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Abstract

We develop a data-sparse and accurate approximation of the normalised hyperbolic operator sine family generated by a strongly P-positive elliptic operator defined in [4, 7].

In the preceding papers [14]-[18], a class of $\mathcal{H}$-matrices has been analysed which are data-sparse and allow an approximate matrix arithmetic with almost linear complexity. An $\mathcal{H}$-matrix approximation to the operator exponent with a strongly P-positive operator was proposed in [5]. In the present paper, we apply the $\mathcal{H}$-matrix techniques to approximate the elliptic solution operator on cylindric domains $\Omega \times [a, b]$ associated with the elliptic operator $\frac{d^2}{dx^2} - \mathcal{L}$, $x \in [a, b]$. It is explicitly presented by the operator-valued normalised hyperbolic sine function $\sinh^{-1}(\sqrt{\mathcal{L}}) \sinh(x\sqrt{\mathcal{L}})$ of an elliptic operator $\mathcal{L}$ defined in Ω.

Starting with the Dunford-Cauchy representation for the hyperbolic sine operator, we then discretise the integral by the exponentially convergent quadrature rule involving a short sum of resolvents. The latter are approximated by the $\mathcal{H}$-matrix techniques. Our algorithm inherits a two-level parallelism with respect to both the computation of resolvents and the treatment of different values of the spatial variable $x \in [a, b]$.

The approach is applied to elliptic partial differential equations in domains composed of rectangles or cylinders. In particular, we consider the $\mathcal{H}$-matrix approximation to the interface Poincaré-Steklov operators with application in the Schur-complement domain decomposition method.

AMS Subject Classification: 65F50, 65F30
Key words: operator-valued sinh function, domain decomposition, Poincaré-Steklov operators

1 Introduction

There are several sparse $(n \times n)$-matrix approximations which allow to construct optimal iteration methods for solving 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 finite element methods. In the latter case the inverse of a sparse FEM matrix is a full matrix. A class of hierarchical matrices ($\mathcal{H}$-matrices) has been recently introduced and developed in [14]-[18]. 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. It is of important practical interest to find hierarchical $\mathcal{H}$-matrix approximations of the operator exponentials, operator $\sinh(x\sqrt{\mathcal{L}})$ and the operator $\cos(t\sqrt{\mathcal{L}})$ functions, which solve evolution differential equations with operator coefficients of the first and second order (parabolic, elliptic and hyperbolic cases) respectively.

Concerning the second order evolution problems and the operator $\cos(t\sqrt{\mathcal{L}})$ function new discretisation methods were recently developed in [4]-[6] 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 (see [5, 6] and the literature cited therein).

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 normalised $\sinh(x\sqrt{\mathcal{L}})$ operator representing the elliptic solution operator. Starting with the Dunford-Cauchy representation for the hyperbolic operator sine family and essentially using the strong P-positivity of the elliptic operator involved we discretise the integral by the exponentially convergent quadrature rule involving a short sum of resolvents. Approximating the resolvents by $\mathcal{H}$-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 space-variable values. Our parallel method has exponential convergence due to the optimal quadrature rule in the contour integration for holomorphic functions providing the explicit representation of the fractional operator powers and exponential operator in terms of data-sparse matrices of linear-logarithmic complexity.

As an application, we consider the data-sparse factorised representation to the Poincaré-Steklov operators associated with elliptic problems in tube domains. Then, we discuss the solution algorithm by reduction to the interface for model elliptic problems in domains composed of many stretched rectangles. This example is related to the model problem considered in [22], where the robust preconditioners for elliptic equations with jumping anisotropic coefficients in many subdomains have been developed. Note that in certain special cases the multilevel preconditioners for anisotropic problems have been developed in [2].

2 Representation of $\sinh^{-1}(\sqrt{\mathcal{L}})\sinh(x\sqrt{\mathcal{L}})$ by a Sum of Resolvents

In this section we outline the description of the normalised hyperbolic operator sine family generated by 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 [26], 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 $\gamma_0 \equiv \Gamma_0 = \{z = \xi + i\eta : \xi = a\eta^2 + \gamma_0\}$ be a parabola, which 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 $\Omega_{\Gamma_0} = \{z = \xi + i\eta : \xi > a\eta^2 + \gamma_0\}$ the domain inside of the parabola. Now, we are in the position to give the following definition.

Definition 2.1 *An operator $A : X \to X$ is called* strongly P-positive *if there exist positive constants a, γ_0 such that its spectrum $sp(A)$ lies in the domain Ω_{Γ_0} and the estimate*

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

holds with a positive constant M.

It was shown in [5] 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 $\|u\|_X \le c_e\|u\|_V$ for all $u \in V$. Assume that $a(\cdot,\cdot)$ is bounded, i.e.,

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

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

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

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

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

guarantee that the numerical range $\{a(u, u) : \ u \in X,\ \|u\|_X = 1\}$ of A (and $sp(A)$) lies in Ω_{Γ_0}, where the parabola Γ_0 depends on the constants $\delta_0, \delta_1, \kappa, c_e$. In the following, the operator A is assumed to be strongly P-positive. In the typical applications, we are going to discuss, this may be the second order strongly elliptic operator or its finite element Galerkin approximation.

2.2 Integral Representation of $\sinh^{-1}(\sqrt{\mathcal{L}})\sinh(x\sqrt{\mathcal{L}})$

Let $\mathcal{L}$ be a linear, densely defined, closed, strongly P-positive operator in a Banach space X. The operator value function (hyperbolic sine family of bounded operators; cf. [7])[1]

$$E(x) \equiv E(x;\mathcal{L}) := \sinh^{-1}(\sqrt{\mathcal{L}})\sinh(x\sqrt{\mathcal{L}})$$

satisfies the elliptic differential equation

$$\frac{d^2E}{dx^2} - \mathcal{L}E = 0, \quad E(0) = \Theta, \quad E(1) = I \tag{2.2}$$

where I is the identity and Θ the zero operator. Given the normalised hyperbolic operator sine family $E(x)$, the solution of the elliptic differential equation (elliptic equation)

$$\frac{d^2u}{dx^2} - \mathcal{L}u = 0, \quad u(0) = 0, \quad u(1) = u_1$$

with a given vector u_1 and unknown vector valued function $u(x) : (0,1) \to X$ can be represented as

$$u(x) = E(x;\mathcal{L})\, u_1.$$

Let $\Gamma_0 = \{z = \xi + i\eta : \xi = a\eta^2 + \gamma_0\}$ be the parabola (called the spectral 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* $b \in (0, \gamma_0)$*. Then the operator family* $E(x;\mathcal{L})$ *can be represented by the Dunford-Cauchy integral [3]*

$$E(x;\mathcal{L}) = \frac{1}{2\pi i}\int_\Gamma \sinh^{-1}(\sqrt{z})\sinh(x\sqrt{z})(zI - \mathcal{L})^{-1}dz = \frac{1}{2\pi i}\int_{-\infty}^{\infty} F(\eta, x)d\eta, \tag{2.3}$$

where

$$F(\eta, x) = -\sinh^{-1}(\sqrt{z})\sinh(x\sqrt{z})(2\tilde{a}\eta - i)(zI - \mathcal{L})^{-1}, \; z = \tilde{a}\eta^2 + b - i\eta.$$

Moreover, $E(x) = \sinh^{-1}(\sqrt{\mathcal{L}})\sinh(x\sqrt{\mathcal{L}})$ *satisfies the differential equation (2.2).*

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

$$\begin{aligned}
E(x;\mathcal{L}) &= \sinh^{-1}(\sqrt{\mathcal{L}})\sinh\left(x\sqrt{\mathcal{L}}\right) \\
&= \frac{1}{2\pi i}\int_\infty^0 \frac{\sinh\left(x\sqrt{a\eta^2 + b + i\eta}\right)}{\sinh(\sqrt{a\eta^2 + b + i\eta})}((\tilde{a}\eta^2 + b + i\eta)I - \mathcal{L})^{-1}(2\tilde{a}\eta + i)d\eta \\
&+ \frac{1}{2\pi i}\int_0^\infty \frac{\sinh\left(x\sqrt{a\eta^2 + b - i\eta}\right)}{\sinh)\sqrt{a\eta^2 + b - i\eta})}((\tilde{a}\eta^2 + b - i\eta)I - \mathcal{L})^{-1}(2\tilde{a}\eta - i)d\eta \\
&= \frac{1}{2\pi i}\int_{-\infty}^{\infty} F(\eta, x)d\eta
\end{aligned}$$

with $F(\eta, x) = -\sinh^{-1}(\sqrt{z})\sinh\left(x\sqrt{z}\right)(2\tilde{a}\eta - i)(zI - \mathcal{L})^{-1}$, $z = \tilde{a}\eta^2 + b - i\eta$.

We introduce polar coordinates of $\tilde{a}\eta^2 + b - i\eta = re^{i\varphi}$, where

$$r = \sqrt{(\tilde{a}\eta^2 + b)^2 + \eta^2}, \qquad \cos\varphi = \frac{\tilde{a}\eta^2 + b}{r}, \qquad \sin\varphi = \frac{-\eta}{r}.$$

[1] The operator $\sinh^{-1}(A) := (\sinh A)^{-1}$ means the inverse to the operator $\sinh A$.

