

Max-Planck-Institut
für Mathematik
in den Naturwissenschaften
Leipzig

\mathcal{H} -matrix approximation for the operator
exponential with applications

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Preprint no.: 42

2000



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Abstract

We develop a data-sparse and accurate approximation to parabolic solution operators in the case of a rather general elliptic part given by a strongly P -positive operator [3].

In the preceding papers [11]-[16], a class of matrices (\mathcal{H} -matrices) has been analysed which are data-sparse and allow an approximate matrix arithmetic with almost linear complexity. In particular, the matrix-vector/matrix-matrix product with such matrices as well as the computation of the inverse have linear-logarithmic cost. In the present paper, we apply the \mathcal{H} -matrix techniques to approximate the exponent of an elliptic operator.

Starting with the Dunford–Cauchy representation for the operator exponent, we then discretise the integral by the exponentially convergent quadrature rule involving a short sum of resolvents. The latter are approximated by the \mathcal{H} -matrices. Our algorithm inherits a two-level parallelism with respect to both the computation of resolvents and the treatment of different time values. In the case of smooth data (coefficients, boundaries), we prove the linear-logarithmic complexity of the method.

AMS Subject Classification: 65F50, 65F30, 15A09, 15A24, 15A99

1 Introduction

There are several sparse ($n \times n$)-matrix approximations which allow to construct optimal iteration methods to solve the elliptic/parabolic boundary value problems with $\mathcal{O}(n)$ arithmetic operations. But in many applications one has to deal with full matrices arising when solving various problems discretised by the boundary element (BEM) or FEM methods. In the latter case the inverse of a sparse FEM matrix is a full matrix. A class of hierarchical (\mathcal{H}) matrices has been recently introduced and developed in [11]-[16]. These full matrices allow an approximate matrix arithmetic (including the computation of the inverse) of almost linear complexity and can be considered as "data-sparse". Methods for approximating the action of matrix exponentials have been investigated since the 1970s, see [19]. The most commonly used algorithms are based on Krylov subspace methods [21, 17]. A class of effective algorithms based on the Cayley transform was developed in [7].

Concerning the second order evolution problems and the operator cosine family new discretisation methods were recently developed in [3]-[4] in a framework of strongly P -positive operators in a Banach space. This framework turns out to be useful also for constructing efficient parallel exponentially convergent algorithms for the operator exponent and the first order evolution differential equations [4]. Parallel methods with a polynomial convergence order 2 and 4 based on a contour integration for symmetric and positive definite operators were proposed in [23].

The aim of this paper is to combine the \mathcal{H} -matrix techniques with the contour integration to construct an explicit data-sparse approximation for the operator exponent. Starting with the Dunford-Cauchy representation for the operator exponent and essentially using the strong P -positivity of the elliptic operator involved we discretise the integral by the exponentially convergent trapezoidal rule involving a short sum of resolvents. Approximating the resolvents by the \mathcal{H} -matrices, we obtain an algorithm with almost linear cost representing the non-local operator in question. This algorithm possesses two levels of parallelism with respect to both the computation of resolvents for different quadrature points and the treatment of numerous time values. Our parallel method has the exponential convergence due to the optimal quadrature rule in the contour integration for holomorphic function providing an explicit representation of the exponential operator in terms of data-sparse matrices of linear-logarithmic complexity.

Our method applies to the matrix exponentials $\exp(A)$ for the class of matrices with $\Re(sp(A)) < 0$, which allow the hierarchical data-sparse \mathcal{H} -matrix approximation to the resolvent $(zI - A)^{-1}$, $z \notin sp(A)$. First, we

discuss an application for solving linear parabolic problems with P-positive elliptic part. Further applications of our method for the fast parallel solving of linear dynamical systems of equations and for the stationary Lyapunov-Sylvester matrix equation $AX + XB + C = 0$ will also be discussed, see §4.

2 Representation of $\exp(t\mathcal{L})$ by a Sum of Resolvents

In this section we outline the description of the operator exponent with a strongly P-positive operator. As a particular case a second order elliptic differential operator will be considered. We derive the characteristics of this operator which are important for our representation and give the approximation results.

2.1 Strongly P-positive Operators

Strongly P-positive operators were introduced in [3] and play an important role in the theory of the second order difference equations [22], evolution differential equations as well as the cosine operator family in a Banach space X [3].

Let $A : X \rightarrow X$ be a linear, densely defined, closed operator in X with the spectral set $sp(A)$ and the resolvent set $\rho(A)$. Let $\Gamma_0 = \{z = \xi + i\eta : \xi = a\eta^2 + \gamma_0\}$ be a parabola, whose interior contains $sp(A)$. In what follows we suppose that the parabola lies in the right half-plane of the complex plane, i.e., $\gamma_0 > 0$. We denote by $\Omega_{\Gamma_0} = \{z = \xi + i\eta : \xi > a\eta^2 + \gamma_0\}$, $a > 0$, the domain inside of the parabola. Now, we are in the position to give the following definition.

Definition 2.1 *We say that an operator $A : X \rightarrow X$ is strongly P-positive if its spectrum $sp(A)$ lies in the domain Ω_{Γ_0} and the estimate*

$$\|(zI - A)^{-1}\|_{X \rightarrow X} \leq \frac{M}{1 + \sqrt{|z|}} \quad \text{for all } z \in \mathbb{C} \setminus \Omega_{\Gamma_0} \quad (2.1)$$

holds true with a positive constant M .

Next, we show that there exist classes of strongly P-positive operators which have important applications. Let $V \subset X \equiv H \subset V^*$ be a triple of Hilbert spaces and let $a(\cdot, \cdot)$ be a sesquilinear form on V . We denote by c_e the constant from the imbedding inequality $\|u\|_X \leq c_e \|u\|_V$, $\forall u \in V$. Assume that $a(\cdot, \cdot)$ is bounded, i.e.,

$$|a(u, v)| \leq c \|u\|_V \|v\|_V \quad \text{for all } u, v \in V.$$

The boundedness of $a(\cdot, \cdot)$ implies the well-posedness of the continuous operator $A : V \rightarrow V^*$ defined by

$$a(u, v) = {}_{V^*} \langle Au, v \rangle_V \quad \text{for all } u \in V.$$

As usual, one can restrict A to a domain $D(A) \subset V$ and consider A as an (unbounded) operator in H . The assumptions

$$\begin{aligned} \Re a(u, u) &\geq \delta_0 \|u\|_V^2 - \delta_1 \|u\|_X^2 & \text{for all } u \in V, \\ |\Im a(u, u)| &\leq \kappa \|u\|_V \|u\|_X & \text{for all } u \in V \end{aligned}$$

guarantee that the numerical range $\{a(u, u) : u \in X \text{ with } \|u\|_X = 1\}$ of A (and $sp(A)$) lies in Ω_{Γ_0} , where the parabola Γ_0 depends on the constants $\delta_0, \delta_1, \kappa, c_e$. Actually, if $a(u, u) = \xi_u + i\eta_u$ then we get

$$\begin{aligned} \xi_u &= \Re a(u, u) \geq \delta_0 \|u\|_V^2 - \delta_1 \geq \delta_0 c_e^{-2} - \delta_1, \\ |\eta_u| &= |\Im a(u, u)| \leq \kappa \|u\|_V. \end{aligned}$$

It implies

$$\xi_u > \delta_0 c_e^{-2} - \delta_1, \quad \|u\|_V^2 \leq \frac{1}{\delta_0} (\xi_u + \delta_1), \quad |\eta_u| \leq \kappa \sqrt{\frac{\xi_u + \delta_1}{\delta_0}}. \quad (2.2)$$

The first and the last inequalities in (2.2) mean that the parabola $\Gamma_\delta = \{z = \xi + i\eta : \xi = \frac{\delta_0}{\kappa} \eta^2 - \delta_1\}$ contains the numerical range of A . Supposing that $\Re sp(A) > \gamma_1 > \gamma_0$ one can easily see that there exists another parabola $\Gamma_0 = \{z = \xi + i\eta : \xi = a\eta^2 + \gamma_0\}$ with $a = \frac{(\gamma_1 - \gamma_0)\delta_0}{(\gamma_1 + \delta_1)\kappa}$ in the right-half plane containing $sp(A)$, see Fig. 1. Note that $\delta_0 c_e^{-2} - \delta_1 > 0$ is the sufficient condition for $\Re sp(A) > 0$ and in this case one can choose $\gamma_1 = \delta_0 c_e^{-2} - \delta_1$. Analogously to [3] it can be shown that inequality (2.1) holds true in $\mathbb{C} \setminus \Omega_{\Gamma_0}$ (see the discussion in [3, pp. 330-331]). In the following, the operator A is strongly P-positive.

