods (see, e.g., [9, 23]) or on updates of preconditioners (of inexact constraint type [24, 25] or of approximate inverse type [26], respectively). Our main objective in this paper is to propose an extension of the LMPs to be used when the coefficient matrices are symmetric indefinite. To the best of our knowledge, we are unaware of any proposition in this direction. This setting is highly relevant, because sequences of symmetric indefinite matrices arise in many applications (solution of certain nonlinear systems of partial differential equations (PDE), numerical optimization, partial differential equations-constrained optimization to name a few). As in the symmetric positive definite case, this limited memory preconditioner can be either directly applied to the original linear system or in combination with an existing preconditioner. In this paper, we simply aim at providing a first theoretical analysis and at showing the relevance of the proposed approach on practical large-scale applications in structural mechanics, when a first-level preconditioner is already available.

The paper is organized as follows. In Section 2, we first present the class of LMPs developed in the symmetric positive definite case studied in [19] and [22]. We extend their definition to the symmetric negative definite case and briefly introduce the variant of LMP, where approximated spectral information based on Ritz vectors is used. In Section 3, the main theoretical section of the paper, we extend the class of LMPs to the symmetric indefinite case and expose our three main contributions. First, we derive a formula to characterize the spectrum of the preconditioned operator. A spectral analysis of the preconditioned matrix shows that the eigenvalues are all real and that the LMPs class is able to cluster at least k eigenvalues at 1. Secondly, we show that the eigenvalues of the preconditioned matrix enjoy interlacing properties with respect to the eigenvalues of the original matrix provided that the k linearly independent vectors have been prior projected onto the invariant subspaces associated with the eigenvalues of the original matrix in the open right and left half-plane, respectively. Third, we focus on theoretical properties of the Ritz-LMP variant, where Ritz information is used to determine the k vectors. We explore in Section 4 the numerical performance of the limited memory preconditioner on possibly large-scale applications in structural mechanics. In this particular context, sequences of linear systems with indefinite matrices of saddle-point structure have to be solved. We show that the limited memory preconditioner based on Ritz information yields a significant decrease in terms of computational operations when solving such sequences of large-scale linear systems. A saving of up to 43% in terms of computational effort - at approximately the same memory cost - is obtained with respect to the original method on one of these applications. Concluding remarks and perspectives are finally proposed in Section 5.

2. LIMITED MEMORY PRECONDITIONERS FOR SYMMETRIC DEFINITE MATRICES

In this section, we briefly review the main properties of the LMPs for linear systems involving symmetric (positive or negative) definite matrices. Then, we recall the notion of Ritz limited memory preconditioner, which will play a central role in the analysis. First, we detail notation used throughout the paper.

2.1. *Notation*

We denote $\|.\|_2$ the Euclidean norm, $I_k \in \mathbb{R}^{k\times k}$ the identity matrix of dimension k and $0_{i,j} \in \mathbb{R}^{i\times j}$ the zero rectangular matrix with i rows and j columns. In addition, the superscript ^{T} denotes the transpose operation, whereas $\Lambda(A)$ corresponds to the set of eigenvalues of a given square matrix A, $A \in \mathbb{R}^{N\times N}$. Given a subspace $\mathscr{S}$ of finite dimension, we denote the range of $\mathscr{S}$ by $\mathcal{R}(\mathscr{S})$, the null space of $\mathscr{S}$ by $\mathcal{N}(\mathscr{S})$, the orthogonal complement of $\mathscr{S}$ by $\mathscr{S}^\perp$ and $A|_{\mathscr{S}}$ the restriction of the matrix A to the subspace $\mathscr{S}$. If $\mathcal{V}$ and $\mathcal{W}$ denote complementary subspaces of a vector space, we denote $\mathcal{P}_{\mathcal{V},\mathcal{W}}$ the projection operator onto $\mathcal{V}$ along $\mathcal{W}$. $\mathcal{P}_{\mathcal{V},\mathcal{W}}$ is the unique projection operator with range $\mathcal{R}(\mathcal{P}_{\mathcal{V},\mathcal{W}}) = \mathcal{V}$ and null space $\mathcal{N}(\mathcal{P}_{\mathcal{V},\mathcal{W}}) = \mathcal{W}$ [27].

2.2. *Limited memory preconditioners for symmetric positive definite matrices*

Many problems in computational science and engineering require the solution of a sequence of linear systems of type $Ax_i = b_i, i = 1, \ldots, I$ with $A \in \mathbb{R}^{N\times N}$ being symmetric positive definite, $x_i \in \mathbb{R}^N$ and $b_i \in \mathbb{R}^N$. For large-scale problems, the conjugate gradient method [28] is generally the method of choice for solving such a sequence, where A could represent either the original or an already preconditioned operator. The convergence behaviour of the conjugate gradient method can be potentially improved with the notion of limited memory preconditioner defined next [19, Definition 2.1].

Definition 1
Let A be a symmetric positive definite matrix of order N and assume that $S \in \mathbb{R}^{N\times k}$ is of full column rank, with $k \leqslant N$. The symmetric matrix H of order N defined as

$$H = \left(I_N - S\left(S^TAS\right)^{-1}S^TA\right)\left(I_N - AS\left(S^TAS\right)^{-1}S^T\right) + S\left(S^TAS\right)^{-1}S^T \qquad (1)$$

is called the limited memory preconditioner (LMP).

H is a symmetric positive definite preconditioner [19, Lemma 3.3] satisfying $HAS = S$, that is, the limited memory preconditioner is able to cluster at least k eigenvalues of HA at 1. In addition, the eigenvalues of the preconditioned matrix HA enjoy interlacing properties with respect to the eigenvalues of the original matrix A. This central result on the clustering of the spectrum of the preconditioned matrix HA is stated in Theorem 1 given next [19, Theorem 3.4].

Theorem 1
Let the positive real numbers $\sigma_1, \cdots, \sigma_N$ denote the eigenvalues of A sorted in nondecreasing order. Then, the set of eigenvalues $\mu_1, \cdots, \mu_N$ of HA can be split in two subsets

$$\sigma_j \leqslant \mu_j \leqslant \sigma_{j+k} \quad \text{for } j \in \{1, \cdots, N-k\},$$
$$\mu_j = 1 \quad \text{for } j \in \{N-k+1, \cdots, N\}.$$

In addition, the condition number of HA can be bounded as follows

$$\frac{\max_{j=1,\cdots,N} \mu_j}{\min_{j=1,\cdots,N} \mu_j} \leqslant \frac{\max\{1, \sigma_N\}}{\min\{1, \sigma_1\}}. \tag{2}$$

2.3. Limited memory preconditioners for symmetric negative definite matrices

As required later in Section 3, we consider the extension of LMPs to the case of symmetric negative definite matrices. A straightforward adaptation of Theorem 1 is given next as a corollary.

Corollary 1
Let A be a symmetric negative definite matrix of order N and assume that $S \in \mathbb{R}^{N \times k}$ is of full column rank, $\leqslant N$. Let H denote a symmetric matrix of order N given by (1) in Definition 1. Let the negative real numbers $\sigma_1, \cdots, \sigma_N$ denote the eigenvalues of A, sorted in nondecreasing order. Then, the set of eigenvalues $\mu_1, \cdots, \mu_N$ of HA can be split in two subsets

$$\sigma_j \leqslant \mu_j \leqslant \sigma_{j+k} \quad \text{for } j \in \{1, \cdots, N-k\},$$
$$\mu_j = 1 \quad \text{for } j \in \{N-k+1, \cdots, N\}.$$

In addition, the condition number of HA can be bounded as follows

$$\frac{\max_{j=1,\cdots,N} |\mu_j|}{\min_{j=1,\cdots,N} |\mu_j|} \leqslant \frac{\max\{1, |\sigma_1|\}}{\min\{1, |\sigma_N|\}}. \tag{3}$$

2.4. Ritz limited memory preconditioner (Ritz-LMP)

In Theorem 1, we note that the nonexpansion of the spectrum of HA is valid for any set of k linearly independent vectors. In [19], three particular forms of LMPs have been proposed and analyzed (the spectral-LMP, the Ritz-LMP, and the quasi-Newton-LMP, respectively). These preconditioners are either based on eigenvectors, Ritz vectors or descent directions, respectively. Ritz vectors are approximations of eigenvectors that are particularly useful when considering the solution of large-scale linear systems or eigenproblems; see, for example, [29, Section 5.7.1], [30] and the references therein. For sake of clarity, we recall their definition next [31].

Definition 2
A scalar θ is called a Ritz value of A with respect to a subspace $\mathcal{L}$ if there exists a nonzero vector $z \in \mathcal{L}$, called a Ritz vector, such that $Az - \theta z \perp \mathcal{L}$, where orthogonality is considered with respect to the canonical inner product.

Ritz pairs (θ, z) can be cheaply obtained from the Lanczos process and we refer the reader to [31] for further details related to their computation.

3. LIMITED MEMORY PRECONDITIONERS FOR SYMMETRIC INDEFINITE MATRICES

In this section, we expose the main theoretical properties of the LMP applied to the solution of symmetric indefinite linear systems.

3.1. Definition

We address the solution of a sequence of linear systems of type $Ax_i = b_i, i = 1, \ldots, I$ with $A \in \mathbb{R}^{N \times N}$ being symmetric indefinite, $x_i \in \mathbb{R}^N$ and $b_i \in \mathbb{R}^N$. Preconditioned iterative methods will be considered for such a purpose. In this setting, our main interest will be to analyze the class of LMPs defined next.

Definition 3
Let A be a symmetric indefinite matrix of order N. Assume that $S \in \mathbb{R}^{N \times k}$, with $k \leqslant N$, is such that $S^T AS$ is nonsingular and denote $\mathscr{S} = \mathcal{R}(S)$. The symmetric matrix H defined as

$$H = \left(I_N - S\left(S^T AS\right)^{-1} S^T A\right)\left(I_N - AS\left(S^T AS\right)^{-1} S^T\right) + S\left(S^T AS\right)^{-1} S^T \tag{4}$$

is called the limited memory preconditioner in the indefinite case.

3.2. *Spectrum of AH*

We aim at characterizing the spectrum of the preconditioned operator AH in the indefinite case. This first contribution is stated in Theorem 2.