It is easy to see that

$$
\begin{gathered}
\tilde{a}\eta^2 + b \le r \le \tilde{a}(\eta^2+1) + b, \\
\sqrt{\frac{1}{2}\min\{\tilde{a},b\}}\,|\eta-1| \le \sqrt{r} \le \sqrt{\frac{1}{2}\min\{\tilde{a},b\}}(|\eta+\sqrt{2}|) \quad \text{for all } \eta \gg 1,\ \sqrt{r} \ge \sqrt{b}, \\
\sqrt{\tilde{a}\eta^2+b-i\eta} = \sqrt{r}e^{i\varphi/2}, \\
\frac{1}{\sqrt{2}} \le \cos\frac{\varphi}{2} = \frac{\sqrt{\sqrt{(\tilde{a}\eta^2+b)^2+\eta^2}+\tilde{a}\eta^2+b}}{\sqrt{2}\sqrt[4]{(\tilde{a}\eta^2+b)^2+\eta^2}} \le 1, \\
-\frac{1}{\sqrt{2}} \le \sin\frac{\varphi}{2} = \frac{\eta}{\sqrt{2}\sqrt[4]{(\tilde{a}\eta^2+b)^2+\eta^2}\sqrt{\sqrt{(\tilde{a}\eta^2+b)^2+\eta^2}+\tilde{a}\eta^2+b}} \le \frac{1}{\sqrt{2}},
\end{gathered}
$$

which implies

$$
-\frac{\pi}{4} \le \frac{\varphi}{2} \le \frac{\pi}{4}. \tag{2.4}
$$

Furthermore, we have due to (2.4) and $\cos\frac{\varphi}{2} \ge \sin\frac{\varphi}{2}$ that

$$
\begin{aligned}
&\sinh(x\sqrt{\tilde{a}\eta^2+b\pm i\eta}) \\
&= \frac{1}{2}\left(e^{x\sqrt{r}\cos\frac{\varphi}{2}}\left(\cos(x\sqrt{r}\sin\frac{\varphi}{2}) \pm i\sin(x\sqrt{r}\sin\frac{\varphi}{2})\right) \pm e^{x\sqrt{r}\cos\frac{\varphi}{2}}\left(\cos(x\sqrt{r}\sin\frac{\varphi}{2}) \mp i\sin(x\sqrt{r}\sin\frac{\varphi}{2})\right)\right).
\end{aligned}
$$

Abbreviating $\sin^2 = \sin^2\left(x\sqrt{r}\sin\frac{\varphi}{2}\right)$, $\cos^2 = \cos^2\left(x\sqrt{r}\sin\frac{\varphi}{2}\right)$, $\sinh = \sinh\left(x\sqrt{r}\cos\frac{\varphi}{2}\right)$ and $\cosh = \cosh\left(x\sqrt{r}\cos\frac{\varphi}{2}\right)$, we have

$$
\begin{aligned}
\left|\sinh(x\sqrt{\tilde{a}\eta^2+b\pm i\eta})\right|^2 &= \cos^2\sinh^2 + \sin^2\cosh^2 = \sinh^2 + \sin^2(\cosh-\sinh)(\cosh+\sinh) \\
&\le \sinh^2 + \sin^2\cosh(\cosh+\sinh)
\end{aligned} \tag{2.5}
$$

for all $x \in [0,1]$. Since

$$
\begin{aligned}
\cosh(\sqrt{r}\cos\frac{\varphi}{2}) &= e^{\sqrt{r}\cos\frac{\varphi}{2}}\frac{1+e^{-2\sqrt{r}\cos\frac{\varphi}{2}}}{2} \le e^{\sqrt{r}\cos\frac{\varphi}{2}}, \\
\cosh(\sqrt{r}\cos\frac{\varphi}{2}) &= e^{\sqrt{r}\cos\frac{\varphi}{2}}\frac{1+e^{-2\sqrt{r}\cos\frac{\varphi}{2}}}{2} \ge e^{\sqrt{r}\cos\frac{\varphi}{2}}/2, \\
\sinh(\sqrt{r}\cos\frac{\varphi}{2}) &= e^{\sqrt{r}\cos\frac{\varphi}{2}}\frac{1-e^{-2\sqrt{r}\cos\frac{\varphi}{2}}}{2} \le e^{\sqrt{r}\cos\frac{\varphi}{2}}/2, \\
\sinh(\sqrt{r}\cos\frac{\varphi}{2}) &= e^{\sqrt{r}\cos\frac{\varphi}{2}}\frac{1-e^{-2\sqrt{r}\cos\frac{\varphi}{2}}}{2} \ge e^{\sqrt{r}\cos\frac{\varphi}{2}}\frac{1-e^{-\sqrt{2b}}}{2},
\end{aligned}
$$

the relations (2.5) yield

$$
\begin{aligned}
\left|\sinh(x\sqrt{\tilde{a}\eta^2+b\pm i\eta})\right| &\le e^{x\sqrt{r}\cos\frac{\varphi}{2}}\left[\left(\frac{1-e^{-2x\sqrt{r}\cos\frac{\varphi}{2}}}{2}\right)^2 + \frac{1-e^{-2x\sqrt{r}\cos\frac{\varphi}{2}}}{2} + e^{-2x\sqrt{r}\cos\frac{\varphi}{2}}\right] \\
&\le e^{x\sqrt{r}\cos\frac{\varphi}{2}}\frac{1-e^{-2x\sqrt{r}\cos\frac{\varphi}{2}}}{2} \qquad \text{for all } x \in [0,1], \\
\left|\sinh(\sqrt{\tilde{a}\eta^2+b\pm i\eta})\right| &\ge \sinh\left(\sqrt{r}\cos\frac{\varphi}{2}\right) \ \ge\ e^{\sqrt{r}\cos\frac{\varphi}{2}}\frac{1-e^{-2\sqrt{r}\cos\frac{\varphi}{2}}}{2}.
\end{aligned} \tag{2.6}
$$

From (2.6) we get

$$
|\sinh^{-1}(\sqrt{\tilde{a}\eta^2+b\pm i\eta})\sinh(x\sqrt{\tilde{a}\eta^2+b\pm i\eta})| \le ce^{-\alpha|\eta|} \tag{2.7}
$$

with

$$
\alpha(x) = (1-x)\sqrt{\min\{\tilde{a},b\}/2} > 0,\ c = \frac{e^{\alpha(x)}}{1-e^{-\sqrt{2b}}} \quad \text{for all } x \in (0,1).
$$

Now, using the inequality

$$\|(\tilde{a}\eta^2 + b - i\eta - \mathcal{L})^{-1}(2\tilde{a}\eta - i)\| \leq M \frac{\sqrt{4\tilde{a}^2\eta^2 + 1}}{1 + \sqrt[4]{(\tilde{a}\eta^2 + b)^2 + \eta^2}},$$

imposed by the strong P-positivity, we can estimate

$$\| \sinh^{-1}(\sqrt{\mathcal{L}}) \sinh(x\sqrt{\mathcal{L}})\| \lesssim \int_0^\infty e^{-\alpha(x)\eta} d\eta < +\infty \qquad \text{for all } x \in (0,1).$$

Analogously, applying (2.1), we have for the second derivative of $E(x) = \sinh^{-1}(\sqrt{\mathcal{L}})\sinh(x\sqrt{\mathcal{L}})$ that

$$\|E''(x)\| = \|\mathcal{L}\sinh^{-1}(\sqrt{\mathcal{L}})\sinh(x\sqrt{\mathcal{L}})\| = \left\| \frac{1}{2\pi i} \int_\Gamma z \frac{\sinh(x\sqrt{z})}{\sinh(\sqrt{z})}(zI - \mathcal{L})^{-1} dz \right\| \leq +\infty,$$

where the integrals converge for $x \in (0,1)$. Furthermore, we have

$$\begin{aligned} \frac{d^2E}{dx^2} - \mathcal{L}E &= \frac{1}{2\pi i} \int_\Gamma \frac{\sinh(x\sqrt{z})}{\sinh(\sqrt{z})}(zI - \mathcal{L})^{-1} dz - \mathcal{L}\left(\frac{1}{2\pi i} \int_\Gamma \frac{\sinh(x\sqrt{z})}{\sinh(\sqrt{z})}(zI - \mathcal{L})^{-1} dz \right) \\ &= \frac{1}{2\pi i} \int_\Gamma z \frac{\sinh(x\sqrt{z})}{\sinh(\sqrt{z})}(zI - \mathcal{L})^{-1} dz - \frac{1}{2\pi i} \int_\Gamma z \frac{\sinh(x\sqrt{z})}{\sinh(\sqrt{z})}(zI - \mathcal{L})^{-1} dz = 0, \end{aligned}$$

i.e., $E(x) = \sinh^{-1}(\sqrt{\mathcal{L}})\sinh(x\sqrt{\mathcal{L}})$ satisfies the differential equation (2.2). ■

2.3 Computational Scheme and Convergence Analysis

Following [29, 5], we construct a quadrature rule for the second integral in (2.3) by using the Sinc approximation on $(-\infty, \infty)$. For $1 \leq p \leq \infty$, introduce the family $\mathbf{H}^p(D_d)$ of all operator-valued functions, which are analytic in the infinite strip D_d,

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

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

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

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

$$\|\mathcal{F}\|_{\mathbf{H}^p(D_d)} = \begin{array}{ll} \lim_{\epsilon\to 0}(\int_{\partial D_d(\epsilon)} \|\mathcal{F}(z)\|^p |dz|)^{1/p} & \text{if } 1 \leq p < \infty, \\ \lim_{\epsilon \to 0} \sup_{z \in D_d(\epsilon)} \|\mathcal{F}(z)\| & \text{if } p = \infty. \end{array}$$

Let

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

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, we use the notations

$$\begin{aligned} I(\mathcal{F}) &= \int_{\mathbb{R}} \mathcal{F}(\xi) d\xi, \\ T(\mathcal{F}, h) &= h \sum_{k=-\infty}^{\infty} \mathcal{F}(kh), \qquad & T_N(\mathcal{F}, h) &= h \sum_{k=-N}^{N} \mathcal{F}(kh), \\ C(\mathcal{F}, h) &= \sum_{k=-\infty}^{\infty} \mathcal{F}(kh) S(k,h), \\ \eta_N(\mathcal{F}, h) &= I(\mathcal{F}) - T_N(\mathcal{F}, h), \qquad & \eta(\mathcal{F}, h) &= I(\mathcal{F}) - T(\mathcal{F}, h). \end{aligned} \tag{2.8}$$

By $f(\xi \pm id^-) = \lim_{\delta \to d; \delta < d} f(\xi \pm i\delta)$ we denote the one-sided limits. Adapting the ideas of [29, 6, 5], we 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*

$$\eta(f,h) = \frac{i}{2}\int_{\mathbb{R}} \left\{ \frac{f(\xi - id^-)e^{-\pi(d+i\xi)/h}}{\sin\left[\pi(\xi - id)/h\right]} - \frac{f(\xi + id^-)e^{-\pi(d-i\xi)/h}}{\sin\left[\pi(\xi + d)/h\right]} \right\} d\xi \tag{2.9}$$

providing the estimate

$$\|\eta(f,h)\| \leq \frac{e^{-\pi d/h}}{2\sinh\left(\pi d/h\right)} \|f\|_{\mathbf{H}^1(D_d)}. \tag{2.10}$$

If, in addition, f satisfies the condition

$$\|f(\xi)\| < ce^{-\alpha|\xi|} \qquad \text{with } \alpha, c > 0 \tag{2.11}$$

on $\mathbb{R}$, then

$$\|\eta_N(f,h)\| \leq \frac{2c}{\alpha}\left[\frac{h}{2\pi d}e^{-2\pi d/h} + e^{-\alpha N h}\right]. \tag{2.12}$$

Applying the quadrature rule T_N with the operator valued function

$$F(\eta, x; \mathcal{L}) = (2\tilde{a}\eta - i)\,\varphi(\eta)\,\left(\psi(\eta)I - \mathcal{L}\right)^{-1},$$

where

$$\varphi(\eta) = -\sinh^{-1}\left(\sqrt{\psi(\eta)}\right)\sinh\left(x\sqrt{\psi(\eta)}\right), \quad \psi(\eta) = \tilde{a}\eta^2 + b - i\eta,$$

we obtain for the integral (2.3) that

$$E(x) \approx E_N(x) = h\sum_{k=-N}^{N} F(kh, x; \mathcal{L}).$$

Note that (2.7) implies that F satisfies (2.11) with $c = c(\tilde{a}, b)$, $\alpha(x) = (1-x)\sqrt{\max\{\tilde{a}, b\}}$. The error analysis is given by the following Theorem (see Appendix for the proof).

