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Global symplectic Lanczos method with application to matrix exponential approximation

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Abstract. It is well-known that the symplectic Lanczos method is an efficient tool for computing a few eigenvalues of large and sparse Hamiltonian matrices. A variety of block Krylov subspace methods were introduced by Lopez and Simoncini to compute an approximation of $\exp(M)V$ for a given large square Hamiltonian matrix M and a tall and skinny matrix V that preserves the geometric property of V. For the same purpose, in this paper, we have proposed a new method based on a global version of the symplectic Lanczos algorithm, called the global J-Lanczos method (GJ-Lanczos). To the best of our knowledge, this is probably the first adaptation of the symplectic Lanczos method in the global case. Numerical examples are given to illustrate the effectiveness of the proposed approach.

Keywords: Hamiltonian matrix, skew-Hamiltonian matrix, symplectic matrix, global symplectic Lanczos method.
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1 Introduction

Global Krylov subspace methods have received considerable attention in recent years, due to their efficiency for solving large and sparse linear systems. Some classes of these methods have been introduced in [22, 23], such as the global Lanczos-based method, the global full orthogonalization method (Gl-FOM), and the global generalized minimal residual (Gl-GMRES) based on the global Arnoldi process to solve a linear system of equations with multiple right-hand sides. Heyouni in [19] proposed the global Hessenberg (Gl-Hess) method and the global changing minimal residual method based on the Hessenberg process (Gl-CMRH). The global bi-conjugate gradient method (Gl-BCG) and global BiCGSTAB algorithm (Gl-BiCGSTAB) based on global oblique projections of the initial residual onto a matrix Krylov subspace have also been developed in [24, 31]. Later, in 2016, improved variants of the global methods for the simultaneous solutions of large and sparse linear systems whose coefficient matrix

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is non-Hermitian were discussed in [30]. Other global versions of Krylov subspace methods can be found in [2, 11, 17–19, 25, 26, 29, 33–37]. In this paper, motivated by some ideas, we propose a new approach of global Krylov subspace methods. More precisely, we introduce a global version of the symplectic Lanczos algorithm (also called global J-Lanczos) based on a J-tridiagonalization procedure that reduces a large sparse $2n \times 2n$ Hamiltonian matrix to a small $2m \times 2m$, ($m \ll n$) Hamiltonian J-tridiagonal matrix in the form

$$\left(\begin{array}{cccc|cccc}
* & * & & & * & & & \\
* & \ddots & \ddots & & & \ddots & & \\
& \ddots & \ddots & * & & & \ddots & \\
& & * & * & & & & * \\
\hline
* & & & & * & * & & \\
& \ddots & & & * & \ddots & \ddots & \\
& & \ddots & & & \ddots & \ddots & * \\
& & & * & & & * & *
\end{array}\right).$$

Many applications in several engineering areas adopt the Hamiltonian structure of matrices in the numerical solution of large systems. Especially the related problems of solving Riccati algebraic equations [21], such as Gerstner and Mehrmann proposed in [6] an algorithm to reduce a Hamiltonian matrix to the J-Hessenberg Hamiltonian form based on symplectic transformations of type QR via an SR factorization with symplectic similarity transformations to solve an algebraic Riccati equation. The Hamiltonian form is also used by Lin, and Wang [13, 14] to construct a J-Lanczos algorithm for solving large sparse Hamiltonian eigenvalue problem which arises in both continuous-time and discrete-time optimal control applications. Inspired by certain results, we have presented in this work an approach to approximate the exponential Hamiltonian matrix operator $\exp(M)V$ for a given large square Hamiltonian matrix M and a tall-and-skinny matrix V preserving the geometric property of V by using the proposed global J-Lanczos method whose corresponding orthogonalization process is shorter due to the reduction of the number of multiplications performed "matrix-vector" or "matrix-matrix" and easier to implement compared to the one used in the block J-Lanczos Krylov method, which makes the algorithm less costly and thus moderately increases the numerical stability. The approximation procedure for $\exp(M)V$ that preserves structural properties of the associated matrices plays an important role in several areas of applied mathematics. It can be exploited to solve systems of ordinary differential equations (ODEs) or time-dependent partial differential equations (PDEs). Many researchers have been interested in the approximation of the given matrix-vector product $\exp(M)v$ and its applications, via Krylov subspace methods, for example, Friesner and his collaborators [15], and Gallopoulos and Saad [16] have presented some ways to apply this approximation to solve systems of ordinary differential equations.

The main difference between the standard global Lanczos method and the global J-Lanczos method is that the first one uses a Euclidean space structure on $\mathbb{R}$ with Frobenius inner product while the second uses $\mathbb{R}^{2n\times 2s}$ as free $\mathbb{K}$-module with a Frobenius inner-like product on the ring $\mathbb{K} = \mathbb{R}^{2\times 2}$, to generate a J^s-orthonormal basis of the Krylov subspace $K_k(M,V) = span\{V, MV, \ldots, M^{k-1}V\}$ for a given $2n$-by-$2n$ Hamiltonian matrix M and a $2n$-by-$2s$ rectangular matrix V where $s \ll n$. The remainder of this paper is organized as follows. We start by introducing some definitions related to the J-structure matrices. Some basic notation and terminology are reviewed in Section 2. In Section 3, we present, in detail, our proposed approach of the global J-Lanczos method. To describe the process, we develop a new variant of the symplectic normalization, which is named "the global J^s-normalization". In Section 4, we are interested in finding an approximation of $\exp(M)V$ using the proposed global J-Lanczos algorithm. Numerical comparisons are made with other known iterative methods in Section 5 to show the performance of the method presented in this work.

2 Terminology, notation, and some basic facts

In this section, we present some basic concepts and notions that will be used throughout this paper. Some of the results in this paragraph are borrowed from [1, 3]. The J-transpose of any $2n$-by-$2p$ real matrix M is defined from the usual transpose T by $M^J = J_{2p}^T M^T J_{2n} \in \mathbb{R}^{2p\times 2n}$ where the skew-symmetric matrix $J_{2n} = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix}$, I_n and 0_n denote the $n\times n$ identity and zero matrices, respectively. It is obvious that J_{2n} is a real orthogonal skew-symmetric matrix, that is, $J_{2n}^{-1} = J_{2n}^T = -J_{2n}$. We will drop the subscripts n and $2n$ whenever the dimension is clear from its context. Any matrix $M \in \mathbb{R}^{2n\times 2n}$ has the explicit block structure $M = \begin{pmatrix} A & R \\ G & -A^T \end{pmatrix}$, where $A, G, R \in \mathbb{R}^{n\times n}$ and $G = G^T$, $R = R^T$ is called Hamiltonian. By a simple algebraic manipulation, we can show that a Hamiltonian matrix M is equivalently defined by $M^J = -M$. Similarly, a matrix $M \in \mathbb{R}^{2n\times 2n}$ is skew-Hamiltonian if and only if $M^J = M$, and it has the form $M = \begin{pmatrix} A & R \\ G & A^T \end{pmatrix}$, where $A, G, R \in \mathbb{R}^{n\times n}$ and $G = -G^T$, $R = -R^T$. Any matrix $S \in \mathbb{R}^{2n\times 2p}$ satisfying $S^T J_{2n} S = J_{2p}$ or equivalently, $S^J S = I_{2p}$ is called a symplectic matrix.

