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

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Summary. 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 [4].

In the preceding papers [12]–[17], 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.

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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 $O(n)$ 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 [12]-[17]. 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 [20]. The most commonly used algorithms are based on Krylov subspace methods [22,18]. A class of effective algorithms based on the Cayley transform was developed in [8].

Concerning the second order evolution problems and the operator cosine family new discretisation methods were recently developed in [4]- [5] 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 [5]. Parallel methods with a polynomial convergence order 2 and 4 based on a contour integration for symmetric and positive definite operators were proposed in [24].

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 based on the Sinc-approximation of integrals in infinite strip and 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 $\Re e(sp(A)) < 0$, 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 Sect. 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 [4] and play an important role in the theory of the second order difference equations [23], evolution differential equations as well as the cosine operator family in a Banach space X [4] .

Let $A : X \to X$ 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 $A : X \to X$ is strongly P-positive if its spectrum $sp(A)$ lies in the domain Ω_{Γ_0} and the estimate*

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

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 $\|u\|_X \le c_e \|u\|_V$, $\forall u \in V$. Assume that $a(\cdot,\cdot)$ is bounded, i.e.,

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

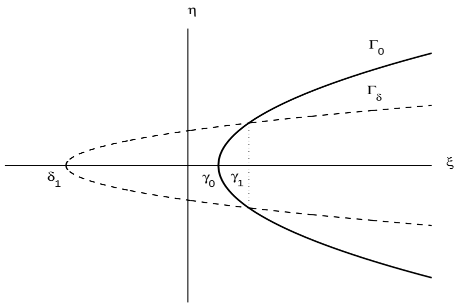


Fig. 1. Parabolae Γ_δ and Γ_0

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

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

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

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

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

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

It implies

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

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 $\Re e\, sp(A) > \gamma_1 > \gamma_0$ 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 $\Re e\, sp(A) > 0$ and in this case one can choose $\gamma_1 = \delta_0 c_e^{-2} - \delta_1$. Analogously to [4] it can be shown that inequality (2.1) holds true in $\mathbb{C} \backslash \Omega_{\Gamma_0}$ (see the discussion in [4, pp. 330-331]). In the following, the operator A is strongly P-positive.

2.2 Examples

As the *first example* let us consider the one-dimensional operator $A : L_1(0,1) \to L_1(0,1)$ 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

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

Here we set $X = L_1(0,1)$ (see Definition 2.1). The eigenvalues $\lambda_k = k^2\pi^2$ $(k = 1, 2, \ldots)$ 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

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

i.e., we have

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

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 $\|u\|_{L_1} = \|(zI - A)^{-1} f\|_{L_1} \le \frac{M}{1+\sqrt{|z|}} \|f\|_{L_1}$ $(f \in L_1(0,1),\ z \in \mathbb{C} \setminus \Omega_{\Gamma_0})$, i.e., the operator $A : L_1 \to L_1$ 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 [5] for details).

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

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

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

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

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

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

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

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

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 $\xi_u\geq C_1|u|_1^2-C_2\|u\|_0\geq C_1C_F-C_2,\ |\eta_u|\leq C_3|u|_1\leq C_3\sqrt{(\xi_u+C_2)/C_1}$, 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 $\gamma_1=C_1C_F-C_2>\gamma_0$. 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 Sect. 2.1.

The *third example* is given by a matrix $A\in\mathbb{R}^{n\times n}$ whose spectrum satisfies $\Re e\, sp(A)>0$. 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 $C_i=\{z:\,|z-a_{ii}|\leq\sum\limits_{j=1,j\neq i}^{n}a_{ij}\}$, $D_j=\{z:\,|z-a_{jj}|\leq\sum\limits_{i=1,i\neq j}^{n}a_{ij}\}$. Then by Gershgorin's theorem,

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

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

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., [21]) satisfies the differential equation

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

where I is the identity operator (the last equality means that $\lim_{t\to+0} T(t)$ $u_0 = u_0$ for all $u_0 \in X$). 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 $u(t)$: $\mathbb{R}_+ \to X$ 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 (called the integration parabola)* $\Gamma = \{z = \xi + i\eta : \xi = \tilde{a}\eta^2 + b\}$ *with* $\tilde{a} \le a,\ b \le \gamma_0$. *Then the exponent* $\exp(-t\mathcal{L})$ *can be represented by the Dunford-Cauchy integral [2]*

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

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

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

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

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

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

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

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

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

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

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

with

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

2.4 The computational scheme and the convergence analysis

Following [25], we construct a quadrature rule for the integral in (2.6) by using the Sinc approximation on $(-\infty, \infty)$. For $1 \le p \le \infty$, introduce the family $\mathbf{H}^p(D_d)$ of all operator-valued functions, which are analytic in the infinite strip D_d,

$$D_d = \{z \in \mathbb{C} : -\infty < \Re e\, z < \infty, |\Im m\, z| < d\}, \tag{2.7}$$

such that if $D_d(\epsilon)$ is defined for $0 < \epsilon < 1$ by

$$D_d(\epsilon) = \{z \in \mathbb{C} : |\Re e\, z| < 1/\epsilon, |\Im m\, z| < d(1-\epsilon)\} \tag{2.8}$$

then for each $\mathcal{F} \in \mathbf{H}^p(D_d)$ there holds $\|\mathcal{F}\|_{\mathbf{H}^p(D_d)} < \infty$ with

$$\|\mathcal{F}\|_{\mathbf{H}^p(D_d)} = \begin{cases} \lim\limits_{\varepsilon\to 0}\left(\int_{\partial D_d(\varepsilon)} \|\mathcal{F}(z)\|^p\,|dz|\right)^{1/p} & \text{if } 1 \le p < \infty, \\ \lim\limits_{\varepsilon\to 0}\sup\limits_{z\in\partial D_d(\varepsilon)} \|\mathcal{F}(z)\| & \text{if } p = \infty. \end{cases} \tag{2.9}$$

Let

$$S(k,h)(x) = \frac{\sin\left[\pi(x-kh)/h\right]}{\pi(x-kh)/h} \tag{2.10}$$

be the kth Sinc function with step size h, evaluated at x. Given $\mathcal{F} \in \mathbf{H}^p(D_d)$, $h > 0$, and a positive integer N, let us use the notations

$$\begin{aligned} I(\mathcal{F}) &= \int_{\mathbb{R}} \mathcal{F}(x)dx, \\ T(\mathcal{F},h) &= h \sum_{k=-\infty}^{\infty} \mathcal{F}(kh), \qquad T_N(\mathcal{F},h) = h \sum_{k=-N}^{N} \mathcal{F}(kh), \\ C(\mathcal{F},h) &= \sum_{k=-\infty}^{\infty} \mathcal{F}(kh)S(k,h), \\ \eta_N(\mathcal{F},h) = I(\mathcal{F}) - T_N(\mathcal{F},h), &\quad \eta(\mathcal{F},h) = I(\mathcal{F}) - T(\mathcal{F},h). \end{aligned}$$

Adapting the ideas of [25,5], one can prove (see Appendix) the following approximation results for functions from $\mathbf{H}^1(D_d)$.