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

$$\|E(x) - E_N(x)\| \leq c_1\left[\frac{e^{-s\sqrt{N}}}{1 - e^{-s\sqrt{N}}} + he^{-s(1-x)\sqrt{N}}\right],$$

where

$$\begin{aligned} s &= \sqrt{2\pi d}\sqrt[4]{\min\{\frac{a}{k}, b\}}, & d &= (1 - \frac{1}{\sqrt{k}})\frac{k}{2a}, \\ c_1 &= \frac{2MM_1e^{\alpha}}{(1 - e^{-x\sqrt{2b}})(1-x)\sqrt{\min\{\frac{a}{k}, b\}}}, & c_2 &= \frac{1}{\sqrt{2\pi d}\sqrt[4]{\min\{\frac{a}{k}, b\}}}, \\ M_1 &= \sup_{z \in \overline{D}_d} \frac{|2\frac{a}{k}z - i|}{1 + \sqrt{|\frac{a}{k}z^2 + b - iz|}}, \end{aligned}$$

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 space-variable value $x \in (0,1)$.

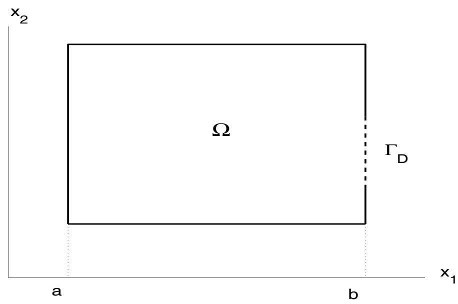

Figure 1: To the definition of Poincaré-Steklov operators

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

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

3. Find the approximation $E_N(x; \mathcal{L})$ for the normalised hyperbolic operator sine $E(x; \mathcal{L})$ in the form

$$E_N(x; \mathcal{L}) = \frac{h}{2\pi i} \sum_{p=-N}^{N} \sinh^{-1}(\sqrt{z_p}) \sinh(x\sqrt{z_p}) \, [2\frac{a}{k}ph - i] \, (z_pI - \mathcal{L})^{-1}.$$

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 values of x (provided that we apply the operator function for a given vector $(x_1, x_2, \dots, x_M)$).*

3 $\mathcal{H}$-Matrix Approximation to the Poincaré-Steklov Map

First considerations of the Dirichlet-Neumann map associated with elliptic problems (now called by Poincaré-Steklov operators) go back to the early works of Poincaré [25] and Steklov [28]. The reneval of interest in applying the Poincaré-Steklov operators is due to recent developments of the domain decomposition methods and fast solvers to the discrete Laplace, biharmonic, Lamé and Stokes equations [1, 20, 21, 19]. These operators were used also in recently developed efficient Cayley transform methods applied to the first order evolution equations [10, 11].

Let $\Omega_c \subset \mathbb{R}^{d+1}$ be a cylinder $\Omega \times [a_0, b_0]$ with the boundary $\Gamma_c = \Gamma_* \cup \Gamma_-$, $\Gamma_- = \partial\Omega \times [a_0, b_0]$ which is partitioned into two non-overlapping pieces Γ_* and Γ_-, where Γ_- is the lateral surface and Γ_* contains its top and bottom bases. Let $\mathcal{L}_0$ be an elliptic second order differential operator of the form $\mathcal{L}_0 = \mathcal{L}_1 + \mathcal{L}$, where

$$\mathcal{L}_1 = \frac{\partial^2}{\partial x_1^2}, \qquad \mathcal{L} = a_{2,2}(x_2)\frac{\partial^2}{\partial x_2^2} + a_{0,1}(x_2)\frac{\partial}{\partial x_2} + a_{0,0}(x_2), \qquad x_2 \in \mathbb{R}^d. \tag{3.1}$$

We consider the model boundary value problem

$$\begin{aligned} \mathcal{L}_0 u = 0 \quad & \text{in } \Omega, \\ u = 0 \quad & \text{on } \Gamma_-, \qquad \gamma_1 u = \psi \quad \text{on } \Gamma_*, \end{aligned} \tag{3.2}$$

where $\gamma_1 = \partial/\partial n = \partial_1$ is the normal derivative operator. The Poincaré-Steklov operator $S : H^{-1/2}(\Gamma_*) \to \tilde{H}^{1/2}(\Gamma_*)$ is defined as the Neumann-Dirichlet mapping

$$S : \psi \to \gamma_0 u|_{\Gamma_*}$$

where γ_0 is the continuous trace operator $\gamma_0 : H^1(\Omega_c) \to H^{1/2}(\Gamma_c)$. One can also introduce the inverse to the operator S by $T = S^{-1} : \tilde{H}^{1/2}(\Gamma_*) \to H^{-1/2}(\Gamma_*)$, which provides the Dirichlet-Neumann mapping associated with the solution of the equation $\mathcal{L}_0 u = 0$ subject to (3.2). In the case of constant coefficients in 2D, the details on sparse finite element approximation of the elliptic Poincaré-Steklov operators on polygonal boundaries may be found in [19].

3.1 Explicit Representation on Cylindric Domains

Let $\Omega_c = \Omega \times [a_0, b_0]$ as above. We consider the boundary value problem (3.2) and suppose that $\Gamma_* = \Gamma_l + \Gamma_r$, where Γ_l, Γ_r stay for the left and right facets of Ω, respectively. Denoting $\psi_i = \psi|_{\Gamma_i}, \varphi_i = \varphi|_{\Gamma_i}, i = l, r$, we have the following solutions for various combinations of the boundary conditions on Γ_l and Γ_r:

$$u(x_1) = \cosh^{-1}\left((b_0 - a_0)\sqrt{\mathcal{L}}\right)\left\{\mathcal{L}^{-1/2}\sinh((b_0 - x_1)\sqrt{\mathcal{L}})\psi_l + \cosh((x_1 - a_0)\sqrt{\mathcal{L}})\varphi_r\right\}, \tag{3.3}$$

$$u(x_1) = \cosh^{-1}\left((b_0 - a_0)\sqrt{\mathcal{L}}\right)\left\{\cosh((b_0 - x_1)\sqrt{\mathcal{L}})\varphi_l + \mathcal{L}^{-1/2}\sinh((x_1 - a_0)\sqrt{\mathcal{L}})\psi_r\right\}, \tag{3.4}$$

$$u(x_1) = \sinh^{-1}\left((b_0 - a_0)\sqrt{\mathcal{L}}\right)\left\{\mathcal{L}^{-1/2}\cosh((b_0 - x_1)\sqrt{\mathcal{L}})\psi_l + \mathcal{L}^{-1/2}\cosh((x_1 - a_0)\sqrt{\mathcal{L}})\psi_r\right\}. \tag{3.5}$$

Given the Dirichlet boundary conditions φ_l on Γ_l and φ_r on Γ_r, we get for the solution of the boundary value problem

$$\begin{aligned} \mathcal{L}u &= 0 \quad \text{in } \Omega, \\ u &= \varphi_l \quad \text{on } \Gamma_l, \qquad u \;=\; \varphi_r \quad \text{on } \Gamma_r, \end{aligned}$$

the following representation

$$u(x_1) = \sinh^{-1}\left((b_0 - a_0)\sqrt{\mathcal{L}}\right)\left\{\sinh^{-1}\left((x_1 - a)\sqrt{\mathcal{L}}\right)\varphi_r + \sinh\left((b - x_1)\sqrt{\mathcal{L}}\right)\varphi_l\right\}. \tag{3.6}$$

Let $\Gamma_0 = \{z = \xi + i\eta : \xi = a\eta^2 + \gamma_0\}$ be the spectral parabola defined as above and containing the spectrum $sp(\mathcal{L})$ of the strongly P-positive operator $\mathcal{L}$ and $\Gamma_{\mathcal{L}} = \{z = \xi + i\eta : \xi = \tilde{a}\eta^2 + b\}$ be the integration parabola containing Γ_0. Using equations (3.3)-(3.6) with $x_1 = a_0$ and $x_1 = b_0$, we obtain (formally) the integral representations for the Poincaré-Steklov operators $S,\ M : H^{-1/2}(\Gamma_l) \times \widetilde{H}^{1/2}(\Gamma_r) \to \widetilde{H}^{1/2}(\Gamma_l) \times H^{-1/2}(\Gamma_r)$ and their inverse $G = M^{-1}$, $T = S^{-1}$ defined in the block form. In particular, introducing

$$S\begin{pmatrix}\psi_\ell \\ \psi_r\end{pmatrix} := \begin{pmatrix} S_{\ell\ell} & S_{r\ell} \\ S_{r\ell}^T & S_{rr}\end{pmatrix}\begin{pmatrix}\psi_\ell \\ \psi_r\end{pmatrix} = \begin{pmatrix}\varphi_\ell \\ \varphi_r\end{pmatrix},$$

we obtain

$$\begin{aligned} S_{\ell\ell} &= \mathcal{L}^{-1/2}\coth\left((b_0 - a_0)\sqrt{\mathcal{L}}\right) &&= \frac{\mathcal{L}}{2\pi i}\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\coth\left((b_0 - a_0)\sqrt{\mathcal{L}}\right)(zI - \mathcal{L})^{-1}dz, \\ S_{r\ell} &= \mathcal{L}^{-1/2}\sinh^{-1}\left((b_0 - a_0)\sqrt{\mathcal{L}}\right) &&= \frac{1}{2\pi i}\int_{\Gamma_{\mathcal{L}}} z^{-1/2}\sinh^{-1}\left((b_0 - a_0)\sqrt{\mathcal{L}}\right)(zI - \mathcal{L})^{-1}dz, \\ S_{rr}^T &= S_{r\ell}, \quad S_{rr} = S_{\ell\ell}. \end{aligned}$$

