HAL
open science

Parallel approximation of the exponential of Hermitian matrices

Frédéric Hecht, Sidi-Mahmoud Kaber, Lucas Perrin, Alain Plagne, Julien Salomon

To cite this version:

Frédéric Hecht, Sidi-Mahmoud Kaber, Lucas Perrin, Alain Plagne, Julien Salomon. Parallel approximation of the exponential of Hermitian matrices. 2023. hal-03948509v2

HAL Id: hal-03948509

https://hal.science/hal-03948509v2

Preprint submitted on 28 Jun 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

PARALLEL APPROXIMATION OF THE EXPONENTIAL OF HERMITIAN MATRICES

FRÉDÉRIC HECHT*, SIDI-MAHMOUD KABER†, LUCAS PERRIN‡, ALAIN PLAGNE§, AND JULIEN SALOMON¶

Abstract. In this work, we consider a rational approximation of the exponential function to design an algorithm for computing matrix exponential in the Hermitian case. Using partial fraction decomposition, we obtain a parallelizable method, where the computation reduces to independent resolutions of linear systems. We analyze the effects of rounding errors on the accuracy of our algorithm. We complete this work with numerical tests showing the efficiency of our method and a comparison of its performances with Krylov algorithms.

Key words. Matrix exponential, Parallel computing, Truncation error, Taylor series, Partial fraction decomposition, Padé approximation, MATLAB, Octave, `expm`, Roundoff error.

AMS subject classifications. 15A16, 65F60, 65L99, 65Y05.

1. Introduction.

Given a square matrix A, the differential equation $u'(t) = Au(t)$ appears in many models, either directly or as an elementary component of more complicated differential systems. To solve this equation with a good accuracy, it is useful to have an algorithm computing matrix exponential. This algorithm must be efficient, both for the accuracy and for the computational efficiency. Such an algorithm is presented in this paper.

Many algorithms for computing the exponential of a matrix are available. We refer to the celebrated review by Moler and Van Loan [23] for a comparison of these methods. None of them is clearly more efficient than the others if we take into account various important criteria such as accuracy, computing time, memory space requirements, complexity, properties of the matrices under consideration, etc.

As is the case with our method, several algorithms are based on rational approximation of the exponential function e^z ($z \in \mathbb{C}$), such as Padé or uniform Chebyshev approximations. Let $R_{m,n}(z)$ denotes such an approximation (m and n are the degrees of the numerator $N_{m,n}$ and denominator $D_{m,n}$ respectively), the considered approximation of $\exp(A)$ is given by $R_{m,n}(A) = [D_{m,n}(A)]^{-1}N_{m,n}(A)$.

In the literature, such approximations are combined with scaling or reduction techniques, which mainly consider the so called *diagonal case*, i.e., $m = n$. In [1], the authors use the scaling and squaring method [17] to compute $\exp(A) \simeq [R_{n,n}(A/\ell)]^\ell$ where $R_{n,n}(z)$ is accurate enough near the origin to guarantee high order approximation of $\exp(A/\ell)$ with $\ell \in \mathbb{N}$. This strategy avoids the conditioning problem of $D_{n,n}$ that can occur when n is large [23]. Rational approximation can also be applied to, e.g., reduced or simpler forms of A, as in [20] where an orthogonal factorization $A = Q^T TQ$ is used to compute $\exp(A) \simeq Q^T R_{n,n}(T)Q$ with T a tridiagonal matrix.

*Laboratoire Jacques-Louis Lions, Sorbonne Université, CNRS, 75005 Paris and INRIA Paris, ALPINES Project-Team, 75589 Paris Cedex 12, France(frederic.hecht@sorbonne-universite.fr).

†Laboratoire Jacques-Louis Lions, Sorbonne Université, CNRS, 75005 Paris, France (sidi-mahmoud.kaber@sorbonne-universite.fr).

‡INRIA Paris, ANGE Project-Team, 75589 Paris Cedex 12, France and Sorbonne Université, CNRS, Laboratoire Jacques-Louis Lions, 75005 Paris, France (lucas.perrin@inria.fr).

§Centre de Mathématiques Laurent Schwartz, École polytechnique, F-91128 Palaiseau, France. (alain.plagne@polytechnique.edu).

¶INRIA Paris, ANGE Project-Team, 75589 Paris Cedex 12, France and Laboratoire Jacques-Louis Lions, Sorbonne Université, CNRS, 75005 Paris, France (julien.salomon@inria.fr).

In the case $n = 0$, properties of orthogonal polynomials have been used to define approximations of the matrix exponential, see [4] for the Chebyshev case (orthogonality on a bounded interval) and [26] for the Laguerre case (orthogonality on the half real line). The interest, in both cases, relies on saving in storage of Ritz vectors during the Krylov iterations.

Our algorithm is based on an independent approach which aims at decomposing the computation in view of parallelization. As a consequence, it can be combined with all the previous algorithms which require the computation of the exponential of a transformed matrix. It shares some features with the one presented in [11] and [12], where diagonal approximations are used to define implicit numerical schemes for linear parabolic equations. The parallelization is obtained using partial fraction decomposition, which is also the case in our method, as explained below. A similar approach is considered in [13], where the author focus on matrices arising from stiff systems of ordinary differential equations, associated with matrices whose numerical range is negative. A specific rational approximation where the poles are constrained to be equidistant in a part of the complex plane is presented. These approximations are related to the functions[1] φ_ℓ ($\ell > 0$) which do not include the exponential (which corresponds to φ_0). Moreover, the proposed approximation appears to be more efficient for large ℓ, whereas our method is designed and efficient in the case $\ell = 0$. Various approximations of some matrix functions (including the exponential) based on rational Krylov methods with fixed denominator are presented in [14]. A posteriori bounds and stopping criterion in a similar framework are given in [10].

Note however that these references mainly focus on the reduction obtained by Krylov approaches and can be combined with our method. The convergence properties of Krylov methods related to matrix functions is widely documented in the literature. Among the more recent papers on this topic, we refer to [3, 7, 8, 18, 19].

In the present work, we focus on the parallelization strategy associated with the rational approximation defined by $R_{0,n}(z) = 1/\exp_n(-z)$ (which we simply denote by $\mathcal{R}_n(z)$ hereafter), where $\exp_n$ denotes the truncated Taylor series of order n associated with the exponential, i.e., $m = 0$. The poles of $\mathcal{R}_n(z)$ are all distinct (and well documented) allowing a partial fraction decomposition with affine denominators. All terms in the decomposition are independent hence their computation can be achieved efficiently in parallel.

To see how these results can be used to compute matrix exponential, consider $\mathcal{E}_n$ an approximation of the complex exponential function depending on one parameter $n \in \mathbb{N}^*$. This approximation naturally extends to the exponential of diagonal matrices by setting $\mathcal{E}_n(\mathrm{diag}(d_i)_i) := (\mathrm{diag}(\mathcal{E}_n(d_i))_i$, thus to any diagonalizable matrix $A = PDP^{-1}$ by $\mathcal{E}_n(A) := P\mathcal{E}_n(D)P^{-1}$. The latter definition is actually a property of usual matrix functions, see [16, Chap. 1]. The approximation error for a diagonalizable matrix $A = PDP^{-1}$, with eigenvalues located in a domain of the complex plane Λ can then be estimated as follows

$$\| \exp(A) - \mathcal{E}_n(A)\|_2 \leq \varepsilon_n \, \kappa_2(P) \tag{1.1}$$

where $\kappa_2(P) = \|P\|_2 \, \|P^{-1}\|_2$ is the condition number of P in the matrix norm associated with the usual Euclidean vector norm $\|\cdot\|_2$ and $\varepsilon_n := \max_{z\in\Lambda} |\mathcal{E}_n(z) - \exp(z)|$. The approximation of $\exp(A)$ is then reduced to the approximation of the exponential on the complex plane. If we further assume A to be Hermitian (or, more generally,

[1] These functions are defined by $\varphi_\ell(x) := \sum_{k=0} \frac{x^k}{(k+\ell)!}$.

normal), then P is a unitary matrix and $\kappa_2(P) = 1$. This is the case for Hermitian matrices that arise, e.g. from the space discretization of the Laplace operator, and more generally for normal matrices. Note, however, that for an arbitrary matrix, the term $\kappa_2(P)$ may be too large and significantly deteriorate the estimate (1.1).