Theorem 2
Let A be a symmetric indefinite matrix of order N and H be given by (4) in Definition 3. Assume that the columns of $Z \in \mathbb{R}^{N \times k}$ form an orthonormal basis for $\mathscr{S}$ and that the columns of $Z_\perp \in \mathbb{R}^{N \times (N-k)}$ form an orthonormal basis for $\mathscr{S}^\perp$. The spectrum of the preconditioned operator AH is then given by

$$\Lambda(AH) = \{1\} \cup \Lambda\left(Z_\perp^T P_{\mathscr{S}^\perp, A\mathscr{S}} A Z_\perp\right).$$

Proof
A direct calculation leads to

$$AH = P_{\mathscr{S}^\perp, A\mathscr{S}} A P_{\mathscr{S}^\perp, A\mathscr{S}} + I_N - P_{\mathscr{S}^\perp, A\mathscr{S}},$$

with $P_{\mathscr{S}^\perp, A\mathscr{S}} = I_N - AS(S^T AS)^{-1} S^T$ the oblique projection onto $\mathscr{S}^\perp$ along $A\mathscr{S}$. To determine the spectrum of AH we consider the matrix $[Z, Z_\perp]^T\ AH\ [Z, Z_\perp]$ which is congruent to AH

$$[Z, Z_\perp]^T\ AH\ [Z, Z_\perp] = \begin{pmatrix} Z^T AHZ & Z^T AHZ_\perp \\ Z_\perp^T AHZ & Z_\perp^T AHZ_\perp \end{pmatrix}.$$

Because $\mathcal{R}(P_{\mathscr{S}^\perp, A\mathscr{S}}) = \mathscr{S}^\perp$, $\mathcal{N}(I_N - P_{\mathscr{S}^\perp, A\mathscr{S}}) = \mathscr{S}^\perp$ and the fact that Z has orthonormal columns, we obtain

$$[Z, Z_\perp]^T\ AH\ [Z, Z_\perp] = \begin{pmatrix} I_k & 0_{k, N-k} \\ Z_\perp^T AHZ & Z_\perp^T P_{\mathscr{S}^\perp, A\mathscr{S}} AZ_\perp \end{pmatrix}, \tag{5}$$

which completes the proof. We deduce that 1 is an eigenvalue of AH at least of multiplicity k. Furthermore, we note that the spectrum of $P_{\mathscr{S}^\perp, A\mathscr{S}} A$ can be characterized via the inverse of A as recently shown in [9, Corollary 3.25]

$$\Lambda\left(P_{\mathscr{S}^\perp, A\mathscr{S}} A\right) = \{0\} \cup \Lambda\left(\left(Z_\perp^T A^{-1} Z_\perp\right)^{-1}\right).$$

Because $\mathcal{N}(P_{\mathscr{S}^\perp, A\mathscr{S}} A) = \mathscr{S}$, $\Lambda\left(Z_\perp^T P_{\mathscr{S}^\perp, A\mathscr{S}} AZ_\perp\right)$ can be also characterized by the relation

$$\Lambda\left(Z_\perp^T P_{\mathscr{S}^\perp, A\mathscr{S}} AZ_\perp\right) = \Lambda\left(\left(Z_\perp^T A^{-1} Z_\perp\right)^{-1}\right).$$

□

Theorem 2 is valid for any set of k linearly independent vectors such that $S^T AS$ is nonsingular. We further note that the characterization of the spectrum of AH given in Theorem 2 holds for any invertible operator A, see [9, Theorem 3.24]. As shown in Theorem 2, the eigenvalues of AH are located on the real axis. The question of the sign of the eigenvalues of AH is addressed more precisely next.

3.3. Sign of the eigenvalues of AH and inertia of H

In light of (5), the spectrum of AH is made of at least k eigenvalues equal to one and of eigenvalues of $Z_\perp^T P_{\mathscr{S}^\perp, A\mathscr{S}} A Z_\perp$. Hence, to investigate the sign of the eigenvalues of AH, we need to determine the inertia of $Z_\perp^T P_{\mathscr{S}^\perp, A\mathscr{S}} A Z_\perp$ as stated next in Theorem 3. Similarly, the inertia of H is characterized in Theorem 4. We recall that the inertia of a symmetric matrix B is a triplet of nonnegative integers (denoted as $\text{In}(B) = (m, z, p)$), where m, z and p are the number of negative, zero, and positive elements of $\Lambda(B)$ [32].

Theorem 3
Let A be a symmetric indefinite matrix of order N and H be given by (4) in Definition 3. The inertia of $Z_\perp^T P_{\mathscr{S}^\perp, A\mathscr{S}} A Z_\perp$ is then given by

$$In\left(Z_\perp^T P_{\mathscr{S}^\perp, A\mathscr{S}} A Z_\perp\right) = In(A) - In\left(S^T A S\right).$$

Proof
We consider the symmetric matrix B defined as

$$B = [Z, Z_\perp]^T \; A \; [Z, Z_\perp],$$

or equivalently

$$B = \begin{pmatrix} Z^T A Z & Z^T A Z_\perp \\ Z_\perp^T A Z & Z_\perp^T A Z_\perp \end{pmatrix}.$$

We remark that B and A have the same inertia due to Sylvester's law of inertia [32]. Because $Z^T A Z$ is nonsingular due to Definition 3, we can apply the Haynsworth inertia additivity formula [33] to obtain

$$In(B) = In\left(Z^T A Z\right) + In\left(Z_\perp^T A Z_\perp - Z_\perp^T A Z \left(Z^T A Z\right)^{-1} Z^T A Z_\perp\right),$$

that also reads

$$In(B) = In\left(Z^T A Z\right) + In\left(Z_\perp^T P_{\mathcal{Z}^\perp, A\mathcal{Z}} A Z_\perp\right).$$

Because $Z^T A Z$ and $S^T A S$ have the same inertia and $P_{\mathcal{Z}^\perp, A\mathcal{Z}} A = P_{\mathscr{S}^\perp, A\mathscr{S}} A$, we obtain the final result. □

Theorem 3 is helpful if the symmetric and indefinite operator A admits l negative eigenvalues where $l \leqslant k << N$. In such a case, if $S \in \mathbb{R}^{N \times k}$ is known such that $S^T A S$ admits l negative eigenvalues, Theorem 3 states that AH admits only real positive eigenvalues. We conclude this section by characterizing the inertia of H.

Theorem 4
Let A be a symmetric indefinite matrix of order N and H be given by (4) in Definition 3. Assume that the columns of $W \in \mathbb{R}^{N \times k}$ form an orthonormal basis for $A\mathscr{S}$ and that the columns of $W_\perp \in \mathbb{R}^{N \times (N-k)}$ form an orthonormal basis for $(A\mathscr{S})^\perp$. The inertia of H is then given by

$$In(H) = In\left(S^T A S\right) + In\left(W_\perp^T P_{\mathscr{S}^\perp, A\mathscr{S}}^T P_{\mathscr{S}^\perp, A\mathscr{S}} W_\perp\right).$$

Proof
Similarly as in Theorem 3, we consider the symmetric matrix C defined as

$$C = [W, W_\perp]^T \; H \; [W, W_\perp],$$

or equivalently

$$C = \begin{pmatrix} W^T S(S^T AS)^{-1} S^T W & W^T S(S^T AS)^{-1} S^T W_\perp \\ W_\perp^T S(S^T AS)^{-1} S^T W & W_\perp^T H W_\perp \end{pmatrix}.$$

C and H have the same inertia due to Sylvester's law of inertia. By applying the Haynsworth inertia additivity formula, we obtain after calculation

$$In(H) = In\left(S^T AS\right) + In\left(W_\perp^T \left(H - S\left(S^T AS\right)^{-1} S^T\right) W_\perp\right).$$

Because

$$H = P^T_{\mathscr{S}^\perp, A\mathscr{S}} P_{\mathscr{S}^\perp, A\mathscr{S}} + S\left(S^T AS\right)^{-1} S^T,$$

the proof is complete. □

An important consequence of Theorem 4 is that the number of negative eigenvalues of H is equal to the number of negative eigenvalues of $S^T AS$, because $W_\perp^T P^T_{\mathscr{S}^\perp, A\mathscr{S}} P_{\mathscr{S}^\perp, A\mathscr{S}} W_\perp$ is symmetric positive definite.

3.4. *Nonexpansion of the spectrum of AH*

In this section, we investigate the question related to the nonexpansion of the spectrum of AH. In general, this property does not hold any longer in the indefinite case as illustrated by this simple example

$$A = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}, \quad S = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad H = \begin{pmatrix} 3 & 5 \\ 5 & 9 \end{pmatrix}, \quad \Lambda(AH) = \{-4\} \cup \{1\}.$$

The second contribution of this paper is to show that a nonexpansion property of the spectrum of AH holds provided that the k linearly independent vectors defining S have been prior projected onto the *invariant* subspaces associated with the eigenvalues of A in the open right and left half-plane, respectively. This second contribution is stated in Theorem 5 with help of preparatory Lemmas 1-4. These projection operators involving the matrix sign function of A are defined next [34].

Definition 4
Let $A \in \mathbb{R}^{N\times N}$ be a symmetric indefinite matrix of order N and let $X \in \mathbb{R}^{N\times N}$ denote the matrix sign function[‡] of A defined as $X = (A^2)^{-\frac{1}{2}} A$. Let $\mathcal{I}_+(A)$ and $\mathcal{I}_-(A)$ denote the invariant subspaces associated with the eigenvalues in the right and left half-plane, respectively. We define $P_+(A) = (I_N + X)/2$ as the projection operator onto $\mathcal{I}_+(A)$ and $P_-(A) = (I_N - X)/2$ as the projection operator onto $\mathcal{I}_-(A)$, respectively.