Proposition 1. *Let $E_i = [e_i, e_{n+i}]$ for $i = 1, \dots, n$, where e_i denotes the i-th unit vector of length $2n$. Then*

$$E_i J_2 = J_{2n} E_i,\ E_i^J = E_i^T \text{ and } E_i^T E_j = \delta_{ij} I_2,$$

where

$$E_i^J = J_2^T E_i^T J_{2n} \text{ and } \delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

More generally, given k, s $\in \mathbb{N}$ such that $n = ks$, we define the set $(F_i)_{1\le i\le k}$ as

$$F_i = [e_{(i-1)s+1}, e_{(i-1)s+2}, \dots, e_{is}, e_{n+(i-1)s+1}, e_{n+(i-1)s+2}, \dots, e_{n+is}] \in \mathbb{R}^{2n\times 2s}.$$

Then, we have

$$F_i J_{2s} = J_{2n} F_i,\ F_i^J = F_i^T \text{ and } F_i^T F_j = \delta_{ij} I_{2s},$$

where

$$F_i^J = J_{2s}^T F_i^T J_{2n} \text{ and } \delta_{ij} = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases}$$

Proposition 2. *Any matrix $\tilde{U} \in \mathbb{R}^{2n\times 2s}$ can be uniquely expressed as a finite linear combination of*

$(F_i)_{1\le i\le k}$, *in form* $\tilde{U}=\sum_{i=1}^k F_iU_i$, *with*

$$U_i=\left(\begin{array}{ccc|ccc} u_{(i-1)s+1,1} & \cdots & u_{(i-1)s+1,s} & u_{(i-1)s+1,s+1} & \cdots & u_{(i-1)s+1,2s}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ u_{is,1} & \cdots & u_{is,s} & u_{is,s+1} & \cdots & u_{is,2s}\\ \hline u_{n+(i-1)s+1,1} & \cdots & u_{n+(i-1)s+1,s} & u_{n+(i-1)s+1,s+1} & \cdots & u_{n+(i-1)s+1,2s}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ u_{n+is,1} & \cdots & u_{n+is,s} & u_{n+is,s+1} & \cdots & u_{n+is,2s} \end{array}\right)\in\mathbb{R}^{2s\times 2s}.$$

Proposition 3. *Let M be a $2n$-by-$2n$ real matrix, where $n=ks$ with k, $s\in\mathbb{N}$. Then M can be represented uniquely as $M=\sum_{i=1}^k\sum_{j=1}^k F_iM_{ij}F_j^T$, where $M_{ij}\in\mathbb{R}^{2s\times 2s}$ is given by*

$$\left(\begin{array}{ccc|ccc} m_{(i-1)s+1,(j-1)s+1} & \cdots & m_{(i-1)s+1,js} & m_{(i-1)s+1,n+(j-1)s+1} & \cdots & m_{(i-1)s+1,n+js}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ m_{is,(j-1)s+1} & \cdots & m_{is,js} & m_{is,n+(j-1)s+1} & \cdots & m_{is,n+js}\\ \hline m_{n+(i-1)s+1,(j-1)s+1} & \cdots & m_{n+(i-1)s+1,js} & m_{n+(i-1)s+1,n+(j-1)s+1} & \cdots & m_{n+(i-1)s+1,n+js}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ m_{n+is,(j-1)s+1} & \cdots & m_{n+is,js} & m_{n+is,n+(j-1)s+1} & \cdots & m_{n+is,n+js} \end{array}\right).$$

Proposition 4. *A matrix M given by $M=\sum_{i=1}^k\sum_{j=1}^k F_iM_{ij}F_j^T$ is Hamiltonian (respectively, skew-Hamiltonian) if $M_{ij}^J=-M_{ji}$ (respectively, $M_{ij}^J=M_{ji}$).*

Proof. This result is obvious since $M^J=\sum_{i=1}^k\sum_{j=1}^k F_iM_{ji}^JF_j^T$. □

Definition 1. *A matrix $M=\sum_{i=1}^k\sum_{j=1}^k F_iM_{ij}F_j^T\in\mathbb{R}^{2n\times 2n}$ is called in block upper J-triangular form if $M_{ij}=0_{2s}$ for $i>j$ and M_{ii} is upper triangular. It is called in block J-Hessenberg form if $M_{ij}=0_{2s}$ for $i>j+1$, and in block J-tridiagonal form if $M_{ij}=0_{2s}$ when $i<j-1$ or $i>j+1$.*

Remark 1. *A Hamiltonian block J-Hessenberg matrix is in block J-tridiagonal form.*

Let us now define and give some properties of what we will call the J^s-diamond product $\diamond_{J^s}$ and the s-star product $*_s$ that we will use to describe our approach to the global J-Lanczos method. Note that the s-star product is used here instead of the Kronecker product only for notational convenience.

Definition 2. (s-star product) *For a given s, let $X=[X_1,X_2,\ldots,X_k]\in\mathbb{R}^{n\times ks}$, where the blocks X_i for $1\le i\le k$ are $n\times s$ matrices, and let ν be a vector in $\mathbb{R}^k$. Then the s-star product of X and ν, which we denote by $X*_s\nu$, is defined as follows*

$$X*_s\nu=\sum_{i=1}^k \nu_iX_i.$$

Given now a matrix $H\in\mathbb{R}^{k\times r}$, the $*_s$-product of H and X is defined by

$$X*_sH=[X*_sH(:,1),X*_sH(:,2),\ldots,X*_sH(:,r)],$$

where $H(:,i)$ denotes the i-th column of H.

Remark 2. *It can be readily verified that*

$$X *_s \nu = X(\nu \otimes I_s),$$

$$X *_s H = X(H \otimes I_s),$$

where the symbol $\otimes$ denotes the Kronecker product.

Proposition 5. *Let $A, B \in \mathbb{R}^{n \times ks}$, $H \in \mathbb{R}^{k \times r}$, $G \in \mathbb{R}^{r \times t}$ and let $\alpha \in \mathbb{R}$. Then we have the following properties:*

$$\begin{aligned} (A+B) *_s H &= A *_s H + B *_s H, \\ A *_s (\alpha H) &= \alpha (A *_s H), \\ (A *_s H) *_s G &= A *_s (HG). \end{aligned} \tag{1}$$

The main ingredient to describe our method is the J^s-diamond product $\diamond_{J^s}$ which we define below and then give some interesting properties.