The paper is organized as follows. Section 2 is devoted to the approximation of the scalar exponential function. As explained above, this approximation, denoted by $\mathcal{R}_n(z)$ is in our approach a rational function whose poles are all simple. In Section 3, we present the approximation of the exponential of a matrix. In practise, the partial fraction decomposition of $\mathcal{R}_n(z)$ raises some specific numerical issues related to floating-point arithmetic ; these are discussed in Section 4. We finally demonstrate the efficiency of our method on some examples in Section 5.

2. The scalar case. For $n \in \mathbb{N}^*$, let us define $\exp_n(z) := \sum_{k=0}^{n} \frac{1}{k!} z^k$, i.e., the exponential Taylor series truncated at order n. It is readily seen that for all $x \in \mathbb{R}$ and even values of n, $\exp_n(x)$ is positive. Since $\exp_n' = \exp_{n-1}$, it follows that $\exp_n$ is strictly increasing for n odd and strictly convex for n even.

2.1. Roots of the truncated exponential series. We denote by $(\theta_k^{(n)})_{k=1,\cdots,n}$ the roots of the polynomial $\exp_n$. If n is even, the roots are pairs of conjugate complex numbers and none of them is a real number. If n is odd, there is one and only one real root of $\exp_n$ and the others are pairwise conjugate. Some roots of $\exp_n$ are represented on the figure 1 (left panel). We see that the norm of the roots increases with n, which intuitively follows from the fact that the exponential function has no roots on the whole complex plane. However, this growth is moderate since (see [30], for example)

$$1 \leq |\theta_k^{(n)}| \leq n. \tag{2.1}$$

G. Szegő has shown in [27] that the *normalized roots*, i.e., the roots of $\exp_n(nz)$,

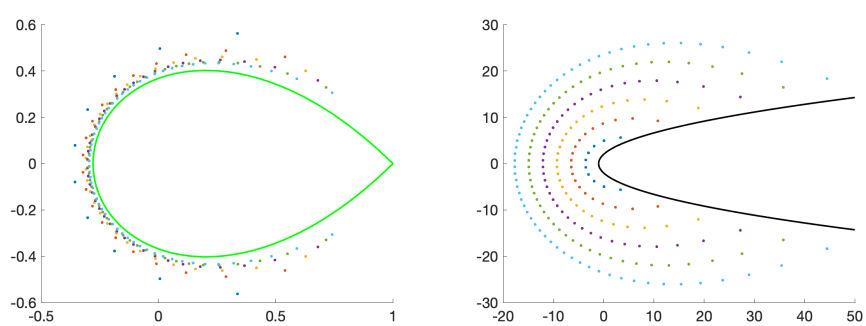

Figure 1: Left: the roots of $z \longmapsto \exp_n(z)$, $n = 10, 20, 30, 40, 50, 60$. The parabola $y^2 = 4(x+1)$ delimits an area containing no roots. Right: the Szegő curve.

approach, when $n \to \infty$, the so-called Szegő curve, defined by

$$\{z \in \mathbb{C}, \quad |ze^{1-z}| = 1, \quad |z| \leq 1\}.$$

Some normalized roots and the Szegő curve are presented in Figure 1 (left panel). In view of (1.1), it is interesting to determine regions of the complex plane which do not

contain any roots. An example is given by the interior of the parabola of equation $y^2 = 4(x+1)$, which thus includes the positive real half-axis. This surprising result has been obtained by Saff and Varga in [24], see Figure 1 (right panel).

2.2. Approximation of the exponential. We propose the following approximation of the exponential function defined for any complex number z by

$$\exp(z) \simeq \mathcal{R}_n(z) := \frac{1}{\exp_n(-z)},$$

which reflects the identity $\exp(z) = \frac{1}{\exp(-z)}$. Note that $\mathcal{R}_n(0) = 1$ and that $\mathcal{R}_n$ has no real root if n is even, which we will always assume in the rest of this paper.

This approach opens the way to a good approximation of the exponential on the half axis $(-\infty, 0]$. We present on Figure 2 a graph of the exponential function, its polynomial approximation $\exp_n$, and the rational approximation $\mathcal{R}_n$, on the interval $[-5, 0]$. Though the two approximations seem to fit well with the exponential function for $n = 20$, we observe that for $n = 10$, the rational approximation is clearly more accurate. Given $n, m \in \mathbb{N}$, the Padé approximant [2] of index (m, n) of the exponential

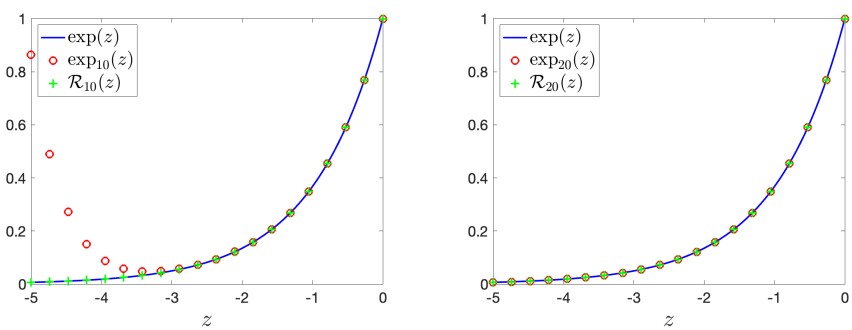

Figure 2: The exponential function and its polynomial and rational approximations rational $\exp_n$ and $\mathcal{R}_n$ on $[-5, 0]$, for $n = 10$ (left) and $n = 20$ (right).

function is explicitly known; it is the rational function with numerator $P_{m,n}$ and denominator $Q_{m,n}$:

$$P_{m,n}(z) = \sum_{k=0}^{m} \frac{(m+n-k)!m!}{(m+n)!(m-k)!k!} z^k, \quad Q_{m,n}(z) = \sum_{k=0}^{n} \frac{(m+n-k)!n!}{(m+n)!(n-k)!k!} (-z)^k.$$

The function $\mathcal{R}_n$ is therefore the Padé approximant of index $(0, n)$ of the exponential function, i.e., its Taylor expansion at the origin coincides with this function up to order n. More precisely, we have

$$\mathcal{R}_n^{(j)}(0) = 1, \qquad j \in \mathbb{N},\ 0 \le j \le n, \tag{2.2}$$

and, in the neighborhood of the origin,

$$\mathcal{R}_n(z) = \exp(z) + \mathcal{O}(z^{n+1}).$$

We can slightly refine this result. Let us decompose $\mathcal{R}_n(z)$ as

$$\mathcal{R}_n(z) = \exp_n(z) + \sum_{k=n+1}^{+\infty} \frac{\lambda_{n,k}}{k!} z^k.$$

A simple calculation shows that (recall that n is supposed to be even) $\lambda_{n,n+1} = 0$ and $\lambda_{n,n+2} = -2(n+1)$. In other words, at $z = 0$, the derivatives of $\mathcal{R}_n(z)$ of order greater than n are not at all close to the derivatives of the exponential function.

The partial fraction decomposition of $\mathcal{R}_n$ is the foundation of our numerical method to compute the exponential of a matrix.

PROPOSITION 2.1. *We have, for all $z \in \mathbb{C}$*

$$\mathcal{R}_n(z) = \sum_{k=1}^{n} \frac{a_k^{(n)}}{z + \theta_k^{(n)}}, \tag{2.3}$$

where $\theta_k^{(n)}$ are the roots of $\exp_n$ and

$$a_k^{(n)} = -\frac{n!}{\prod_{j \neq k} (\theta_k^{(n)} - \theta_j^{(n)})}. \tag{2.4}$$

One should not be alarmed in the calculation of the coefficients $a_k^{(n)}$ by the relation (2.4) whose denominator is a product of the differences $\theta_k^{(n)} - \theta_j^{(n)}$ since the difference between two roots of $\exp_n$ is uniformly lower bounded with respect to n (see [30, Theorem 4])

$$\inf_{n \geq 2} \min_{j \neq k} |\theta_j^{(n)} - \theta_k^{(n)}| \geq \gamma := 0.29044 \cdots \tag{2.5}$$

thus avoiding to divide by too small numbers in (2.4). Note also that other expressions can be used to compute the coefficients $a_k^{(n)}$, e.g.,

$$a_k^{(n)} = \frac{-1}{\exp_n'(\theta_k^{(n)})} = \frac{n!}{(\theta_k^{(n)})^n}. \tag{2.6}$$

Numerical properties of these formula are investigated in Section 4.