We denote by $Q_+ \in \mathbb{R}^{N\times N_+}$ ($Q_- \in \mathbb{R}^{N\times N_-}$) an orthonormal basis of $\mathcal{I}_+(A)$ ($\mathcal{I}_-(A)$, respectively) and by $Q \in \mathbb{R}^{N\times N}$ the orthonormal matrix defined as $Q = [Q_+, Q_-]$ with $N = N_+ + N_-$. Given $\tilde{S} \in \mathbb{R}^{N\times k}$, $S = [S_+, S_-]$ ($S_+ \in \mathbb{R}^{N\times k_+}$, $S_- \in \mathbb{R}^{N\times k_-}$ with $k = k_+ + k_-$, $k \leqslant N$) consists of k projected vectors obtained as

$$S_+ = Q_+ Q_+^T \left[\tilde{s}_{i_1}, \cdots, \tilde{s}_{i_{k_+}}\right], \tag{6}$$

$$S_- = Q_- Q_-^T \left[\tilde{s}_{j_1}, \cdots, \tilde{s}_{j_{k_-}}\right], \tag{7}$$

where $\left[\tilde{s}_{i_1}, \cdots, \tilde{s}_{i_{k_+}}\right]$ ($\left[\tilde{s}_{j_1}, \cdots, \tilde{s}_{j_{k_-}}\right]$) corresponds to k_+ (k_-, respectively) distinct columns of $\tilde{S}$. Equivalently, we can write

[‡] A (being symmetric indefinite) has no eigenvalues on the imaginary axis, so that the matrix sign function of A is defined.

$$S_+ = Q_+ \tilde{S}_+, \quad \tilde{S}_+ \in \mathbb{R}^{N_+ \times k_+}, \quad \tilde{S}_+ = Q_+^T \left[\tilde{s}_{i_1}, \cdots, \tilde{s}_{i_{k_+}}\right], \tag{8}$$

$$S_- = Q_- \tilde{S}_-, \quad \tilde{S}_- \in \mathbb{R}^{N_- \times k_-}, \quad \tilde{S}_- = Q_-^T \left[\tilde{s}_{j_1}, \cdots, \tilde{s}_{j_{k_-}}\right]. \tag{9}$$

The main goal of the next developments is to show that a property of nonexpansion of the spectrum of HA can be obtained by solving two tractable subproblems related to either $\mathcal{I}_+(A)$ or $\mathcal{I}_-(A)$. We first prove that $\mathcal{I}_+(A)$ and $\mathcal{I}_-(A)$ are H-invariant, by showing Lemma 1 and Lemma 2 successively.

Lemma 1
Define $T \in \mathbb{R}^{N \times N}$ as $T = S(S^T AS)^{-1} S^T$, $T_+ \in \mathbb{R}^{N \times N}$ as $T_+ = S_+ \left(S_+^T AS_+\right)^{-1} S_+^T$ and $T_- \in \mathbb{R}^{N \times N}$ as $T_- = S_-(S_-^T AS_-)^{-1} S_-^T$, respectively. T can be decomposed as

$$T = T_+ + T_-.$$

Proof
Because $\mathcal{I}_+(A)$ and $\mathcal{I}_-(A)$ are A-invariant and orthogonal subspaces, the relation $S_-^T AS_+ = 0_{k_-,k_+}$ holds. Hence, $S^T AS$ can be written as

$$S^T AS = [S_+, S_-]^T A [S_+, S_-] = \begin{pmatrix} S_+^T AS_+ & 0_{k_+,k_-} \\ 0_{k_-,k_+} & S_-^T AS_- \end{pmatrix}.$$

Because $S_+^T AS_+$ and $S_-^T AS_-$ are nonsingular, we deduce

$$\begin{aligned} S(S^T AS)^{-1} S^T &= [S_+, S_-] \begin{pmatrix} \left(S_+^T AS_+\right)^{-1} & 0_{k_+,k_-} \\ 0_{k_-,k_+} & \left(S_-^T AS_-\right)^{-1} \end{pmatrix} [S_+, S_-]^T, \\ &= S_+ \left(S_+^T AS_+\right)^{-1} S_+^T + S_- \left(S_-^T AS_-\right)^{-1} S_-^T, \end{aligned}$$

which completes the proof. □

Lemma 2
$\mathcal{I}_+(A)$ and $\mathcal{I}_-(A)$ are H-invariant

$$\forall v \in \mathcal{I}_+(A) \quad Hv \in \mathcal{I}_+(A), \tag{10}$$

$$\forall v \in \mathcal{I}_-(A) \quad Hv \in \mathcal{I}_-(A). \tag{11}$$

Proof
Because of Lemma 1 and orthogonality of $\mathcal{I}_+(A)$ and $\mathcal{I}_-(A)$, we obtain

$$\forall v \in \mathcal{I}_+(A) \quad Tv = T_+ v,$$

meaning that $Tv \in \mathcal{I}_+(A)$. We also deduce that $ATv \in \mathcal{I}_+(A)$ because $\mathcal{I}_+(A)$ is A-invariant. Furthermore, Hv can be simply written as

$$Hv = (I_N - TA)(I_N - AT)v + Tv.$$

Hence, we deduce relation (10), that is, $\mathcal{I}_+(A)$ is H-invariant. A similar proof leads to the H-invariance of $\mathcal{I}_-(A)$. □

Lemma 3 states a similarity property that is central in the analysis of $\Lambda(HA)$.

Lemma 3
Let $A_+ = Q_+^T A Q_+ \in \mathbb{R}^{N_+ \times N_+}$ $\left(A_- = Q_-^T A Q_- \in \mathbb{R}^{N_- \times N_-}\right)$ denote the orthogonally projected restriction of A with respect to the basis Q_+ (Q_-, respectively). Let $H_+ = Q_+^T H Q_+ \in \mathbb{R}^{N_+ \times N_+}$ $\left(H_- = Q_-^T H Q_- \in \mathbb{R}^{N_- \times N_-}\right)$ denote the orthogonally projected restriction of H with respect to the basis Q_+ (Q_-, respectively). Then $Q^T HAQ$ admits the following decomposition

$$Q^T HAQ = \begin{pmatrix} H_+A_+ & 0_{N_+,N_-} \\ 0_{N_-,N_+} & H_-A_- \end{pmatrix}.$$

As a consequence, $\Lambda(HA) = \Lambda(H_+A_+) \cup \Lambda(H_-A_-)$.

Proof
Because $\mathcal{I}_+(A)$ and $\mathcal{I}_-(A)$ are A-invariant and orthogonal subspaces, the relation $Q_-^T AQ_+ = 0_{N_-,N_+}$ holds. $Q^T AQ$ can then be written as

$$Q^T AQ = \begin{pmatrix} A_+ & 0_{N_+,N_-} \\ 0_{N_-,N_+} & A_- \end{pmatrix}.$$

Furthermore, due to the H-invariance of $\mathcal{I}_+(A)$ (Lemma 2) and the orthogonality of Q, we deduce that $Q_-^T HQ_+ = 0_{N_-,N_+}$. Thus, we obtain

$$Q^T HQ = \begin{pmatrix} H_+ & 0_{N_+,N_-} \\ 0_{N_-,N_+} & H_- \end{pmatrix},$$

which leads to

$$Q^T HAQ = \begin{pmatrix} H_+A_+ & 0_{N_+,N_-} \\ 0_{N_-,N_+} & H_-A_- \end{pmatrix}.$$

This similarity relation immediately implies that $\Lambda(HA) = \Lambda(H_+A_+) \cup \Lambda(H_-A_-)$. □

Consequently, we must now focus on the analysis of H_+A_+ and H_-A_-, respectively. In Lemma 4, we show that H_+ and H_- are both of limited memory preconditioner type.

Lemma 4
Define $\tilde{T}_+ \in \mathbb{R}^{N_+ \times N_+}$ as $\tilde{T}_+ = \tilde{S}_+ \left(\tilde{S}_+^T A_+ \tilde{S}_+\right)^{-1} \tilde{S}_+^T$ and $\tilde{T}_- \in \mathbb{R}^{N_- \times N_-}$ as $\tilde{T}_- = \tilde{S}_- \left(\tilde{S}_-^T A_- \tilde{S}_-\right)^{-1} \tilde{S}_-^T$, respectively, with $\tilde{S}_+, \tilde{S}_-$ given by relations (8, 9), respectively. H_+ and H_- can be written as

$$H_+ = (I_{N_+} - \tilde{T}_+A_+)(I_{N_+} - A_+\tilde{T}_+) + \tilde{T}_+, \tag{12}$$

$$H_- = (I_{N_-} - \tilde{T}_-A_-)(I_{N_-} - A_-\tilde{T}_-) + \tilde{T}_-. \tag{13}$$

As a consequence, H_+ and H_- are both LMP.

Proof
Using successively Lemma 1, equations (8) and (9), the definition of $\tilde{T}_+$ and A_+, and the orthogonality of Q, we obtain

$$\begin{aligned}
H_+ &= \left(Q_+^T - Q_+^T T_+ A\right)\left(Q_+ - AT_+Q_+\right) + Q_+^T T_+ Q_+, \\
H_+ &= \left(Q_+^T - \tilde{T}_+ Q_+^T A\right)\left(Q_+ - AQ_+\tilde{T}_+\right) + \tilde{T}_+, \\
H_+ &= \left(Q_+^T - \tilde{T}_+ Q_+^T A\right) QQ^T \left(Q_+ - AQ_+\tilde{T}_+\right) + \tilde{T}_+, \\
H_+ &= \left(I_{n_+} - \tilde{T}_+A_+\right)\left(I_{n_+} - A_+\tilde{T}_+\right) + \tilde{T}_+.
\end{aligned}$$

Relation (13) can be obtained by a similar proof. Because A_+ is symmetric positive definite, relation (12) reveals that H_+ is a limited memory preconditioner related to the symmetric positive definite case (see Definition 1). Similarly, A_- being symmetric negative definite, H_- defines a limited memory preconditioner related to the symmetric negative definite case (see Corollary 1). □

Based on the previous developments (Lemmas 1–4), we finally state the main result related to the nonexpansion of the spectrum of HA.