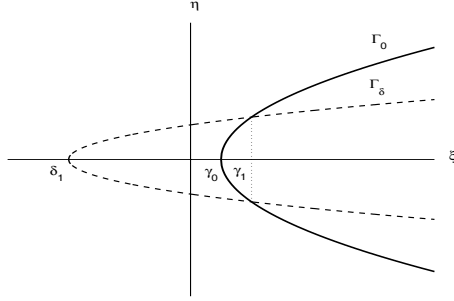


Figure 1: Parabolae Γ_δ and Γ_0 .

2.2 Several Examples

As the *first example* let us consider the one-dimensional operator $A : L_1(0, 1) \rightarrow L_1(0, 1)$ with the domain $D(A) = H_0^2(0, 1) = \{u : u \in H^2(0, 1), u(0) = 0, u(1) = 0\}$ in the Sobolev space $H^2(0, 1)$ defined by

$$Au = -u'' \quad \text{for all } u \in D(A).$$

Here we set $X = L_1(0, 1)$ (see Definition 2.1). The eigenvalues $\lambda_k = k^2\pi^2$ ($k = 1, 2, \dots$) of A lie on the real axis inside of the domain Ω_{Γ_0} enveloped by the path $\Gamma_0 = \{z = \eta^2 + 1 \pm i\eta\}$. The Green function for the problem

$$(zI - A)u \equiv u''(x) + zu(x) = -f(x), \quad x \in (0, 1); \quad u(0) = u(1) = 0$$

is given by

$$G(x, \xi) = \frac{1}{\sqrt{z} \sin \sqrt{z}} \begin{cases} \sin \sqrt{z}x \sin \sqrt{z}(1 - \xi) & \text{if } x \leq \xi, \\ \sin \sqrt{z}\xi \sin \sqrt{z}(1 - x) & \text{if } x \geq \xi, \end{cases}$$

i.e., we have

$$u(x) = (zI - A)^{-1}f = \int_0^1 G(x, \xi)f(\xi)d\xi.$$

Estimating the absolute value of the Green function on the parabola $z = \eta^2 + 1 \pm i\eta$ for $|z|$ large enough we get that $\|u\|_{L_1} = \|(zI - A)^{-1}f\|_{L_1} \leq \frac{M}{1 + \sqrt{|z|}} \|f\|_{L_1}$ ($f \in L_1(0, 1)$, $z \in \mathbb{C} \setminus \Omega_{\Gamma_0}$), i.e., the operator $A : L_1 \rightarrow L_1$ is strongly P-positive in the sense of Definition 2.1. Similar estimates for the Green function imply the strong positiveness of A also in $L_\infty(0, 1)$ (see [4] for details).

As the *second example* of a strongly P-positive operator one can consider the strongly elliptic differential operator

$$\mathcal{L} := - \sum_{j,k=1}^d \partial_j a_{jk} \partial_k + \sum_{j=1}^d b_j \partial_j + c_0 \quad (\partial_j := \frac{\partial}{\partial x_j}) \quad (2.3)$$

with smooth (in general complex) coefficients a_{jk}, b_j and c_0 in a domain Ω with a smooth boundary. For the ease of presentation, we consider the case of Dirichlet boundary conditions. We suppose that $a_{pq} = a_{qp}$ and the following ellipticity condition holds

$$\sum_{i,j=1}^d a_{ij} y_i y_j \geq C_1 \sum_{i=1}^d y_i^2.$$

This operator is associated with the sesquilinear form

$$a(u, v) = \int_{\Omega} \left(\sum_{i,j=1}^d a_{ij} \partial_i u \overline{\partial_j v} + \sum_{j=1}^d b_j \partial_j u \overline{v} + c_0 u \overline{v} \right) d\Omega.$$

Our algorithm needs explicit estimates for the parameters of the parabola which in this example have to be expressed by the coefficients of the differential operator. Let

$$C_2 := \inf_{x \in \Omega} \left| \frac{1}{2} \sum_j \frac{\partial b_j}{\partial x_j} - c_0 \right|, \quad C_3 := \sqrt{d} \max_{x,j} |b_j(x)|,$$

$|u|_1^2 = \sum_j |\partial_j u|^2$ be the semi-norm of the Sobolev space $H^1(\Omega)$, $\|\cdot\|_k$ be the norm of the Sobolev space $H^k(\Omega)$ ($k = 0, 1, \dots$) with $H^0(\Omega) = L_2(\Omega)$, and C_F the constant from the Friedrichs inequality

$$|u|_1^2 \geq C_F \|u\|_0^2 \quad \text{for all } u \in H_0^1(\Omega).$$

This constant can be estimated by $C_F = 1/(4B^2)$, where B is the edge of the cube containing the domain Ω . It is easy to show that in this case with $V = H_0^1(\Omega)$, $H = L_2(\Omega)$ it holds $\xi_u \geq C_1 |u|_1^2 - C_2 \|u\|_0 \geq C_1 C_F - C_2$, $|\eta_u| \leq C_3 |u|_1 \leq C_3 \sqrt{(\xi_u + C_2)/C_1}$, so that the parabola Γ_δ is defined by the parameters $\delta_0 = C_1$, $\delta_1 = C_2$, $\kappa = C_3$ and the lower bound of $sp(A)$ can be estimated by $\gamma_1 = C_1 C_F - C_2 > \gamma_0$. Now, the desired parabola Γ_0 is constructed as above by putting $a = \frac{(\gamma_1 - \gamma_0)\delta_0}{(\gamma_1 + \delta_1)\kappa}$, see §2.1.

The *third example* is given by a matrix $A \in \mathbb{R}^{n \times n}$ whose spectrum satisfies $\Re sp(A) > 0$. In this case, the parameters of the parabola Γ_0 can be determined by means of the Gershgorin circles. Let $A = \{a_{ij}\}_{i,j=1}^n$, define $C_i = \{z : |z - a_{ii}| \leq \sum_{j=1, j \neq i}^n a_{ij}\}$, $D_j = \{z : |z - a_{jj}| \leq \sum_{i=1, i \neq j}^n a_{ij}\}$. Then by Gershgorin's theorem,

$$sp(A) \subset \mathcal{C}_A := (\cup_i C_i) \cap (\cup_j D_j).$$

The corresponding parabola Γ_0 is obtained as the enveloping one for the set \mathcal{C}_A with simple modifications in the case $\Re(\mathcal{C}_A) \cap (-\infty, 0] \neq \emptyset$.

2.3 Representation of the Operator Exponent

Let \mathcal{L} be a linear, densely defined, closed, strongly P-positive operator in a Banach space X . The operator exponent $T(t) \equiv \exp(-t\mathcal{L})$ (operator-valued function or a continuous semigroup of bounded linear operators on X with the infinitesimal generator \mathcal{L} , see, e.g., [20]) satisfies the differential equation

$$\frac{dT}{dt} + \mathcal{L}T = 0, \quad T(0) = I, \quad (2.4)$$

where I is the identity operator. Given the operator exponent $T(t)$ the solution of the first order evolution equation (parabolic equation)

$$\frac{du}{dt} + \mathcal{L}u = 0, \quad u(0) = u_0$$

with a given initial vector u_0 and unknown vector valued function $u(t) : \mathbb{R}_+ \rightarrow X$ can be represented as

$$u(t) = \exp(-t\mathcal{L})u_0.$$

Let $\Gamma_0 = \{z = \xi + i\eta : \xi = a\eta^2 + \gamma_0\}$ be the parabola defined as above and containing the spectrum $sp(\mathcal{L})$ of the strongly P-positive operator \mathcal{L} .