2.3. Convergence and error estimate. The rational approximation of a real or complex function is a well-documented problem. Results concerning existence of best approximation, uniqueness, computation can be found, e.g., in [22]. In this section, we focus on the convergence properties of $\mathcal{R}_n(z)$ on $]-\infty, 0]$. This interval includes the spectrum of negative Hermitian matrices that we consider in this paper. Note however that results on others domains are available. Indeed, let $\mathbb{P}_k$ denotes the set of polynomials of degree at most k, $\mathbb{P}_{m,n}$ the set of rational functions p/q, $p \in \mathbb{P}_m$, $q \in \mathbb{P}_n$, and

$$E_{m,n}(\exp, \Lambda) := \min_{r \in \mathbb{P}_{m,n}(\Lambda)} \max_{z \in \Lambda} |\exp(z) - r(z)|,$$

the error of best uniform approximation of the exponential on $\Lambda \subset \mathbb{C}$. On bounded domains, we have for example [5]

$$E_{m,n}(\exp, [-1, 1]) \underset{n+m \to \infty}{\simeq} \frac{n!m!}{2^{n+m}(n+m)!(n+m+1)!}.$$

The analog of this result on the disk $B(0,\varrho)$ of radius ϱ centered in 0 is [28]

$$E_{m,n}(\exp, B(0,\varrho)) \underset{n+m\to\infty}{\simeq} \frac{n!m!\varrho^{n+m+1}}{(n+m)!(n+m+1)!}.$$

In both cases, we observe a fast decreasing of the error when Λ is bonded. This is not the case in the applications which have motivated our study. The case $\Lambda =]-\infty, 0]$ is discussed in the pioneering work of [6]. The authors show that the best approximation error $E_{0,n}(\exp,]-\infty, 0])$ decays linearly and exhibit a particular function, which just happens to be our rational approximation $\mathcal{R}_n$.

PROPOSITION 2.2. *([6, Lemma 1]) We have for any real $x \leq 0$*

$$|\mathcal{R}_n(x) - \exp(x)| \leq M_1(n) := \frac{1}{2^n}. \tag{2.7}$$

The convergence of $\mathcal{R}_n(x)$ to $\exp(x)$ is therefore linear on the real negative half-line[2]. The error on this interval is represented in Figure 3 for various values of n. Figure 4 shows iso-curves of the norm of the error for $n = 32$ as well as points $-\theta_k^{(n)}$. The values presented in the graphics for $n = 32$ are the 10^{-k} for $k = 0, \cdots, 14$. One observes there the rapid decay of the approximation along the real half-axis. We also observe a remarkable decay in the whole left half-plane.

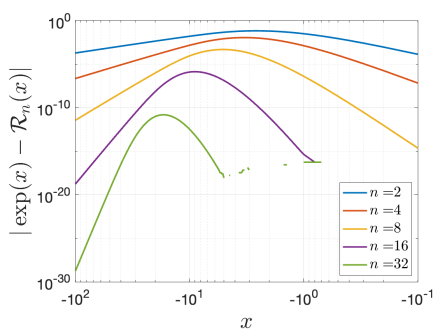

Figure 3: The error $|\mathcal{R}_n(x) - \exp(x)|$ for $n \in \{4, 8, 16, 32\}$.

Before going further, let us state a technical result.

LEMMA 2.3. *The function $f_n(x) := \exp_n(x)\exp(-x)$ satisfies*

$$f_n(n+1) < \frac{1}{2} \tag{2.8}$$

$$f_n^2(x) \leq \frac{n+1}{n} f_{n-1}(x) f_{n+1}(x). \tag{2.9}$$

Proof. We first show that

$$\exp_n(n+1) = \sum_{k=0}^{n} \frac{(n+1)^k}{k!} < \exp(n+1) - \exp_n(n+1) = \sum_{k=n+1}^{+\infty} \frac{n^k}{k!}, \tag{2.10}$$

[2]For the sake of completeness, let us note that the optimal linear decrease is given by Schönhage in [25] who showed that $\lim_{n\to+\infty} E_{0,n}^{1/n}(\exp,]-\infty, 0]) = 1/3$.

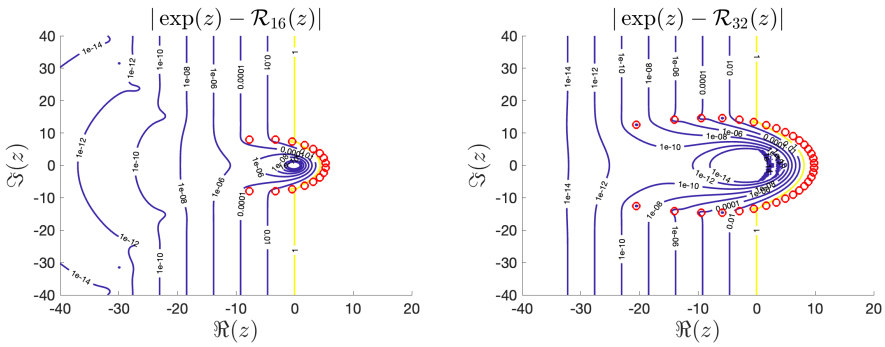

Figure 4: Norm of error $\mathcal{R}_n(z) - \exp(z)$ and poles of $\mathcal{R}_n$ for $n = 16$ (left) and $n = 32$ (right).

which directly leads to (2.8). To get (2.10), we compare the terms $k = n - j$ and $k = n + j - 1$ of the respective sums. Precisely, we have

$$\frac{n^{n-j}}{(n-j)!} \leq \frac{n^{n+j-1}}{(n+j-1)!}.$$

The proof is by induction on j. For $j = 1$, we actually have equality. Assuming that the property is true at rank j, we have

$$\begin{aligned}\frac{n^{n-(j+1)}}{(n-(j+1))!} =& \frac{n^{n-j}}{(n-j)!}\frac{n-j}{n} < \frac{n^{n+j-1}}{(n+j-1)!}\frac{n-j}{n} = \frac{n^{n+j}}{(n+j)!}(1-(\frac{j}{n})^2) \\ <& \frac{n^{n+j}}{(n+j)!},\end{aligned}$$

hence the result. Inequality (2.9) simply follows from the Cauchy-Schwarz inequality applied to

$$\int_x^{+\infty} \exp(-t)t^n dt = \int_x^{+\infty} (\exp(-t/2)t^{\frac{n-1}{2}})\,(\exp(-t/2)t^{\frac{n+1}{2}})\,dt,$$

since $f_n(x) = \int_x^{+\infty} \exp(-t)\frac{t^n}{n!}dt$. ∎

In the following proposition, we summarize some properties of the function $err_n : x \in]-\infty, 0] \longmapsto \mathcal{R}_n(x) - \exp(x) > 0$.

Proposition 2.4. *For $n \geq 1$, the function err_n reaches its maximum at a single point $\xi_n < 0$, is increasing on $]-\infty, \xi_n]$ and decreasing on $[\xi_n, 0]$. Moreover, we have*

$$\frac{n}{2} \leq -\xi_n \leq n + 2. \tag{2.11}$$

Proof. To simplify the notation, we introduce $y = -x$ and study the error $err_n(y) = \mathcal{R}_n(-y) - \exp(-y)$ on the half-axis $(0, +\infty[$, in which we have excluded $y = 0$ where the error cancels. Since

$$\begin{aligned} err_n'(y) =& \exp(2y)\frac{(\exp_n(y)\exp(-y))^2 - \exp_{n-1}(y)\exp(-y)}{\exp_n(y)^2} \\ =& y^n \frac{\exp(-y)}{\exp_n(y)^2}\left(\frac{1}{n!}\exp_n(y) - \exp_{n-1}(y)\frac{\exp(y) - \exp_n(y)}{y^n}\right),\end{aligned} \tag{2.12}$$

the variations on err_n are determined by the sign of

$$g_n(y) := \frac{1}{n!}\exp_n(y) - \exp_{n-1}(y)\frac{\exp(y)-\exp_n(y)}{y^n}. \tag{2.13}$$