Theorem 5
Let A be a symmetric indefinite matrix of order N, H be given by (4) in Definition 3 based on $S = [S_+, S_-]$ consisting of k_+ (k_-) vectors projected onto the positive (negative, respectively) invariant subspace of A, $\mathcal{I}_+(A)$ ($\mathcal{I}_-(A)$, respectively). Then the following properties hold

(a) Let the positive real numbers $\sigma_1^+, \cdots, \sigma_{N_+}^+$ denote the eigenvalues of A_+ sorted in nondecreasing order. Then, the set of eigenvalues $\mu_1^+, \cdots, \mu_{N_+}^+$ of $H_+ A_+$ can be split in two subsets

$$\begin{aligned} &\sigma_j^+ \leqslant \mu_j^+ \leqslant \sigma_{j+k_+}^+ \text{ for } j \in \{1, \cdots, N_+ - k_+\}, \\ &\mu_j^+ = 1 \text{ for } j \in \{N_+ - k_+ + 1, \cdots, N_+\}. \end{aligned} \tag{14}$$

(b) Let the negative real numbers $\sigma_1^-, \cdots, \sigma_{n_-}^-$ denote the eigenvalues of A_- sorted in nondecreasing order. Then, the set of eigenvalues $\mu_1^-, \cdots, \mu_{N_-}^-$ of $H_- A_-$ can be split in two subsets

$$\begin{aligned} &\sigma_j^- \leqslant \mu_j^- \leqslant \sigma_{j+k_-}^- \text{ for } j \in \{1, \cdots, N_- - k_-\}, \\ &\mu_j^- = 1 \text{ for } j \in \{N_- - k_- + 1, \cdots, N_-\}. \end{aligned} \tag{15}$$

(c) In addition, the condition number of HA, $\kappa(HA)$, can be bounded as follows

$$\kappa(HA) \leqslant \frac{\max\left\{1, \sigma_{N_+}^+, |\sigma_1^-|\right\}}{\min\left\{1, \sigma_1^+, |\sigma_{N_-}^-|\right\}}. \tag{16}$$

Proof
Because H_+ and H_- are LMP (see Lemma 4), Properties (a) and (b) are direct consequences of Theorem 1 and Corollary 1, respectively. Furthermore, a direct application of Theorem 1 and Corollary 1 leads to the following inequalities

$$\begin{aligned} \mu_{max}^+ &= \max_{j=1,\cdots,N_+} \mu_j^+ \leqslant \max\left\{1, \sigma_{N_+}^+\right\}, \\ \mu_{min}^+ &= \min_{j=1,\cdots,N_+} \mu_j^+ \geqslant \min\left\{1, \sigma_1^+\right\}, \\ \mu_{max}^- &= \max_{j=1,\cdots,N_-} |\mu_j^-| \leqslant \max\left\{1, |\sigma_1^-|\right\}, \\ \mu_{min}^- &= \min_{j=1,\cdots,N_-} |\mu_j^-| \geqslant \min\left\{1, |\sigma_{N_-}^-|\right\}. \end{aligned}$$

Property (c) is then easily deduced from Lemmas 3 and 4, because

$$\frac{\max\left\{\mu_{max}^+, \mu_{max}^-\right\}}{\min\left\{\mu_{min}^+, \mu_{min}^-\right\}} \leqslant \frac{\max\left\{1, \sigma_{N_+}^+, |\sigma_1^-|\right\}}{\min\left\{1, \sigma_1^+, |\sigma_{N_-}^-|\right\}}.$$

□

3.5. Ritz limited memory preconditioner

As shown in Theorem 5, the use of projected vectors in the limited memory preconditioner insures a nonexpansion property of the spectrum of the preconditioned operator, which is an attractive feature. Nevertheless, using the exact sign function of A or matrix functions that approximate $\text{sign}(A)\tilde{S}$ can be computationally too expensive for large-scale problems. Consequently, approximate spectral information based on Ritz vectors (information that is cheaply available) is usually chosen to select the k columns of $\tilde{S}$. This leads to the Ritz limited memory preconditioner (Ritz-LMP) that is analyzed in Theorem 6 and Corollary 2, respectively. In Section 4.2, we will later numerically investigate the performance of the Ritz-LMP preconditioner and of the LMPs preconditioner based on either exact spectral information (spectral-LMP) or projected Ritz information (Projected Ritz-LMP). First, we detail a property of the Ritz vectors in Lemma 5.

3.5.1. Characterization of the Ritz vectors. Given $A \in \mathbb{R}^{N\times N}$ symmetric, the application of the Lanczos method [15, 16] leads to the Lanczos relation

$$AV_l = V_l T_l + v_{l+1}\left(t_{l+1,l}e_l^T\right), \quad v_1 = b/\|b\|_2 \tag{17}$$

where $V_l = [v_1, \cdots, v_l]$ has orthonormal columns and $T_l \in \mathbb{R}^{l\times l}$ is a symmetric tridiagonal matrix. Determining the Ritz pairs of A with respect to $\mathcal{R}(V_l)$ requires the solution of the standard eigenvalue problem

$$T_l Y = Y\Theta \tag{18}$$

with $Y^T Y = I_l$, $Y = [y_1, \cdots, y_l]$ and $\Theta \in \mathbb{R}^{l\times l}$ diagonal. $(\theta_i, V_l y_i)$ is called a Ritz pair, θ_i a Ritz value and $V_l y_i$ the corresponding Ritz vector. Given $1 \leqslant k \leqslant l$, we select k Ritz pairs and define $\tilde{S} \in \mathbb{R}^{N\times k}$ as

$$\tilde{S} = V_l Y_{l,k} \tag{19}$$

with $Y_{l,k} \in \mathbb{R}^{l\times k}$ as $Y_{l,k} = [y_1, \cdots, y_k]$. We note that $\tilde{S}$ has orthonormal columns, that is, $\tilde{S}^T\tilde{S} = I_k$. We prove in the next lemma that $\mathcal{R}(\tilde{S})$ is an invariant subspace of a matrix different from A.

Lemma 5
Assume that l iterations of the Lanczos method have been performed so that the Lanczos relation (17) holds. Define the symmetric matrix $\Delta A \in \mathbb{R}^{N\times N}$ as

$$\Delta A = -v_{l+1}\left(t_{l+1,l}e_l^T\right)V_l^T - V_l\left(t_{l+1,l}e_l\right)v_{l+1}^T. \tag{20}$$

Assume that $\tilde{S} \in \mathbb{R}^{N\times k}$ has been defined as in relation (19). Then, $\tilde{\mathscr{S}} = \mathcal{R}(\tilde{S})$ is an invariant subspace of $(A + \Delta A)$ and

$$(A + \Delta A)\tilde{S} = \tilde{S}\Theta_k,$$

with $\Theta_k = diag(\theta_1, \cdots, \theta_k)$.

Proof
A simple calculation gives

$$(A + \Delta A)V_l = V_l T_l.$$

Postmultiplying by $Y_{l,k}$ leads to

$$(A + \Delta A)\tilde{S} = \tilde{S}\Theta_k,$$

with $\Theta_k = diag(\theta_1, \cdots, \theta_k)$. □

3.5.2. Characterization of the Ritz limited memory preconditioner. According to relation (5) of Theorem 2, we need to analyze $(P_{\tilde{\mathscr{S}}^\perp, A\tilde{\mathscr{S}}}A)|_{\tilde{\mathscr{S}}^\perp}$ to characterize the Ritz-LMP. This is detailed next in Theorem 6. A consequence is then stated in Corollary 2.

Theorem 6
Let A be a symmetric indefinite matrix of order N and ΔA be given by (20) in Lemma 5. Assume that $\tilde{S} \in \mathbb{R}^{N\times k}$ has been defined as in relation (19). Then,

$$\|(P_{\tilde{\mathscr{S}}^\perp,(A+\Delta A)\tilde{\mathscr{S}}}A - P_{\tilde{\mathscr{S}}^\perp,A\tilde{\mathscr{S}}}A)|_{\tilde{\mathscr{S}}^\perp}\|_2 = t_{l+1,l}^2 \left|\sum_{i=1}^{k}\frac{y_{l,i}^2}{\theta_i}\right|,$$

with $y_{l,i} = e_l^T y_i$.

Proof
We consider the oblique projection $P_{\tilde{\mathscr{S}}^\perp,(A+\Delta A)\tilde{\mathscr{S}}}$ onto $\tilde{\mathscr{S}}^\perp$ along $(A+\Delta A)\tilde{\mathscr{S}}$ defined as

$$P_{\tilde{\mathscr{S}}^\perp,(A+\Delta A)\tilde{\mathscr{S}}} = I_N - (A+\Delta A)\tilde{S}\left(\tilde{S}^T(A+\Delta A)\tilde{S}\right)^{-1}\tilde{S}^T.$$

Because $\left(\tilde{S}^T(A+\Delta A)\tilde{S}\right)^{-1} = \Theta_k^{-1}$ we obtain

$$P_{\tilde{\mathscr{S}}^\perp,(A+\Delta A)\tilde{\mathscr{S}}} = I_N - \tilde{S}\tilde{S}^T = P_{\tilde{\mathscr{S}}^\perp}.$$

Furthermore, $P_{\tilde{\mathscr{S}}^\perp,(A+\Delta A)\tilde{\mathscr{S}}}A$ can be written as

$$\begin{aligned} P_{\tilde{\mathscr{S}}^\perp,(A+\Delta A)\tilde{\mathscr{S}}}A &= P_{\tilde{\mathscr{S}}^\perp,A\tilde{\mathscr{S}}}A - \Delta A\tilde{S}(\Theta_k)^{-1}\tilde{S}^T A, \\ &= P_{\tilde{\mathscr{S}}^\perp,A\tilde{\mathscr{S}}}A - \Delta A\tilde{S}\left(\tilde{S}^T - \Theta_k^{-1}\tilde{S}^T\Delta A\right). \end{aligned}$$

We note that $\tilde{S}^T\Delta A\tilde{S} = 0_k$ because $[V_l, v_{l+1}]$ is an orthonormal basis. Hence, $P_{\tilde{\mathscr{S}}^\perp}(\Delta A\tilde{S}) = \Delta A\tilde{S}$ which leads to

$$\left(P_{\tilde{\mathscr{S}}^\perp,(A+\Delta A)\tilde{\mathscr{S}}}A - P_{\tilde{\mathscr{S}}^\perp,A\tilde{\mathscr{S}}}A\right)|_{\tilde{\mathscr{S}}^\perp} = \Delta A\tilde{S}\Theta_k^{-1}\tilde{S}^T\Delta A. \tag{21}$$

Relation (20) yields

$$\Delta A\tilde{S}\Theta_k^{-1}\tilde{S}^T\Delta A = t_{l+1,l}^2\left(e_l^T Y_{l,k}\Theta_k^{-1}Y_{l,k}^T e_l\right)v_{l+1}v_{l+1}^T.$$

Using the relations $\|uv^T\|_2 = \|u\|_2\|v\|_2$ and $\|v_{l+1}\|_2 = 1$ yields

$$\left\|\Delta A\tilde{S}\Theta_k^{-1}\tilde{S}^T\Delta A\right\|_2 = t_{l+1,l}^2\left|\sum_{i=1}^{k}\frac{y_{l,i}^2}{\theta_i}\right|,$$

which completes the proof. □

Corollary 2
There exist nonnegative scalar quantities $m_1, \cdots, m_{N-k}$ and $\tau \in \mathbb{R}$ such that

$$\lambda_i\left(\left(P_{\tilde{\mathscr{S}}^\perp,A\tilde{\mathscr{S}}}A\right)|_{\tilde{\mathscr{S}}^\perp}\right) = \lambda_i\left((P_{\tilde{\mathscr{S}}^\perp}A)|_{\tilde{\mathscr{S}}^\perp}\right) + m_i\tau, \quad i = 1, \cdots, N-k, \tag{22}$$

with $m_1 + \cdots + m_{N-k} = 1$ and $\tau = t_{l+1,l}^2 e_l^T Y_{l,k}\Theta_k^{-1}Y_{l,k}^T e_l$.