Lemma 2.2 *Choose a parabola $\Gamma = \{z = \xi + i\eta : \xi = a\eta^2 + b\}$ with $b \in (0, \gamma_0)$. Then the exponent $\exp(-t\mathcal{L})$ can be represented by the Dunford-Cauchy integral [1]*

$$\exp(-t\mathcal{L}) = \frac{1}{2\pi i} \int_{\Gamma} e^{-zt} (zI - \mathcal{L})^{-1} dz. \quad (2.5)$$

Moreover, $T(t) = \exp(-t\mathcal{L})$ satisfies the differential equation (2.4).

Proof. In fact, using the parameter representation $z = a\eta^2 + b \pm i\eta$, $\eta \in (0, \infty)$, of the path Γ and the estimate (2.1), we have

$$\begin{aligned} \|\exp(-t\mathcal{L})\| &= \left\| \frac{1}{2\pi i} \int_{-\infty}^0 e^{-(a\eta^2 + b + i\eta)t} ((a\eta^2 + b + i\eta)I - \mathcal{L})^{-1} (2a\eta + i) d\eta \right. \\ &\quad \left. + \frac{1}{2\pi i} \int_0^{\infty} e^{-(a\eta^2 + b - i\eta)t} ((a\eta^2 + b - i\eta)I - \mathcal{L})^{-1} (2a\eta - i) d\eta \right\| \\ &\leq C \int_0^{\infty} e^{-(a\eta^2 + b)t} \frac{\sqrt{4a^2\eta^2 + 1}}{1 + [(a\eta^2 + b)^2 + \eta^2]^{1/4}} d\eta. \end{aligned}$$

Analogously, applying (2.1) we have for the derivative of $T(t) = \exp(-t\mathcal{L})$

$$\begin{aligned} \|\mathcal{L} \exp(-t\mathcal{L})\| &= \left\| \frac{1}{2\pi i} \int_{\Gamma} z e^{-zt} (tI - \mathcal{L})^{-1} dz \right\| \\ &\leq C \int_0^{\infty} \sqrt{(a\eta^2 + b)^2 + \eta^2} e^{-(a\eta^2 + b)t} \frac{\sqrt{4a^2\eta^2 + 1}}{1 + [(a\eta^2 + b)^2 + \eta^2]^{1/4}} d\eta, \end{aligned}$$

where the integrals are finite for $t > 0$. Furthermore, we have

$$\begin{aligned} \frac{dT}{dt} + \mathcal{L}T &= \frac{1}{2\pi i} \int_{\Gamma} -z e^{-zt} (zI - \mathcal{L})^{-1} dz + \mathcal{L} \left(\frac{1}{2\pi i} \int_{\Gamma} e^{-zt} (zI - \mathcal{L})^{-1} dz \right) \\ &= -\frac{1}{2\pi i} \int_{\Gamma} z e^{-zt} (zI - \mathcal{L})^{-1} dz + \frac{1}{2\pi i} \int_{\Gamma} z e^{zt} (zI - \mathcal{L})^{-1} dz = 0, \end{aligned}$$

i.e., $T(t) = \exp(-t\mathcal{L})$ satisfies the differential equation (2.4). This completes the proof. \blacksquare

The parametrised integral (2.5) can be represented in the form

$$\exp(-t\mathcal{L}) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} F(\eta, t) d\eta \quad (2.6)$$

with

$$F(\eta, t) = e^{-zt} (zI - \mathcal{L})^{-1} \frac{dz}{d\eta}, \quad z = a\eta^2 + b - i\eta.$$

After the change of variables $\eta = \eta(\xi)$, $\eta : (0, 2\pi) \rightarrow (-\infty, \infty)$, we get the integral representation

$$\exp(-t\mathcal{L}) = \frac{1}{2\pi i} \int_0^{2\pi} F_1(\xi, t) d\xi \quad (2.7)$$

with a 2π -periodic analytic operator-valued function $F_1(\xi, t) = F(\eta, t) \frac{d\eta}{d\xi}$ of ξ , where $F_1(0, t) = 0$. In the following we shall use the parametrisation

$$\eta = \frac{\xi - \pi}{[\xi(2\pi - \xi)]^\alpha} \quad \text{for } \xi \in (0, 2\pi), \alpha \in (0, 1). \quad (2.8)$$

2.4 The Computational Scheme and the Convergence Analysis

Let $\Phi(\xi)$ be an analytical 2π -periodic operator-valued function and $\xi_j = j\pi/N$ ($j = 0, \dots, 2N - 1$) be an equidistant grid. Denote the (unique) trigonometric polynomial by $(P_N\Phi)(\xi) \equiv \Phi_N(\xi) := \sum_{j=0}^N \alpha_j \cos j\xi + \sum_{j=1}^N \beta_j \sin j\xi$ providing the interpolation property $\Phi(\xi_j) \equiv \Phi_j = \Phi_N(\xi_j)$. The coefficients of this polynomial are the linear operators

$$\begin{aligned} \alpha_0 &= \frac{1}{2N} \sum_{k=0}^{2N-1} \Phi_k, & \alpha_N &= \frac{1}{2N} \sum_{k=0}^{2N-1} (-1)^k \Phi_k, \\ \alpha_j &= \frac{1}{N} \sum_{k=0}^{2N-1} \Phi_k \cos j\xi_k, & \beta_j &= \frac{1}{N} \sum_{k=0}^{2N-1} \Phi_k \sin j\xi_k, \quad j = 1, \dots, N - 1. \end{aligned}$$

The representation with respect to the Lagrange basis is

$$(P_N\Phi)(\xi) = \frac{1}{2N} \sin N\xi \sum_{k=0}^{2N-1} (-1)^k \Phi(\xi_k) \cot \frac{\xi - \xi_k}{2} \quad (0 \leq \xi < 2\pi, \xi \neq \xi_k, k = 0, \dots, 2N - 1).$$

Integrating the interpolation polynomial $\Phi_N(\xi)$, we get the usual trapezoidal rule for the integral $\int_0^{2\pi} \Phi(\xi) d\xi$ similar to the case of real-valued functions. Thus, we have for the integral (2.7)

$$T(t) \equiv \exp(-t\mathcal{L}) \approx T_N(t) \equiv \exp_N(-t\mathcal{L}) := \sum_{k=0}^{2N-1} \theta_k F_1(\xi_k, t) = \sum_{k=1}^{2N-1} \theta_k F_1(\xi_k, t),$$

where $\xi_k = \frac{k\pi}{N}$, $\theta_k = \frac{\pi}{N}$, $k = 0, 1, \dots, 2N - 1$. This introduces the following algorithm for the approximation of the operator exponent at a given time value t .

Algorithm 2.3 1. Determine z_k ($k = 1, \dots, 2N - 1$) by $z_k = a\eta_k^2 + b - i\eta_k$, $\xi_k = \frac{k\pi}{N}$, $\eta_k = \eta(\xi_k)$.

2. Find the resolvents $(z_k I - \mathcal{L})^{-1}$, $k = 1, \dots, 2N - 1$ (note that it can be done in parallel).

3. Find the approximation $\exp_N(-t\mathcal{L})$ for the operator exponent $\exp(-t\mathcal{L})$ in the form

$$\exp_N(-t\mathcal{L}) = \frac{1}{2Ni} \sum_{k=1}^{2N-1} e^{-z_k t} (z_k I - \mathcal{L})^{-1} \frac{dz(\eta(\xi_k))}{d\eta} \frac{d\eta(\xi_k)}{d\xi}, \quad (2.9)$$

where $\frac{dz}{d\eta} = 2a\eta - i$.