Definition 3. ***(J^s-diamond product)*** *For a given s, let $U = [U_1 \,,\, U_2] \in \mathbb{R}^{2n \times 2s}$ and $V = [V_1 \,,\, V_2] \in \mathbb{R}^{2n \times 2s}$ where U_i and V_i are $2n \times s$ matrices, for $i = 1, 2$. The J^s-diamond product of U and V denoted $V \diamond_{J^s} U$ is defined by*

$$V \diamond_{J^s} U = \begin{pmatrix} -tr(V_2^T J U_1) & -tr(V_2^T J U_2) \\ tr(V_1^T J U_1) & tr(V_1^T J U_2). \end{pmatrix}$$

Remark 3. *1) $U \diamond_{J^s} U = tr(U_1^T J U_2) I_2$.*

2) If $s = 1$, assuming that $U = [u_1 \;\; u_2]$ and $V = [v_1 \;\; v_2] \in \mathbb{R}^{2n \times 2}$, the J^s-diamond product $V \diamond_{J^s} U$ is nothing else than the matrix product $V^J U$. Indeed,

$$\begin{aligned} V \diamond_{J^s} U &= \begin{pmatrix} -v_2^T J u_1 & -v_2^T J u_2 \\ v_1^T J u_1 & v_1^T J u_2 \end{pmatrix} \\ &= J^T V^T J U \\ &= V^J U. \end{aligned}$$

Proposition 6. *Let $A = [A_1, A_2, \ldots, A_{2p}] \in \mathbb{R}^{2n \times 2ps}$ and $B = [B_1, B_2, \ldots, B_{2l}] \in \mathbb{R}^{2n \times 2ls}$, where A_i and B_j are blocks of size $2n \times s$, for $1 \le i \le 2p$ and $1 \le j \le 2l$. Then, the J^s-diamond product $A \diamond_{J^s} B$ is the $2p$-by-$2l$ real matrix given by*

$$A \diamond_{J^s} B = \sum_{i=1}^{p} \sum_{j=1}^{l} E_i \begin{pmatrix} -tr(A_{p+i}^T J B_j) & -tr(A_{p+i}^T J B_{l+j}) \\ tr(A_i^T J B_j) & tr(A_i^T J B_{l+j}) \end{pmatrix} E_j^T.$$

Note that $E_i = [e_i, e_{p+i}]$ for $i = 1, \ldots, p$ and $E_j = [e_j, e_{l+j}]$ for $j = 1, \ldots, l$, where e_i, e_{p+i} denote the i-th and $(p+i)$-th unit vector of length $2p$, respectively, and e_j, e_{l+j} correspond to the j-th and $(l+j)$-th unit vector of length $2l$, respectively.

Lemma 1. *According to the definition of the J^s-diamond product, we have*

$$A \diamond_{J^s} B = \sum_{i=1}^{p}\sum_{j=1}^{l} E_i\left([A_i, A_{p+i}] \diamond_{J^s} [B_j, B_{l+j}]\right) E_j^T.$$

Moreover, it is easy to see that

$$(A \diamond_{J^s} B)^J = B \diamond_{J^s} A. \tag{2}$$

Proposition 7. *Let $A \in \mathbb{R}^{2n\times 2ps}$, $B, C \in \mathbb{R}^{2n\times 2ls}$ and let $\alpha \in \mathbb{R}$. It's easy to prove that*

$$\begin{aligned} A \diamond_{J^s} (B+C) &= A \diamond_{J^s} B + A \diamond_{J^s} C, \\ A \diamond_{J^s} (\alpha B) &= \alpha (A \diamond_{J^s} B). \end{aligned} \tag{3}$$

Proposition 8. *Let $A = [A_1, A_2, \ldots, A_{2p}] \in \mathbb{R}^{2n\times 2ps}$ and $B = [B_1, B_2, \ldots, B_{2l}] \in \mathbb{R}^{2n\times 2ls}$, where A_i and B_j are $2n \times s$ matrices, for $1 \le i \le 2p$ and $1 \le j \le 2l$, respectively, and let $v \in \mathbb{R}^{2l\times 2}$, $G \in \mathbb{R}^{2p\times 2r}$, $H \in \mathbb{R}^{2l\times 2t}$ and $M \in \mathbb{R}^{2n\times 2n}$. Then we have the following relations*

$$A \diamond_{J^s} (B *_s v) = (A \diamond_{J^s} B) v, \tag{4}$$

$$A \diamond_{J^s} (B *_s H) = (A \diamond_{J^s} B) H, \tag{5}$$

$$(MA) \diamond_{J^s} B = A \diamond_{J^s} (M^J B), \tag{6}$$

$$(A *_s G) \diamond_{J^s} (B *_s H) = G^J (A \diamond_{J^s} B) H, \tag{7}$$

where the superscript J refers to the J-transpose.

Proof. Formulas (4), (5) and (6) are easy to get. However, formula (7) can be proved using formulas (2), (5) and (6). □

In the following, we define the orthogonality and the normalization on $\mathbb{R}^{2n\times 2s}$ in the global symplectic context.

Definition 4. *For a given s, let $U = [U_1\ ,\ U_2]$ and $V = [V_1\ ,\ V_2]$ be two $2n \times 2s$ matrices, with U_i, $V_i \in \mathbb{R}^{2n\times s}$ for $i = 1,\ 2$. Then,*

1) *U and V are J^s-orthogonal if their inner-like product $V \diamond_{J^s} U = 0_{2\times 2}$.*

2) *V is said to be J^s-normed if $V \diamond_{J^s} V = I_2$.*

3) *U is said non-isotropic if $tr(U_1^T J U_2) \neq 0$.*

Lemma 2. (Global J^s-normalization) *Let $U = [U_1\ ,\ U_2] \in \mathbb{R}^{2n\times 2s}$ be a non-isotropic matrix (i.e. $tr(U_1^T J U_2) \neq 0$; $U_i \in \mathbb{R}^{2n\times s}$ for $i = 1,\ 2$). The $2n \times 2s$ matrix $V = U *_s C^{-1}$, where*

$$C = \begin{cases} \sqrt{\alpha} I_2, & \text{if } \alpha > 0, \\ \sqrt{-\alpha}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, & \text{if } \alpha < 0, \end{cases} \qquad \text{with } \alpha = tr(U_1^T J U_2), \tag{8}$$

is called the J^s-normalized matrix associated to U, which satisfies $V \diamond_{J^s} V = I_2$. The 2-by-2 diagonal matrix C is called the global J^s-norm of U and verifies $U \diamond_{J^s} U = C^J C = \alpha I_2$.