Lemma 2.3 *For any operator-valued function $f \in \mathbf{H}^1(D_d)$, there holds*

$$\eta(f,h) = \frac{i}{2} \int_{\mathbb{R}} \left\{ \frac{f(\xi - id)\exp(-\pi(d+i\xi)/h)}{\sin[\pi(\xi - id)/h]} - \frac{f(\xi + id)\exp(-\pi(d-i\xi)/h)}{\sin[\pi(\xi + d)/h]} \right\} d\xi \tag{2.11}$$

providing the estimate

$$\|\eta(f,h)\| \le \frac{\exp(-\pi d/h)}{2\sinh(\pi d/h)} \|f\|_{\mathbf{H}^1(D_d)}. \tag{2.12}$$

If, in addition, f satisfies on $\mathbb{R}$ the condition

$$\|f(x)\| < ce^{-\alpha x^2}, \quad \alpha, c > 0, \tag{2.13}$$

then

$$\|\eta_N(f,h)\| \le c\sqrt{\pi} \left[\frac{\exp(-2\pi d/h)}{\sqrt{\alpha}(1 - \exp(-2\pi d/h))} + \frac{\exp[-\alpha(N+1)^2h^2]}{\alpha h(N+1)} \right]. \tag{2.14}$$

Applying the quadrature rule T_N with the operator-valued function

$$F(\eta, t; \mathcal{L}) = (2\tilde{a}\eta - i)\varphi(\eta)(\psi(\eta)I - \mathcal{L})^{-1} \tag{2.15}$$

where

$$\varphi(\eta) = e^{-t\psi(\eta)}, \quad \psi(\eta) = \tilde{a}\eta^2 + b - i\eta, \tag{2.16}$$

we obtain for integral (2.6)

$$\begin{aligned} T(t) &\equiv exp(-t\mathcal{L}) \approx T_N(t) \equiv exp_N(-t\mathcal{L}) \\ &= h \sum_{k=-N}^{N} F(kh,t;\mathcal{L}). \end{aligned} \tag{2.17}$$

Note that F satisfies (2.13) with $\alpha = t\,\tilde{a}$. The error analysis is given by the following Theorem (see Appendix for the proof).

Theorem 2.4 *Choose* $k > 1,\ \tilde{a} = a/k,\ h = \sqrt[3]{2\pi dk/((N+1)^2 a)},\ b = b(k) = \gamma_0 - (k-1)/(4a)$ *and the integration parabola* $\Gamma_{b(k)} = \{z = \tilde{a}\eta^2 + b(k) - i\eta : \eta \in (-\infty,\infty)\}$. *Then there holds*

$$\begin{aligned} \|T(t) - T_N(t)\| &\equiv \|\exp(-t\mathcal{L}) - \exp_N(-t\mathcal{L})\| \\ &\le Mc\sqrt{\pi}\left[\frac{2\sqrt{k}\, exp[-s(N+1)^{2/3}]}{\sqrt{at}(1-exp(-s(N+1)^{2/3}))}\right. \\ &\qquad \left. + \frac{k\, exp[-ts(N+1)^{2/3}]}{t(N+1)^{1/3}\sqrt[3]{2\pi dka^2}}\right], \end{aligned} \tag{2.18}$$

where

$$\begin{aligned} s &= \sqrt[3]{(2\pi d)^2 a/k}\,, \\ c &= M_1 e^{t[ad^2/k+d-b]}\,, \qquad d = (1-\frac{1}{\sqrt{k}})\frac{k}{2a}, \\ M_1 &= \max_{z\in\overline{D}_d} \frac{|2\frac{a}{k}z - i|}{1+\sqrt{|\frac{a}{k}z^2 + b - iz|}} \end{aligned} \tag{2.19}$$

and M *is the constant from the inequality of the strong P-positiveness.*

The exponential convergence of our quadrature rule allows to introduce the following algorithm for the approximation of the operator exponent at a given time value t.

Algorithm 2.5 *1. Choose* $k > 1$, $d = (1-\frac{1}{\sqrt{k}})\frac{k}{2a}$, N *and determine* z_p $(p = -N,\ldots,N)$ *by* $z_p = \frac{a}{k}(ph)^2 + b - iph$, *where* $h = \sqrt[3]{\frac{2\pi dk}{a}}(N+1)^{-2/3}$ *and* $b = \gamma_0 - \frac{k-1}{4a}$.

2. *Find the resolvents* $(z_pI - \mathcal{L})^{-1},\ p = -N,\ldots,N$ *(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*

$$\exp_N(-t\mathcal{L}) = \frac{h}{2\pi i}\sum_{p=-N}^{N} e^{-tz_p}\left[2\frac{a}{k}ph - i\right](z_pI - \mathcal{L})^{-1}. \tag{2.20}$$

Remark 2.6 The above algorithm possesses *two sequential levels of parallelism*: first, one can compute all resolvents at Step 2 in parallel and, second, each operator exponent at different time values (provided that we apply the operator exponential for a given time vector $(t_1, t_2, \ldots, t_M)$).

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 2.5, which converges much faster than (2.20).

Algorithm 2.7 *1′. Determine* $h = \sqrt[3]{\frac{2\pi dk}{a}}(N+1)^{-2/3}$, $z_p(t)$ $(p = -N,$ $\ldots, N)$ *by* $z_p(t) = \frac{a}{k}(ph)^2 + b(t) - iph$, *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 $(z_p(t)I - t\mathcal{L})^{-1}$, $p = -N, \ldots, N$ *(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*

$$\exp_N(-t\mathcal{L}) = \frac{h}{2\pi i} \sum_{p=-N}^{N} e^{-tz_p(t)} \left[2\frac{a}{k}ph - i\right] (z_p(t)I - t\mathcal{L})^{-1}.$$

Though the above algorithm allows only a 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 $t_i = i\Delta t$, $i = 1, \ldots, n_t$. Then the exponentials for $i = 2, \ldots, n_t$ are easily obtained as the corresponding monomials from $\exp_N(-\Delta t\mathcal{L})$.