Proof
Relation (21) in Theorem 6 reveals that

$$(P_{\tilde{\mathscr{S}}^\perp,A\tilde{\mathscr{S}}}A)|_{\tilde{\mathscr{S}}^\perp} = \left(P_{\tilde{\mathscr{S}}^\perp,(A+\Delta A)\tilde{\mathscr{S}}}A\right)|_{\tilde{\mathscr{S}}^\perp} - \tau v_{l+1}v_{l+1}^T, \tag{23}$$

with the scalar quantity τ defined by $\tau = t_{l+1,l}^2 e_l^T Y_{l,k}\Theta_k^{-1}Y_{l,k}^T e_l$. This shows that $(P_{\tilde{\mathscr{S}}^\perp,A\tilde{\mathscr{S}}}A)|_{\tilde{\mathscr{S}}^\perp}$ is equal to $(P_{\tilde{\mathscr{S}}^\perp}A)|_{\tilde{\mathscr{S}}^\perp}$ perturbed by a rank-one matrix. Hence, the application of Theorem 8.1.8 [32] shows the existence of nonnegative scalar quantities m_i such that

$$\lambda_i\left(\left(P_{\tilde{\mathscr{S}}^\perp,A\tilde{\mathscr{S}}}A\right)|_{\tilde{\mathscr{S}}^\perp}\right) = \lambda_i\left((P_{\tilde{\mathscr{S}}^\perp}A)|_{\tilde{\mathscr{S}}^\perp}\right) + m_i\tau, \quad i = 1, \cdots, N-k,$$

with $m_1 + \cdots + m_{N-k} = 1$, which completes the proof. □

If the columns of $\tilde{Z}_\perp \in \mathbb{R}^{N\times(N-k)}$ form an orthonormal basis for $\tilde{\mathscr{S}}^\perp$, the spectrum of $P_{\tilde{\mathscr{S}}^\perp} A|_{\tilde{\mathscr{S}}^\perp}$ is then given by

$$\Lambda(P_{\tilde{\mathscr{S}}^\perp} A|_{\tilde{\mathscr{S}}^\perp}) = \Lambda\left(\tilde{Z}_\perp^T A \tilde{Z}_\perp\right). \tag{24}$$

Relations (22) and (24) yield a simple characterization of the Ritz-LMP preconditioner which reveals that the scalar τ is an important quantity to monitor numerically. Indeed, when $|\tau|$ is small, $\left(P_{\tilde{\mathscr{S}}^\perp, A\tilde{\mathscr{S}}} A\right)|_{\tilde{\mathscr{S}}^\perp}$ is spectrally close to $(P_{\tilde{\mathscr{S}}^\perp} A)|_{\tilde{\mathscr{S}}^\perp}$.

3.5.3. Computational cost and memory requirements of the Ritz-LMP. Finally, we briefly detail the computational cost related to the application of the Ritz-LMP to a given vector and also specify the memory requirements. It is known that an application of the standard limited memory preconditioner to a vector has a complexity of $8kN$ operations [19]. Nevertheless, by exploiting the Lanczos relation (17), a significant reduction of this complexity can be obtained. Indeed, Theorem 4.3 in [19] shows that the Ritz-LMP H reads as

$$H = I_N + S\left(\Theta_k^{-1} - I_k\right)S^T - S\omega v_{l+1}^T - v_{l+1}\omega^T S^T + S\omega\omega^T S^T, \tag{25}$$

where the components of $\omega = (\omega_1, \cdots, \omega_k)^T$ are defined as

$$\omega_i = \frac{t_{l+1,l}\, y_{l,i}}{\theta_i}, (i = 1, \cdots, k). \tag{26}$$

Later, we define the vector $s_\omega \in \mathbb{R}^N$ as $s_\omega = S\omega$. Hence, the application of the preconditioner H to a given vector of length N costs $(4k + 9)N$ floating point operations as detailed in Algorithm 1. In addition, the storage requirements related to the Ritz-LMP variant consist of $k + 2$ vectors of length N (v_{l+1}, s_ω and $S \in \mathbb{R}^{N\times k}$) and of k scalars (corresponding to the Ritz values).

Algorithm 1 Application of the Ritz Limited Memory Preconditioner H to a given vector x: $y = Hx$

1: $\alpha_1 = s_\omega^T x$ (costs $2N$ flops)
2: $\alpha_2 = -\alpha_1 + v_{l+1}^T x$ (costs $2N$ flops)
3: $z = S(\Theta_k^{-1} - I_k)S^T x$ (costs $4kN$ flops)
4: $y = x + z - \alpha_2 s_\omega - \alpha_1 v_{l+1}$. (costs $5N$ flops)

4. APPLICATIONS TO SOLID AND STRUCTURAL MECHANICS

We illustrate the numerical behaviour of LMPs on applications in solid and structural mechanics that require the solution of symmetric saddle-point linear systems. Numerical simulations have been performed within the framework of the open-source software *Code_Aster*[§] (version 12.3.0), which is a general purpose finite element code developed at EDF (Electricité de France). For more than 20 years, *Code_Aster* serves as the simulation tool used by the engineering departments of EDF to analyze the various components of the power generation facilities and to produce safety analysis. To solve nonlinear problems in structural mechanics, *Code_Aster* mostly relies on Newton-type methods, where the approximate solution of linear systems by preconditioned Krylov subspace methods is handled through the PETSc[¶] (version 3.4.3) library. We first detail relevant properties of the saddle-point linear systems to be solved, before presenting detailed numerical results.

[§] http://www.code-aster.org
[¶] http://www.mcs.anl.gov/petsc/

4.1. Sequence of saddle-point systems

We consider a sequence of linear systems of saddle-point type

$$\mathcal{K}_i\ y_i = c_i \Longleftrightarrow \begin{pmatrix} G_i & B^T \\ B & 0_{m,m} \end{pmatrix} \begin{pmatrix} u_i \\ v_i \end{pmatrix} = \begin{pmatrix} f_i \\ g_i \end{pmatrix}, \quad i = 1, \cdots, I, \tag{27}$$

where $G_i \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{m\times n}$, $f_i \in \mathbb{R}^n$, $g_i \in \mathbb{R}^m$ and $m < n$. Later we call u_i the physical unknowns and v_i the Lagrange multipliers. The stiffness matrices G_i $(i = 1, \cdots, I)$ are symmetric positive semidefinite because they are related to the discretization of an unconstrained mechanical problem (i.e., with no essential boundary conditions). The deficiency of G_i can be large. Indeed, it is known that an upper bound of the dimension of $\mathcal{N}(G_i)$ corresponds to the number of rigid body motions of subbodies of materials contained within the finite element mesh. Here, these motions correspond to three translations and three rotations for each subbody [35]. We further assume that B is of full row rank ($rank(B) = m$) and that $\mathcal{N}(G_i) \cap \mathcal{N}(B) = \{0\}$, $\forall i \in \{1, \cdots, I\}$. These assumptions make sure the existence and uniqueness of the solution of each linear system in the sequence [36]. We also note that B is a very sparse matrix in our setting. Indeed, B is usually related to the dualization of the boundary conditions. These relations are local in the sense that they involve adjacent nodes of the mesh. Unless stated, B admits only one nonzero coefficient per row due to Dirichlet boundary conditions. In this case, $B^T B$ is a diagonal matrix.

In general, Krylov subspace methods are only feasible in combination with a preconditioner when considering large-scale problems [37]. In this study, we consider a specific block diagonal symmetric positive definite preconditioner based on the augmented Lagrangian method [36, 38–40]

$$\mathcal{M}_1 = \begin{pmatrix} G_1 + \gamma B^T B & 0_{n,m} \\ 0_{m,n} & \dfrac{1}{\gamma} I_m \end{pmatrix}, \quad \gamma > 0. \tag{28}$$

We note that the (1,1) block of $\mathcal{M}_1$ in (28) is positive definite because G_1 is positive definite on $\mathcal{N}(B)$. The choice $\gamma = \dfrac{\|G_1\|_2}{\|B\|_2^2}$ has been found to perform well in practice [38] and approximation of this quantity will be used later. Spectral studies of the preconditioned operator have been performed notably in [39, 41]. $\mathcal{M}_1^{-1}\mathcal{K}_1$ has eigenvalues 1 of multiplicity n, -1 of multiplicity $dim(\mathcal{N}(G_1))$ with remaining eigenvalues lying in the interval $(-1, 0)$ [39, Theorem 2.1]. Because inverting exactly $G_1 + \gamma B^T B$ is too demanding in terms of both computational operations and memory requirements for large-scale problems, we consider a factorized approximate preconditioner of the form $\mathcal{M}_1 \approx \mathcal{L}\mathcal{L}^T$ based on the incomplete Cholesky factorization of $G_1 + \gamma B^T B$ written as $G_1 + \gamma B^T B \approx LL^T$ [37]. We deduce the final formulation of the symmetric preconditioned linear system $\mathcal{A}_i\ x_i = b_i$ denoted as

$$\mathcal{A}_i\ x_i = b_i \Longleftrightarrow \begin{pmatrix} L^{-1} & 0 \\ 0 & \sqrt{\gamma} I_m \end{pmatrix} \begin{pmatrix} G_i & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} L^{-T} & 0 \\ 0 & \sqrt{\gamma} I_m \end{pmatrix} \begin{pmatrix} w_i \\ z_i \end{pmatrix} = \begin{pmatrix} L^{-1} & 0 \\ 0 & \sqrt{\gamma} I_m \end{pmatrix} \begin{pmatrix} f_i \\ g_i \end{pmatrix}. \tag{29}$$