In this formula, the last term as well as all its derivatives is positive on $I =]0,+\infty[$ so that $g_n^{(n+1)}(y) < 0$ on this interval. To prove that g_n has an unique zero ξ_n in I, we shall show that for some $a_1 > 0$, g_n' is strictly positive on in interval $]0, a_1[$ and strictly negative on $]a_1, +\infty[$. That guarantees the result since $g_n(0) > 0$ and $\lim_{y\to+\infty} g_n(y) = -\infty$. The values of $g_n^{(k)}$ $(k = 1, \cdots, n)$ on both sides of interval I are of importance in the analysis. Note first that $\lim_{y\to+\infty} g_n^{(k)}(y) = -\infty$ for all $k \in \mathbb{N}$ and that the sequence $u_k := g_n^{(k)}(0) = \frac{1}{n!} - \sum_{\ell=1}^{k} \frac{k!}{(k-\ell)!(n+\ell)!}$ is decreasing. Indeed, for $k = 1, \cdots, n-1$ we have

$$\begin{aligned} u_{k+1} - u_k &= -\frac{(k+1)!}{(n+k+1)!} + \sum_{\ell=1}^{k} \frac{k!}{(k-\ell)!(n+\ell)!} - \frac{(k+1)!}{(k+1-\ell)!(n+\ell)!} \\ &= -\frac{(k+1)!n!}{(n+k+1)!} - k!\sum_{\ell=1}^{k} \frac{1}{(k-\ell)!(n+\ell)!}\frac{\ell}{k+1-\ell} < 0. \end{aligned}$$

Since the first term in the right hand side of (2.13) is a polynomial of order n, we have $g_n^{(n+1)}(y) < 0$ on I. Hence $g_n^{(n)}$ is strictly decreasing on this interval. If $u_n > 0$, then for some $a_n > 0$, $g_n^{(n)} > 0$ on some interval $[0, a_n[$ and $g_n^{(n)} < 0$ on $]a_n, +\infty[$. Hence function $g_n^{(n-1)}$ is strictly increasing on the first interval and decreasing on the second one. It follows that there exists a unique $a_{n-1} > a_n$ where this function vanishes. This property clearly spreads to g_n. Otherwise, $u_n \le 0$, and the previous reasoning can be applied to the largest n' such that $u_{n'} > 0$.

To prove (2.11), we first show that $err_n'(n/2) < 0$, i.e., $g_n(n/2) > 0$. Set $y = n\theta$, with $0 < \theta < 1$. We have

$$\begin{aligned} \frac{\exp(y)-\exp_n(y)}{y^n} &= \frac{1}{(n\theta)^n}\sum_{\ell=n+1}^{+\infty}\frac{\theta^\ell}{\ell!/n^\ell} \\ &\le \frac{1}{(n\theta)^n}\frac{n^{n+1}}{(n+1)!}\sum_{\ell=n+1}^{+\infty}\theta^\ell = \frac{n}{(n+1)!}\frac{\theta}{1-\theta}. \end{aligned}$$

As a consequence, we get

$$g_n(n\theta) \ge \frac{(n\theta)^n}{(n!)^2} + \frac{\exp_{n-1}(n\theta)}{n!}\left(1 - \frac{n}{n+1}\frac{\theta}{1-\theta}\right),$$

which is positive when $\theta = 1/2$.

We then prove that $err_n'(n+2) < 0$. Rewriting (2.12) with the notation of Lemma 2.3, we get $err_n'(y) = \exp(2y)\frac{(f_n(y))^2 - f_{n-1}(y)}{\exp_n(y)^2}$. The task is now to find the sign of $(f_n(n+2))^2 - f_{n-1}(n+2)$. Because of Lemma 2.3, we have

$$\begin{aligned} (f_n(n+2))^2 - f_{n-1}(n+2) &\le \left(\frac{n+1}{n}f_{n+1}(n+2) - 1\right) f_{n-1}(n+2) \\ &\le \left(\frac{n+1}{2n} - 1\right) f_{n-1}(n+2), \end{aligned}$$

where the former inequality follows from (2.9) and the latter from (2.8). This shows that $(f_n(n+2))^2 - f_{n-1}(n+2) < 0$. Hence $err_n'(n+2) < 0$. ∎

3. Approximation of the exponential of Hermitian matrices. Let A be a square matrix of $\mathcal{M}_d(\mathbb{C})$. Given $n > 1$, we suppose that all matrices $A - \theta_k^{(n)} I$ are invertible, i.e., their spectrum does not contain any root of any $\exp_n$. This is the case if the matrix A is Hermitian (recall that n is supposed to be even). The same is true for any matrix provided that n is large enough. We propose the following approximation of the exponential of A

$$\exp(A) \simeq \mathcal{R}_n(A) := \sum_{k=1}^{n} a_k^{(n)} (A + \theta_k^{(n)} I)^{-1}, \tag{3.1}$$

where I denotes the identity matrix.

REMARK 3.1. *Note that $\mathcal{R}_n(0) = I$ and that if the matrix $D \in \mathcal{M}_d(\mathbb{C})$ is diagonal, so is matrix $\mathcal{R}_n(D)$ with $(\mathcal{R}_n(D))_{i,i} = \mathcal{R}_n(D_{i,i})$. On the other hand, for any invertible matrix $P \in \mathcal{M}_d(\mathbb{C})$, we have*

$$\mathcal{R}_n(PAP^{-1}) = P\mathcal{R}_n(A)P^{-1}.$$

From now on, we restrict our attention to negative Hermitian matrices. In view of Proposition 2.4, we can state a specific estimate in this case.

THEOREM 3.2. *Assume that $Spec(A) \subset \mathbb{R}^-$ and let $\varrho(A) := \max_{\lambda \in Spec(A)} |\lambda|$. If $n > 2\varrho(A)$, then*

$$\| \exp(A) - \mathcal{R}_n(A) \|_2 \leq \varepsilon,$$

where $\varepsilon = \mathcal{R}_n(-\varrho(A)) - \exp(-\varrho(A))$.

REMARK 3.3 (Shifting method for nonnegative Hermitian matrices). *Since the spectrum of a real-valued matrix can be localized everywhere in the complex plane, we cannot guarantee that (2.7) holds in the general case. This problem can be solved by a shifting method in the case of Hermitian matrices. Let A be an Hermitian matrix and $c \in \mathbb{R}$ a bound of its spectrum, $c \geq \alpha(A) := \max_i \lambda_i$. Since $Spec(A - cI) \subset \mathbb{R}^-$, we can consider the approximation*

$$\exp(A) = e^c \exp(A - cI) \simeq e^c \mathcal{R}_n(A - cI).$$

But the term e^c can be very large so that the approximation is only relevant for moderate values of c. However, we have

$$\frac{\| \exp(A) - e^c \mathcal{R}_n(A - cI) \|_2}{\| \exp(A) \|_2} \leq \frac{e^c}{\| \exp(A) \|_2} \| \exp(A - cI) - \mathcal{R}_n(A - cI) \|_2.$$

Assuming that A is Hermitian, we have $\| \exp(A) \|_2 = e^{\alpha(A)}$, so that the relative error can be controlled in this case. Some numerical results about this strategy are presented in Section 5.

Many applications require in practice to compute a matrix-vector product instead of assembling the full matrix. In such a case, given $v \in \mathbb{C}^d$, $y = \exp(A)v$ is computed by

$$y \simeq \mathcal{R}_n(A)v = \sum_{k=1}^{n} a_k^{(n)} y_k^{(n)}, \tag{3.2}$$

with $y_k^{(n)}$ the solution to the linear system $(A + \theta_k^{(n)} I) y_k^{(n)} = v$. Each $y_k^{(n)}$ could be computed separately from the others leading to significant savings in computing time as illustrated by our numerical tests, see Section 5.