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

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

where $L = O(\log N)$, $N = \dim V_h$, 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 $\widetilde{\mathbf{A}}_{\mathcal{H}}$ to the exact fully populated matrix $\mathbf{L}_{\mathcal{H}}^{-1}$. The difference $||\mathbf{A}_{\mathcal{H}} - \widetilde{\mathbf{A}}_{\mathcal{H}}||$ will not be analysed in this paper. In turn, the numerical results in [9] exhibit the approximation $||\mathbf{L}_{\mathcal{H}}^{-1} - \widetilde{\mathbf{A}}_{\mathcal{H}}|| = O(\varepsilon)$ with the block rank $r = O(\log^{d-1} \varepsilon^{-1})$ 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 $(zI - \mathcal{L})^{-1} : H^{-1}(\Omega) \to H_0^1(\Omega)$, $\Omega \in \mathbb{R}^d$, $d \geq 1$, where $z \in \mathbb{C}$, $z \notin sp(\mathcal{L})$, is given in Step 1 of Algorithm 2.5. 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 $(zI - \mathcal{L})^{-1}$,

$$(zI - \mathcal{L})^{-1}u = \int_\Omega G(x, y; z)u(y)dy, \qquad u \in H^{-1}(\Omega), \tag{3.1}$$

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

$$\begin{aligned} &(zI - \mathcal{L})_x G(x, y; z) = \delta(x - y) \qquad &&(x, y \in \Omega), \\ &G(x, y; z) = 0 &&(x \in \partial\Omega,\ y \in \Omega). \end{aligned} \tag{3.2}$$

Together with an adjoint system of equations in the second variable y, equation (3.2) 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 [12,13].

The error analysis for the $\mathcal{H}$-matrix approximation to the integral operator from (3.1) may be based on using degenerate expansions of the kernel, see Sect. 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 $G(x, y; z)$ 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 $G(x, y; z)$ 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 $|\alpha| = \alpha_1 + \ldots + \alpha_d$ there holds $|\partial_x^\alpha \partial_y^\beta G(x, y; z)| \leq c(|\alpha|, |\beta|; z)|x - y|^{2-|\alpha|-|\beta|-d}$ for all $|\alpha|, |\beta| \leq m$.*

The smoothness of Green's function $G(x, y; z)$ is determined by the regularity of the problem (3.2).

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)

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

Let I be the index set of unknowns (e.g., the FE-nodal points) and $T(I)$ be the hierarchical cluster tree [12]. For each $i \in I$, the support of the corresponding basis function φ_i is denoted by $X(i) := \mathrm{supp}(\varphi_i)$ 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 finite elements defined on the quasi-uniform grid.

In a canonical way (cf. [13]), 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,*

$$\min\{\mathrm{diam}(\sigma), \mathrm{diam}(\tau)\} \leq 2\,\eta\; \mathrm{dist}(\sigma, \tau), \tag{3.3}$$

$(\sigma, \tau) \in P_2$, $\eta < 1$, 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

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

With the splitting $P_2 = P_{far} \cup P_{near}$, where $P_{far} := \{\sigma \times \tau \in P_2 : \mathrm{dist}(X(\tau), X(\sigma)) > 0\}$, 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,

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

of the order $k \ll N = \dim V_h$ for $\sigma \times \tau \in P_{far}$, see [13]. 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

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

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

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

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

3.3 The error analysis

For the error analysis, we consider the uniform hierarchical cluster tree $T(I)$ (see [12,13] 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 $\ell = 0, 1, \ldots, L$. 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

$$m_\ell = a\, L^{1-q}(L-\ell)^q + b, \qquad 0 \le q \le 1, \qquad a, b > 0. \tag{3.4}$$

Note that for $q = 0$, we arrive at the constant order $m = O(L)$, which leads to the exponential convergence of the $\mathcal{H}$-matrix approximation, see [16].

Introduce

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

For the ease of exposition, we consider the only two special cases $q = 0$ and $q = 1$. Denote by $A_h : V_h \to V_h'$ 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 [15, Lemma 2.4].

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

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

for each $\tau \times \sigma \in P_2^{(\ell)}$*, where the order of expansion* m_ℓ *is defined by (3.4) 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*

$$\langle (A_h - A_{\mathcal{H}})u, v\rangle \lesssim h^2 N_0 \delta(L, q)||u||_0||v||_0, \tag{3.5}$$

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

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

for any a in (3.4).

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 $|| \cdot ||_{H^{-1}\to H^1}$ may be proven for any $0 \le q < 1$, see [15].

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*

$$||A_h - A_{\mathcal{H}}||_{H^{-1}\to H_0^1} \lesssim N_0\delta(L, q), \qquad q = 0, 1. \tag{3.6}$$

Proof. The estimate (3.5) and the inverse inequality imply

$$||(A_h - A_{\mathcal{H}})u_h||_{H^1(\Omega)} = \sup_{v\in V_h} \frac{\langle (A_h - A_{\mathcal{H}})u_h, v\rangle}{||v||_{-1,\Omega}} \lesssim hN_0\delta(L, q)||u_h||_0,$$

for any $u_h \in V_h$. Finally, the repeated application of the inverse inequality now to the term $||u_h||_0$ implies (3.6). ■

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 $k_{const} = O(m^{d-1}) = O(1)$ which again leads to linear complexity.

We further discuss an important aspect of our scheme related to the uniformity of the error estimate with respect to the choice of quadrature points $z_\nu,\ \nu = -N, ..., N$. The point is that the following asymptotic estimate holds (see Algorithm 2.5)

$$\max_\nu |z_\nu| = O(N^{2/3}) = O\left(\log \frac{1}{\varepsilon}\right), \tag{3.7}$$

where N is the number of quadrature points and ε is the given tolerance. In fact, due to Theorem 2.4, there holds $N^{2/3} = \log \varepsilon^{-1}$. Therefore, the corresponding Green function in (3.1), (3.2) has oscillating features like in the case of Helmholtz' equation, which potentially may lead to a "deterioration of data-sparsity" in the $\mathcal{H}$-matrix approximation. We further give arguments explaining that this is not the case.