Application of a Krylov subspace method (without any second level preconditioner) for the solution of (29) is later referred to as 'No-LMP'. We note that the same approximate first-level preconditioner $\mathcal{M}_1 \approx \mathcal{L}\mathcal{L}^T$ is used through the sequence. LMPs combined with Krylov subspace methods will be used to solve the sequence of linear systems (29) approximately. As mentioned in Section 3.5, we extract k approximations of eigenvectors known as Ritz vectors when solving the first linear system in this sequence to deduce $S \in \mathbb{R}^{N\times k}$. We note that S is used in the whole sequence, even in the case of changing matrices (as in Section 4.4). Hence, with this choice, the limited memory preconditioner H is then defined once for all as

$$H = \left(I_{n+m} - S\left(S^T\mathcal{A}_1 S\right)^{-1} S^T\mathcal{A}_1\right)\left(I_{n+m} - \mathcal{A}_1 S\left(S^T\mathcal{A}_1 S\right)^{-1} S^T\right) + S\left(S^T\mathcal{A}_1 S\right)^{-1} S^T. \tag{30}$$

In all the applications considered, we always select the Ritz vectors corresponding to the smallest in modulus Ritz values. Because positive or negative Ritz values can occur in practice, H is a symmetric indefinite preconditioner due to Theorem 4. Hence, we use the symmetric indefinite matrix H as a right preconditioner of GMRES(ℓ) for the approximate solution of the remaining linear systems in the sequence (29). We consider a value for the restart parameter equal to $\ell = 30$. A zero initial guess x_i^0 is always chosen and the iterative method is stopped when the Euclidean norm of the residual normalized by the Euclidean norm of the right-hand side satisfies the following relation

$$\frac{||b_i - \mathcal{A}_i x_i^k||_2}{||b_i||_2} \leqslant 10^{-8}. \tag{31}$$

The numerical results have been obtained on Aster5, a IBM IDATAPLEX computer located at EDF R&D Data Center (each node of Aster5 is equipped with 2 Intel Xeon $E5 - 2600$, each running 12 cores at 2.7 Ghz). Physical memory available on a given node (24 cores) of Aster5 ranges from 64 GB to 1 TB. This code was compiled by the Intel compiler suite with the best optimization options and linked with the Intel MKL BLAS and LAPACK subroutines. Both iteration counts and measure of computational effort will be reported. This numerical study has been performed in a serial environment and we refer the reader to [42] for additional numerical experiments on a parallel distributed memory computer. Our main interest is to analyze the efficiency of the limited memory preconditioner for the solution of the sequence of saddle-point systems where both the matrices and the right-hand sides may change. A small-scale problem is considered first, while two large-scale configurations will be analyzed later in Sections 4.3 and 4.4. Problems with a given matrix and multiple right-hand sides are considered in Sections 4.2 and 4.3, while a sequence of linear systems with varying matrices is addressed in Section 4.4.

4.2. Mechanical bearing

We first focus on a linear problem in solid mechanics related to the computation of the displacement of a mechanical bearing. In this experiment, the bearing is subject to an external pressure on its left part, while embedded on the right part. The computational mesh is shown in Figure 1.

The moderate dimension of the problem ($n = 7305$, $m = 228$, $N = 7533$) allows us to compute the spectrum of $\mathcal{A}$ and the matrix sign function of $\mathcal{A}$. Thus, we will be able to investigate the behaviour of the limited memory preconditioner with S based either on exact eigenvectors (spectral-LMP), Ritz vectors (Ritz-LMP) or projected Ritz vectors (Projected Ritz-LMP) as introduced in Section 3.5. As shown in Figure 2 (left part), the spectrum of $\mathcal{A}$ exhibits clusters at -1 and 1 (in agreement with the theory) and eigenvalues close to 0. Exact eigenvectors related to eigenvalues of smallest modulus and Ritz vectors related to Ritz values of smallest modulus are considered next. As an illustration, Figure 2 (right part) shows the spectrum of $\mathcal{A}H$, when a limited memory preconditioner based on $k = 20$ Ritz vectors (Ritz LMP) is selected.

Figure 3 shows the convergence history of GMRES(30) for these different variants of LMPs with increasing values of k ($k = 5, 20, 30$, respectively). We note that the use of the limited memory preconditioner leads to a significant decrease in terms of numbers of iterations. The combination of the augmented Lagrangian preconditioner with the limited memory preconditioner is thus successful

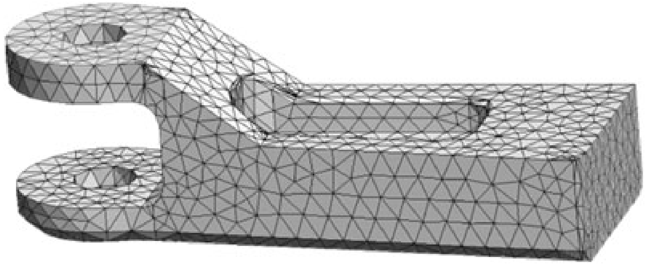

Figure 1. Mesh of the mechanical bearing.

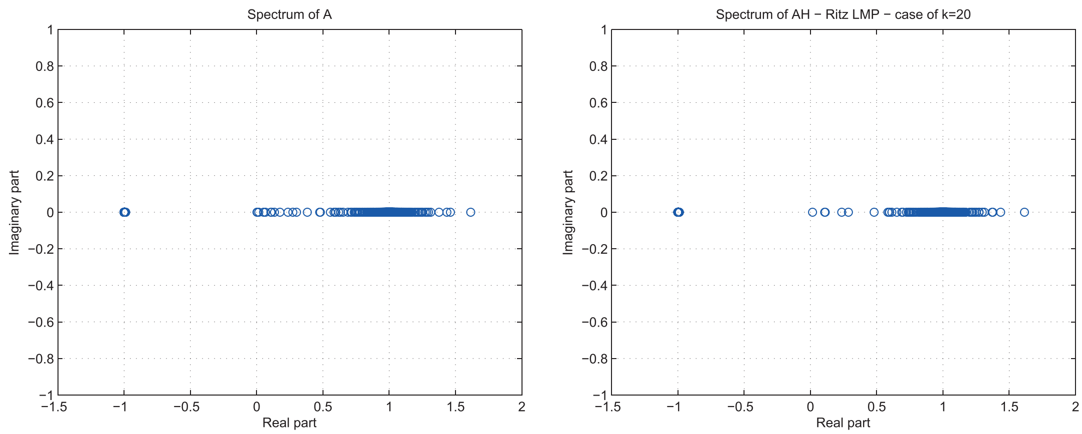

Figure 2. Mechanical bearing: spectrum of $\mathcal{A}$ (left part) and spectrum of $\mathcal{A}H$ (right part), where H corresponds to a limited memory preconditioner (Ritz LMP) with $k = 20$ Ritz vectors.

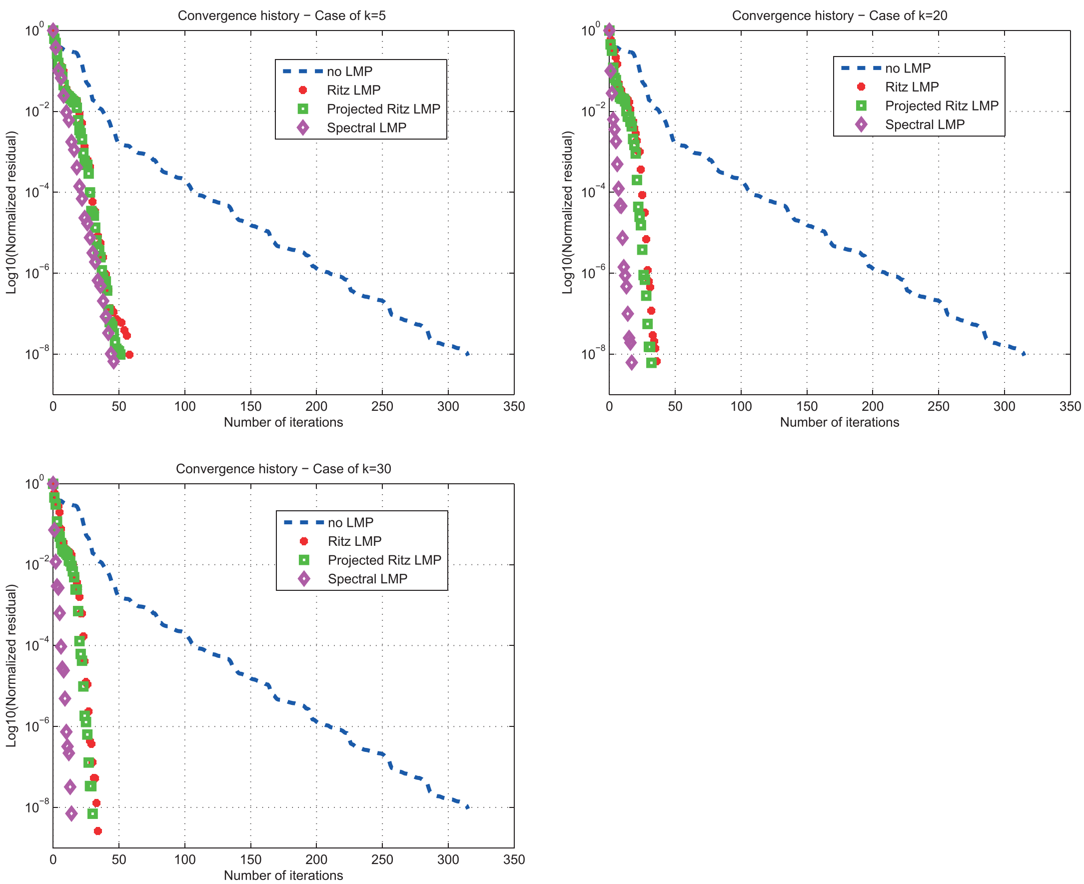

Figure 3. Mechanical bearing: convergence history of GMRES(30). Four preconditioning methods are compared: no second level preconditioning (No LMP, dashed line), limited memory preconditioners based on Ritz vectors (Ritz LMP, circle), on projected Ritz vectors (projected Ritz LMP, square) and on exact eigenvectors (spectral LMP, diamond).

on this application. Using eigenvectors of $\mathcal{A}$ for S leads to the minimal number of iterations in all situations. More interestingly, we also note that using Ritz or projected Ritz vectors for S leads to a very similar convergence behaviour on this model example. This fact is in agreement with the theory presented in Section 3.5 and illustrates that in practice it is sufficient to consider Ritz vectors only, because they are good approximations of projected Ritz vectors. We further note that the value of $|\tau|$ given in relation (23) is equal to 0.0335, 0.075, and 0.079 for $k = 5, 20, 30$, respectively. We will thus consider only the Ritz-LMP variant based on Ritz vectors related to Ritz values of smallest modulus in the next sections.