Furthermore, setting

$$M\begin{pmatrix}\psi_\ell \\ \varphi_r\end{pmatrix} := \begin{pmatrix} M_{\ell\ell} & M_{r\ell} \\ M_{r\ell}^t & M_{rr}\end{pmatrix}\begin{pmatrix}\psi_\ell \\ \varphi_r\end{pmatrix} = \begin{pmatrix}\varphi_\ell \\ \psi_r\end{pmatrix},$$

and using (3.3) we obtain the explicit representations of blocks

$$\begin{aligned} M_{\ell\ell} &= \mathcal{L}^{-1/2}\tanh\left((b_0 - a_0)\sqrt{\mathcal{L}}\right) &&= \frac{\mathcal{L}}{2\pi i}\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\tanh\left((b_0 - a_0)\sqrt{\mathcal{L}}\right)(zI - \mathcal{L})^{-1}dz, \\ M_{r\ell} &= \cosh^{-1}\left((b_0 - a_0)\sqrt{\mathcal{L}}\right) &&= \frac{1}{2\pi i}\int_{\Gamma_{\mathcal{L}}} \frac{1}{\cosh\left((b_0 - a_0)\sqrt{\mathcal{L}}\right)}(zI - \mathcal{L})^{-1}dz, \\ M_{r\ell}^T &= -\cosh^{-1}\left((b_0 - a_0)\sqrt{\mathcal{L}}\right), \qquad M_{rr} = \mathcal{L}M_{\ell\ell}. \end{aligned}$$

The representation for

$$T\begin{pmatrix}\varphi_\ell \\ \varphi_r\end{pmatrix} := \begin{pmatrix} T_{\ell\ell} & T_{r\ell} \\ T_{r\ell}^T & T_{rr}\end{pmatrix}\begin{pmatrix}\varphi_\ell \\ \varphi_r\end{pmatrix} = \begin{pmatrix}\psi_\ell \\ \psi_r\end{pmatrix}$$

is similar:

$$T_{\ell\ell} = \sqrt{\mathcal{L}}\coth\left((b_0 - a_0)\sqrt{\mathcal{L}}\right) \equiv \mathcal{L}S_{\ell\ell}, \qquad T_{r\ell} = -\mathcal{L}S_{r\ell},$$
$$T_{r\ell}^T = -T_{r\ell}, \qquad T_{rr} = T_{\ell\ell}.$$

We can summarise the representation of the blocks of Poincaré-Steklov operators S, M and T. Further, we consider the case $\Im m\, sp(\mathcal{L}) = 0$ though the analysis for off-diagonal terms holds true for the general P-positive operators. In particular, the following result holds.

Lemma 3.1 *Let $\mathcal{L} \geq \gamma_0 I$, $\gamma_0 > 0$, be a selfadjoint, positive definite operator in a Hilbert space H or a strongly P-positive operator with discrete spectrum in a Banach space X such that its eigenfunctions are a basis of X. Choose a parabola $\Gamma_{\mathcal{L}} = \{z = \xi + i\eta : \xi = \tilde{a}\eta^2 + b\}$ with $b \in (0, \gamma_0)$. Then the bounded operators $M_{\ell\ell}, M_{r\ell}, S_{\ell\ell}, S_{r\ell}$ can be represented by*

$$\begin{aligned}
\mathcal{L}^{-1}M_{\ell\ell} &= \tfrac{1}{2\pi i}\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\tanh((b_0-a_0)\sqrt{z})\,(zI-\mathcal{L})^{-1}dz &&= \tfrac{1}{2\pi i}\int_{-\infty}^{\infty} F_{M_{\ell\ell}}(\eta)d\eta,\\
M_{r\ell} &= \tfrac{1}{2\pi i}\int_{\Gamma_{\mathcal{L}}} \cosh^{-1}((b_0-a_0)\sqrt{z})\,(zI-\mathcal{L})^{-1}dz &&= \tfrac{1}{2\pi i}\int_{-\infty}^{\infty} F_{M_{r\ell}}(\eta)d\eta\\
\mathcal{L}^{-1}S_{\ell\ell} &= \tfrac{1}{2\pi i}\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\coth((b_0-a_0)\sqrt{z})\,(zI-\mathcal{L})^{-1}dz &&= \tfrac{1}{2\pi i}\int_{-\infty}^{\infty} F_{S_{\ell\ell}}(\eta)d\eta,\\
S_{r\ell} &= \tfrac{1}{2\pi i}\int_{\Gamma_{\mathcal{L}}} z^{-1/2}\sinh^{-1}((b_0-a_0)\sqrt{z})\,(zI-\mathcal{L})^{-1}dz &&= \tfrac{1}{2\pi i}\int_{-\infty}^{\infty} F_{S_{r\ell}}(\eta)d\eta
\end{aligned}$$

with

$$\begin{aligned}
F_{M_{\ell\ell}}(\eta) &= (2\tilde{a}\eta - i)z^{-3/2}(\eta)\tanh((b_0-a_0)\sqrt{z(\eta)})\,(z(\eta)I-\mathcal{L})^{-1},\\
F_{M_{r\ell}}(\eta) &= (2\tilde{a}\eta - i)\cosh^{-1}((b_0-a_0)\sqrt{z(\eta)})\,(z(\eta)I-\mathcal{L})^{-1},\\
F_{S_{\ell\ell}}(\eta) &= (2\tilde{a}\eta - i)z^{-3/2}(\eta)\coth((b_0-a_0)\sqrt{z(\eta)})\,(z(\eta)I-\mathcal{L})^{-1},\\
F_{S_{r\ell}}(\eta) &= (2\tilde{a}\eta - i)z^{-1/2}(\eta)\sinh^{-1}((b_0-a_0)\sqrt{z(\eta)})\,(z(\eta)I-\mathcal{L})^{-1},
\end{aligned}$$

where $z = \tilde{a}\eta^2 + b - i\eta$.

Proof. We consider, for example, the case of a Hilbert space and the operator $S_{\ell\ell}$. Then we have

$$\begin{aligned}
\mathcal{L}^{-1}S_{\ell\ell} &= \frac{1}{2\pi i}\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\coth((b_0-a_0)\sqrt{z})\,(zI-\mathcal{L})^{-1}dz\\
&= \frac{1}{2\pi i}\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\coth((b_0-a_0)\sqrt{z})\int_{\gamma_0}^{\infty}(z-\lambda)^{-1}dE_\lambda dz\\
&= \frac{1}{2\pi i}\int_{\lambda_0}^{\infty}\left(\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\coth((b_0-a_0)\sqrt{z})(z-\lambda)^{-1}dz\right)dE_\lambda,
\end{aligned}$$

where E_λ denotes the spectral family associated with $\mathcal{L}$. Since $\lambda \in \mathbb{R}$, $|\tilde{a}\eta^2 + b - i\eta - \lambda| \geq \eta$, the integral

$$\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\coth((b_0-a_0)\sqrt{z})(z-\lambda)^{-1}dz = \int_{-\infty}^{\infty}\frac{(2\tilde{a}\eta - i)\coth\left((b_0-a_0)\sqrt{\tilde{a}\eta^2+b-i\eta}\right)}{(\tilde{a}\eta^2+b-i\eta)^{3/2}(\tilde{a}\eta^2+b-i\eta-\lambda)}d\eta < \infty$$

converges and the operator $S_{\ell\ell}$ is well defined. Due to (2.5-2.7) and the strong P-positiveness of $\mathcal{L}$ one can see that there exist constants c_1, M_1, α such that

$$|F_{S_{r\ell}}(\eta)| = \left|(2\tilde{a}\eta - i)z^{-1/2}(\eta)\sinh^{-1}\left((b_0-a_0)\sqrt{z(\eta)}\right)\right| \leq c_1 M_1 e^{-\alpha|\eta|},$$

where

$$\alpha_1 = \sqrt{\frac{\min\{\tilde{a}, b\}}{2}} > 0,\ c_1 = M_1\frac{2e^{\alpha}}{1-e^{-\sqrt{2b}}},\ M_1 = \max_{\eta\in(-\infty,\infty)}\frac{|2\tilde{a}\eta - i|}{\sqrt{|\tilde{a}\eta^2+b-i\eta|}(1+\sqrt{|\tilde{a}\eta^2+b-i\eta|}\,)},$$

i.e., the integral defining $S_{r\ell}$ converges. Analogously, one can prove that other blocks are well defined. If the operator $\mathcal{L}$ possesses a discrete spectrum $\lambda_j = \mu_j + i\nu_j$, $j = 1, 2, \ldots$, and P_j denotes the projector onto the subspace defined by the corresponding eigenfunction e_j, then the representation holds

$$(zI - \mathcal{L})^{-1} = \sum_{j=1}^{\infty}(z-\lambda_j)^{-1}P_j$$

yielding

$$\begin{aligned}\mathcal{L}^{-1}S_{\ell\ell} &= \frac{1}{2\pi i}\sum_{j=1}^{\infty}\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\coth\left((b_0-a_0)\sqrt{z}\right)(zI-\mathcal{L})^{-1}dzP_j\\ &= \frac{1}{2\pi i}\sum_{j=1}^{\infty}\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\coth\left((b_0-a_0)\sqrt{z}\right)(zI-\lambda_j)^{-1}dzP_j.\end{aligned}$$

Analogously as above one can show that all integrals converge and $S_{\ell\ell}$ is the well defined bounded operator. The same holds also for other blocks of S. ∎

3.2 Discretisation of the Poincaré-Steklov Operators

In order to get an appropriate discretisation to the Poincaré-Steklov operators we use the integral representations from Lemma 3.1. First of all we consider the operator $S_{r\ell}$. Applying the quadrature rule T_N with the operator valued function

$$F_{S_{r\ell}}(\eta) = (2\tilde{a}\eta - i)z^{-1/2}(\eta)\sinh^{-1}\left((b-a)\sqrt{z(\eta)}\right)(z(\eta)I-\mathcal{L})^{-1}, \qquad z = a\eta^2+b-i\eta, \tag{3.7}$$

we obtain for the operator $S_{r\ell}$ that

$$S_{r\ell} \approx S_{r\ell}^{(N)} = h\sum_{k=-N}^{N} F_{S_{r\ell}}(kh).$$

The error analysis is given by the following Theorem.