4. Floating-point arithmetic and numerical implementation. In this section, we examine the efficiency of the approximation

$$\exp(x) \simeq \sum_{k=1}^{n} \frac{a_k^{(n)}}{x+\theta_k^{(n)}},$$

where x is assume to be a real number. We decompose the error according to

$$\underbrace{\exp(x) - \sum_{k=1}^{n} \frac{a_k^{(n)}}{x+\theta_k^{(n)}}}_{e_1(x)} = \underbrace{\left(\exp(x) - \frac{1}{\exp_n(-x)}\right)}_{e_2(x)} + \underbrace{\left(\frac{1}{\exp_n(-x)} - \sum_{k=1}^{n} \frac{a_k^{(n)}}{x+\theta_k^{(n)}}\right)}_{e_3(x)}.$$

The latter cancels in exact arithmetic. However, working for example in a finite

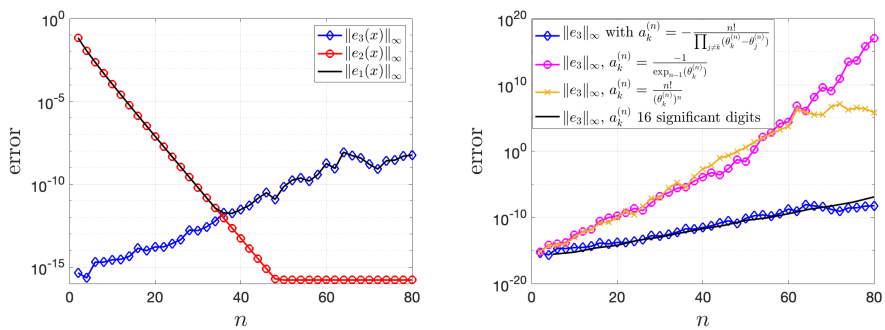

Figure 5: Left: uniform norm of e_1, e_2, and e_3 over $[-100, 0]$ as a function of n. Right: norm of e_3 using various definitions of $a_k^{(n)}$, the black curve computation is done with $a_k^{(n)}$ computed with 32 significant digits and truncated to 16 significant digits.

precision of 16 significant digits, we see on Figure 5 (left panel) that in practise e_1 decreases until approximately $n = 34$ and then increases. This observation shows that our approximation is not relevant in practice for large values of n. This behavior can be explained by an analysis of e_2 and e_3. The former decreases as predicted by Proposition 2.2. The latter increases with respect to n. The increase in e_3 is related to the partial fraction decomposition in floating-point arithmetic which is our framework hereafter, since we use MATLAB [21] and Octave [9] with double precision. The accuracy actually deteriorates for larger values of n. Indeed, the three equivalent definitions of the coefficients $a_k^{(n)}$ given by (2.4) and (2.6) lead in practise to different numerical results. The uniform norm of e_3 obtained with each of these definitions is shown on Figure 5 (right panel). The formula given in (2.4) gives the most precise result, which is actually very similar to the one obtained by keeping the exact 16 first digits. Hence, we use (2.4) in the sequel.

In order to understand the influence of the floating-point arithmetic, we give in the next proposition a bound which guarantees a certain precision for a given n when working with a floating-point arithmetic of D significant digits.

PROPOSITION 4.1. *Denote by $\widetilde{a}_k^{(n)}$ and $\widetilde{\theta}_k^{(n)}$, the D-significant digits approximations of $a_k^{(n)}$ and $\theta_k^{(n)}$, and assume that*

$$\gamma > n10^{(1-D)} \tag{4.1}$$

with γ defined in (2.5). We have the following upper bound, for $x \in \mathbb{R}$:

$$\left| \frac{1}{\exp_n(-x)} - \sum_{k=1}^{n} \frac{\widetilde{a}_k^{(n)}}{\widetilde{\theta}_k^{(n)} + x} \right| \leq M_2(n, D) := (C_1(D) + C_2(n, D)) \sum_{k=1}^{n} \left| \widetilde{a}_k^{(n)} \right|, \tag{4.2}$$

where

$$C_1(D) := \frac{2 \cdot 10^{(1-D)}}{\gamma \left(1 - 10^{(1-D)}\right)}, \quad C_2(n, D) := \frac{4n \cdot 10^{(1-D)}}{\gamma(\gamma - n \cdot 10^{(1-D)})}.$$

Note that the condition given in (4.1) is not restrictive: it holds for example in the case of 16 significant digits even in the case where $n \approx 10^{10}$.

This result is illustrated in Figure 6. We see in this example that with 16 significant digits, the bound obtained in (4.2) implies that working with $n = 30$ guarantees an error of order 10^{-8} and get an actual order of 10^{-10}. We see however that to increase the accuracy, we could work up to $n \approx 36$.

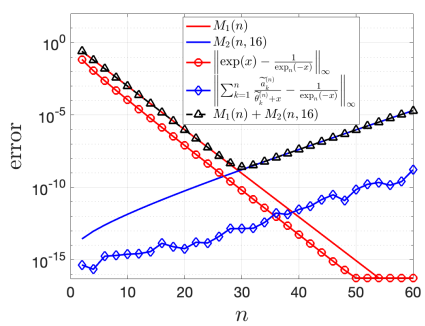

Figure 6: Uniform norm of e_2 and e_3 over $[-100, 0]$, in 16 significant digits, and upper bounds : $M_1(n) := 1/2^n$ (see Proposition 2.2) and $M_2(n, D = 16)$ given by (4.2).

Proof. (Proposition 4.1) Since we are dealing with numerical approximations based on D significant digits, we consider the first D digits of $\widetilde{a}_k^{(n)}$ and $\widetilde{\theta}_k^{(n)}$ to be exact. Then, for any complex number z and its approximation $\widetilde{z}$ we have:

$$\widetilde{z} = z(1 + \varepsilon_z), \quad |\varepsilon_z| \in \left[10^{-D}, 10^{(1-D)}\right]. \tag{4.3}$$

Writing $r_k^{(n)}(x) = \frac{1}{\theta_k^{(n)}+x}$ and $\widetilde{r}_k^{(n)}(x) = \frac{1}{\widetilde{\theta}_k^{(n)}+x}$, we see that finding an upper bound for the left side of (4.2) amounts to finding an upper bound for:

$$\sum_{k=1}^{n} r_k^{(n)}(x) \left(\widetilde{a}_k^{(n)} - a_k^{(n)}\right) + \widetilde{a}_k^{(n)} \left(\widetilde{r}_k^{(n)}(x) - r_k^{(n)}(x)\right)$$
$$= \sum_{k=1}^{n} r_k^{(n)}(x) a_k^{(n)} \left(\frac{\varepsilon_{a_k^{(n)}}}{1 + \varepsilon_{a_k^{(n)}}}\right) + \sum_{k=1}^{n} \widetilde{a}_k^{(n)} \left(\widetilde{r}_k^{(n)}(x) - r_k^{(n)}(x)\right),$$

where the equality follows from (4.3). Combining (2.1) with (4.3), we get $|\widetilde{\theta}_k^{(n)} - \theta_k^{(n)}| = |\varepsilon_{\theta_k^{(n)}} \theta_k^{(n)}| \leq n \cdot 10^{(1-D)}$. Combining (2.5) with the fact that for n even, $\theta_k^{(n)}$ are strictly

not real, we obtain that $\left|\theta_k^{(n)}+x\right| \geq \left|\mathcal{I}m(\theta_k^{(n)})\right| \geq \frac{\gamma}{2}$ when $x \in \mathbb{R}$. As a consequence $\left|r_k^{(n)}(x)\right| \leq \frac{2}{\gamma}$ for all $x \in \mathbb{R}$. In the same manner, we can see that

$$\left|\widetilde{\theta}_k^{(n)}+x\right| \geq \left|\mathcal{I}m(\widetilde{\theta}_k^{(n)})\right| \geq \left||\mathcal{I}m(\theta_k^{(n)})| - |\mathcal{I}m(\varepsilon_{\theta_k^{(n)}}\theta_k^{(n)})|\right| \geq \frac{\left|\gamma - n10^{(1-D)}\right|}{2}$$

which follows from (4.1). Consequently, $\left|\widetilde{r}_k^{(n)}(x)\right| \leq \frac{2}{\gamma - n10^{(1-D)}}$ for all $x \in \mathbb{R}$.

Finally, we have $|\widetilde{r}_k^{(n)}(x) - r_k^{(n)}(x)| = |\widetilde{r}_k^{(n)}(x)||r_k^{(n)}(x)||\widetilde{\theta}_k^{(n)} - \theta_k^{(n)}|$ so that $|\widetilde{r}_k^{(n)}(x) - r_k^{(n)}(x)| \leq \frac{4n\cdot 10^{(1-D)}}{\gamma(\gamma - n10^{(1-D)})}$. Combining all theses inequalities with $|\varepsilon_{a_k^{(n)}}| \leq 10^{(1-D)}$, and $\left|\frac{\varepsilon_{a_k^{(n)}}}{1+\varepsilon_{a_k^{(n)}}}\right| \leq \frac{10^{(1-D)}}{1-10^{(1-D)}}$, we get (4.2). ∎

The graphs of $e_1(x)$ for $x = -10$ obtained with various number of significant digits is given in Figure 7. We see that the larger the number of significant digits, the later e_1 starts increasing. It follows that floating-point arithmetic precision must be adapted to n which is in practise the number of processor used in the computation.