4.3. Containment building of a nuclear reactor

In this section, we investigate the mechanical properties of a containment building of a nuclear reactor of a Water Pressurized Reactor power plant. This building protects both the reactor from external aggressions and the environment if an internal accident occurs. Robust and accurate numerical simulations are thus required for both design and safety analysis. We consider an advanced mechanical modeling that takes into account numerous prestressing tendons, whose role is to improve the global resistivity of the structure (see Figure 4). The containment building is subject to gravity and to an internal pressure. The whole loading is gradually applied into four successive steps. Each pitch of loading then corresponds to a specific linear system in the sequence, where only the right-hand side has changed (i.e., $\mathcal{A}_1 = \cdots = \mathcal{A}_4$). The physical part of the solution consists of gridded fields of displacement. The introduction of Lagrange multipliers stems from the imposition of kinematic relations modeling perfect adhesion between the prestressing tendons and the concrete [43] and to the dualization of the boundary conditions. In this setting, B admits either five or one nonzero entries per row, respectively. This study is known to be complex for different reasons. First, from a mechanical point of view, the modeling is rather advanced with a mixing of three-dimensional elements for the concrete and of one-dimensional elements for the wires. Moreover, because the prestressing tendons are attached to the concrete thanks to dualized linear relations, the number of Lagrange multipliers is really important ($m = 158,928$ for a global size of $N = 442,725$). The number of nonzero entries of G_1 and $G_1 + \gamma B^T B$ is 7079238 and 8343685, respectively. Secondly, the occurrence of a large number of prestressing tendons (more than 600 here) induces a nullspace of large dimension for the stiffness matrix (larger than 3600, see Section 4.1). This numerical study is thus challenging and serves as a relevant realistic test case in structural mechanics to investigate the efficiency of preconditioners for Krylov subspace methods.

In this experiment, we set γ to $2,4684 \times 10^{11}$ and consider a level of fill equal to 8 in the incomplete Cholesky factorization of the $(1,1)$ block of $\mathcal{M}_1$. Actually, with a lower level of fill

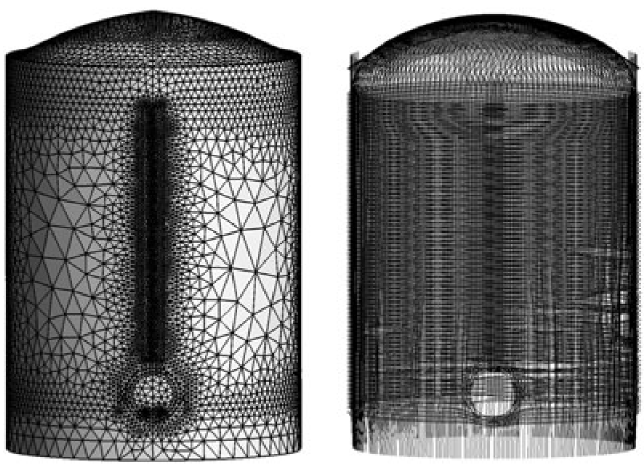

Figure 4. Containment building: three-dimensional mesh (left part) and location of the prestressing tendons on the surface (right part).

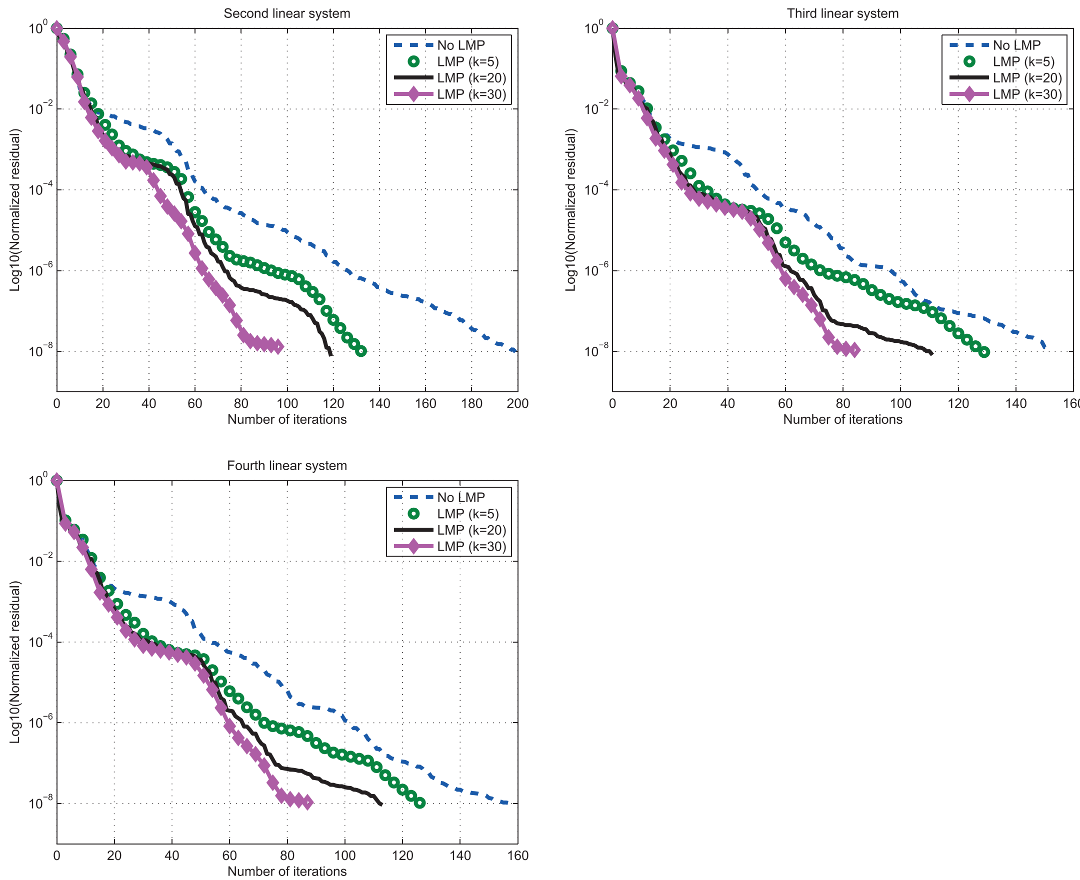

Figure 5. Containment building: convergence history of preconditioned GMRES(30) for the last three linear systems in the sequence. Case of limited memory preconditioners (Ritz LMP) with $k = 5$, 20, or 30 Ritz vectors associated to the smallest in modulus Ritz values.

the preconditioned Krylov subspace method can hardly converge. However, even with this value of fill, the required memory is around 7 Go, while state-of-the-art sparse direct solvers require at least 10 Go for the complete factorization of the $(1,1)$ block of $\mathcal{M}_1$.

Figure 5 shows the evolution of the Euclidean norm of the relative residual for the last three linear systems in the sequence ($I = 2, 3, 4$). In this experiment, we consider LMP with a varying number of Ritz vectors ($k = 5, 20, 30$, respectively). Whatever the linear system considered in the sequence, the smallest number of iterations is obtained when selecting a large value of Ritz vectors ($k = 30$). In addition, we show in Table I the cumulative iteration count over the last three linear systems, the total number of floating point operations[‖] and the memory requirements, both provided by PETSc, respectively. We note that selecting S based on $k = 30$ Ritz vectors leads to a decrease of 47% in terms of cumulative iteration count and to a decrease of 43% in terms of computational operations. This satisfactory result comes at a price of a very moderate increase in memory requirements (3%), because the limited memory preconditioner only needs the storage of $(k + 2)$ vectors of size N as detailed in Section 3.5.3.

4.4. *Polycrystalline aggregate*

The polycrystalline aggregate problem is especially used as an homogenization method to obtain macroscopic constitutive laws of a material from microscopic considerations only. In this

[‖]In PETSc one floating point operation corresponds to one operation of any of the following types: multiplication, division, addition, or subtraction.

Table I. Containment building: cumulative iteration count over the sequence of linear systems, floating point operations and memory requirements for different limited memory preconditioners. Case of $k = 5$, 20 or 30 Ritz vectors.

	No LMP	LMP, $k = 5$	LMP, $k = 20$	LMP, $k = 30$
Total iteration count	509	389	343	272
Iteration count decrease (%)	×	24	33	47
Flops ($\times 10^{11}$)	4.764	3.6946	3.342	2.7041
Flops decrease (%)	×	22	29	**43**
Memory (Mo)	6686	6722	6823	6891
Memory increase (%)	×	0.5	2	3

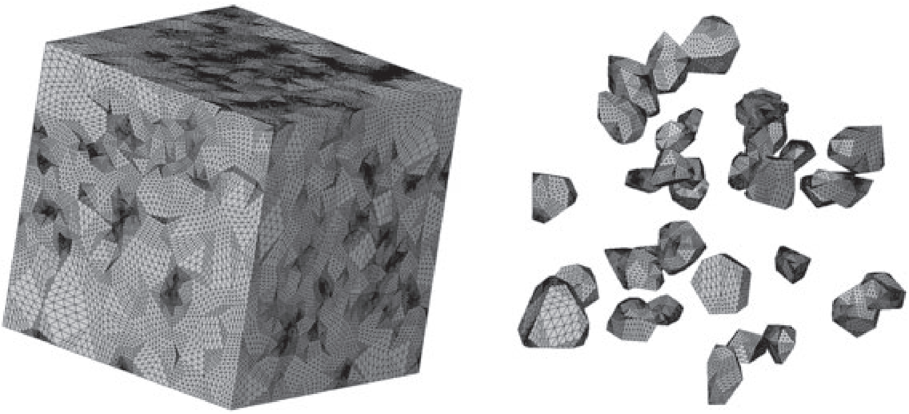

Figure 6. Polycrystalline aggregate: unstructured mesh of the representative elementary volume (left part) and detailed view of some grains of the polycrystalline aggregate (right part).