Proof. Since $U \diamond_{J^s} U = C^J C = \alpha I_2$, and using formula (7), we have

$$\begin{aligned} V \diamond_{J^s} V &= (U *_s C^{-1}) \diamond_{J^s} (U *_s C^{-1}) \\ &= C^{-J} (U \diamond_{J^s} U) C^{-1} \\ &= I_2. \end{aligned}$$

□

Proposition 9. *If $V = [V_1,\, V_2] \in \mathbb{R}^{2n\times 2s}$ is a symplectic matrix, then $V \diamond_{J^s} V = sI_2$ (i.e. $\frac{1}{\sqrt{s}}V$ is J^s-normed).*

Proof. Since V is symplectic, we have

$$V^J V = \begin{pmatrix} -V_2^T J V_1 & -V_2^T J V_2 \\ V_1^T J V_1 & V_1^T J V_2 \end{pmatrix} = I_{2s},$$

which implies that

$$V \diamond_{J^s} V = \begin{pmatrix} -tr(V_2^T J V_1) & -tr(V_2^T J V_2) \\ tr(V_1^T J V_1) & tr(V_1^T J V_2) \end{pmatrix} = sI_2.$$

□

3 Global J-Lanczos method

In this section, we propose a global version of the symplectic Lanczos method that relies on simple recurrence formulas based on the global J^s-normalization defined above. In the following, the dimension of the elements of the basis $(E_i)_{1\le i\le n}$ and $(F_i)_{1\le i\le k}$ are given according to the context. In analogy to the standard Lanczos, the scheme proposed here is that for a given Hamiltonian matrix $M \in \mathbb{R}^{2n\times 2n}$, we construct a J^s-orthonormal basis $Q_k = [q_1,\ldots,q_k,q_{k+1},\ldots,q_{2k}] \in \mathbb{R}^{2n\times 2ks}$ ($k \le n$) of the Krylov subspace $K_k(M,V) = span\{V, MV, \ldots, M^{k-1}V\}$, where the matrix $V \in \mathbb{R}^{2n\times 2s}$ is such that $s << n$. The column blocks q_i for $i = 1,\ldots,2k$ are in $\mathbb{R}^{2n\times s}$. We also construct the $2k$-by-$2k$ Hamiltonian J-tridiagonal matrix H_k satisfying the global symplectic Lanczos relationship $MQ_k = Q_k *_s H_k + (V_{k+1} *_s C_k) F_{k+1}^T$, where $V_{k+1} \in \mathbb{R}^{2n\times 2s}$ is J^s-orthogonal to Q_k (i.e., $Q_k \diamond_{J^s} V_{k+1} = 0_{2k\times 2}$). Note that the reduced matrix H_k remains Hamiltonian and has the following J-tridiagonal form

$$H_k = \left(\begin{array}{ccccc|ccccc} a_1 & c_1 & & & & \beta_1 & & & & \\ b_1 & a_2 & c_2 & & & & \beta_2 & & & \\ & \ddots & \ddots & \ddots & & & & \ddots & & \\ & & \ddots & \ddots & c_{k-1} & & & & \ddots & \\ & & & b_{k-1} & a_k & & & & & \beta_k \\ \hline \gamma_1 & & & & & -a_1 & -b_1 & & & \\ & \gamma_2 & & & & -c_1 & -a_2 & -b_2 & & \\ & & \ddots & & & & \ddots & \ddots & \ddots & \\ & & & \ddots & & & & \ddots & \ddots & -b_{k-1} \\ & & & & \gamma_k & & & & -c_{k-1} & -a_k \end{array}\right), \quad (9)$$

with γ_i, β_i, a_i, b_i, c_i, $\in \mathbb{R}$, where $b_i \ne 0$ and $c_i \ne 0$ for $i = 1,\ldots,k$.

3.1 Global J-Lanczos process

We start by identifying on both sides of the equality $MQ_k = Q_k *_s H_k + (V_{k+1} *_s C_k) F_{k+1}^T$, the i-th and $(k+i)$-th s-block columns q_i and q_{k+i}, respectively. Then we get, for $i = 1, \dots, k$,

$$\begin{cases} Mq_i = c_{i-1}q_{i-1} + a_i q_i + b_i q_{i+1} + \gamma_i q_{k+i}, \\ Mq_{k+i} = \beta_i q_i - b_{i-1}q_{k+i-1} - a_i q_{k+i} - c_i q_{k+i+1}. \end{cases} \tag{10}$$

Note that $b_0 = 0$ and $c_0 = 0$. The J^s-orthonormality of the matrix Q_k which is expressed by

$$Q_k \diamond_{J^s} Q_k = \sum_{i=1}^{k} \sum_{j=1}^{k} E_i \begin{pmatrix} -tr(q_{k+i}^T J q_j) & -tr(q_{k+i}^T J q_{k+j}) \\ tr(q_i^T J q_j) & tr(q_i^T J q_{k+j}) \end{pmatrix} E_j^T = I_{2k},$$

leads to $tr(q_i^T J q_{k+i}) = 1$ for all $i = 1, \dots k$, while the other traces are equal to zero. Using equations (3) and (5), we find

$$Q_k \diamond_{J^s} MQ_k = Q_k \diamond_{J^s} \left(Q_k *_s H_k + (V_{k+1} *_s C_k) F_{k+1}^T\right) = H_k.$$

Therefore, the coefficients a_i, γ_i and β_i can be determined as follows,

$$\begin{cases} a_i = -tr(q_{k+i}^T JMq_i), \\ \beta_i = -tr(q_{k+i}^T JMq_{k+i}), \qquad \text{for } \ i = 1, \dots, k. \\ \gamma_i = tr(q_i^T JMq_i), \end{cases}$$

On the other hand, if we combine the two equations of system (10), we obtain

$$\begin{aligned} M[q_i, q_{k+i}] = {} & [q_{i-1}, q_{k+i-1}] *_s \underbrace{\begin{pmatrix} c_{i-1} & 0 \\ 0 & -b_{i-1} \end{pmatrix}}_{h_{i-1,i}} + [q_i, q_{k+i}] *_s \underbrace{\begin{pmatrix} a_i & \beta_i \\ \gamma_i & -a_i \end{pmatrix}}_{h_{i,i}} \\ & + [q_{i+1}, q_{k+i+1}] *_s \underbrace{\begin{pmatrix} b_i & 0 \\ 0 & -c_i \end{pmatrix}}_{h_{i+1,i}}. \end{aligned} \tag{11}$$

Setting

$$\begin{cases} V_{i-1} = [q_{i-1} \ , \ q_{k+i-1}], \\ V_i = [q_i \ , \ q_{k+i}], \\ V_{i+1} = [q_{i+1} \ , \ q_{k+i+1}], \end{cases}$$

and

$$\begin{cases} T_i = h_{i,i} = \begin{pmatrix} a_i & \beta_i \\ \gamma_i & -a_i \end{pmatrix}, \\ C_i = h_{i+1,i} = -h_{i,i+1}^J = \begin{pmatrix} b_i & 0 \\ 0 & -c_i \end{pmatrix}. \end{cases} \tag{12}$$

The relation (11) can thus be reformulated as follows

$$MV_i = -V_{i-1} *_s C_{i-1}^J + V_i *_s T_i + V_{i+1} *_s C_i.$$

The main steps of the global J-Lanczos algorithm can be illustrated as follows.