For the ease of exposition, consider the 3D Laplacian, $\mathcal{L} = -\Delta$. We use the representation

$$G(x, y; z) = s(x, y; z) + G_0(x, y; z),$$

where the fundamental solution $s(x, y; z)$ is given by

$$s(x, y; z) = \frac{1}{4\pi} \frac{e^{-\sqrt{z}|x-y|}}{|x-y|} \qquad (x, y \in \mathbb{R}^3) \tag{3.8}$$

and the remainder G_0 satisfies the equation

$$\begin{aligned} (zI - \mathcal{L})_x G_0(x, y; z) &= 0 \quad (x, y \in \Omega), \\ G_0(x, y; z) &= -s(x, y; z) \quad (x \in \partial\Omega,\ y \in \Omega). \end{aligned} \tag{3.9}$$

Here we assume that the principal singularity of $G(x, y; z)$ is described by the fundamental solution $s(x, y; z)$ though the component $G_0(x, y; z)$ also has a singular behaviour on the submanifold $x = y,\ x, y \in \Gamma$. The complexity of the $\mathcal{H}$-matrix approximation to integral operators with the Helmholtz kernel $\frac{1}{4\pi}\frac{\exp(-\kappa|x-y|)}{|x-y|}$ was analysed in [15] in the case of $\Re e\, \kappa = 0$. However, the result remains verbatim in the general situation $\kappa \in \mathbb{C}$. In our case, we set $|\kappa| = N^{1/3}$ and obtain that the order of expansion to approximate the matrix blocks with the accuracy $O(\eta^L)$ will be estimated by $O(L + |\kappa|)$ (see [15] for more details). Taking into account that $L = O(\log \varepsilon^{-1})$, we arrive at $|\kappa| = O(L^{1/3})$. This relation shows that one may expect a certain growth of the local rank; however, the total cost has the same asymptotical estimate as in the case $\kappa = 0$.

Finally, we support these arguments by the numerical results presented in Tables 1-3 below. Table 1 shows the approximation error for the different resolvents depending on the local rank k and actually indicates that, with fixed $\varepsilon > 0$, the local rank k does not grow with respect to ν. Table 2 illustrates the exponential convergence of the quadrature rule T_N with respect to k. Table 3 presents the weights γ_p in front of the resolvents in the quadrature formula (2.20), decaying exponentially with respect to $p\,(= \nu)$.

Further numerical results will be presented in Sect. 5.

3.4 Complexity estimate and further discussion of $\mathcal{H}$-matrices

The linear-logarithmic complexity $O(kN \log N)$ of the $\mathcal{H}$-matrix arithmetic is proven in [12–14]. 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

Table 1. Approximation the resolvents for different z_ν, $\nu = 0, ..., 10$, vs. the local rank k

ν	0	1	2	3	4	6	8	10
$k=1$	19.0	6.4	1.1	0.29	0.08	0.09	0.03	0.02
$k=3$	0.71	0.33	0.07	0.02	0.00	0.00	0.00	0.00
$k=5$	0.06	0.03	0.00	0.00	0.00	0.00	0.00	0.00
$k=10$	3.4e-4	1.6e-4	3.3e-5	8.7e-6	5.4e-6	1.3e-6	9.3e-7	7.0e-7

Table 2. Approximation the exponent $T = \exp(-\mathcal{L})$ vs. local rank k

k	1	2	3	4	5	6	10
$\frac{\|\|T-T_N\|\|}{\|\|T\|\|}$	3.47	2.73	0.53	0.046	0.011	0.0045	0.00011

Table 3. Coefficients $\gamma\nu$ in front of the resolvents in (2.20) for $\nu = 0, ..., 10$

ν	0	1	2	4	6	8	10
z_ν	(0.29,0)	(0.35,0.28)	(0.54,0.56)	(1.31,1.13)	(2.58,1.69)	(4.36,2.26)	(6.65,2,82)
$\Re e\, \gamma_\nu$	-0.03	-0.026	-0.009	0.015	0.009	0.0019	0.0001
$\Im m\, \gamma_\nu$	0.00	0.022	0.034	0.020	0.002	-0.0008	-0.0002

blocks the storage and matrix-vector multiplication complexity is bounded by

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

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 (3.3) and responsible for the approximation.

The complexity of the variable order $\mathcal{H}$-matrices with m_ℓ given by (3.4) and for $d = 2, 3$ depends on the representation of matrix blocks. Using the representation of blocks in a fixed basis, see [17], we have

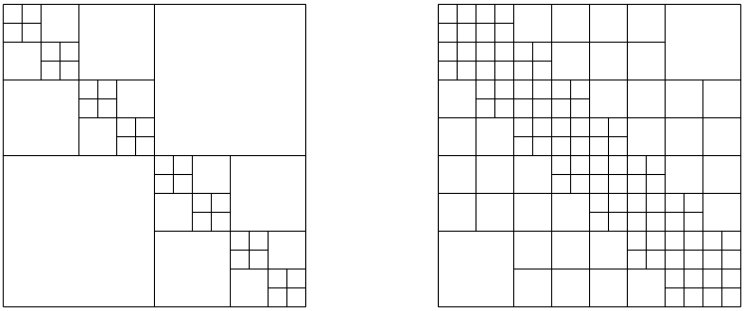
$$\text{(3.10)} \quad \mathbf{A}_{\mathcal{H}}^{\tau\times\sigma} = \sum\nolimits_{i,j=1}^{k_\ell} a_{ij}(a_i \cdot c_j^T) \in \mathcal{V}_a \otimes \mathcal{V}_c, \quad a_i \in \mathbb{R}^{n_\tau},\ c_j \in \mathbb{R}^{n_\sigma},$$

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

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

As result, we arrive at a linear complexity bound with the choice $q = 1$ in (3.4). It is easy to see that for $q = 1$ the matrix-vector product has linear complexity as well, see [17,16].

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 [12,13]. In the general case of quasiuniform meshes the complexity $O(k^2 N)$ 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 $-\frac{d^2}{dx^2} : H_0^1(\Omega) \to H^{-1}(\Omega)$, $\Omega = (0,1)$, 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 [12] for more details).