Remark 2.4 The above algorithm possesses two sequential levels of parallelism: one can compute all resolvents in Step 2 in parallel and then each operator exponent at different time values provided that we apply the operator exponential for a given time vector (t_1, t_2, \dots, t_M) .

Note that for small parameters $t \ll 1$, the numerical tests indicate that Step 3 in the algorithm above has slow convergence. In this case, we propose the following modification of Algorithm 2.3, which converges much faster than (2.9).

Algorithm 2.5 1'. Determine $z_k(t)$ ($k = 1, \dots, 2N - 1$) by $\xi_k = \frac{k\pi}{N}$, $\eta_k = \eta(\xi_k)$, $z_k(t) = a\eta_k^2 + b(t) - i\eta_k$, where the parameter $b(t)$ is defined with respect to the location of $sp(t\mathcal{L})$, i.e., $b(t) = tb$.

2'. Find the resolvents $(z_k(t)I - t\mathcal{L})^{-1}$, $k = 1, \dots, 2N - 1$ (it can be done in parallel).

3'. Find the approximation $\exp_N(-t\mathcal{L})$ for the operator exponent $\exp(-t\mathcal{L})$ in the form

$$\exp_N(-t\mathcal{L}) = \frac{1}{2Ni} \sum_{k=1}^{2N-1} e^{-z_k(t)t} (z_k(t)I - t\mathcal{L})^{-1} \frac{dz(\eta(\xi_k))}{d\eta} \frac{d\eta(\xi_k)}{d\xi}, \quad \text{where } \frac{dz}{d\eta} = 2a\eta - i.$$

Though the above algorithm allows only sequential treatment of different time values close to $t = 0$, in many applications (e.g., for integration with respect to the time variable) we may choose the time-grid as $t_i = i\Delta t$, $i = 1, \dots, n_t$. Then the exponentials for $i = 2, \dots, n_t$ are easily obtained as the corresponding monomials from $\exp_N(-\Delta t\mathcal{L})$.

Adapting the ideas of [18] it is easy to prove the following approximation result for any fixed $t \in (0, \infty)$.

Lemma 2.6 There holds

$$\|T(t) - T_N(t)\| \equiv \|\exp(-t\mathcal{L}) - \exp_N(-t\mathcal{L})\| \leq M_1 \frac{\coth(s/2)}{\sinh sN}, \quad (2.10)$$

where s is the width of a strip in which $F_1(\xi, t)$ can be extended holomorphically and $M_1 = M_1(s, t)$ is the bound on $F_1(\xi, t)$.

Proof. First of all we note that $\Phi(\xi) = F_1(\xi, t)$ is a bounded operator for all ξ, t . Let Γ_R be the counterclockwise oriented boundary of the rectangle $[\frac{\pi}{2N}, 2\pi + \frac{\pi}{2N}] \times [-\sigma, \sigma]$ containing all interpolation points where $\sigma \in (0, s)$ is arbitrary. By a simple modification of the results from [18] for operator-valued functions one gets for the interpolation error

$$\begin{aligned} \Phi(\xi) - \Phi_N(\xi) &= \frac{\sin N\xi}{4\pi i} \int_{\Gamma_R} \frac{\cot \frac{z-\xi}{2}}{\sin Nz} \Phi(z) dz \\ &= \frac{\sin N\xi}{4\pi i} \left[\int_{\Gamma_u} \frac{\cot \frac{z-\xi}{2}}{\sin Nz} \Phi(z) dz + \int_{\Gamma_l} \frac{\cot \frac{z-\xi}{2}}{\sin Nz} \Phi(z) dz \right], \quad \xi \neq \xi_j, \quad j = 0, \dots, 2N - 1, \end{aligned}$$

where we have used the periodicity of the integrand and Γ_u, Γ_l denote the top and the bottom sides of the rectangle Γ_R corresponding to the values $z = \sigma$ and $z = -\sigma$. Using the inequalities $|\sin Nz| \geq \sinh N\sigma$, $|\cot \frac{z}{2}| \leq \coth \frac{\sigma}{2}$ for $\Im m z = \pm\sigma$ and passing to the limit $\sigma \rightarrow s$, we get the statement of the lemma. ■

The specific dependence of $M_1(s, t)$ on the time variable t in (2.10) will be investigated in §5. In accordance with (5.1) there holds

$$\|\exp(-t\mathcal{L}) - \exp_N(-t\mathcal{L})\| \lesssim s^{-1} \exp(-[b - a\alpha_2^2 s^2 + \alpha_1 s]t - sN),$$

where α_1, α_2 denote generic constants independent of the parameters involved.

3 On the \mathcal{H} -Matrix Approximation to the Resolvent $(zI - \mathcal{L})^{-1}$

Below, we briefly discuss the main features of the \mathcal{H} -matrix techniques to be used for data-sparse approximation of the operator resolvent in question. We recall the complexity bound for the \mathcal{H} -matrix arithmetic and prove the existence of the accurate \mathcal{H} -matrix approximation to the resolvent of elliptic operator in the case of smooth data.

Note that there are different strategies to construct the \mathcal{H} -matrix approximation to the inverse $A = \mathcal{L}^{-1}$ of the elliptic operator \mathcal{L} . The existence result is obtained for the direct Galerkin approximation \mathbf{A}_h to the operator A provided that the Green function is given explicitly (we call this \mathcal{H} -matrix approximation by $\mathbf{A}_{\mathcal{H}}$). In this paper, such an approximation has only the theoretical significance. However, using this construction we prove the *density* of \mathcal{H} -matrices for approximation to the inverse of elliptic operators in the sense that there exists the \mathcal{H} -matrix $\mathbf{A}_{\mathcal{H}}$ such that

$$\|\mathbf{A}_h - \mathbf{A}_{\mathcal{H}}\| \leq c\eta^L, \quad \eta < 1, \quad (3.1)$$

where $L = \mathcal{O}(\log N)$, $N = \dim V_h$, cf. Corollary 3.4.

In practice, we start from certain FE Galerkin stiffness matrix \mathbf{L}_h corresponding to the elliptic operator involved, which has already the \mathcal{H} -matrix format, i.e., we set $\mathbf{L}_{\mathcal{H}} := \mathbf{L}_h$. Then using the \mathcal{H} -matrix arithmetic, we compute the approximate \mathcal{H} -matrix inverse $\tilde{\mathbf{A}}_{\mathcal{H}}$ to the exact fully populated matrix $\mathbf{L}_{\mathcal{H}}^{-1}$. The difference $\|\mathbf{A}_{\mathcal{H}} - \tilde{\mathbf{A}}_{\mathcal{H}}\|$ will not be analysed in this paper. In turn, the numerical results in [8] exhibit the approximation $\|\mathbf{L}_{\mathcal{H}}^{-1} - \tilde{\mathbf{A}}_{\mathcal{H}}\| = \mathcal{O}(\varepsilon)$ with the block rank $r = \mathcal{O}(\log^{d-1} \varepsilon^{-1})$ for $d = 2$.

We end up with a simple example of the hierarchical block partitioning to build the \mathcal{H} -matrix inverse for the 1D Laplacian and for a singular integral operator.

3.1 Problem Classes

Suppose we are given the second order elliptic operator (2.3). In our application, we look for a sufficiently accurate data-sparse approximation of the operator $(zI - \mathcal{L})^{-1} : H^{-1}(\Omega) \rightarrow H_0^1(\Omega)$, $\Omega \in \mathbb{R}^d$, $d \geq 1$, where $z \in \mathbb{C}$, $z \notin \text{sp}(\mathcal{L})$, is given in Step 1 of Algorithm 2.3. Assume that Ω is a domain with smooth boundary. To prove the existence of an \mathcal{H} -matrix approximation to $\exp(-t\mathcal{L})$, we use the classical integral representation for $(zI - \mathcal{L})^{-1}$,

$$(zI - \mathcal{L})^{-1}u = \int_{\Omega} G(x, y)u(y)dy, \quad u \in H^{-1}(\Omega), \quad (3.2)$$

where Green's function $G(x, y) = G(x, y; z)$ solves the equation

$$(zI - \mathcal{L})_x G(x, y) = \delta(x - y) \quad (x, y \in \Omega), \quad G(x, y) = 0 \quad (x \in \partial\Omega, y \in \Omega). \quad (3.3)$$

Together with an adjoint system of equations in the second variable y , equation (3.3) provides the base to prove the existence of the \mathcal{H} -matrix approximation of $(zI - \mathcal{L})^{-1}$ which then can be obtained by using the *\mathcal{H} -matrix arithmetic* from [11, 12].