Algorithm 1 The global J-Lanczos method (GJ-Lanczos)

Input: A Hamiltonian matrix $M \in \mathbb{R}^{2n\times 2n}$ and a J^s-normed matrix $V_1 = [q_1, q_{k+1}] \in \mathbb{R}^{2n\times 2s}$ (i.e. $V_1 \diamond_{J^s} V_1 = I_2$) with $k << n$ and $q_1,\ q_{k+1} \in \mathbb{R}^{2n\times s}$.

Output: The J^s-orthonormal matrix $Q_k = [q_1, \dots, q_k, q_{k+1}, \dots, q_{2k}] \in \mathbb{R}^{2n\times 2ks}$ and the Hamiltonian J-tridiagonal matrix $H_k \in \mathbb{R}^{2k\times 2k}$ such that $Q_k \diamond_{J^s} M Q_k = H_k$.

Initialize: $V_0 = 0_{2n\times 2s}$, $h_{0,1} = C_0 = 0_{2\times 2}$,

for $i = 1, 2, \dots, k$ **do**

$h_{i,i} = T_i = V_i \diamond_{J^s} M V_i$

$\Lambda_i = MV_i + V_{i-1} *_s C^J_{i-1} - V_i *_s T_i$.

Global J^s-Normalization step (see, lemma 2) $\begin{cases} \Lambda_i = V_{i+1} *_s C_i \\ with\ \ [q_{i+1}, q_{k+i+1}] = V_{i+1}\ \ and\ \ h_{i+1,i} = -h^J_{i,i+1} = C_i. \end{cases}$

end for

Set $Q_k = \sum_{i=1}^{k} V_i F_i^T$ and $H_k = \sum_{j=1}^{k} \sum_{i=\max(j-1,1)}^{\min(j+1,k)} E_i h_{ij} E_j^T$.

Remark 4. *It should be noted that the algorithm outlined above may suffer from breakdown if the matrix Λ_i is isotropic at a certain step i. Otherwise, the basis generated by this algorithm is J^s-orthonormal which means that $Q_k \diamond_{J^s} Q_k = I_{2k}$. This comes from the fact that, by construction, $V_i \diamond_{J^s} V_j = \delta_{i,j} I_2$ for $i, j = 1, \dots k$, where*

$$\delta_{i,j} = \begin{cases} 1, & if\ j = i, \\ 0, & if\ j \neq i, \end{cases}$$

denotes Kronecker's symbol.

The results presented in the following lemma will be useful later to derive some basic relations of our new method.

Lemma 3. *Suppose $Q_k = [q_1, \dots, q_k, q_{k+1}, \dots, q_{2k}] \in \mathbb{R}^{2n\times 2ks}$, and $H_k \in \mathbb{R}^{2k\times 2k}$ are defined as above, and let $V \in \mathbb{R}^{2n\times 2s}$. Then*

$$Q_k \diamond_{J^s} (V F_i^T) = (Q_k \diamond_{J^s} V) E_i^T, \tag{13}$$

$$(Q_k *_s H_k) F_i = Q_k *_s (H_k E_i). \tag{14}$$

Proof. It is obvious, $F_i = E_i \otimes I_s$, which gives

$$\begin{aligned} Q_k \diamond_{J^s} (V F_i^T) &= Q_k \diamond_{J^s} (V(E_i^T \otimes I_s)), \\ &= Q_k \diamond_{J^s} (V *_s E_i^T), \\ &= (Q_k \diamond_{J^s} V) E_i^T. \end{aligned}$$

On the other hand, we have

$$\begin{aligned} (Q_k *_s H_k) F_i &= (Q_k (H_k \otimes I_s)) F_i, \\ &= Q_k ((H_k \otimes I_s) F_i), \\ &= Q_k ((H_k E_i) \otimes I_s), \\ &= Q_k *_s (H_k E_i). \end{aligned}$$

□

Theorem 1. *According to Algorithm 1, the following relationships are derived*

$$\begin{aligned} MQ_k &= Q_k *_s H_k + (V_{k+1} *_s h_{k+1,k})F_k^T, \\ Q_k \diamond_{J^s} MQ_k &= H_k, \end{aligned}$$

where H_k has the same Hamiltonian structure as the matrix M.

Proof. From Algorithm 1, we have

$$MQ_kF_i = MV_i = V_{i-1} *_s h_{i-1,i} + V_i *_s h_{i,i} + V_{i+1} *_s h_{i+1,i}.$$

Given that $Q_k = \sum_{j=1}^{k} V_j F_j^T$, $H_k = \sum_{j=1}^{k} \sum_{i=\max(j-1,1)}^{\min(j+1,k)} E_i h_{ij} E_j^T$ and with formula (13) of Lemma 3, we obtain

$$\begin{aligned} MQ_kF_i &= V_{i-1} *_s h_{i-1,i} + V_i *_s h_{i,i} + V_{i+1} *_s h_{i+1,i}, \\ &= Q_k *_s H_k E_i, \\ &= (Q_k *_s H_k)F_i \quad for\ i = 1,\dots,k-1. \end{aligned}$$

It follows that, for $i = k$,

$$\begin{aligned} MQ_kF_k &= MV_k, \\ &= Q_k *_s H_k E_k + V_{k+1} *_s h_{k+1,k}, \\ &= (Q_k *_s H_k)F_k + V_{k+1} *_s h_{k+1,k}, \end{aligned}$$

from which, we deduce that

$$MQ_k = Q_k *_s H_k + (V_{k+1} *_s h_{k+1,k})F_k^T.$$

The second relationship is proven using formulas (4) and (5). Indeed,

$$\begin{aligned} Q_k \diamond_{J^s} MQ_k &= Q_k \diamond_{J^s} (Q_k *_s H_k) + Q_k \diamond_{J^s} (V_{k+1} *_s h_{k+1,k})F_k^T, \\ &= \underbrace{(Q_k \diamond_{J^s} Q_k)}_{I_{2k}} H_k + [Q_k \diamond_{J^s} (V_{k+1} *_s h_{k+1,k})]E_k^T, \\ &= H_k + [\underbrace{(Q_k \diamond_{J^s} V_{k+1})}_{0_{2k\times 2}} h_{k+1,k}]E_k^T, \\ &= H_k. \end{aligned}$$