(a) (b)

Fig. 2a,b. 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 an 1D index set. In the case $d = 2, 3$ the admissible block partitioning is defined recursively, see [13], using the block cluster tree $T(I \times I)$. The numerical experiments for the 2D Laplacian illustrate the efficiency of the $\mathcal{H}$-matrix inversion. Improved data-sparsity is achieved by using the $\mathcal{H}^2$-matrix approximation [17] based on the block representation (3.10) with fixed bases 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 [21] 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

$$(4.1) \quad u(t) = \exp(-t\mathcal{L})u_0 + \int_0^t \exp(-(t-s)\mathcal{L})f(s)ds \quad \text{for } t \in (0,T]\,.$$

The uniform approximation to $e^{-t\mathcal{L}}$ with respect to the integration parameter $t \in [0,\infty)$ is based on a decomposition $[0,\infty) = \cup_{\alpha=0}^{J}\delta_\alpha$ by a hierarchical time grid defined as follows. Let $\Delta t = 2^{-J} > 0$ be the minimal time step, then we define $\delta_0 := [0, \Delta t]$, $\delta_\alpha := [\Delta t 2^\alpha, \Delta t 2^{\alpha+1}]$, $\alpha = 1, ..., J-1$ and $\delta_J := [1,\infty)$. Let $\mathbf{M}_{j\alpha}$ be the $\mathcal{H}$-matrix approximation of the resolvent $(z_{j\alpha}I - \mathcal{L})^{-1}$ in (2.20) associated with the Galerkin ansatz space $V_h \subset L^2(\Omega)$, where we choose different parabolas Γ_α for different time intervals δ_α. Careful analysis of the error estimate (2.18) ensures the uniform $\mathcal{H}$-matrix approximation to the operator exponential in the form

$$\exp_{\mathcal{H}}(-t\mathcal{L}) = \sum_{j=-N}^{N} \gamma_{j\alpha} e^{-z_{j\alpha}t}\mathbf{M}_{j\alpha}, \qquad \gamma_{j\alpha} = \frac{h}{2\pi i}\left(2\frac{a_\alpha}{k_\alpha}jh - i\right),$$
$$t \in \delta_\alpha, \quad \alpha = 1, ..., J.$$

Now, we consider the following semi-discrete scheme. Let $\mathbf{u}_0$, $\mathbf{f}$ be the vector representations of the corresponding Galerkin projections of u_0 and f onto the spaces V_h and $V_h \times [0,T]$, respectively, and let $[0,t] = \cup_{\alpha=0}^{J_0}\delta_\alpha$, $J_0 \le J$. Substitution of the above representations into (4.1) leads to the entirely parallelisable scheme

$$(4.2) \qquad u_{\mathcal{H}}(t) = \sum_{j=-N}^{N} \left(\gamma_{jJ_0} e^{-z_{jJ_0}t}\mathbf{M}_{jJ_0}\mathbf{u}_0 + \sum_{\alpha=1}^{J_0} \gamma_{j\alpha} e^{-z_{j\alpha}t}\mathbf{M}_{j\alpha} \int_{\delta_\alpha} e^{z_{j\alpha}s}\mathbf{f}(s)ds \right)$$

with respect to $j = -N, \ldots, N$, 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 values.

4.2 Dynamical systems and control theory

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

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

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

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

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

$$X_{\mathcal{H}}(t) = \sum_{l,j=-N}^{N} \Bigg[\gamma_{a_{lJ_0}} \gamma_{b_{jJ_0}} e^{-(a_{lJ_0}+b_{jJ_0})t} \mathbf{A}_{lJ_0} X_0 \mathbf{B}_{jJ_0}$$
$$+ \sum_{\alpha=1}^{J_0} \gamma_{a_{l\alpha}} \gamma_{b_{j\alpha}} e^{-(a_{l\alpha}+b_{j\alpha})t} \mathbf{A}_{l\alpha} \int_{\delta_\alpha} e^{(a_{l\alpha}+b_{j\alpha})s} C(s) ds \mathbf{B}_{j\alpha} \Bigg].$$

Let C be constant and the eigenvalues of A, B have negative real parts, then $X(t) \to X_\infty$ as $t \to \infty$, 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 hierarchical approximations to e^{tA} and e^{tB} on each time interval δ_α as above. Then there holds

$$X_{\mathcal{H},\infty} = \int_0^\infty \sum_{\alpha=1}^{J_0} \left[\left(\sum_{l=-N}^{N} \gamma_{a_{l\alpha}} e^{-a_{l\alpha} t} \mathbf{A}_{l\alpha} \right) \mathbf{C}_{\mathcal{H}} \left(\sum_{j=-N}^{N} \gamma_{b_{j\alpha}} e^{-b_{j\alpha} t} \mathbf{B}_{j\alpha} \right) \right] dt$$

$$= \sum_{\alpha=1}^{J_0} \sum_{l,j=-N}^{N} \gamma_{a_{l\alpha}} \gamma_{b_{j\alpha}} \int_{\delta_\alpha} e^{-(a_{l\alpha}+b_{j\alpha})t} dt \, \mathbf{A}_{l\alpha} \mathbf{C}_{\mathcal{H}} \mathbf{B}_{j\alpha}, \tag{4.3}$$

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 $O(k^2 n)$, we then obtain a fully parallelisable scheme of complexity $O(NJ_0\, k\, n)$ (but not $O(n^3)$ 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, $\operatorname{rank}(C) = k \ll n$. 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*

$$X_{\mathcal{H}} = \sum_{\beta=1}^{k} \sum_{l,j=-N}^{N} \sum_{\alpha=1}^{J} \frac{e^{-(a_{l\alpha}+b_{j\alpha})\Delta t 2^\alpha} - e^{-(a_{l\alpha}+b_{j\alpha})\Delta t 2^{\alpha+1}}}{a_{l\alpha}+b_{j\alpha}} \cdot (\mathbf{A}_{l\alpha}\mathbf{a}_\beta) \cdot (\mathbf{A}_{j\alpha}\mathbf{c}_\beta)^T, \tag{4.4}$$

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

Proof. In fact, substitution of the rank-k matrix C into (4.3) leads to (4.4). Due to the exponential convergence in (2.18), we obtain $N = O(\log \varepsilon^{-1})$, where ε is the approximation error. Combining all terms in (4.4) corresponding to the same index $l = -N, \ldots, N$ proves that $X_{\mathcal{H}}$ has the rank $k(2N-1)J$. ∎

Various techniques were considered for numerical solution of the Lyapunov equation, see, e.g., [3], [7], [20] 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 [9] for a more detailed analysis and numerical results concerning the $\mathcal{H}$-matrix techniques for solving the matrix Riccati and Lyapunov equations.