The error analysis for the \mathcal{H} -matrix approximation to the integral operator from (3.2) may be based on using degenerate expansions of the kernel, see §3.2. In this way, we use different smoothness prerequisites. In the case of smooth boundaries and analytic coefficients the analyticity of the Green's function $G(x, y)$ for $x \neq y$ is applied:

Assumption 3.1 *For any $x_0, y_0 \in \Omega$, $x_0 \neq y_0$, the kernel function $G(x, y)$ is analytic with respect to x and y at least in the domain $\{(x, y) \in \Omega \times \Omega : |x - x_0| + |y - y_0| < |x_0 - y_0|\}$.*

An alternative (and weaker) assumption requires that the kernel function G is asymptotically smooth, i.e.,

Assumption 3.2 *For any $m \in \mathbb{N}$, for all $x, y \in \mathbb{R}^d$, $x \neq y$, and all multi-indices α, β with $|\alpha| = \alpha_1 + \dots + \alpha_d$ there holds $|\partial_x^\alpha \partial_y^\beta G(x, y)| \leq c(|\alpha|, |\beta|)|x - y|^{2-|\alpha|-|\beta|-d}$ for all $|\alpha|, |\beta| \leq m$.*

The smoothness of Green's function $G(x, y)$ is determined by the regularity of the problem (3.3).

3.2 On the Existence of \mathcal{H} -Matrix Approximation

Let $A := (zI - \mathcal{L})^{-1}$. Given the Galerkin ansatz space $V_h \subset L^2(\Omega)$, consider the existence of a data-sparse approximation $\mathbf{A}_{\mathcal{H}}$ to the exact stiffness matrix (which is not computable in general)

$$\mathbf{A}_h = \langle A\varphi_i, \varphi_j \rangle_{i,j \in I}, \quad \text{where } V_h = \text{span}\{\varphi_i\}_{i \in I}.$$

Let I be the index set of unknowns (e.g., the FE-nodal points) and $T(I)$ be the hierarchical cluster tree [11]. For each $i \in I$, the support of the corresponding basis function φ_i is denoted by $X(i) := \text{supp}(\varphi_i)$ and for each cluster $\tau \in T(I)$ we define $X(\tau) = \bigcup_{i \in \tau} X(i)$. In the following we use only piecewise constant/linear FEs defined on the quasi-uniform grid.

In a canonical way (cf. [12]), a block-cluster tree $T(I \times I)$ can be constructed from $T(I)$, where all vertices $b \in T(I \times I)$ are of the form $b = \tau \times \sigma$ with $\tau, \sigma \in T(I)$. Given a matrix $M \in \mathbb{R}^{I \times I}$, the block-matrix corresponding to $b \in T(I \times I)$ is denoted by $M^b = (m_{ij})_{(i,j) \in b}$. An *admissible block partitioning* $P_2 \subset T(I \times I)$ is a set of disjoint blocks $b \in T(I \times I)$, satisfying the *admissibility condition*,

$$\min\{\text{diam}(\sigma), \text{diam}(\tau)\} \leq 2\eta \text{dist}(\sigma, \tau), \quad (3.4)$$

$(\sigma, \tau) \in P_2$, $\eta < 1$, whose union equals $I \times I$ (see an example in Fig. 2b related to the 1D case). Let a block partitioning P_2 of $I \times I$ and $k \ll N$ be given. The set of complex \mathcal{H} -matrices induced by P_2 and $k = k(b)$ is

$$\mathcal{M}_{\mathcal{H},k}(I \times I, P_2) := \{M \in \mathbb{Z}^{I \times I} : \text{for all } b \in P_2 \text{ there holds } \text{rank}(M^b) \leq k(b)\}.$$

With the splitting $P_2 = P_{far} \cup P_{near}$, where $P_{far} := \{\sigma \times \tau \in P_2 : \text{dist}(X(\tau), X(\sigma)) > 0\}$, the standard \mathcal{H} -matrix approximation of the nonlocal operator $A = (zI - \mathcal{L})^{-1}$ is based on using a separable expansion of the exact kernel,

$$G_{\tau,\sigma}(x, y) = \sum_{\nu=1}^k a_{\nu}(x)c_{\nu}(y), \quad (x, y) \in X(\sigma) \times X(\tau),$$

of the order $k \ll N = \dim V_h$ for $\sigma \times \tau \in P_{far}$, see [12]. The reduction with respect to the operation count is achieved by replacing the full matrix blocks $\mathbf{A}^{\tau \times \sigma}$ ($\tau \times \sigma \in P_{far}$) by their low-rank approximation

$$\mathbf{A}_{\mathcal{H}}^{\tau \times \sigma} := \sum_{\nu=1}^k \mathbf{a}_{\nu} \cdot \mathbf{c}_{\nu}^T, \quad \mathbf{a}_{\nu} \in \mathbb{R}^{n_{\tau}}, \quad \mathbf{c}_{\nu} \in \mathbb{R}^{n_{\sigma}},$$

where $\mathbf{a}_{\nu} = \left\{ \int_{X(\tau)} a_{\nu}(x)\varphi_i(x)dx \right\}_{i \in \tau}$, $\mathbf{c}_{\nu} = \left\{ \int_{X(\sigma)} c_{\nu}(y)\varphi_j(y)dy \right\}_{j \in \sigma}$. Therefore, we obtain the following storage and matrix-vector multiplication cost for the matrix blocks

$$\mathcal{N}_{st}(\mathbf{A}_{\mathcal{H}}^{\tau \times \sigma}) = k(n_{\tau} + n_{\sigma}), \quad \mathcal{N}_{MV}(\mathbf{A}_{\mathcal{H}}^{\tau \times \sigma}) = 2k(n_{\tau} + n_{\sigma}),$$

where $n_{\tau} = \#\tau$, $n_{\sigma} = \#\sigma$. On the other hand, the approximation of the order $\mathcal{O}(N^{-\alpha})$, $\alpha > 0$, is achieved with $k = \mathcal{O}(\log^{d-1} N)$.

3.3 The Error Analysis

For the error analysis, we consider the uniform hierarchical cluster tree $T(I)$ (see [11, 12] for more details) with the depth L such that $N = 2^{dL}$. Define $P_2^{(\ell)} := P_2 \cap T_2^{\ell}$, where T_2^{ℓ} is the set of clusters $\tau \times \sigma \in T_2$ such that blocks τ, σ belong to level ℓ , with $\ell = 0, 1, \dots, L$. We consider the expansions with the local rank k_{ℓ} depending only on the level number ℓ and defined by $k_{\ell} := \min\{2^{d(L-\ell)}, m_{\ell}^{d-1}\}$, where $m = m_{\ell}$ is given by

$$m_{\ell} = aL^{1-q}(L - \ell)^q + b, \quad 0 \leq q \leq 1, \quad a, b > 0. \quad (3.5)$$

Note that for $q = 0$, we arrive at the constant order $m = \mathcal{O}(L)$, which leads to the exponential convergence of the \mathcal{H} -matrix approximation, see [15].

Introduce

$$N_0 = \max_{0 \leq \ell \leq p} \max \left\{ \max_{\tau \in T(\ell)} \sum_{\tau: \tau \times \sigma \in P_2^{(\ell)}} 1, \max_{\sigma \in T(\ell)} \sum_{\sigma: \tau \times \sigma \in P_2^{(\ell)}} 1 \right\}.$$

For the ease of exposition, we consider the only two special cases $q = 0$ and $q = 1$. Denote by $A_h : V_h \rightarrow V'_h$ the restriction of A onto the Galerkin subspace $V_h \subset L^2(\Omega)$ defined by $\langle A_h u, v \rangle = \langle Au, v \rangle$ for all $u, v \in V_h$. The operator $A_{\mathcal{H}}$ has the similar sense. The following statement is the particular case of [14, Lemma 2.4].