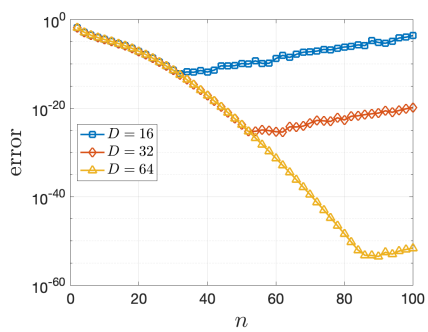

Figure 7: Error (e_1) on the approximation of $\exp(x)$ vs n ($x = -10$) computed with Maple, with 16, 32 and 64 significant digits, respectively.

5. Numerical efficiency. In this section, we test the performance of our method on MATLAB and Octave, and compare it with several other algorithms: the `expm` functions available in these softwares, and a rational Krylov method. Recall that `expm` is based on the combination of a Padé approximation with a scaling and squaring technique. MATLAB uses the variant described in [17] and [1] whereas Octave uses the variant described in [29].

Remark 5.1. *If n is even and $x \in \mathbb{R}$, we can compute twice as fast $\mathcal{R}_n(x)$. Indeed, the complex numbers $\theta_k^{(n)}$ are in this case a set of conjugate pairs as well as $a_k^{(n)}$, and $\frac{1}{\theta_k^{(n)}+x}$. Assuming that the labelling is such that $\theta_{2\ell+1}^{(n)} = \overline{\theta_{2\ell}^{(n)}}$, we get*

$$\sum_{k=1}^{n} \frac{a_k^{(n)}}{x+\theta_k^{(n)}} = \sum_{\ell=1}^{n/2} 2\mathcal{R}e\left(\frac{a_{2\ell}^{(n)}}{x+\theta_{2\ell}^{(n)}}\right).$$

It follows that the number of computations can be divided by two. The same holds for the computation of $\mathcal{R}_n(A)$ when Spec(A) is real, e.g., in the Hermitian case that we consider in this paper.

5.1. Setting. Because of the results obtained in Section 4, we consider cases where $n \leq 32$ so that floating arithmetic does not affect our results. All computational times are measured thanks to the MATLAB/Octave `tic` / `toc` functions. The simulated parallel computational times for our method are estimated as follows: $t_{para} = \max_{1 \leq i \leq n} t_i$ where t_i is the computational time of the i-th matrix inversion or linear system resolution. We denote by t_{seq} the sequential computing time of the approximation via `expm` and by t_{Krylov} the time taken by a rational Krylov approximation to get the same absolute error as the one of our method using $n = 32$.

We first show that the error of our method does not depend on the dimension of the matrix by considering a symmetric $d \times d$ real matrix A, with spectrum randomly chosen within a fixed range. We then compare with the above mentioned algorithms, using matrices $B = \Delta_d^1 \in \mathcal{M}_d(\mathbb{R})$ and $C = \Delta_d^2 \in \mathcal{M}_d(\mathbb{R})$ corresponding respectively to the usual Finite Difference discretization of the Laplace operator in one and two dimensions. We consider both approximations $\exp(\cdot)$ and $\exp(\cdot)v$ where v is a random vector of size d and norm 1.

5.2. Stability of the error with respect to the dimension. Given a matrix A, we consider either the absolute error $\| \exp(A) - \mathcal{R}_n(A)\|_2$ or the relative error $\frac{\| \exp(A) - \mathcal{R}_n(A)\|_2}{\| \exp(A)\|_2}$ when the spectrum of A is non-positive or include positive eigenvalues, respectively. This choice follows from the fact that relative error is relevant for large numbers whereas small numbers are correctly analysed with absolute error. Both cases occur when using exp.

As a first example, we consider the matrix A described previously. The absolute error $\| \exp(A) - \mathcal{R}_n(A)\|_2$ as a function of the dimension d is represented in Figure 8 (left panel). The results are smoothed by using the mean of the error for various random spectra included in $[-1, 0]$. We use the approximation (3.1) where the inverse matrix is computed using the functions `inv` of MATLAB and Octave. We note that the error does not depend on d, which is an expected result since the spectrum remains in a fixed interval. In a second example, we consider a matrix with positive spectrum

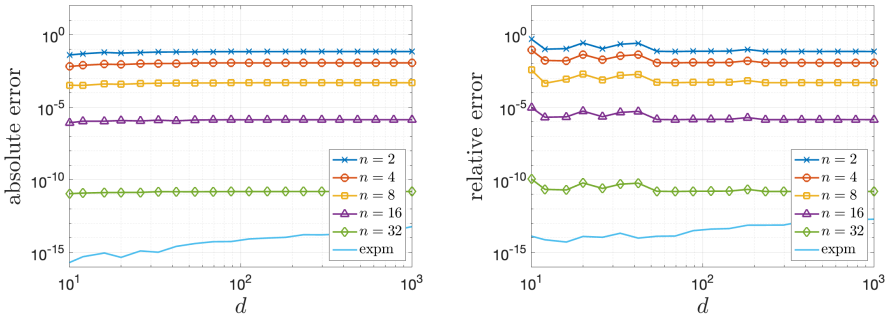

Figure 8: Error versus the dimension of the matrix. Left: absolute error, matrices with negative spectra. Right: relative error, matrices with positive spectra using the shift method from Remark 3.3.

included in $[0, 20]$. We use the shift method presented in Remark 3.3 to compute the exponential, and the relative error $\frac{\| \exp(A) - \mathcal{R}_n(A)\|_2}{\| \exp(A)\|_2}$. We see that the error still not depends on the dimension of the problem.

5.3. Computation of $\exp(\cdot)$ **for the Laplace operator.** From now on, we focus on matrices B and C described previously.

The absolute error is computed in practise by $\|\texttt{expm}(\cdot)-\mathcal{R}_n(\cdot)\|_2$. The results are presented in Figure 9 (bottom) for B and in Figure 10 for C (bottom). Here again, the error does not depend on the dimension of the problem, but only on the degree of truncation n. Note that increasing n only expands the spectrum of these matrices on the left side, hence does not deteriorate our approximations.

Next, we compare the computing times t_{seq} and t_{para}. The results are presented in Figure 9 for B and in Figure 10 for C. In these tests, the matrices $(B+\theta_k^{(n)}I)^{-1}$ are computed with the MATLAB and Octave functions `inv` in parallel and, as explained previously t_{para} is defined as the maximum time taken to compute one of the $a_k^{(n)}(A+\theta_k^{(n)}I)^{-1}$. We can see that t_{para} is slightly larger than t_{seq} in the case of MATLAB and almost ten times larger in the case of Octave.

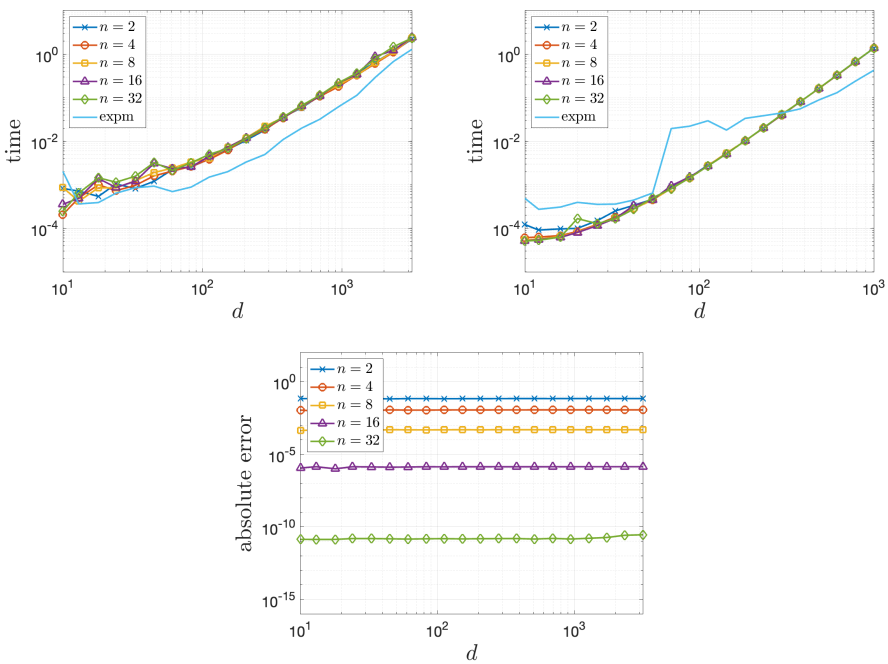

Figure 9: Performance of the approximation of $\exp(B)$ for matrix $B = \Delta_d^1$. Top: CPU time required to compute `expm` and approximation $\mathcal{R}_n$ for various values of n using MATLAB (left) and Octave (right). Bottom: relative error in the computation of $\exp(B)$ as a function of d.