Theorem 3.2 *Choose $k>1$, $\tilde{a}=a/k$, $h=\frac{\sqrt{2\pi d/N}}{\sqrt[4]{\min\{\frac{a}{k},b\}/2}}$, $b=b(k)=\gamma_0-\frac{k-1}{4a}$ and the integration parabola $\Gamma_{b(k)}=\{z=\tilde{a}\eta^2+b(k)-i\eta : \eta\in(-\infty,\infty)\}$, then there holds*

$$\|S_{r\ell}-S_{r\ell}^{(N)}\| \le c_3\left[c_2N^{-1/2}+1\right]e^{-s\sqrt{N}},$$

where

$$\begin{aligned} s &= \sqrt{2\pi d}\sqrt[4]{\min\{\frac{a}{k},b\}/2}, & d &= (1-\frac{1}{\sqrt{k}})\frac{k}{2a},\\ c_2 &= \frac{1}{\sqrt{2\pi d}\sqrt[4]{\frac{1}{2}\min\{\frac{a}{k},b\}}}, & c_3 &= \frac{2MM_2e^{\alpha}}{(1-e^{-\sqrt{2b}})\sqrt{\frac{1}{2}\min\{\frac{a}{k},b\}}},\\ M_2 &= \max_{z\in\overline{D}_d}\frac{|2\frac{a}{k}z-i|}{\sqrt{|\frac{a}{k}z^2+b-iz|}(1+\sqrt{|\frac{a}{k}z^2+b-iz|})}, \end{aligned}$$

M is the constant from the inequality of the strong P-positivity.

Proof. We choose the integration path similar to Theorem 2.4. The integrand can be analytically extended onto a strip D_d with the width $d=\left(1-\frac{1}{\sqrt{k}}\right)\frac{k}{2a}$. Set

$$\alpha_1 = \sqrt{\frac{a}{k}(\eta^2-\nu^2)+b+\nu+i(\frac{2a\nu}{k}-1)\eta}.$$

Due to the strong P-positivity of $\mathcal{L}$ there holds for $z=\eta+i\nu\in D_d$ that

$$\begin{aligned} F_{S_{r\ell}}(z;\mathcal{L})\| &\le M\frac{|(2\frac{a}{k}z-i)|\sinh^{-1}\left((b-a)\sqrt{\frac{a}{k}z^2+b-iz}\right)}{\sqrt{|\frac{a}{k}z^2+b-iz|}(1+\sqrt{|\frac{a}{k}z^2+b-iz|})}\\ &= \frac{M|2\frac{a}{k}z-i|}{\alpha(\alpha+1)\ \sinh\left((b_0-a_0)\sqrt{\frac{a}{k}(\eta^2-\nu^2)+b+\nu+i(\frac{2a\nu}{k}-1)\eta}\right)}\\ &\le MM_2\sinh^{-1}\left((b-a)\sqrt{\frac{a}{k}(\eta^2-\nu^2)+b+\nu+i(\frac{2a\nu}{k}-1)\eta}\right) \end{aligned}$$

and the estimate (2.7) implies that $F(z,t;\mathcal{L}) \in \mathbf{H}^1(D_d)$. We have also

$$\|F_{S_{r\ell}}(\eta,x;\mathcal{L})\| < ce^{-\alpha|\eta|} \qquad \text{for } \eta \in \mathbb{R}$$

with

$$\alpha = \sqrt{\min\{\frac{a}{k}, b\}/2} > 0, \qquad c = MM_2 \frac{e^{\alpha}}{1-e^{-\sqrt{2b}}}. \tag{3.8}$$

Using Lemma 2.3 and setting in (2.12) α as in (3.8), we get

$$\|\eta_N(F,h)\| \le \frac{2c}{\alpha}\left[\frac{h}{2\pi d}\exp(-2\pi d/h) + \exp(-\alpha\, h\, N)\right]. \tag{3.9}$$

Equalising the exponents by setting $2\pi d/h = \alpha\, hN$, we get $h = \frac{\sqrt{2\pi d/N}}{\sqrt[4]{\frac{1}{2}\min\{\frac{a}{k},b\}}}$. Substitution of this value into (3.9) leads to the estimate

$$\|\eta_N(F,h)\| \le c_3\left[c_2 N^{-1/2}e^{-s\sqrt{N}} + e^{-s(1-x)\sqrt{N}}\right], \text{ where } c_3 = \frac{2MM_2e^{\alpha}}{(1-e^{-\sqrt{2b}})\alpha},\ c_2 = \frac{1}{s},\ s = \sqrt{2\pi d\alpha}.$$

This complete the proof. ∎

This introduces the following algorithm with an exponential convergence rate for computing the approximation $S_{r\ell}^{(N)}$ to the operators $S_{r\ell}$.

Algorithm 3.3 *1. Choose $k > 1, N$ and set $d = (1-\frac{1}{\sqrt{k}})\frac{k}{2a}$, $z_p = \frac{a}{k}(ph)^2 + b - iph$ $(p = -N,\dots,N)$, where $h = \frac{\pi d_1}{2N}$ and $b = \gamma_0 - \frac{k-1}{4a}$.*

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

3. Given $F_{S_{r\ell}}$ from (3.7), find the approximation $S_{r\ell}^{(N)}$ for the operator $S_{r\ell}$ in the form

$$S_{r\ell}^{(N)} = h\sum_{p=-N}^{N} F_{S_{r\ell}}(ph).$$

Applying Algorithm 3.3 to the operator-valued function $F_{S_{\ell\ell}}$ allows to compute the diagonal block $S_{\ell\ell}$ with polynomial accuracy. For the sake of simplicity, we consider a selfadjoint, positive definite operator $\mathcal{L}$ and obtain

$$\mathcal{L}^{-1}S_{\ell\ell} = \frac{1}{2\pi i}\int_{\lambda_0}^{\infty}\left(\int_{\Gamma_{\mathcal{L}}} z^{-3/2}\coth\left((b_0-a_0)\sqrt{z}\right)(z-\lambda)^{-1}dz\right)dE_{\lambda}.$$

Substituting the function $F_{S_{\ell\ell}}$ instead of $F_{S_{r\ell}}$ in Algorithm 3.3, we obtain the approximation to $S_{\ell\ell}$. The convergence rate of the corresponding Algorithm 3.3 depends on the estimate of the following quantity

$$\eta_{S_{\ell\ell}}^{(N)}(\lambda) = \left|\int_{-\infty}^{\infty}\Phi(\eta,\lambda)d\eta - \sum_{p=-N}^{N}\Phi(ph,\lambda)\right| = \eta_1 + \eta_2 + \eta_3,$$

with $\Phi(\eta,\lambda) = (2\tilde{a}\eta - i)z^{-3/2}\coth((b_0-a_0)\sqrt{z})(z-\lambda)^{-1}$, $z = \tilde{a}\eta^2 + b - i\eta$ and

$$\begin{aligned}
\eta_1 &= \int_{-\infty}^{-Nh}\Phi(\eta,\lambda)d\eta,\\
\eta_2 &= \int_{-Nh}^{(N+1)h}\Phi(\eta,\lambda)d\eta - \sum_{p=-N}^{N}\Phi(ph,\lambda) \;=\; \sum_{p=-N}^{N}\left[\int_{ph}^{(p+1)h}\Phi(\eta,\lambda)d\eta - h\Phi(ph,\lambda)\right]\\
&= \sum_{p=-N}^{N}\int_{ph}^{(p+1)h}\int_{ph}^{\eta}\Phi'_{\eta}(\eta,\lambda)d\eta,\\
\eta_3 &= \int_{(N+1)h}^{\infty}\Phi(\eta,\lambda)d\eta.
\end{aligned}$$

It is easy to see that

$$|\eta_1| \lesssim \int_{-\infty}^{-Nh} \eta^{-2} d\eta \lesssim N^{-1}h^{-1} \lesssim N^{-1/2}.$$

Analogously we get $|\eta_3| \lesssim N^{-1/2}$. The second summand is estimated by

$$|\eta_2| = \left| \sum_{p=-N}^{N} \int_{ph}^{(p+1)h} \int_{ph}^{\eta} \Phi'_\eta(\eta,\lambda) d\eta \right| \le h \int_{-Nh}^{(N+1)h} |\Phi'(\eta,\lambda)| d\eta \lesssim N^{-1/2}.$$

Thus, we finally get

$$|\eta^{(N)}_{S_{\ell\ell}}(\lambda)| \lesssim N^{-1/2}.$$

Note that applying the construction to the discrete case, we obtain that the operator $S_{\ell\ell}$ admits the integral representation without any factorisation as above due to the estimate $\|(zI - \mathcal{L}_h)^{-1}\| \le c|z|^{-1}$ for $|z|$ big enough.

3.3 Approximation by Additive Splitting and Nonlinear Iteration

As an alternative to the polynomially convergent algorithm for approximation of $S_{\ell\ell}$, below we discuss the approach based on the additive splitting

$$S_{\ell\ell} = S_0(\mathcal{L}) + \mathcal{L}^{-1/2}, \qquad S_0(\mathcal{L}) = \mathcal{L}^{-1/2}\left(coth\left((b_0 - a_0)\sqrt{\mathcal{L}} \right) - I \right), \tag{3.10}$$

where the complex function $S_0(\xi)$ has the exponential decay as $\xi \in \mathbb{R}$, $|\xi| \to \infty$. Therefore, the idea is to apply the exponentially convergent quadrature rule to the integral representation of $S_0(\mathcal{L})$, as for the off-diagonal term $S_{r\ell}$, and then construct the $\mathcal{H}$-matrix approximation to $\mathcal{L}^{-1/2}$ by an iterative process. Since the matrix iterations converge quadratically, we obtain also the linear-logarithmic complexity for the $\mathcal{H}$-matrix approximation of the second term in the right-hand side of (3.10).