Lemma 3.3 Let $\eta = 2^{-\alpha}$, $\alpha > 0$, and

$$|s(x, y) - s_{\tau\sigma}(x, y)| \lesssim \eta^{m_\ell} \ell^{3-d} \text{dist}(\tau, \sigma)^{2-d}$$

for each $\tau \times \sigma \in P_2^{(\ell)}$, where the order of expansion m_ℓ is defined by (3.5) with $q = 0, 1$ and with a given $a > 0$ such that $-\alpha a + 2 < 0$. Then, for all $u, v \in V_h$ there holds

$$\langle (A_h - A_{\mathcal{H}})u, v \rangle \lesssim h^2 N_0 \delta(L, q) \|u\|_0 \|v\|_0, \quad (3.6)$$

where $\delta(L, 0) = \eta^L$ and $\delta(L, 1) = 1$ and $d = 2, 3$.

Note that in the case of constant order expansions, i.e., for $q = 0$, we obtain the exponential convergence

$$\langle (A_h - A_{\mathcal{H}})u, v \rangle \lesssim N_0 L^{4-d} \eta^L \|u\|_0 \|v\|_0 \quad (u, v \in V_h)$$

for any a in (3.5).

The first important consequence of Lemma 3.3 is that for the variable order expansions with $q = 1$ the asymptotically optimal convergence is verified only for trial functions from $L^2(\Omega)$. On the other hand, the exponential convergence in the operator norm $\|\cdot\|_{H^{-1} \rightarrow H^1}$ may be proven for any $0 \leq q < 1$, see [14].

Corollary 3.4 Suppose that the inverse inequality $\|v\|_{0,\Omega} \lesssim h^{-1} \|v\|_{-1,\Omega}$ is valid for all $v \in V_h$. Then there holds

$$\|A_h - A_{\mathcal{H}}\|_{H^{-1} \rightarrow H_0^1} \lesssim N_0 \delta(L, q), \quad q = 0, 1. \quad (3.7)$$

Proof. The estimate (3.6) and the inverse inequality imply

$$\|(A_h - A_{\mathcal{H}})u_h\|_{H^1(\Omega)} = \sup_{v \in V_h} \frac{\langle (A_h - A_{\mathcal{H}})u_h, v \rangle}{\|v\|_{-1,\Omega}} \lesssim h N_0 \delta(L, q) \|u_h\|_0,$$

for any $u_h \in V_h$. Finally, the repeated application of the inverse inequality now to the term $\|u_h\|_0$ implies (3.7). \blacksquare

Remark 3.5 In the case $q = 1$ and $d = 2, 3$, we obtain the optimal error estimate for functions $u \in L^2(\Omega)$. However, if $d = 1$, we have the local rank of constant order $k_{const} = \mathcal{O}(m^{d-1}) = \mathcal{O}(1)$ which again leads to linear complexity.

3.4 Complexity Estimate and Further Discussion of \mathcal{H} -Matrices

The linear-logarithmic complexity $\mathcal{O}(kN \log N)$ of the \mathcal{H} -matrix arithmetic is proven in [11, 12, 13]. In the special case of regular tensor-product grids the following sharp estimate is valid: for any \mathcal{H} -matrix $\mathbf{M} \in \mathbb{R}^{I \times I}$ with rank- k blocks the storage and matrix-vector multiplication complexity is bounded by

$$\mathcal{N}_{st}(\mathbf{M}) \leq (2^d - 1)(\sqrt{d}\eta^{-1} + 1)^d kLN, \quad \mathcal{N}_{MV}(\mathbf{M}) \leq 2\mathcal{N}_{st}(\mathbf{M}).$$

Here, as above, L denotes the depth of the hierarchical cluster tree $T(I)$ with $N = \#I = 2^{dL}$ and $\eta < 1$ is the fixed admissibility parameter defined in (3.4) and responsible for the approximation.

The complexity of the variable order \mathcal{H} -matrices with m_ℓ given by (3.5) and for $d = 2, 3$ depends on the representation of matrix blocks. Using the representation of blocks in a fixed basis, see [16], we have

$$\mathbf{A}_{\mathcal{H}}^{\tau \times \sigma} = \sum_{i,j=1}^{k_\ell} a_{ij} (a_i \cdot c_j^T) \in \mathcal{V}_a \otimes \mathcal{V}_c, \quad a_i \in \mathbb{R}^{n_\tau}, \quad c_j \in \mathbb{R}^{n_\sigma}, \quad (3.8)$$

where $\mathcal{V}_a = \text{span}\{a_i\}_{1 \leq i \leq k_\ell}$, $\mathcal{V}_c = \text{span}\{c_j\}_{1 \leq j \leq k_\ell}$ with $k_\ell = \mathcal{O}(m_\ell^{d-1})$. We then obtain the following storage estimate

$$\mathcal{N}_{st}(\mathbf{A}_{\mathcal{H}}) \lesssim N_0 \sum_{\ell=0}^L k_\ell^2 2^{d\ell} \lesssim N_0 L^{2(1-q)(d-1)} N.$$

As result, we arrive at a linear complexity bound with the choice $q = 1$ in (3.5). It is easy to see that for $q = 1$ the matrix-vector product has linear complexity as well, see [16, 15].

In what follows, we discuss simple examples of block partitionings P_2 and the corresponding \mathcal{H} -matrix approximations for the integral operators with asymptotically smooth kernels. The inversion in the \mathcal{H} -matrix arithmetic to the given $M \in \mathcal{M}_{\mathcal{H},k}(I \times I, P_2)$ is discussed in [11, 12]. In the general case of quasiuniform meshes the complexity $\mathcal{O}(k^2 N)$ of matrix inversion is proven. It is worth to note that the FE Galerkin matrix for the second order elliptic operator in \mathbb{R}^d , $d \geq 1$, belongs to $\mathcal{M}_{\mathcal{H},k}(I \times I, P_2)$ for each $k \in \mathbb{N}$. In particular, for $d = 1$ the tridiagonal stiffness matrix corresponding to the operator $-\frac{d^2}{dx^2} : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$, $\Omega = (0, 1)$, belongs to $\mathcal{M}_{\mathcal{H},1}(I \times I, P_2)$ with the partitioning P_2 depicted in Fig. 2a. Therefore, each matrix block involved in the above partitioning has the rank equals one. It is a particular 1D-effect that the inverse to this tridiagonal matrix has the same format, i.e., the inverse is exactly reproduced by an \mathcal{H} -matrix (see [11] for more details).

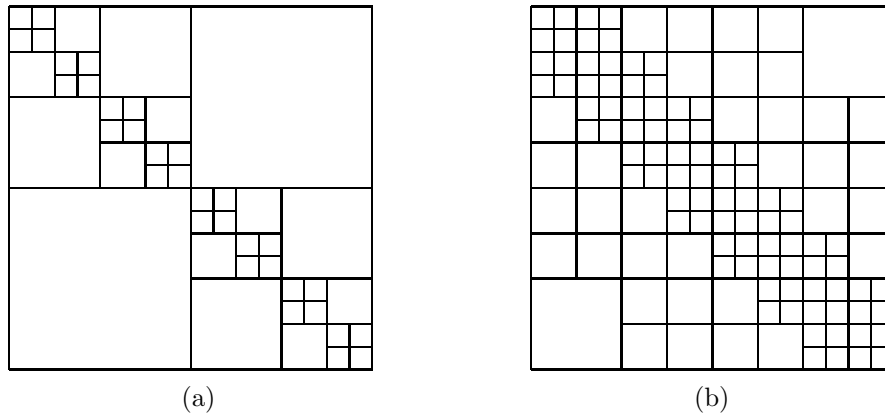


Figure 2: Block partitioning P_2 in the case of 1D differential operator (a) and for the integral operator with a singular kernel (b)

In general, the admissibility condition is intended to provide the hierarchical approximation for the asymptotically smooth kernel $G(x, y)$, see Assumption 3.2, which is singular on the diagonal $x = y$. Thus, an admissible block partitioning includes only “nontouching blocks” belonging to P_{far} and leaves of $T(I \times I)$, see Fig. 2b corresponding to the case $\eta = \frac{1}{2}$, $N = 2^4$ for 1D index set. In the case $d = 2, 3$ the admissible block partitioning is defined recursively, see [12], using the block cluster tree $T(I \times I)$. The numerical experiments for 2D Laplacian illustrate the efficiency of the \mathcal{H} -matrix inversion. Improved data-sparsity is achieved by using the \mathcal{H}^2 -matrix approximation [16] based on the block representation (3.8) with fixed basis of \mathcal{V}_a and \mathcal{V}_c for all admissible matrix blocks.