5.4. Computation of $\exp(\cdot)v$ **for the Laplace operator.** Still considering matrices B and C, we finally consider the action of the matrix exponential on vectors. For $v \in \mathbb{R}^d$, the vector $w = \exp(B)v$ is approximated by (3.2) where $(B+\theta_k^{(n)}I)y_k^{(n)} = v$ is solved using the solvers `mldivide` of MATLAB and Octave. We evaluate the mean of the error and the mean of t_{para} for a series of random vectors v of norm 1.

Rational Krylov methods being the state of the art for this type of computation, we first look at the method proposed in [14] to compare it with our approximation. All

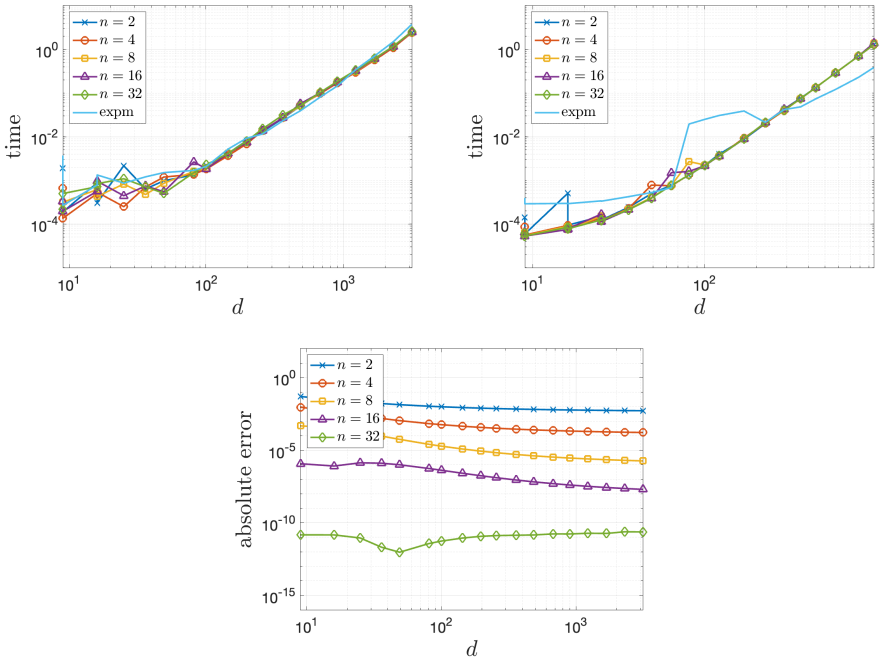

Figure 10: Same as Figure 9 for matrix $C = \Delta_d^2$.

our results related to rational Krylov methods are obtained using Guettel's toolbox [15], with parameter $\xi = -1$ as in [14]. Figure 11 shows the absolute error of the two methods, as a function of the computational time. We see that in both cases, for a prescribed accuracy, our method outperforms rational Krylov method.

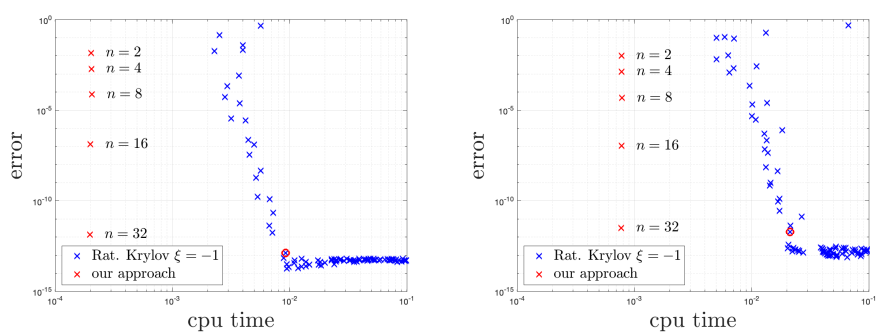

Figure 11: Error and CPU time comparison of the approximation $\exp(B)v$ using rational Krylov method (blue) and our approach (red). Vector v is randomly chosen, $d = 100$ (left) and $d = 400$ (right). Each point of the cloud corresponds to a Krylov rational space of size m with $m \in \{1, ..., d-1\}$. The dimension m for which Krylov method is at least as precise as our method with $n = 32$ is circled in red.

The absolute error $\|\texttt{expm}(B)v - \mathcal{R}_n(B)v\|_2$ together with the computing times

t_{seq}, t_{Krylov} and t_{para} are shown in Figure 12. In this case t_{para} is defined as the maximum time used to compute one of the vectors $a_k^{(n)} y_k^{(n)}$ (see (3.2)). We note that t_{seq} and t_{Krylov} are larger than t_{para} for all values of the dimension d of the matrix, with MATLAB as well as Octave. For example, with $d = 10^3$, $t_{seq} \approx 10^2 t_{para}$ and $t_{seq} \approx 10^4 t_{para}$ with MATLAB and Octave, respectively, and $t_{Krylov} \approx 10 t_{para}$ and $t_{Krylov} \approx 10^3 t_{para}$.

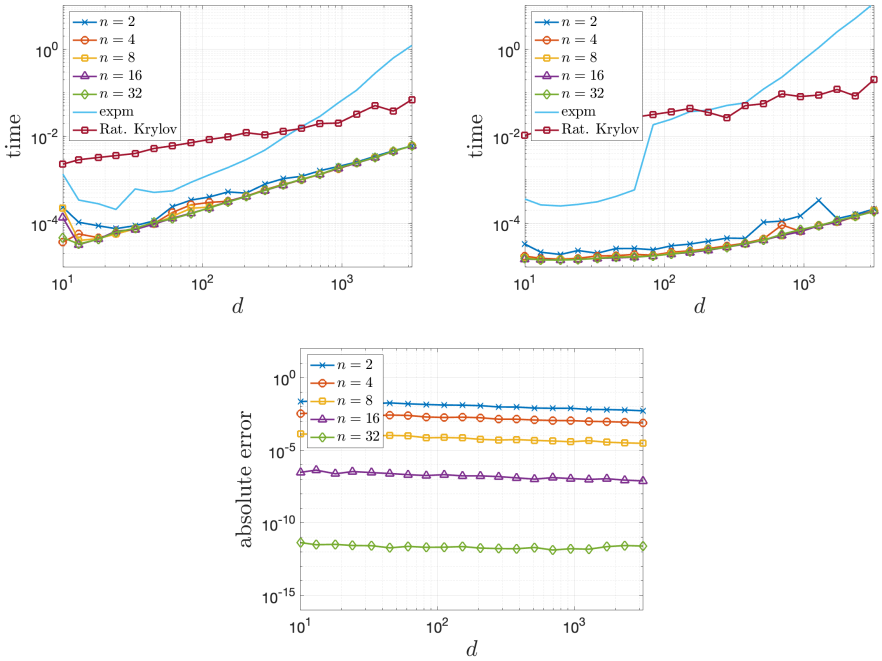

Figure 12: Top: CPU time required to compute $Av = \exp(\Delta_d^1)v$ for vectors v randomly chosen using rational Krylov method and our method for various values of n. Computations are done with MATLAB (left) and Octave (right). Bottom: relative error, as a function of the dimension of the matrix.