Moreover, it is easy to verify via formulas (2) and (6) that H_k has the same Hamiltonian structure as the matrix M. □

Remark 5. *If M is skew-Hamiltonian, the matrix H_k resulting from applying Algorithm1 to M,preserves the same skew-Hamiltonian structure, i.e. $H_k^J = (Q_k \diamond_{J^s} MQ_k)^J = H_k$.*

Theorem 2. *Suppose that the matrix M is Hamiltonian and skew-symmetric. If $V_1 = [q_1\ ,\ q_{k+1}] \in \mathbb{R}^{2n\times 2s}$ is such that $q_{k+1} = -Jq_1$, then the blocks $(q_l)_l$ generated by Algorithm1 are verifying $q_{k+i} = -Jq_i$ for $i = 1,\dots,k$. Moreover, the reduced matrix H_k is also Hamiltonian and skew-symmetric.*

Proof. The matrix M is Hamiltonian and skew-symmetric, this yields $JM = MJ$. We first show, by induction, that $q_{k+i} = -Jq_i$ for $i = 1,\dots,k$ which is true for $i = 1$ according to the hypothesis. From Algorithm1, taking into account that $q_{k+i-1} = -Jq_{i-1}$ and $q_{k+i} = -Jq_i$ for a given $i \leq k-1$, we have

$$\begin{aligned} T_i &= V_i \diamond_{J^s} MV_i \\ &= \begin{pmatrix} -tr(q_{k+i}^T JMq_i) & -tr(q_{k+i}^T JMq_{k+i}) \\ tr(q_i^T JMq_i) & tr(q_i^T JMq_{k+i}) \end{pmatrix} \\ &= \begin{pmatrix} tr(q_i^T Mq_i) & -tr(q_i^T JMq_i) \\ tr(q_i^T JMq_i) & tr(q_i^T Mq_i) \end{pmatrix} \\ &= tr(q_i^T JMq_i) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \end{aligned}$$

This leads to $a_i = 0$ and $\beta_i = -\gamma_i$, and assuming $c_{i-1} = -b_{i-1}$, it follows from system (10)

$$\begin{cases} \Lambda_i^{(1)} = Mq_i + b_{i-1}q_{i-1} - \beta_i Jq_i, \\ \Lambda_i^{(2)} = -MJq_i - b_{i-1}Jq_{i-1} - \beta_i Jq_{k+i} = -J\Lambda_i^{(1)}. \end{cases}$$

This results in $C_i = \begin{pmatrix} b_i & 0 \\ 0 & -c_i \end{pmatrix} = \sqrt{\alpha} I_2$ with $\alpha = tr({\Lambda_i^{(1)}}^T J\Lambda_i^{(2)}) = tr({\Lambda_i^{(1)}}^T \Lambda_i^{(1)}) > 0$ as long as $\Lambda_i^{(1)} \neq 0_{2n\times s}$. Finally, we obtain $V_{i+1} = [q_{i+1}\ ,\ q_{k+i+1}] = \Lambda_i *_s C_i^{-1} = \frac{1}{b_i}[\Lambda_i^{(1)}\ ,\ -J\Lambda_i^{(1)}]$, which means that $q_{k+i+1} = -Jq_{i+1}$. This proves the desired result. Furthermore, according to Theorem 1, H_k is Hamiltonian, while the skew-symmetry is simply obtained from the structure of C_i and T_i. □

4 Approximation of the matrix exponential operator

The approximation of the matrix-matrix product $\exp(M)V$ for a large-scale square matrix M and a given tall matrix V is the focus of this paper. This interest comes from the vast role that approximation of the matrix exponential operator plays in many scientific areas. It's the key element of many exponential integrators to solve systems of ordinary differential equations (ODEs) or time-dependent partial differential equations (PDEs) [4]. The use of Krylov subspace approaches in this context has been proposed in the literature [1, 7, 8, 10, 12, 13, 20, 32]. The approximation procedure for $\exp(M)V$ taking into account structural properties of M and V is more efficient and more accurate when M is a Hamiltonian and skew-symmetric matrix or simply Hamiltonian. The preservation of geometric properties is necessary for the effectiveness of some geometric integration methods [9, 28]. Structure-preserving methods can be used, for example, to compute Lyapunov exponents of dynamical systems and geodesics (see [5, 7]). Our goal in this section is to present a structure-preserving approximation of the matrix-matrix product $\exp(M)V$, applying global J-Lanczos process for a given $2n$-by-$2n$ Hamiltonian, skew-symmetric matrix M and a $2n$-by-$2s$ rectangular matrix V ($s \ll n$). The proposed approach is new, differs from those given in [1, 27], and seems to give better results.

The next lemma provides an important result given in [27] which will be of interest in the later discussion.

Lemma 4. *If M is a $2n \times 2n$ real Hamiltonian matrix, then $\exp(M)$ is symplectic. If M is in addition skew-symmetric, then $\exp(M)$ is orthogonal and symplectic.*

Proof. Indeed, $\exp(M)^J \exp(M) = \exp(M^J)\exp(M) = \exp(-M)\exp(M) = I_{2n}$, and the same result remains true for the superscript T. □

In the following theorem, we will have an approximation of $\exp(M)V$ that preserves the global J^s-norm of V defined in Lemma 2.

Theorem 3. *Let $M \in \mathbb{R}^{2n\times 2n}$ be a Hamiltonian matrix, and $V = \left[\tilde{V_1}, \tilde{V_2}\right] \in \mathbb{R}^{2n\times 2s}$ where $\tilde{V_1}$, $\tilde{V_2} \in \mathbb{R}^{2n\times s}$, and C is its global J^s-norm (defined in Lemma 2). Assuming that Q_k and H_k are generated by Algorithm* 1. *Then, for any polynomial p_{k-1} of degree less than $k-1$, the following formula is satisfied.*

$$p_{k-1}(M)(V) = Q_k *_s (p_{k-1}(H_k)E_1C).$$

It follows that

$$\exp(M)V \simeq Q_k *_s (\exp(H_k)E_1C),$$

which verifies that $W_k \diamond_{J^s} W_k = V \diamond_{J^s} V = tr(\tilde{V_1}^T J\tilde{V_2})I_2$, with $W_k = Q_k *_s (\exp(H_k)E_1C)$.