4 Applications

4.1 Parabolic Problems

In the first example, we consider an application to parabolic problems. Using semigroup theory (see [20] for more details), the solution of the first order evolution equation

$$\frac{du}{dt} + \mathcal{L}u = f, \quad u(0) = u_0,$$

with a known initial vector $u_0 \in L^2(\Omega)$ and with the given right-hand side $f \in L^2(Q_T)$, $Q_T := (0, t) \times \Omega$, can be represented as

$$u(t) = \exp(-t\mathcal{L})u_0 + \int_0^t \exp(-(t-s)\mathcal{L})f(s)ds. \quad (4.1)$$

We consider the following semi-discrete scheme. Let \mathbf{M}_j be the \mathcal{H} -matrix approximation of the resolvent $(z_j I - \mathcal{L})^{-1}$ in (2.9) associated with the Galerkin ansatz space $V_h \subset L^2(\Omega)$ and let \mathbf{u}_0, \mathbf{f} be the vector representations of the corresponding Galerkin projections onto the spaces V_h and $V_h \times [0, T]$, respectively.

Then the \mathcal{H} -matrix approximation of the operator exponential takes the form

$$\exp_{\mathcal{H}}(-t\mathcal{L}) = \sum_{j=1}^{2N_0-1} \gamma_j e^{-z_j t} \mathbf{M}_j, \quad \gamma_j = \frac{1}{2N_0 i} \frac{dz(\eta(\xi_j))}{d\eta} \frac{d\eta(\xi_j)}{d\xi}.$$

Substitution of the above representation into (4.1) leads to the entirely parallelisable scheme

$$u_{\mathcal{H}}(t) = \sum_{j=1}^{2N_0-1} \gamma_j e^{-z_j t} \mathbf{M}_j \left(\mathbf{u}_0 + \int_0^t e^{z_j s} \mathbf{f}(s) ds \right), \quad (4.2)$$

with respect to $j = 1, \dots, 2N_0 - 1$, to compute the approximation $u_{\mathcal{H}}(t)$,

The second level of parallelisation appears if we are interested to calculate the right-hand side of (4.2) for different time steps.

4.2 Dynamical Systems and Control Theory

In the second example, we consider the linear dynamical system of equations

$$\frac{dX(t)}{dt} = AX(t) + X(t)B + C(t), \quad X(0) = X_0,$$

where $X, A, B, C \in \mathbb{R}^{n \times n}$. The solution is given by

$$X(t) = e^{tA} X_0 e^{tB} + \int_0^t e^{(t-s)A} C(s) e^{(t-s)B} ds.$$

Suppose that we can construct the \mathcal{H} -matrix approximations of the corresponding matrix exponents

$$\exp_{\mathcal{H}}(tA) = \sum_{l=1}^{2N_0-1} \gamma_{al} e^{-a_l t} \mathbf{A}_l, \quad \exp_{\mathcal{H}}(tB) = \sum_{j=1}^{2N_0-1} \gamma_{bj} e^{-b_j t} \mathbf{B}_j, \quad \mathbf{A}_l, \mathbf{B}_j \in \mathcal{M}_{\mathcal{H},k}(I \times I, P_2).$$

Then the approximate solution $X_{\mathcal{H}}(t)$ may be computed in parallel as in the first example,

$$X_{\mathcal{H}}(t) = \sum_{l,j=1}^{2N_0-1} \gamma_{al} \gamma_{bj} e^{-(a_l+b_j)t} \mathbf{A}_l \left(X_0 + \int_0^t e^{(a_l+b_j)s} C(s) ds \right) \mathbf{B}_j.$$

Let C be constant and the eigenvalues of A, B have negative real parts, then $X(t) \rightarrow X_{\infty}$ as $t \rightarrow \infty$, where

$$X_{\infty} = \int_0^{\infty} e^{tA} C e^{tB} dt$$

satisfies the *Lyapunov-Sylvester equation*

$$AX_{\infty} + X_{\infty}B + C = 0.$$

Assume we are given the hierarchical approximations to e^{tA} and e^{tB} as above. Then there holds

$$X_{\mathcal{H},\infty} = \int_0^{\infty} \left(\sum_{l=1}^{2N_0-1} \gamma_{al} e^{-a_l t} \mathbf{A}_l \right) \mathbf{C}_{\mathcal{H}} \left(\sum_{j=1}^{2N_0-1} \gamma_{bj} e^{-b_j t} \mathbf{B}_j \right) dt = \sum_{l,j=1}^{2N_0-1} \gamma_{al} \gamma_{bj} \int_0^{\infty} e^{-(a_l+b_j)t} dt \mathbf{A}_l \mathbf{C}_{\mathcal{H}} \mathbf{B}_j, \quad (4.3)$$

where $\mathbf{C}_{\mathcal{H}}$ stands for the \mathcal{H} -matrix approximation to C if available. Taking into account that the \mathcal{H} -matrix multiplication has the complexity $\mathcal{O}(k^2 n)$, we then obtain a fully parallelisable scheme of complexity $\mathcal{O}(N_0 k n)$ (but not $\mathcal{O}(n^3)$ as in the standard linear algebra) for solving the matrix Lyapunov equation.

In many applications the right-hand side is given by a low rank matrix, $\text{rank}(C) = k \ll n$. In this case we immediately obtain the explicit low rank approximation for the solution of the Lyapunov equation.

Lemma 4.1 Let $C = \sum_{\alpha=1}^k \mathbf{a}_\alpha \cdot \mathbf{c}_\alpha^T$. Moreover, we assume $B = A^T$. Then the solution of the Lyapunov-Sylvester equation is approximated by

$$X_{\mathcal{H}} = \sum_{\alpha=1}^k \sum_{l,j=1}^{2N_0-1} \frac{\gamma_{al}\gamma_{bj}}{a_l + b_j} (\mathbf{A}_l \mathbf{a}_\alpha) \cdot (\mathbf{A}_j \mathbf{c}_\alpha)^T, \quad (4.4)$$

such that $\|X_\infty - X_{\mathcal{H}}\|_\infty \leq \varepsilon$, with $N_0 = \mathcal{O}(\log \varepsilon^{-1})$ and $\text{rank}(X_{\mathcal{H}}) = k(2N_0 - 1)$.

Proof. In fact, substitution of the rank- k matrix C into (4.3) leads to (4.4). Due to the exponential convergence in (2.10), we obtain $N_0 = \mathcal{O}(\log \varepsilon^{-1})$, where ε is the approximation error. Combining all terms in (4.4) corresponding to the same index $l = 1, \dots, 2N_0 - 1$ proves that $X_{\mathcal{H}}$ has the rank $k(2N_0 - 1)$. ■

Various techniques were considered for numerical solution of the Lyapunov equation, see, e.g., [2], [6], [19] and the references therein. Among others, Lemma 4.1 proves the non-trivial fact that the solution X_∞ of our matrix equation admits an accurate low rank approximation if this is the case for the right-hand side C . We refer to [8] for a more detailed analysis and numerical results concerning the \mathcal{H} -matrix techniques for solving the Lyapunov equation.