We make the same analysis for the absolute error $\|\texttt{expm}(C)v - \mathcal{R}_n(C)v\|_2$ together with the computing times t_{seq}, t_{Krylov} and t_{para} are shown in Figure 13. We note again that t_{seq} and t_{Krylov} are larger than t_{para} for all values of the dimension d of the matrix, with MATLAB as well as Octave. For $d = 10^3$, we observe that $t_{seq} \approx 10 t_{para}$ and $t_{seq} \approx 10^2 t_{para}$ with MATLAB and Octave, respectively, whereas $t_{para} \lessapprox t_{Krylov}$ and $t_{Krylov} \approx 10 t_{para}$.

Finally, we point out that our method defines a way to approximate the exponential of a matrix, whereas Krylov's rational methods approximate the matrix-vector product. These methods are based on a reduction of dimensionality. For the problems considered in this article they lead in practice to the computation of the exponential of a smaller matrix. Hence rational Krylov can be combined with our method for the computation of the exponential of this smaller matrix.

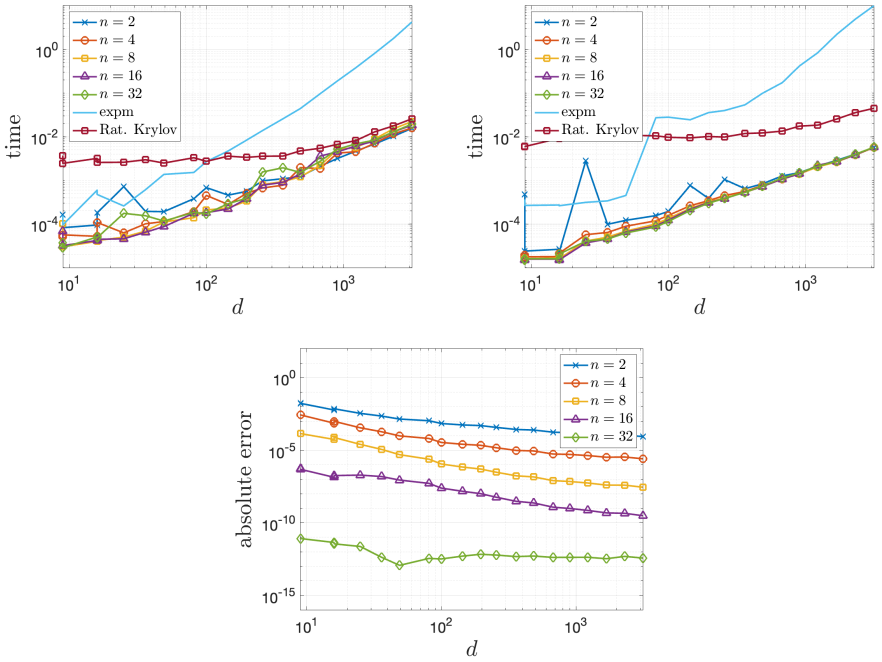

Figure 13: Same as Figure 12 for matrix $B = \Delta_d^2$.

[1] A. H. Al-Mohy and N. J. Higham. Computing the action of the matrix exponential, with an application to exponential integrators. *SIAM Journal on Scientific Computing*, 33(2):488–511, 2011.

[2] G. Baker, P. Graves-Morris, and S. Baker. *Padé Approximants*. Encyclopedia of Mathematics and its Applications. Cambridge University Press, 1996.

[3] B. Beckermann and L. Reichel. Error estimates and evaluation of matrix functions via the faber transform. *SIAM Journal on Numerical Analysis*, 47(5):3849–3883, 2009.

[4] L. Bergamaschi and M. Vianello. Efficient computation of the exponential operator for large, sparse, symmetric matrices. *Numer. Linear Algebra Appl.*, 7(1):27–45, 2000.

[5] D. Braess. On the conjecture of meinardus on rational approximation of $\exp(x)$. *J. Approx. Theory*, 36(4):317–320, 1982.

[6] W. Cody, G. Meinardus, and R. Varga. Chebyshev rational approximations to e^{-x} in $[0, +\infty)$ and applications to heat-conduction problems. *Journal of Approximation Theory*, 2(1):50–65, 1969.

[7] F. Diele, I. Moret, and S. Ragni. Error estimates for polynomial krylov approximations to matrix functions. *SIAM Journal on Matrix Analysis and Applications*, 30(4):1546–1565, 2009.

[8] V. Druskin, L. Knizhnerman, and M. Zaslavsky. Solution of large scale evolutionary problems using rational krylov subspaces with optimized shifts. *SIAM Journal on Scientific Computing*, 31(5):3760–3780, 2009.

[9] J. W. Eaton, D. Bateman, S. Hauberg, and R. Wehbring. *GNU Octave version 5.2.0 manual: a high-level interactive language for numerical computations*, 2020.

[10] A. Frommer and V. Simoncini. Stopping criteria for rational matrix functions of hermitian and symmetric matrices. *SIAM Journal on Scientific Computing*, 30(3):1387–1412, 2008.

[11] E. Gallopoulos and Y. Saad. Efficient parallel solution of parabolic equations: Implicit methods on the cedar multicluster. In J. Dongarra, P. Messina, D. C. Sorensen, and R. G. Voigt, editors, *Proc. of the Fourth SIAM Conf. Parallel Processing for Scientific Computing*, pages 251–256. SIAM, 1989.

[12] E. Gallopoulos and Y. Saad. Efficient solution of parabolic equations by Krylov approximation methods. *SIAM J. Sci. Statist. Comput.*, 13(5):1236–1264, 1992.

[13] T. Göckler and V. Grimm. Uniform approximation of *varphi*-functions in exponential integrators by a rational krylov subspace method with simple poles. *SIAM Journal on Matrix Analysis and Applications*, 35(4):1467–1489, 2014.

[14] S. Güttel. Rational Krylov approximation of matrix functions: numerical methods and optimal pole selection. *GAMM-Mitt.*, 36(1):8–31, 2013.

[15] S. Güttel. Rktoolbox guide, Jul 2020.

[16] N. J. Higham. *Functions of Matrices: Theory and Computation.* Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2008.

[17] N. J. Higham. The scaling and squaring method for the matrix exponential revisited. *SIAM Rev.*, 51(4):747–764, 2009.

[18] L. Knizhnerman and V. Simoncini. A new investigation of the extended krylov subspace method for matrix function evaluations. *Numerical Linear Algebra with Applications*, 17(4):615–638, 2010.

[19] L. Lopez and V. Simoncini. Analysis of projection methods for rational function approximation to the matrix exponential. *SIAM Journal on Numerical Analysis*, 44(2):613–635, 2006.

[20] Y. Y. Lu. Exponentials of symmetric matrices through tridiagonal reductions. *Linear Algebra and its Applications*, 279(1):317–324, 1998.

[21] The Mathworks, Inc., Natick, Massachusetts. *MATLAB version 9.11.0.1769968 (R2021b)*, 2021.

[22] G. Meinardus. *Approximation of Functions: Theory and Numerical Methods.* Springer tracts in natural philosophy. Springer, 1967.

[23] C. Moler and C. Van Loan. Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later. *SIAM Review*, 45(1):3–49, 2003.

[24] E. B. Saff and R. S. Varga. Zero-free parabolic regions for sequences of polynomials. *SIAM Journal on Mathematical Analysis*, 7(3):344–357, 1976.

[25] A. Schönhage. Zur rationalen approximierbarkeit von e^{-x} über $[0, +\infty)$. *Journal of Approximation Theory*, 7(4):395–398, 1973.

[26] B. N. Sheehan, Y. Saad, and R. B. Sidje. Computing $\exp(-\tau A)b$ with Laguerre polynomials. *Electron. Trans. Numer. Anal.*, 37:147–165, 2010.

[27] G. Szegö. Über einige eigenschaften der exponentialreihe. *Sitzungsber. Berl. Math. Ges*, 23:50–64, 1924.

[28] L. N. Trefethen. The asymptotic accuracy of rational best approximations to e^z on a disk. *Journal of Approximation Theory*, 40(4):380–383, 1984.

[29] R. C. Ward. Numerical computation of the matrix exponential with accuracy estimate. *SIAM Journal on Numerical Analysis*, 14(4):600–610, 1977.

[30] S. M. Zemyan. On the zeroes of the $n-th$ partial sum of the exponential series. *The American Mathematical Monthly*, 112(10):891–909, 2005.