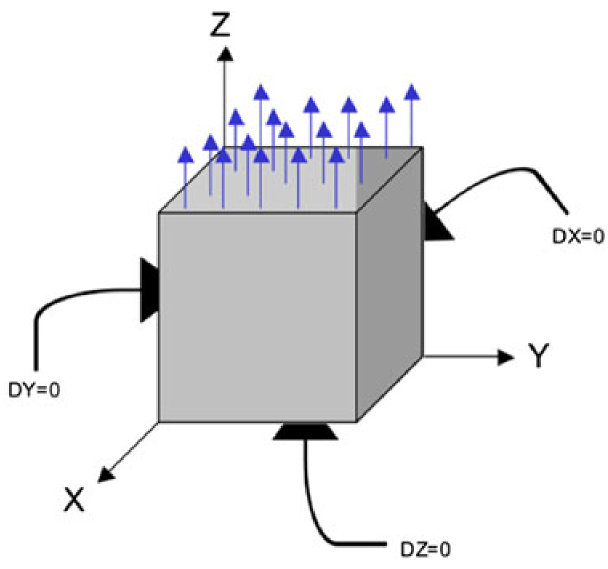

Figure 7. Polycrystalline aggregate: sketch of the boundary conditions.

framework, numerical simulations are performed at a mesoscopic scale in a simple geometry (a cube named representative elementary volume). One thousand points are randomly distributed in this cube and Voronoi cells are created using perpendicular bisector planes. Each cell then represents a grain which has its own constitutive law. The cells are finally discretized with tetrahedra leading to a global three-dimensional unstructured mesh (see Figure 6 for an illustration).

We impose a traction loading on a given face of the cube and specify zero displacement boundary conditions on the other faces as shown in Figure 7.

All these boundary conditions are dualized, leading to a sequence of saddle-point systems of the form (27) with changing matrices. To evaluate the numerical performance of the LMP, we aim at performing these simulations on different meshes. Thus, a coarse mesh ($N = 56561$ with $n = 54567$ and $m = 1994$), an intermediate mesh ($N = 425222$ with $n = 417525$ and $m = 7697$) and a fine mesh ($N = 3298601$ with $n = 3268359$ and $m = 30242$) are considered in this study. We note that the proportion of Lagrange multipliers is always less than 1% and that the simulation on the finest mesh is considered as a real computational challenge in practice. Newton's method is employed because of the nonlinearity of the constitutive law of the structure [44]. As expected, it is found that the total number of Newton's iterations is mesh-dependent (7, 9, 14 iterations are required on the coarse, intermediate and fine mesh, respectively). Finally, we set γ to 1.052×10^5, 7.6101×10^4 and 7.3267×10^4 on the coarse, intermediate and fine mesh, respectively. Similarly, we set the level of fill for the incomplete Cholesky factorization of the $(1, 1)$ block of $\mathcal{M}_1$ to 4 in the three cases.

Table II collects the results for the three different simulations. Using only a first-level preconditioner in combination with GMRES(30) (No LMP) is not a scalable approach due to the strong increase in terms of cumulative number of iterations. Nevertheless, whatever the level of mesh refinement, we observe that the use of the limited memory preconditioner leads to a significant decrease both in terms of cumulative number of iterations over the whole Newton's sequence and of computational operations. A decrease of 18% in terms of floating point operations at a price of a low memory increase (only 0.2%) is indeed obtained on the fine mesh calculation which is a rather satisfactory result. Larger gains are obtained for the simulations on the coarse and intermediate meshes (bold values in Table II). On this application, choosing 5 Ritz vectors leads to the best strategy in terms of floating point operation reduction. Considering a larger number of Ritz vectors reduces the cumulative number of iterations as shown in Figure 8. Nevertheless, this choice leads to a larger cost in terms of computational operations.

Table II. Polycrystalline aggregate: cumulative iteration count over the complete Newton's sequence, floating point operations and memory requirements for different preconditioners. Results are given for three different levels of mesh refinement (coarse, intermediate and fine, respectively).

		No LMP	LMP, $k = 5$	LMP, $k = 20$	LMP, $k = 30$
Coarse mesh	Total iteration count	354	235	227	222
	Iteration count decrease (%)	×	33.5	36	37.5
	Flops ($\times 10^{10}$)	2.0785	1.4293	1.4647	1.4875
	Flops decrease (%)	×	**31**	29.5	28.5
	Memory (Mo)	1137	1140	1146	1151
	Memory increase (%)	×	0.2	0.8	1.2
Interm. mesh	Total iteration count	1316	1033	1027	1019
	Iteration count decrease (%)	×	21.5	22	22.5
	Flops ($\times 10^{11}$)	6.5841	5.3049	5.605	5.686
	Flops decrease (%)	×	**19.5**	15	13.5
	Memory (Mo)	8286	8305	8358	8387
	Memory increase (%)	×	0.2	0.8	1.2
Fine mesh	Total iteration count	6002	4835	4651	4614
	Iteration count decrease (%)	×	20	22.5	23
	Flops ($\times 10^{12}$)	2.4735	2.0414	2.0591	2.1058
	Flops decrease (%)	×	**18**	17	15
	Memory (Mo)	65613	65787	66165	66416
	Memory increase (%)	×	0.2	0.8	1.2

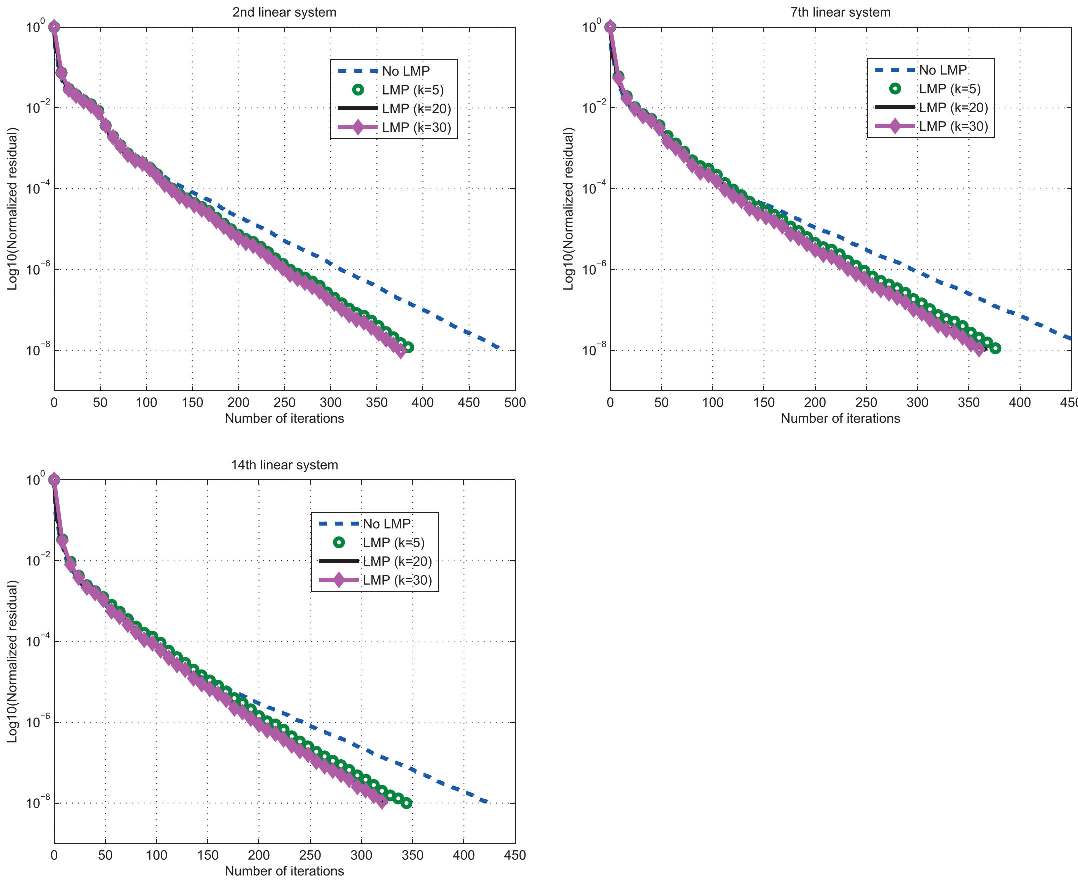

Figure 8. Polycrystalline aggregate (fine mesh calculation): convergence history of preconditioned GMRES(30) at three different iterations of the Newton's method (2nd iteration, 7th iteration and 14th iteration). Case of limited memory preconditioners (Ritz LMP) with $k = 5, 20$, or 30 Ritz vectors associated to the smallest in modulus Ritz values.

5. CONCLUSIONS

We have proposed a class of LMPs for the solution of linear systems with symmetric indefinite matrices and multiple right-hand sides. This preconditioner based on limited memory quasi-Newton formulas can be either directly employed on the original linear system or can improve an existing first-level symmetric preconditioner as well. In addition, this method is especially worth considering when the solution of a sequence of linear systems with slowly varying left-hand sides is considered.

We have derived a formula to characterize the spectrum of the preconditioned operator. We have shown that the eigenvalues of the preconditioned operator are real-valued (with at least k eigenvalues equal to 1). Furthermore, we have shown that the eigenvalues of the preconditioned matrix enjoy interlacing properties with respect to the eigenvalues of the original matrix provided that the k linearly independent vectors have been prior projected onto invariant subspaces associated with the eigenvalues of the original matrix. Then, we have studied the Ritz-LMP variant, where Ritz information is used to determine the k vectors.

Finally, the Ritz-LMP variant has proved to be efficient in terms of both preconditioner applications and computational operations on problems related to structural mechanics, where sequences of large-scale symmetric indefinite saddle-point linear systems have to be solved. Numerical experiments have highlighted the relevance of the proposed preconditioner that leads to a significant decrease in terms of computational operations. A saving of up to 43% in terms of computational effort - at approximately the same memory cost - is obtained with respect to the original method on one of these applications.

Although not reported in the manuscript, the proposed limited memory preconditioner formula has been also implemented in a parallel distributed memory environment within $Code\_Aster$. In practice, this straightforward extension allows us to consider selected large-scale industrial problems in a limited amount of computational time on a moderate number of cores. This is especially useful in an industrial setting. Finally, we would like to mention that current investigations focus on the derivation and analysis of preconditioner update formulas, in the case where the original preconditioned matrix is not symmetric. In addition, when the original matrix is symmetric, this extension would also allow us to consider a broader class of first-level preconditioners and to provide a complete picture of the performance of preconditioned Krylov subspace methods. This is a topic of a forthcoming study.

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