5 On the choice of computational parameters and numerics

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

Let $\varGamma_0 = \{z = \xi \pm i\eta = a\eta^2 + \gamma_0 \pm i\eta\}$ 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 $\varGamma_{b(k)} = \{z = \xi_1 \pm i\eta_1 = \frac{a}{k}\eta_1^2 + b \pm i\eta_1 : \ \eta_1 \in (-\infty, \infty)\}$ with $b(k) = \gamma_0 - \frac{k-1}{4a}$. In this case the integrand can be extended analytically into the strip D_d with $d = \left(1 - \frac{1}{\sqrt{k}}\right) \frac{k}{2a}$ and the estimate (2.18) holds with constants given by (2.19).

First, let us estimate the constant M_1 in (2.19). Since the absolute value of an analytic function attains its maximum on the boundary, we have

$$M_1 = \max\left\{ \sup_{\eta\in(-\infty,\infty)} f_-(\eta), \sup_{\eta\in(-\infty,\infty)} f_+(\eta) \right\}, \tag{5.1}$$

where

$$f_\pm(\eta) = \frac{|2\frac{a}{k}(\eta \pm id) - i|}{1 + \sqrt{\left|\frac{a}{k}(\eta \pm id)^2 + b - i(\eta \pm id)\right|}}. \tag{5.2}$$

It is easy to see that

$$f_\pm^2 \le \frac{(2\frac{a}{k}\eta)^2 + (2\frac{a}{k}d \mp 1)^2}{1 + \left|\frac{a}{k}(\eta^2 \pm 2\eta d i - d^2) + b + d \mp i\eta\right|}. \tag{5.3}$$

Further we have for the function f_+

$$\begin{aligned} f_+^2(\eta) &\le \frac{4\frac{a^2}{k^2}\eta^2 + (2\frac{a}{k}d - 1)^2}{1 + \sqrt{(\frac{a}{k}(\eta^2 - d^2) + b + d)^2 + (2\frac{a}{k}d - 1)^2\eta^2}} \\ &\le \frac{4\frac{a^2}{k^2}\eta^2 + (2\frac{a}{k}d - 1)^2}{1 + \frac{a}{k}(\eta^2 - d^2) + b + d} = \frac{4\frac{a^2}{k^2}\eta^2 + \frac{1}{k}}{\frac{a}{k}\eta^2 + 1 + \gamma_0} \\ &= \frac{4a + 4\gamma_0 - 1}{k(\xi + 1 + \gamma_0)^2}, \end{aligned} \tag{5.4}$$

where $\xi = a\eta^2/k, \ \xi \in (0, \infty)$. The latter function increases monotonically and $\max f_+ = f_+(\infty) = 4a/k$ provided that $4a + 4\gamma_0 > 1$, while it decreases monotonically and $\max f_+ = f_+(0) = \frac{1}{k(1+\gamma_0)}$ provided that $0 < 4a + 4\gamma_0 < 1$. Similarly one can see that $\max f_- = f_-(\infty) = 4a/k$ provided that $4a(1 - \gamma_0)/k > (2 - 1/k)^2$, while $\max f_- = f_-(0) = (2 - 1/\sqrt{k})^2/(1 + \gamma_0)$ if $4a(1 - \gamma_0)/k < (2 - 1/k)^2$. Thus, we have

$$M_1 \le \max\left\{ \frac{4a}{k}, \frac{1}{k(1 + \gamma_0)}, \frac{(2 - 1/\sqrt{k})^2}{1 + \gamma_0} \right\}. \tag{5.5}$$

Other constants can be rewrite as

$$c = M_1 e^{t[ad^2/k+d-b]} = M_1 e^{tk(1-1/\sqrt{k})/a},$$
$$s = \sqrt[3]{\pi^2 k(1-1/\sqrt{k})^2/a} \asymp \sqrt[3]{k/a}. \tag{5.6}$$

One can see that the multiplicative constant c in the estimate (2.18) increases linearly as $a \to \infty$, whereas the multiplicative coefficient s in the front of $(N+1)^{2/3}$ in the exponent tends to zero, i.e., the convergence rate becomes worse. On the other hand, s tends to infinity as a tends to zero, but the constant c tends exponentially to infinity.

Given a, we can influence the efficacy of our method by changing the parameter $k > 1$. Denoting $t_* = \min\{1, t\}$, we see that for k large enough, the leading term of the error is

$$e^{-[\sqrt[3]{k/a}t_*(N+1)^{2/3} - tk/a]}. \tag{5.7}$$

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

$$N \asymp \left(\frac{1}{mt_*} \ln \frac{1}{\varepsilon} + tm^2/t_* \right)^{3/2},$$

where $m = \sqrt[3]{k/a}$. It is easy to find that N (i.e., the number of resolvent inversions for various z_i) becomes minimal if we choose $k \asymp \frac{a}{2t} \ln \frac{1}{\varepsilon}$. In this case the number of resolvent inversions is estimated by

$$N_{min} \asymp \sqrt[3]{t}/t_* \left(\ln \frac{1}{\varepsilon} \right)^{2/3}.$$

To complete this section, we present numerical examples on the $\mathcal{H}$-matrix approximation of the exponential for the finite difference Laplacian Δ_h on $\Omega = (0,1)^d$, $d = 1, 2$ (with zero boundary conditions) defined on the uniform grid with the mesh-size $h = 1/(n+1)$, where n^d is the problem size. Table 4 presents the relative error of the $\mathcal{H}$-matrix approximation for 1D Laplacian by Algorithm 2.3 versus the number N of resolvents involved. The relative error is measured by

$$\| \exp(-t\Delta_h) - \exp_N(-t\Delta_h) \|_2 / \| \exp(-t\Delta_h) \|_2.$$

The local rank is chosen as $k_0 = 8$, while $b = 0.9\,\lambda_{\min}(\Delta_h)$, $a = 4.0$, $k = 5.0$. Our calculations indicate the robust exponential convergence of (2.18) 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 $a_0 = O(1)$ and confirm our analysis. The computational time (in sec.) corresponding to the $\mathcal{H}$-matrix evaluation of each resolvent in (2.18) at a 450MHz SUN-UltraSPARC2 station is presented in the last

Table 4. Approximation to the exponential of $\varDelta_h$ with $d = 1$, where $n = dimV_h$ and N is defined from (2.20)

$n\backslash N$	1	4	7	10	20	30	40	time/N(sec)
256	6.0 e-2	8.7 e-3	1.7 e-3	3.8 e-4	5.6 e-6	1.5 e-7	5.9 e-9	0.5
1024	6.4 e-2	9.6 e-3	1.9 e-3	4.4 e-4	6.9 e-6	2.0 e-7	7.3 e-9	3.7
4096	6.5 e-2	9.8 e-3	1.9 e-3	4.6 e-4	7.4 e-6	2.5 e-7	(3.6 e-8)	21
16384	6.6 e-2	9.9 e-3	2.0 e-3	4.6 e-4	7.0 e-6	(1.3 e-6)	(1.9 e-7)	118