Proof. Suppose that Q_k and H_k are the results of k steps of the global J-Lanczos algorithm. Then we have

$$MQ_k = Q_k *_s H_k + (V_{k+1} *_s h_{k+1,k})F_k^T \quad \text{and} \quad Q_k \diamond_{J^s} MQ_k = H_k.$$

It was shown that the J^s-normalized matrix associated with V is given by $V_1 = V *_s C^{-1}$, which leads to $V = V_1 *_s C = Q_kF_1 *_s C$. We will prove by induction that $M^iV = (Q_k *_s H_k^i)F_1 *_s C$, for $i = 0, 1, \ldots k-1$. The statement is obviously true for $i = 0$, as well as for $i = 1$, indeed,

$$\begin{aligned} MV &= M(Q_kF_1 *_s C), \\ &= MQ_kF_1 *_s C, \\ &= [(Q_k *_s H_k)F_1 + (V_{k+1} *_s h_{k+1,k})\underbrace{F_k^T F_1}_{0_{2s\times 2s}}] *_s C, \\ &= (Q_k *_s H_k)F_1 *_s C. \end{aligned}$$

Suppose that the result is true for a given $i \le k-2$, it implies that,

$$\begin{aligned} M^{i+1}V &= M[(Q_k *_s H_k^i)F_1 *_s C], \\ &= (MQ_k *_s H_k^i)F_1 *_s C, \\ &= \left[(Q_k *_s H_k) *_s H_k^i\right] F_1 *_s C + \underbrace{\left[((V_{k+1} *_s h_{k+1,k})F_k^T) *_s H_k^i\right] F_1}_{=0_{2n\times 2s}} *_s C, \\ &= (Q_k *_s H_k^{i+1})F_1 *_s C. \end{aligned}$$

We therefore conclude that, $p_{k-1}(M)V = (Q_k *_s p_{k-1}(H_k))F_1 *_s C$ for all polynomials p_{k-1} of degree $\le k-1$, which can also be written using formulas (1) and (14)

$$p_{k-1}(M)(V) = Q_k *_s (p_{k-1}(H_k)E_1C).$$

This eventually leads us to the following approximation

$$\exp(M)V \simeq Q_k *_s (\exp(H_k)E_1C).$$

Moreover, using formula (7), we obtain

$$\begin{aligned} W_k \diamond_{J^s} W_k &= \left[Q_k *_s (\exp(H_k)E_1C)\right] \diamond_{J^s} \left[Q_k *_s (\exp(H_k)E_1C)\right], \\ &= (\exp(H_k)E_1C)^J \left[Q_k \diamond_{J^s} Q_k\right] (\exp(H_k)E_1C), \\ &= C^J \left[E_1^J \exp(H_k)^J \underbrace{(Q_k \diamond_{J^s} Q_k)}_{=I_{2k}} \exp(H_k)E_1 \right] C, \\ &= C^J \left[E_1^J \underbrace{\exp(H_k)^J \exp(H_k)}_{=I_{2k}} E_1 \right] C, \\ &= C^J C, \end{aligned}$$

such that, according to Lemma 2, $C^J C = V \diamond_{J^s} V = tr(\tilde{V}_1^T J \tilde{V}_2) I_2$. □

Remark 6. *If V is given by $V = \left[\tilde{V}_1, -J\tilde{V}_1\right] \in \mathbb{R}^{2n\times 2s}$, and according to Theorem 2 and Lemma 4, if M, in addition to being Hamiltonian, is a skew-symmetric matrix, then* $\exp(H_k)$ *is both orthogonal and symplectic.*

5 Numerical experiments

The numerical examples below illustrate the effectiveness of the proposed global J-Lanczos method when applied to approximate an operator of the form $\exp(M)V$ by comparing our approach with those given in [1, 27] which based on the block symplectic Lanczos method. Using the Frobenius norm, we examine the accuracy of $W_k = Q_k *_s (\exp(H_k)E_1C)$ as an approximation of $\exp(M)V$ (i.e. $\|\exp(M)V - Q_k *_s (\exp(H_k)E_1C)\|_F$) when the dimension of Krylov's space k increases. The matrices in Example 1 are constructed similarly to the matrices in Example 3.4 described by Lopez and Simoncini in [27]. The $2n$-by-$2s$ matrix V is given by $V = [X, -JX]$, where $X = \exp(G)I_{2n\times s}$, with G being a $2n$-by-$2n$ skew-symmetric and Hamiltonian matrix derived in the same way as M. Here $I_{2n\times s}$ consists of the first s columns of the identity matrix I_{2n}. The test matrices used in Examples 2 and 3 are taken from the Matrix Market (`http://math.nist.gov/MatrixMarket/`). All our experiments were performed using Matlab 2015a. The vertical axis in all given figures represents $10 * \log_{10}$ of error except in Figures 3 and 6 where the error is represented directly.

Example 1. In this first example, we consider a 10000-by-10000 skew-symmetric and Hamiltonian matrix M defined as

$$M = \begin{pmatrix} M_1 & M_2 \\ -M_2 & M_1 \end{pmatrix},$$

where M_1 and M_2 are the 5000-by-5000 skew-symmetric and symmetric parts, respectively, of two different matrices with normally distributed random entries. For $s = 5$, varying m from 1 to 500,we obtain the error displayed in the Figure 1. In order to make a comparison between our approach and those given in ([1, 27]) simultaneously, we take $n = 1500$ and $s = 2$, we then obtain the error indicated in the Figures 2 and 3.

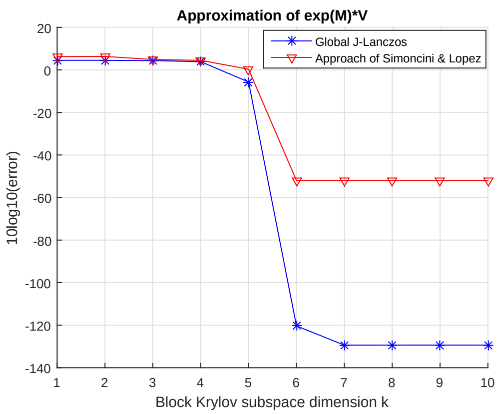

Figure 1: Error of the exponential approximation when $s = 5$ and k varies from 1 to 500.

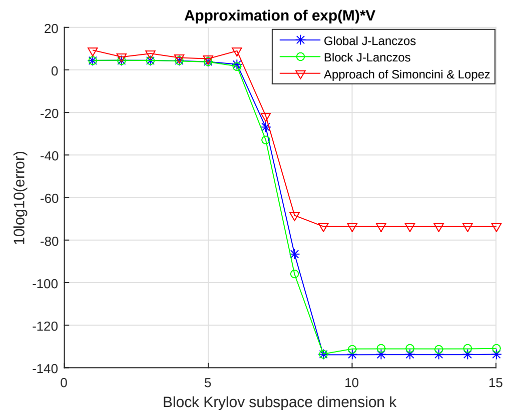

Figure 2: Error of the exponential approximation when $s = 2$ and k varies from 1 to 300.