Our construction of the square root of an $\mathcal{H}$-matrix is based on the iterative solving of the nonlinear matrix equation using formatted matrix-matrix multiplication and inversion. Let L_h be the Galerkin stiffness matrix for the operator $\mathcal{L}$ with respect to the finite element space $V_h \in H^1_0(\Omega)$ with $n = \dim V_h$. We propose to apply the nonlinear iterations for computing symmetric and positive definite matrix $X = A^{1/2}$, where A is defined as the $\mathcal{H}$-matrix approximation to the exact inverse L_h^{-1}. The existence of such an $\mathcal{H}$-matrix A was investigated in [5]. The proper initial guess X_0 may be obtained by the $\mathcal{H}$-matrix approximation applied on the coarse finite element space $V_H \subset V_h$ or from above defined polynomial algorithm based on the factorised representation. We solve the nonlinear operator equation

$$F(X) := X^2 - A = 0, \qquad X \in \mathbf{Y},$$

in the corresponding normed space $\mathbf{Y} := \mathbb{R}^{n\times n}$ of square matrices by the matrix iteration

$$X_{i+1} = \frac{1}{2}(X_i + X_i^{-1} \cdot A), \qquad X_0 \text{ given}, \quad i = 0,1,2,\dots . \tag{3.11}$$

For this scheme, which is well-known from the literature, we give a simple direct convergence analysis. Denote $Y_i = X_i A^{-1/2} \in \mathbf{Y}$ and $\delta_i = Y_i - I$.

Lemma 3.4 *Let A, $X_0 \in \mathbf{Y}$ be symmetric and positive definite matrices and assume that the initial guess X_0 satisfies*

$$||X_0 A^{-1/2} - I|| = q < \frac{1}{2}.$$

Then the iteration (3.11) converges quadratically,

$$||\delta_{i+1}|| \le q_0^{2^i}, \qquad i = 1,2,\dots,$$

where $q_0 = \frac{q}{1-q} < 1$, and the iteration (3.11) yields $X_i = X_i^T$ for all i. Moreover, $X_i > 0$ is valid for any i satisfying $q_0^{2^i} \le \sqrt{\lambda_{max}(A)}$.

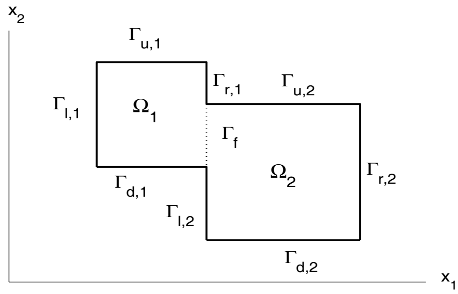

Figure 2: The interface problem

Proof. By definition, (3.11) yields

$$Y_{i+1} - I = (Y_i - I)^2 \, Y_i^{-1}, \qquad i = 0, 1, \dots .$$

It is easy to see that

$$||Y_i^{-1}|| \le ||Y_{i-1}^{-1}|| \le \dots \le ||Y_0^{-1}|| \le \frac{1}{1-q}, \qquad i = 1, 2, \dots .$$

Therefore, the first assertion follows

$$||\delta_{i+1}|| \le ||Y_0^{-1}||^{(1+2+2^2+2^3+\dots+2^{i-1})} \, ||\delta_0||^{2^i} \le q_0^{2^i}.$$

To proceed with, we use the recursion

$$\varepsilon_{i+1} = \varepsilon_i X_i^{-1} \varepsilon_i, \qquad \varepsilon_i = X_i - A^{1/2}, \qquad i = 0, 1, \dots ,$$

which implies the symmetry of X_i, $i \ge 1$, by induction. Since

$$||\varepsilon_{i+1}|| \le \|A^{1/2}\| \, ||A^{-1/2} \, \varepsilon_{i+1}|| = \|A^{1/2}\| \, ||\delta_{i+1}|| \le c \, \|A^{1/2}\| \, q_0^{2^i}$$

implies $||\varepsilon_{i+1}|| \le \sqrt{\lambda_{max}(A)} q_0^{2^i}$, we obtain $X_i > 0$ for any i which satisfies $\sqrt{\lambda_{max}(A)} q_0^{2^i} < 1$. ∎

Due to the quadratic convergence of the scheme proposed, we need only $\log\log \varepsilon^{-1}$ iterative steps to obtain the accuracy $O(\varepsilon)$, which results in an $O(k^2 p^2 n \log\log n)$ complexity of the iterative correction algorithm, see Appendix 5.1 for further details on the $\mathcal{H}$-matrices. Lemma 3.4 applies in the case of exact matrix arithmetic. However, the numerical experiments show that the specific truncation errors of the $\mathcal{H}$-matrix arithmetic can be put under efficient control (see also the discussion in [16]).

4 Application to Elliptic Boundary Value Problems

4.1 Reduction to the Interface: Two Subdomains

Assume the domain Ω with the boundary Γ to be composed of two matching and non-overlapping rectangles Ω_i, $i = 1, 2$, with boundaries $\Gamma_i = \Gamma_{l,i} \cup \Gamma_{t,i} \cup \Gamma_{r,i} \cup \Gamma_{b,i}$, where $\Gamma_{l,i}, \Gamma_{t,i}, \Gamma_{r,i}, \Gamma_{b,i}$ stay for the left, right, top and bottom edges respectively (see Fig. 2). Let $\Gamma_f = \Gamma_{r,1} \cap \Gamma_{l,2}$ (dash line) be the interior matching line. We consider the boundary value problem

$$\begin{aligned} \mathcal{L}u &= 0 \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \Gamma \backslash \Gamma_{r,1} \backslash \Gamma_{l,2}, \qquad \gamma_1 u = 0 \quad \text{on } \Gamma_{r,1} \cup \Gamma_{l,2} \end{aligned}$$

where the operator $\mathcal{L}$ is given by (3.1). We denote by $\mathcal{L}_i$ the operator (3.1) defined in the domains Ω_i, $i = 1, 2$. Introducing the unknown vectors

$$u_{f,r} = \begin{matrix} 0 & \text{on } \Gamma_{r,1} \backslash \Gamma_f, \\ \gamma_1 u & \text{on } \Gamma_f \end{matrix} \qquad \text{and} \qquad u_{f,l} = \begin{matrix} 0 & \text{on } \Gamma_{l,2} \backslash \Gamma_f, \\ \gamma_1 u & \text{on } \Gamma_f, \end{matrix}$$

we can present the solutions $u^{(i)}$ in the domains Ω_i, $i = 1, 2$, in the form

$$u^{(1)}(x_1) = \mathcal{L}^{-1/2} \cosh^{-1}\left((b_0 - a_0)\sqrt{\mathcal{L}_1}\right) \sinh\left((x_1 - a_0)\sqrt{\mathcal{L}_1}\right) u_{f,r},$$
$$u^{(2)}(x_1) = \mathcal{L}^{-1/2} \sinh^{-1}\left((c_0 - b_0)\sqrt{\mathcal{L}_2}\right) \cosh\left((x_1 - b_0)\sqrt{\mathcal{L}_2}\right) u_{f,l}.$$

Setting $u^{(1)}(b_0) = u^{(2)}(b_0)$ on Γ_f, we get the following interface problem

$$\mathcal{L}_1^{-1/2} \tanh\left((b_0 - a_0)\sqrt{\mathcal{L}_1}\right) u_{f,r} = \mathcal{L}_2^{-1/2} \tanh\left((c_0 - b_0)\sqrt{\mathcal{L}_2}\right) u_{f,l}.$$

Substitution of the $\mathcal{H}$-matrix discretisations from Algorithm 3.3 leads to the interface problem which may be solved by the direct method based on the $\mathcal{H}$-matrix arithmetic.

4.2 Anisotropic Domain Decomposition

The elliptic equations with strongly jumping diffusion and anisotropy coefficients as well as the equations defined in the domains involving thin substructures face a wide range of applications in the problems of structural mechanics, porous media, magnetostatics and biology. A robust preconditioning technique for such class of elliptic problems in 2D was developed in [22]. In this section, we demonstrate how in some particular cases the corresponding equation may be efficiently treated as an interface equation using sparse approximations to the Poincaré-Steklov operators. The 3D case may be considered in a similar way.

In the domain $\Omega \in \mathbb{R}^2$ composed of $M \geq 1$ matching and non-overlapping rectangles Ω_i, $\overline{\Omega} = \cup_{i=1}^M \overline{\Omega}_i$, we consider the variational problem with piecewise constant anisotropy and diffusion coefficients:
Given $f \in H^{-1}(\Omega)$, $\psi_i \in H^{-1/2}(\Gamma_i)$ and positive constants μ_i, ε_i, find $u \in V \subset H^1(\Omega)$, such that

$$a(u, v) = F(v) := \sum_{i=1}^{M} (\psi_i, v)_{L^2(\Gamma_i)} + (f, v)_{L^2(\Omega)} \qquad \text{for all } v \in V, \tag{4.1}$$

where the bilinear form $a(\cdot, \cdot) : V \times V \to \mathbb{R}$ is defined by

$$a(u, v) = \sum_{i=1}^{M} a_i(u_{|\Omega_i}, v_{|\Omega_i}) \qquad (u, v \in V), \quad \text{where}$$
$$a_i(u, v) = \mu_i \int\limits_{\Omega_i} \begin{pmatrix} \varepsilon_i & 0 \\ 0 & \varepsilon_i^{-1} \end{pmatrix} \nabla u \cdot \nabla v dx\ , \qquad \mu_i,\ \varepsilon_i > 0, \quad x \in \Omega_i.$$

Our approach remains valid for the following choice of the Hilbert space V:

$$V = H_0^1(\Omega), \quad V = \{u \in H^1(\Omega) : (u, 1)_{L^2(\Omega)} = 0\}, \quad \text{or}$$
$$V = H^1_{\Gamma_D}(\Omega) := \{u \in H^1(\Omega) : u_{|\Gamma_D} = 0\}, \quad \Gamma_D \subset \partial\Omega, \quad \Gamma_D \neq \emptyset,$$

corresponding to the Dirichlet, Neumann and mixed boundary conditions, respectively. We use the notations $\Gamma_i = \partial\Omega_i$ for the subdomain boundaries and $\Gamma = \cup_{i=1}^M \Gamma_i \backslash \Gamma_D$ for the interface.

Our particular example related to the skin-modelling problem from [22] may be viewed either as the isotropic problem with $\varepsilon_i = 1$, but with highly stretched geometries of subdomains or as the strongly anisotropic problem with jumping coefficients μ_i and ε_i, but with regular decomposition. In the following, we consider the isotropic description of the problem.