Table 5. Approximation to the exponential of $\varDelta_h$ with $d = 2$, where $n = dimV_h$ and N is defined from (2.20)

$n\backslash N$	1	4	7	10	20	30	40	time/N(sec)
256	5.5 e-2	7.9 e-3	1.5 e-3	3.3 e-4	4.5 e-6	1.1 e-7	4.3 e-9	0.5
1024	6.3 e-2	9.3 e-3	1.8 e-3	4.2 e-4	6.5 e-6	1.9 e-7	(5.2 e-8)	51
4096	6.5 e-2	9.7 e-3	1.9 e-3	4.5 e-4	7.2 e-6	(4.5 e-7)	(3.0 e-7)	379

column. The numbers in brackets "()" indicate that the best possible accuracy with rank $= 8$ is already achieved.

The results have been obtained using the general **HMA1** code implementing the $\mathcal{H}$-matrix arithmetic, see also [9] for more details.

Table 5 presents the results for the 2D Laplacian on $\Omega = (0,1)^2$ obtained on 300MHz SUN UltraSPARC2. Parameters a, k, b are chosen as in the previous example. In both cases the efficacy appears to be not sensitive to the choice of a and k, but the parameter b has to approach $\lambda_{\min}(\varDelta_h)$ from below.

6 Appendix: Proof of Lemma 2.3 and Theorem 2.4

First, we prove Lemma 2.3.

Proof. Let $E(f,h)$ be defined as follows

$$E(f,h)(z) = f(z) - C(f,h)(z).$$

Analogously to [25] (see Theorem 3.1.2) one can get

$$\begin{aligned} E(f,h)(z) &= f(z) - C(f,h)(z) \\ &= \frac{\sin(\pi z/h)}{2\pi i} \int_{\mathbb{R}} \left\{ \frac{f(\xi - id)}{(\xi - z - id)\sin[\pi(\xi - id)/h]} \right. \end{aligned} \tag{6.1}$$

$$\left. - \frac{f(\xi + id)}{(\xi - z + id)\sin[\pi(\xi + id)/h]} \right\} d\xi \tag{6.2}$$

and upon replacing z by x we have

$$\eta(f,h) = \int_{\mathbb{R}} E(f,h)(x)dx. \tag{6.3}$$

After interchanging the order of integration and using the identities

$$\frac{1}{2\pi i}\int_{\mathbb{R}} \frac{\sin(\pi x/h)}{\pm(\xi - x) - id}dx = \frac{i}{2}e^{-\pi(d\pm i\xi)/h}, \tag{6.4}$$

we obtain (2.11). Using the estimate (see [25], p.133) $\sinh(\pi d/h) \leq |\sin[\pi(\xi \pm id)/h]| \leq \cosh(\pi d/h)$, the assumption $f \in \mathbf{H}^1(D_d)$ and the identity (2.11), we obtain the desired bound (2.12). The assumption (2.13) now implies

$$\begin{aligned} \|\eta_N(f,h)\| &\leq \|\eta(f,h)\| + h\sum_{|k|>N}\|f(kh)\| \\ &\leq \frac{\exp(-\pi d/h)}{2\sinh(\pi d/h)}\|f\|_{\mathbf{H}^1(D_d)} + c\,h\sum_{|k|>N}\exp[-\alpha(kh)^2]. \end{aligned} \tag{6.5}$$

For the last sum we use the simple estimate

$$\begin{aligned} \sum_{|k|>N} e^{-\alpha(kh)^2} &= 2\sum_{k=N+1}^{\infty} e^{-\alpha(kh)^2} \leq 2\int_{N+1}^{\infty} e^{-\alpha h^2 x^2}dx \\ &= \frac{2}{\sqrt{\alpha}h}\int_{\sqrt{\alpha}h(N+1)}^{\infty} e^{-x^2}dx \qquad (6.6) \\ &= \frac{\sqrt{\pi}}{\sqrt{\alpha}h}erfc(\sqrt{\alpha}h(N+1)) \\ &= \frac{\sqrt{\pi}}{\sqrt{\alpha}h}e^{-(N+1)^2\alpha h^2}\psi\left(\frac{1}{2},\frac{1}{2};(N+1)^2\alpha h^2\right), \qquad (6.7) \end{aligned}$$

where $\psi(\frac{1}{2},\frac{1}{2};(N+1)^2\alpha h^2)$ is the Whittecker function with the asymptotics [1]

$$\psi\left(\frac{1}{2},\frac{1}{2};x^2\right) = \sum_{n=0}^{M}\left(\frac{-1}{2}\right)^n x^{-(2n+1)} + O(|x|^{-2M-3}). \tag{6.8}$$

This yields

$$\sum_{|k|>N} e^{-\alpha(kh)^2} \leq \frac{\sqrt{\pi}}{\alpha h^2(N+1)}e^{-\alpha(N+1)^2h^2}. \tag{6.9}$$

It follows from (2.13) that

$$\|f\|_{\mathbf{H}^1(D_d)} \le 2c\int_{-\infty}^{\infty} e^{-\alpha x^2}\,dx = \frac{2c}{\sqrt{\alpha}}\sqrt{\pi} \tag{6.10}$$

which together with (6.5) and (6.9) implies

$$\|\eta_N(f,h)\| \le c\sqrt{\pi}\left[\frac{\exp(-\pi d/h)}{\sqrt{\alpha}\sinh(\pi d/h)} + \frac{\exp[-\alpha(N+1)^2h^2]}{\alpha h(N+1)}\right],$$

which completes the proof. ■

Now, we conclude with the proof of Theorem 2.4.