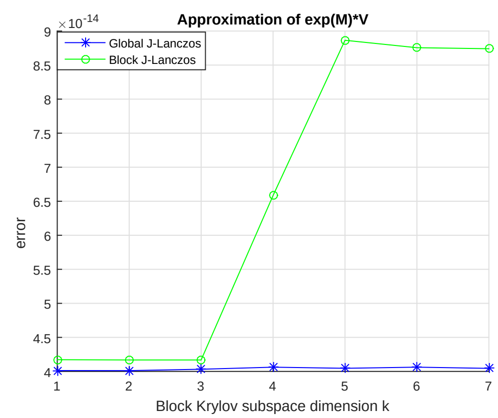

Figure 3: Error of the exponential approximation when $s = 2$ and k varies from 161 to 300.

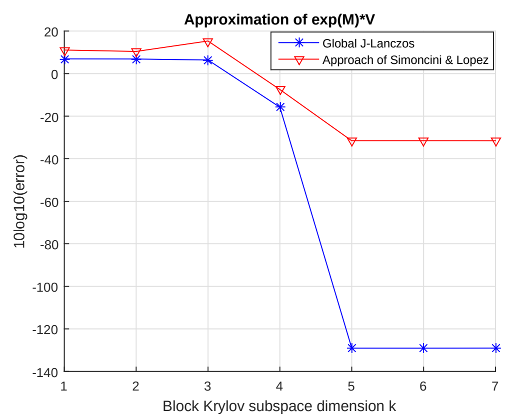

Figure 4: Error of the exponential approximation using GJ-Lanczos method when $s = 6$ and k varies from 1 to 350.

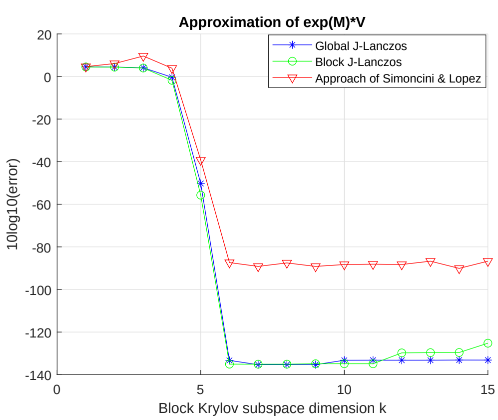

Figure 5: Error of the exponential approximation when $s = 2$ and k varies from 1 to 300.

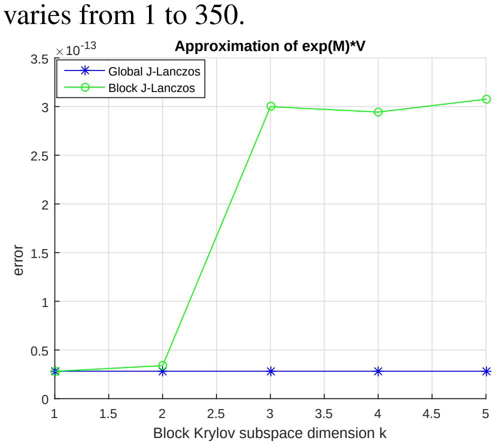

Figure 6: Error of the exponential approximation when $s = 2$ and k varies from 181 to 261.

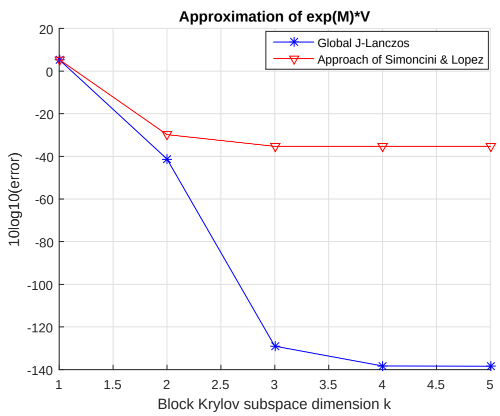

Figure 7: Error of the exponential approximation when $s = 5$ and k varies from 1 to 50.

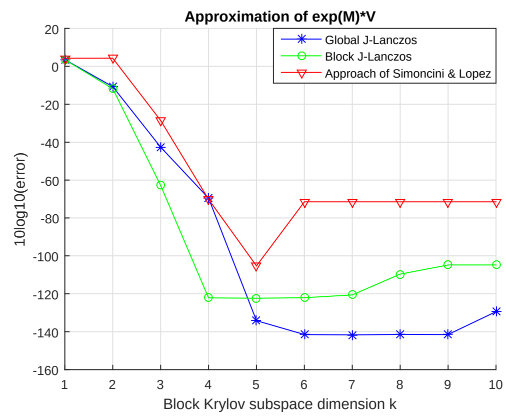

Figure 8: Error of the exponential approximation when $s = 2$ and k varies from 1 to 50.

Example 2. In this example, we consider a 10000×10000 skew-symmetric and Hamiltonian matrix M constructed as follows

$$M = \begin{pmatrix} M_1 & M_2 \\ -M_2 & M_1 \end{pmatrix}.$$

The blocks M_1 and M_2 are the n-by-n skew-symmetric and symmetric parts, respectively. M_1 is taken as a random matrix with normally distributed numbers and $M_2 = gallery('ris', n)$ is a 5000×5000 symmetric Hankel matrix, with elements $M(i, j) = 0.5/(n - i - j + 1.5)$, for $i, j = 1, \ldots, n$. For $s = 6$, we get Figure 4. For a matrix of size 2000-by-2000, with $s = 2$, Figures 5 and 6 and illustrate the performances of the methods proposed in this study.

Example 3. For this example, we wish to examine the evolution of the error relative to the approximation of $\exp(M)V$, when the matrix M is Hamiltonian but not necessarily skew-symmetric, for this reason, we consider a 10000×10000 Hamiltonian matrix M given as follows

$$M = \begin{pmatrix} M_1 & -M_2 \\ -M_3 & M_1 \end{pmatrix},$$

where M_1 and M_2 are the n-by-n skew-symmetric and symmetric parts, respectively. M_1 is taken as Hansen matrix and $M_2 = gallery('ris', n)$ is a 5000×5000 symmetric Hankel matrix, with elements $M(i, j) = 0.5/(n - i - j + 1.5)$, for $i, j = 1, \ldots, n$. $M_3 = shaw(n)$ is a 5000×5000 symmetric Hansen matrix. For $s = 5$, in the Figure 7, we find the error committed when approximating $\exp(A)V$. Let $n = 1000$, $s = 2$, we have the following error shown in the Figure 8.

6 Conclusion

In this paper, we have presented a global approach to the symplectic Lanczos method based on a new version of symplectic global like-orthogonalization and symplectic global like-normalization. The developed global J-Lanczos method, in addition to being robust in particular in terms of computational time which has been observed during the calculations and being easily implementable, presents a considerable numerical efficiency compared to the block J-Lanczos method, when applied to approximate the exponential matrix-matrix operator $\exp(M)V$ for a given large square Hamiltonian matrix M and a tall and skinny matrix V, preserving the geometric property of V.

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