The typical geometry is presented in Fig. 4.2 (left). We consider the limit case with $\mu_i = 0$ in all shaded subdomains and $\mu_i = 1$, otherwise (flow in the "lipid layer" $\Omega_{lip} = \Omega \setminus \cup_{i:\mu_i=0}\Omega_i$). This corresponds to the homogeneous Neumann condition at all interior interfaces and to the choice $V_{lip} := V_{|\Omega_{lip}}$ of the computational space. The corresponding reduction of (4.1) to the *interface* is then given by: *find $\lambda \in Y := \{\lambda = z_{|\Gamma} : z \in V_{lip}\}$ such that*

$$a_\Gamma(\lambda, v) := \sum_{i=1}^{M} \mu_i \langle T_i \lambda_i, v_i \rangle_{\Gamma_i} = F(v) \qquad \text{for all } v \in Y. \tag{4.2}$$

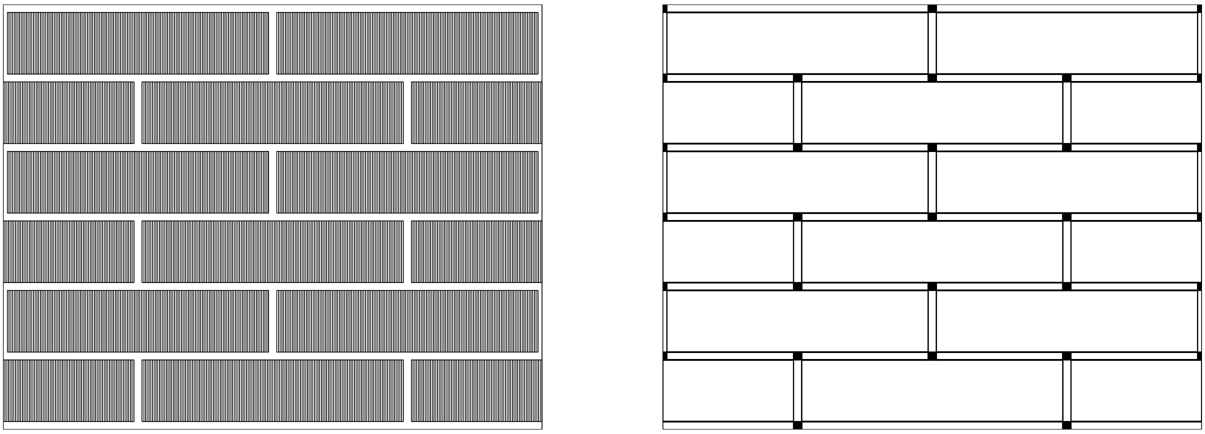

Figure 3: Computational domain (left) and basic decomposition (right) in the model problem.

Here, the (anisotropic) Poincaré-Steklov operator $T_i : Y_i \to Y_i'$, with $Y_i = Y_{|\Gamma_i}$, is defined by

$$\begin{aligned} \langle T_i \lambda, v \rangle_{\Gamma_i} &= a_i(\overline{\lambda}, \widetilde{v}) && \text{for all } \widetilde{v} \in V_i,\ \widetilde{v}_{|\Gamma_i} = v, \\ a_i(\overline{\lambda}, z) &= 0 && \text{for all } z \in V_i \cap H_0^1(\Omega_i), \end{aligned} \tag{4.3}$$

where $\overline{u}_{|\Gamma_i} = \lambda$, $\overline{u} \in V_i = V_{|\Omega_i}$. The trace space Y is equipped with the norm $\|\lambda\|_Y = \inf_{z \in V : z_{|\Gamma} = \lambda} \|z\|_V$. Here $\langle \cdot, \cdot \rangle_{\Gamma_i}$ denotes the L^2-duality on Γ_i.

Lemma 4.1 *The bilinear form $a_\Gamma(\cdot, \cdot) : Y \times Y \to \mathbb{R}$ is symmetric, continuous and positive definite. With any given element $\psi_i \in H^{-1/2}(\Gamma_i)$, equation (4.2) is uniquely solvable in Y providing $\lambda_{|\Gamma} = u$.*

Proof. The first assertion is a consequence of the mapping properties to the local Poincaré-Steklov operators and the definition of the trace norm on Y. We then apply the Lax-Milgram Lemma to equation (4.2) taking into account the continuity of $F(\cdot)$ in Y. The equivalence of equations (4.1) and (4.2) follows from the definition (4.3). ■

We decompose the computational domain onto a set of stretched rectangles and squares (marked by black in Fig. 4.2 (right)). In each stretched subdomain we have to transfer the flux from one short edge to the opposite one with fixed homogeneous Neumann boundary conditions on stretched pieces of the boundary. This may be done by approximating the corresponding Poincaré-Steklov operators as above. Due to the specific geometry, the finite element ansatz space to be used for approximation of $\mathcal{L}$ has relatively small dimension. Thus, one can compute the Schur-complement system of equations associated only with a small number of degrees of freedom related to the "black" subdomains. The resultant Schur-complement system of equations may be then solved by the PCG method with simple block diagonal preconditioner. Note that it is not the scope of our paper to discuss the details of preconditioning techniques for such kind of problems. We refer to [2, 22] for further details on the topic. In fact, here we focus mainly on the data-sparse representation to the interface operator, which allows the almost linear storage and matrix-vector product cost with respect to the number of degrees of freedom associated with the "black squares", see Fig. 4.2 (right).

Note that the coefficients of the differential operator $\mathcal{L}$ may be variable. Similar scheme can be also realised in the 3D case in the presence of thin geometries, see also the next section.

4.3 Elliptic Problems in Cylinder Type Domains

As an example, we consider an application to elliptic problems in cylindrical domains.

Given the normalised hyperbolic sine operator $E(x)$, the solution of the elliptic boundary value problem posed in the domain $\Omega_{\mathcal{L}} \times [0, 1] \in \mathbb{R}^{d+1}$,

$$\frac{d^2 u}{dx^2} - \mathcal{L} u = -f(x), \quad u(0) = u_0, \quad u(1) = u_1, \tag{4.4}$$

with known boundary data $u_0,\ u_1$ and with the given right-hand side $f(x)$, can be represented as

$$u(x) = E(x;\mathcal{L})u_1 + E(1-x;\mathcal{L})u_0 + \int_0^1 G(x,s;\mathcal{L})f(s)ds, \tag{4.5}$$

where

$$G(x,s;\mathcal{L}) \equiv G(x,s) = \left[\sqrt{\mathcal{L}}\sinh\left(\sqrt{\mathcal{L}}\right)\right]^{-1} * \begin{matrix} \sinh(x\sqrt{\mathcal{L}})\sinh\left((1-s)\sqrt{\mathcal{L}}\right) & \text{for } x \le s, \\ \sinh(s\sqrt{\mathcal{L}})\sinh\left((1-s)\sqrt{\mathcal{L}}\right) & \text{for } x \ge s \end{matrix}$$

is Green's function for problem (4.4). It is easy to prove that Green's function can also be represented through the normalised hyperbolic operator sinh-function in the following way

$$G(x,s) = \frac{1}{2} \begin{matrix} \int_{x+s-1}^{x-s+1} E(t;\mathcal{L})dt & \text{for } x \le s, \\ \int_{x+s-1}^{s-x+1} E(t;\mathcal{L})dt & \text{for } x \ge s. \end{matrix}$$

Integration by parts yields

$$\begin{aligned} \int_0^1 G(x,s;\mathcal{L})f(s)ds = & \frac{1}{2}\left[\int_0^x f(t)dt \int_{x+s-1}^{s-x+1} E(t;\mathcal{L})dt + \int_x^1 f(t)dt \int_{x+s-1}^{x-s+1} E(t;\mathcal{L})dt\right] \\ & - \frac{1}{2}\int_0^x (E(s-x+1;\mathcal{L}) - E(x+s-1;\mathcal{L}))\int_0^s f(t)dtds \\ & - \frac{1}{2}\int_x^1 (E(x-s+1;\mathcal{L}) - E(x+s-1;\mathcal{L}))\int_s^1 f(t)dtds. \end{aligned} \tag{4.6}$$

We consider the following semi-discrete scheme. Let $\mathbf{M}_j$ be the $\mathcal{H}$-matrix approximation of the resolvent $(z_jI-\mathcal{L})^{-1}$ (see §5.1) associated with the Galerkin ansatz space $V_h \subset L^2(\Omega_{\mathcal{L}})$ and let $\mathbf{u}_0$, $\mathbf{f}$ be the vector representations of the corresponding Galerkin projections onto the spaces V_h and $V_h \times [0,1]$, respectively. Then the $\mathcal{H}$-matrix approximation of the normalised hyperbolic sinh-function takes the form (set $u_1 = 0$)

$$E_N(x;\mathcal{L})u_0 = \sum_{j=-N}^{N} \gamma_j \sinh^{-1}(\sqrt{z_j})\sinh(\sqrt{z_j}x)\mathbf{M}_j, \qquad \gamma_j = \frac{h}{2\pi i}(2jh - i), \quad z_j = \frac{a}{k}(jh)^2 + b - ijh.$$

Substitution of this representation into (4.5) and taking into account (4.6) leads to the entirely parallelisable scheme

$$\begin{aligned} u_{\mathcal{H}}(x) = & \sum_{j=-N}^{N} \gamma_j \sinh^{-1}(\sqrt{z_j})\sinh(x\sqrt{z_j})\mathbf{M}_j * \\ & \left[\mathbf{u}_0 + \frac{1}{\sqrt{z_j}\sinh(\sqrt{z_j})}\int_0^x \left(\sinh((s-x+1)\sqrt{z_j}) - \sinh((s+x-1)\sqrt{z_j})\right)\mathbf{f}(s)ds \right. \\ & \left. + \frac{1}{\sqrt{z_j}\sinh(\sqrt{z_j})}\int_x^1 \left(\sinh((s-x+1)\sqrt{z_j}) - \sinh((s+x-1)\sqrt{z_j})\right)\mathbf{f}(s)ds\right] \end{aligned} \tag{4.7}$$

with respect to $j = -N, \dots, N$, to compute the approximation $u_{\mathcal{H}}(x)$.

The second level of parallelisation appears if we apply some quadrature rule to calculate the integral term in the right-hand side of (4.7).

5 Appendix

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

For the reader's convenience, we present briefly the main features of the $\mathcal{H}$-matrix techniques to be used for the data-sparse approximation of the operator resolvent in question. The details on the complexity bound and the corresponding approximation results for the $\mathcal{H}$-matrix arithmetic may be found in [14]-[18].