Proof. First, we note that one can choose as integration path any parabola

$$\Gamma_b = \{z = \frac{a}{k}\eta^2 + b + i\eta : \eta \in (-\infty,\infty), k > 1, b < \gamma_0\}, \tag{6.11}$$

which contains the spectral parabola

$$\Gamma_0 = \{z = a\eta^2 + \gamma_0 + i\eta : \eta \in (-\infty,\infty)\}. \tag{6.12}$$

In order to apply Lemma 2.3 for the quadrature rule T_N we have to provide that the integrand $F(\eta,t)$ can be analytically extended in a strip D_d around the real axis η. It is easy to see that it is the case when there exists $d > 0$ such that for $|\nu| < d$ the function (transformed resolvent)

$$R(\eta + i\nu, \mathcal{L}) = [\psi(\eta + i\nu)I - \mathcal{L}]^{-1}, : \eta \in (-\infty,\infty),\ |\nu| < d \tag{6.13}$$

has a bounded norm $\|R\|_{X\to X}$. Due to the strong P-positivity of $\mathcal{L}$, the latter can be easily varified if the parabola set

$$\begin{aligned}\Gamma_b(\nu) &= \left\{z = \frac{a}{k}(\eta + i\nu)^2 + b + i(\eta + i\nu) :\ \eta \in (-\infty,\infty),\ |\nu| < d\right\}\\ &= \left\{z = \frac{a}{k}\eta^2 + b + \frac{k}{4a} - \frac{a}{k}\left(\nu + \frac{k}{2a}\right)^2 + i\eta\left(1 + \frac{2a}{k}\nu\right);\right.\\ &\left.\eta \in (-\infty,\infty),\ |\nu| < d\right\}\end{aligned} \tag{6.14}$$

does not intersect Γ_0. Each parabola from the set $\Gamma_b(\nu)$ can be represented also in the form $\xi = a'\eta^2 + b'$ with

$$a' = a\left(k + 4a\nu + \frac{4a^2}{k}\nu^2\right)^{-1}, b' = b + \frac{k}{4a} - \frac{a}{k}\left(\nu + \frac{k}{2a}\right)^2. \tag{6.15}$$

Now, it is easy to see that if we choose

$$\nu = \left(\frac{1}{\sqrt{k}} - 1\right)\frac{k}{2a} \equiv -d,\ b = b(k) = \gamma_0 - \frac{k-1}{4a} \tag{6.16}$$

then

$$\begin{aligned} \Gamma_{b(k)}(-d) &= \left\{ z = \frac{a}{k}\eta^2 + b + \frac{k-1}{4a} + i\frac{\eta}{\sqrt{k}} : \ \eta \in (-\infty, \infty) \right\} \\ &= \left\{ z = a\eta_*^2 + \gamma_0 + i\eta_* : \ \eta_* \equiv \frac{\eta}{\sqrt{k}} \in (-\infty, \infty) \right\} \\ &\equiv \Gamma_0. \end{aligned} \tag{6.17}$$

From (6.15), one can see that $a' \to 0, \ b' \to 0$ monotonically with respect to ν as $\nu \to \infty$, i.e. the parabolae from $\Gamma_b(\nu)$ move away from the spectral parabola Γ_0 monotonically. This means that the parabolae set $\Gamma_b(\nu)$ for $b = b(k), \ |\nu| < d$ lies outside of the spectral parabola Γ_0, i.e. we can extend the integrand into the strip (2.7) with d given by (6.16). Note, that the choice $\nu = d = (1 - 1/\sqrt{k})\frac{k}{2a}$ selects from the family $\Gamma_{b(k)}(\nu)$ the particular parabola

$$\begin{aligned} \Gamma_{b(k)}(d) &= \left\{ z = a\eta^2/k + b_+ + i\eta(2 - 1/\sqrt{k}) : \eta \in (-\infty, \infty) \right\} \\ &= \left\{ z = a_+\eta_*^2 + b_+ + i\eta_* : \eta_* \equiv \eta(2 - 1/\sqrt{k}) \in (-\infty, \infty) \right\} \end{aligned} \tag{6.18}$$

with

$$a_+ = \frac{a}{k(2 - 1/\sqrt{k})^2}, \ b_+ = b - \frac{3k - 4\sqrt{k} + 1}{4a},$$

which for $|\nu| \le d$ is the most remote from the spectral parabola Γ_0. Due to the strong P-positivity of $\mathcal{L}$ there holds for $z = \eta + i\nu \in D_d$

$$\begin{aligned} \|F(z, t; \mathcal{L})\| &\le M \frac{|(2\frac{a}{k}z - i)| \ \exp[-t(\frac{a}{k}z^2 + b - iz)]}{1 + \sqrt{|\frac{a}{k}z^2 + b - iz|}} \\ &= M \frac{|2\frac{a}{k}z - i| exp\{-t[\frac{a}{k}(\eta^2 - \nu^2) + b + \nu]\}}{1 + \sqrt{|\frac{a}{k}z^2 + b - iz|}} \quad \text{and} \\ &F(z, t; \mathcal{L}) \in \mathbf{H}^1(D_d) \quad \text{for all } t > 0. \end{aligned} \tag{6.19}$$

We have also

$$\|F(\eta, t; \mathcal{L})\| < ce^{-\alpha\eta^2}, \ \eta \in \mathbb{R} \tag{6.20}$$

with

$$\alpha = t\frac{a}{k}, \quad c = M_1 e^{t[ad^2/k + d - b]}, \quad M_1 = \max_{z \in \overline{D}_d} \frac{|2\frac{a}{k}z - i|}{1 + \sqrt{|\frac{a}{k}z^2 + b - iz|}}. \tag{6.21}$$

Using Lemma 2.3 and setting in (2.14) $\alpha = t\frac{a}{k}$, we get

$$\text{(6.22)}\ \|\eta_N(F,h)\| \le \\ Mc\sqrt{\pi}\left[\frac{2\sqrt{k}\,\exp(-2\pi d/h)}{\sqrt{at}(1-\exp(-2\pi d/h))} + \frac{k\,\exp[-(N+1)^2h^2\frac{a}{k}t]}{ath(N+1)}\right].$$

Equalising the exponents by setting $-2\pi d/h = -(N+1)^2h^2a/k$, we get $h = \sqrt[3]{\frac{2\pi dk}{a}}(N+1)^{-2/3}$. Substituting this value into (6.22) leads to the estimate

$$\|\eta_N(F,h)\| \le \\ Mc\sqrt{\pi}\left[\frac{2\sqrt{k}e^{-s(N+1)^{2/3}}}{\sqrt{at}(1-e^{-s(N+1)^{2/3}})} + \frac{ke^{-ts(N+1)^{2/3}}}{t(N+1)^{1/3}\sqrt[3]{2\pi dka^2}}\right], \tag{6.23}$$

which completes our proof. ∎

Note that our estimate implies $\|\eta_N(F,h)\| = O(\frac{1}{t(N+1)^{1/3}})$ as $t \to 0$, but numerical tests even indicate an error order $O(\frac{1}{(N+1)^{1/3}})$ as $t \to 0$.

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