5 On the Choice of Computational Parameters and Numerics

In this section we discuss how the parameters of the parabola influence our method.

Let $\Gamma_0 = \{z = \xi \pm i\eta = a\eta^2 + \gamma_0 \pm i\eta\}$ be the parabola containing the spectrum of \mathcal{L} whose parameters a, γ_0 are determined by the coefficients of \mathcal{L} . Given a , we choose the integration path $\Gamma = \{z = \xi_1 \pm i\eta_1 = a_1\eta_1^2 + b \pm i\eta_1\}$ with $b \in (0, \gamma_0)$, $a_1 \geq a$. It is easy to find that the distance $d(\Gamma, \Gamma_0)$ between Γ and Γ_0 is

$$d(\Gamma, \Gamma_0) = \min_{\eta, \eta_1 \in \mathbb{R}} \{[a(\eta^2 - \eta_1^2) + (b - \gamma_0)]^2 + (\eta - \eta_1)^2\}^{1/2} = \gamma_0 - b.$$

It means that the strip Π_η around the real axis $\eta \in (-\infty, \infty)$ in (2.6), in which the integrand can be extended holomorphically, is of the width $s_\eta = 2(\gamma_0 - b)$. Let $\eta = \eta(\xi)$ be a conformal mapping $\eta : (0, 2\pi) \rightarrow (-\infty, \infty)$ and s_ξ be the width of the strip Π_ξ around the interval $\xi \in (0, 2\pi)$ in which, in turn, the integrand $F_1(\xi, t) \equiv F(\eta, t)$ can be extended holomorphically. It follows from

$$\eta(\xi + is_\xi) = \eta(\xi) + i\eta'(\theta)s_\xi$$

that $\alpha_1 s_\xi \leq s_\eta \leq \alpha_2 s_\xi$ where $\alpha_1 = \min_{\xi \in \Pi_\xi} |\eta'(\xi)|$, $\alpha_2 = \max_{\xi \in \Pi_\xi} |\eta'(\xi)|$ and $s_\xi \rightarrow 0$ together with $s_\eta \rightarrow 0$. The bound of the integrand $F_1(\xi, t) = F(\eta, t)$ on Π_ξ is less or equal to the bound of $F(\eta, t)$ in the strip Π_η . Since the absolute value of an analytic function attains its maximum on the boundary, we have

$$\begin{aligned} M_1 &= \sup_{\xi \in \Pi_\xi} \|F_1(\xi, t)\| = \sup_{\xi \in \Pi_\xi} \|e^{-z(\xi)t} (z(\xi) - \mathcal{L})^{-1} \frac{dz}{d\xi} \frac{d\xi}{d\eta}\| \\ &\leq M\alpha_2 \max_{\eta \in (-\infty, \infty)} \sup_{\eta \in (-\infty, \infty)} |e^{-[a(\eta+is_\eta)^2 + b - i(\eta+is_\eta)]t}| \frac{|2a(\eta + is_\eta) - i|}{1 + \sqrt{|z|}} \leq M\alpha_2 \max\{\theta_+(t), \theta_-(t)\} e^{-[b - as_\eta^2 + s_\eta]t}, \end{aligned}$$

where

$$\theta_\pm(t) = \sup_{\eta \in (-\infty, \infty)} \theta_\pm(\eta, t), \theta_\pm(\eta, t) = e^{-a\eta^2 t} \frac{\sqrt{4a^2\eta^2 + (2as_\eta \mp 1)^2}}{1 + \sqrt{(a\eta^2 + b - as_\eta^2 \pm s_\eta)^2 + \eta^2(2as_\eta \mp 1)^2}}.$$

For the last function we have the estimate $\theta_\pm(\eta, t) \leq \bar{\theta}_\pm(\eta, t)$ with

$$\bar{\theta}_\pm(\eta, t) = e^{-a\eta^2 t} \left[\frac{4a^2\eta^2 + (2as_\eta \mp 1)^2}{1 + (a\eta^2 + b - as_\eta^2 \pm s_\eta)^2 + \eta^2(2as_\eta \mp 1)^2} \right]^{1/2}.$$

Denoting $\zeta = a\eta^2$, we get

$$\bar{\theta}_\pm(\eta, t) \equiv \tilde{\theta}_\pm(\zeta, t) = e^{-\zeta t} \left[\frac{4a\zeta + (2as_\eta \mp 1)^2}{1 + (\zeta + b - as_\eta^2 \pm s_\eta)^2 + \zeta(2as_\eta \mp 1)^2/a} \right]^{1/2}.$$

It is easy to find that there exists a_0 such that $\frac{d\bar{\theta}_{\pm}^2(\zeta, t)}{d\zeta} < 0$ for all $a > a_0$ and $\zeta \in (0, \infty)$, i.e., for such a we have

$$\bar{\theta}_{\pm}(\eta, t) \leq \tilde{\theta}_{\pm}(0, t) = \frac{|2as_{\eta} \mp 1|}{\sqrt{1 + (b - as_{\eta}^2 \pm s_{\eta})^2}} = \frac{|2as_{\eta} \mp 1|}{\sqrt{1 + (b - as_{\eta}^2 \pm s_{\eta})^2}} \lesssim s_{\eta}^{-1}.$$

Thus, we get the estimate

$$\|T(t) - T_N(t)\| \equiv \|\exp(-t\mathcal{L}) - \exp_N(-t\mathcal{L})\| \lesssim s_{\xi}^{-1} \exp(-[b - a\alpha_2^2 s_{\xi}^2 + \alpha_1 s_{\xi}]t - s_{\xi}N). \quad (5.1)$$

In order to arrive at a given tolerance $\varepsilon > 0$ we have to choose

$$N \asymp s_{\xi}^{-1} \ln \frac{1}{\varepsilon} + \ln s_{\xi} - [\gamma_0 - a\alpha_2^2 s_{\xi}^2]t.$$

This rough estimate shows that we can minimise N (i.e., the number of resolvent inversions for various z_i) by maximization of $s_{\xi} \lesssim \gamma_0 - b$ with respect to the parameters a, b and α from (2.8). One can also see that the decreasing of a implies decreasing of N .

To complete this section, we present the numerical example on the \mathcal{H} -matrix approximation of the exponential for the 1D finite difference Laplacian Δ_h on $\Omega = (0, 1)$ (with zero boundary conditions) defined on the uniform grid with the mesh-size $h = 1/(n+1)$, where n is the problem size. Table 1 presents the accuracy of the \mathcal{H} -matrix approximation by Algorithm 2.3 versus the number N of resolvents involved. The local rank is chosen as $k = 5$, while $b = 0.9 \lambda_{\min}(\Delta_h)$, $a = 4$. Our calculations indicate the robust exponential convergence of (2.9) with respect to N for the range of parameters $b \in (0, 0.95\lambda_{\min}(\Delta_h))$ and $a \in (0, a_0)$ with $a_0 = \mathcal{O}(1)$ and confirm our analysis. The computational time corresponding to the \mathcal{H} -matrix evaluation of each resolvent in (2.9) takes 0.16 and 28.1 sec. at a SUN-Ultra1 station for $n = 128$ and $n = 4096$, respectively.

The results have been obtained by L. Grasedyck (University of Kiel) using the general **HMA1** code implementing the \mathcal{H} -matrix arithmetic, see also [8] for more details.

$n \setminus N$	1	4	7	10	20	30	40	50	60	70
128	1.4 e-0	7.1 e-2	3.4 e-2	9.3 e-3	2.4 e-4	1.4 e-5	2.9 e-6	3.4 e-7	8.1 e-8	2.2 e-8
4096	1.4 e-0	7.5 e-2	3.3 e-2	9.0 e-3	2.3 e-4	8.0 e-6	3.2 e-6	1.2 e-7	1.1 e-7	2.6 e-8

Table 1: Approximation to the exponential of 1D discrete Laplacian, where $n = \dim V_h$ and N is defined from (2.9)

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