In our application, we look for a sufficiently accurate data-sparse approximation of the operator $(zI-\mathcal{L})^{-1}$: $H^{-1}(\Omega) \to H_0^1(\Omega)$, $\Omega \in \mathbb{R}^d$, $d = 1, 2, 3$, where $z \in \mathbb{C} \setminus sp(\mathcal{L})$ is given in Step 1 of the Algorithm 2.5. Assume that Ω is a domain with smooth boundary. The existence of the $\mathcal{H}$-matrix approximation to $\exp(-t\mathcal{L})$ is based on the classical integral representation for $(zI - \mathcal{L})^{-1}$,

$$(zI - \mathcal{L})^{-1}u = \int_\Omega G(x, y)u(y)dy, \qquad u \in H^{-1}(\Omega), \tag{5.1}$$

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

$$(zI - \mathcal{L})_x G(x, y) = \delta(x - y) \quad \text{for } x, y \in \Omega, \qquad G(x, y) = 0 \quad \text{for } x \in \partial\Omega,\ y \in \Omega. \tag{5.2}$$

Together with an adjoint system of equations in the second variable y, equation (5.2) provides the base to prove the existence of the $\mathcal{H}$-matrix approximation of $(zI-\mathcal{L})^{-1}$ which then can be obtained by the *$\mathcal{H}$-matrix arithmetic* from [14, 15].

The error analysis for the $\mathcal{H}$-matrix approximation to the integral operator from (5.1) may be based on different smoothness prerequisites. The typical assumption requires that the kernel function G is asymptotically smooth, i.e.,

Assumption 5.1 *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*

$$|\partial_x^\alpha \partial_y^\beta G(x, y)| \leq c(|\alpha|, |\beta|)|x - y|^{2-|\alpha|-|\beta|-d} \qquad \textit{for all } |\alpha|, |\beta| \leq m.$$

In general, the smoothness of Green's function $G(x, y)$ is determined by the regularity of problem (5.2).

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

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

Let I be the index set of unknowns (e.g., the finite element-nodal points) and $T(I)$ be the hierarchical cluster tree [14]. For each $i \in I$, the support of the corresponding basis function φ_i is denoted by $X(i) := \operatorname{supp}(\varphi_i)$ 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. [15]), 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*,

$$\min\{\operatorname{diam}(\sigma), \operatorname{diam}(\tau)\} \leq 2\,\eta \operatorname{dist}(\sigma, \tau), \quad \text{or } \min\{\operatorname{card}(\sigma), \operatorname{card}(\tau)\} = 1,$$

$(\sigma, \tau) \in P_2$, $\eta < 1$, whose union equals $I \times I$. 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 is

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

In our paper, the construction below is applied only for theoretical needs, namely to prove the existence of $\mathcal{H}$-matrix approximation to the operator resolvent. With the splitting $P_2 = P_{far} \cup P_{near}$, where $P_{far} := \{\sigma \times \tau \in P_2 : \operatorname{dist}(\tau, \sigma) > 0\}$, the standard $\mathcal{H}$-matrix approximation of the nonlocal operator A given in (5.1) consists of three essential steps [15]:

(a) construction of the *admissible* block-partitioning $P_2 = P_{far} \cup P_{near}$ of the tensor product index set $I \times I$.

(b) construction of an approximate integral operator $A_\mathcal{H} \in \mathcal{L}(V, V')$ with a kernel $s_\mathcal{H}(\cdot, \cdot)$ defined for each tensor product domain $X(\sigma) \times X(\tau)$ with $\sigma \times \tau \in P_{far}$ by a *separable expansion*

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

of the order $k \ll N = \dim V_h$. In the near-field area, the kernel function is unchanged.

(c) setup of the Galerkin $\mathcal{H}$-matrix $\mathbf{A}_{\mathcal{H}} = \langle A_{\mathcal{H}}\varphi_i, \varphi_j\rangle_{i,j\in I}$ for the operator $A_{\mathcal{H}}$.

The reduction in 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

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

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

$$\mathcal{N}_{st}\left(\mathbf{A}_{\mathcal{H}}\right) = O(kN), \qquad \mathcal{N}_{MV}\left(\mathbf{A}_{\mathcal{H}}\right) = O(kN).$$

On the other hand, the approximation of the order $O(N^{-\alpha})$, $\alpha > 0$, is achieved with $k = O(\log^\beta N)$, where either $\beta = d$ or $\beta = d-1$ depending on the type of separable expansion for the kernel function.

5.2 Proofs 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 [29, Theorem 3.1.2] one can get

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

and upon replacing z by x, we have

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

After interchanging the order of integration and using the identities

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

we obtain (2.9). Using the estimate (see [29, p.133]) $\sinh(\pi d/h) \le |\sin[\pi(\xi \pm id)/h]| \le \cosh(\pi d/h)$, the assumption $f \in \mathbf{H}^1(D_d)$ and the identity (2.9), we obtain the desired bound (2.10). The assumption (2.11) now implies

$$\|\eta_N(f,h)\| \le \|\eta(f,h)\| + h\sum_{|k|>N}\|f(kh)\| \le \frac{\exp(-\pi d/h)}{2\sinh(\pi d/h)}\|f\|_{\mathbf{H}^1(D_d)} + c\,h\sum_{|k|>N}\exp[-\alpha|kh|]. \tag{5.3}$$

For the last sum we use the simple estimate

$$\sum_{|k|>N} e^{-\alpha|kh|} = 2\sum_{k=N+1}^{\infty} e^{-\alpha kh} = \frac{2e^{-\alpha(N+1)h}}{1 - e^{-\alpha h}} < \frac{2}{\alpha}e^{-\alpha N h}. \tag{5.4}$$

It follows from (2.11) that

$$\|f\|_{\mathbf{H}^1(D_d)} \le 2c\int_{-\infty}^{\infty} e^{-\alpha|x|}dx = \frac{4c}{\alpha} \tag{5.5}$$

which together with (5.3), (5.4) and (5.5) implies

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

which completes the proof. ∎

Now we are able to prove Theorem 2.4.

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

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

which contains the spectral parabola

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

In order to apply Lemma 2.3 for the quadrature rule E_N, we have to provide that the integrand $F(\eta, t)$ can be analytically extended onto 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)

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

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

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

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

$$a' = a\left(k + 4a\nu + \frac{4a^2}{k}\nu^2\right)^{-1}, \qquad b' = b + \frac{k}{4a} - \frac{a}{k}\left(\nu + \frac{k}{2a}\right)^2. \tag{5.6}$$

Now, it is easy to see that if we choose

$$\nu = \left(\frac{1}{\sqrt{k}} - 1\right)\frac{k}{2a} \equiv -d, \qquad b = b(k) = \gamma_0 - \frac{k-1}{4a}, \tag{5.7}$$

then

$$\begin{aligned}\Gamma_{b(k)}(-d) &= \{z = \frac{a}{k}\eta^2 + b + \frac{k-1}{4a} + i\frac{\eta}{\sqrt{k}} :\ \eta \in (-\infty, \infty)\}\\ &= \{z = a\eta_*^2 + \gamma_0 + i\eta_* :\ \eta_* \equiv \frac{\eta}{\sqrt{k}} \in (-\infty, \infty)\} \equiv \Gamma_0.\end{aligned} \tag{5.8}$$

From (5.6) 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 D_d with d given by (5.7). Due to the strong P-positivity of $\mathcal{L}$ there holds for $z = \eta + i\nu \in D_d$

$$\begin{aligned}\|F(z, x; \mathcal{L})\| &\le M\frac{|(2\frac{a}{k}z - i)|\,\sinh^{-1}\left(\sqrt{\frac{a}{k}z^2 + b - iz}\right)\sinh\left(x\sqrt{\frac{a}{k}z^2 + b - iz}\right)}{1 + \sqrt{|\frac{a}{k}z^2 + b - iz|}}\\ &= \frac{M|2\frac{a}{k}z - i|\sinh\left(x\sqrt{\frac{a}{k}(\eta^2 - \nu^2) + b + \nu + i(2a\nu/k - 1)\eta}\right)}{\left(1 + \sqrt{|\frac{a}{k}z^2 + b - iz|}\right)\sinh\left(\sqrt{\frac{a}{k}(\eta^2 - \nu^2) + b + \nu + i(2a\nu/k - 1)\eta}\right)}\end{aligned}$$

and the estimate (2.7) implies that $F(z, t; \mathcal{L}) \in \mathbf{H}^1(D_d)$. We have also

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

with

$$\alpha = \alpha(x) = (1 - x)\sqrt{\frac{1}{2}\min\{\frac{a}{k}, b\}} > 0, \qquad c = MM_1\frac{e^{\alpha}}{1 - e^{-\sqrt{2b}}} \qquad \text{for all } x \in (0, 1),$$

$$M_1 = \max_{z\in\overline{D}_d}\frac{|2\frac{a}{k}z - i|}{1 + \sqrt{|\frac{a}{k}z^2 + b - iz|}}.$$

Using Lemma 2.3 and setting in (2.12) α as defined above, we get

$$\|\eta_N(F,h)\| \le c_1 \left[\frac{\exp(-2\pi d/h)}{1-\exp(-2\pi d/h)} + h \exp[-(1-x)\sqrt{\frac{1}{2}\min\{\frac{a}{k},b\}Nh}] \right], \tag{5.9}$$

where $\eta_N(F,h) = E(x) - E_N(x)$ as defined in (2.8) and

$$c_1 = \frac{2MM_1e^{\alpha}}{(1-e^{-\sqrt{2b}})\alpha}.$$

Equalising the exponents by setting $2\pi d/h = \sqrt{\frac{1}{2}\min\{\frac{a}{k},b\}Nh}$, we get $h = \frac{\sqrt{2\pi d/N}}{\sqrt[4]{\frac{1}{2}\min\{\frac{a}{k},b\}}}$. Substitution of this value into (5.9) leads to the estimate

$$\|\eta_N(F,h)\| \le c_1 \left[\frac{e^{-s\sqrt{N}}}{1-e^{-s\sqrt{N}}} + he^{-s(1-x)\sqrt{N}} \right], \text{ where } s = \sqrt{2\pi d}\sqrt[4]{\frac{1}{2}\min\{\frac{a}{k},b\}}.$$

This completes the proof of Theorem 2.4. ■

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