Preconditioned space-time boundary element methods for the one-dimensional heat equation

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1 Introduction

Space–time discretization methods, see, e.g., [8], became very popular in recent years, due to their ability to drive adaptivity in space and time simultaneously, and to use parallel iterative solution strategies for time–dependent problems. But the solution of the global linear system requires the use of some efficient preconditioner.

In this note we describe a space–time boundary element discretization of the heat equation and an efficient and robust preconditioning strategy which is based on the use of boundary integral operators of opposite orders, but which requires a suitable stability condition for the boundary element spaces used for the discretization. We demonstrate the method for the simple spatially one-dimensional case. However, the presented results, particularly the stability analysis of the boundary element spaces, can be used to extend the method to the two- and three-dimensional problem [2].

Let $\Omega = (a,b) \subset \mathbb{R}$, $\Gamma := \partial\Omega = \{a,b\}$ and $T > 0$. As a model problem we consider the Dirichlet boundary value problem for the heat equation,

$$\alpha\partial_t u - \Delta_x u = 0 \text{ in } Q := \Omega \times (0,T),\ u = g \text{ on } \Sigma := \Gamma \times (0,T),\ u = u_0 \text{ in } \Omega \qquad (1)$$

with the heat capacity constant $\alpha > 0$, the given initial datum u_0, and the boundary datum g. The solution of (1) can be expressed by using the representation formula for the heat equation [1], i.e. for $(x,t) \in Q$ we have

$$\begin{aligned} u(x,t) = &\int_\Omega U^\star(x-y,t)u_0(y)\mathrm{d}y + \frac{1}{\alpha}\int_\Sigma U^\star(x-y,t-s)\frac{\partial}{\partial n_y}u(y,s)\mathrm{d}s_y\mathrm{d}s \\ &- \frac{1}{\alpha}\int_\Sigma \frac{\partial}{\partial n_y}U^\star(x-y,t-s)g(y,s)\mathrm{d}s_y\mathrm{d}s, \end{aligned} \qquad (2)$$

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where $U^\star$ denotes the fundamental solution of the heat equation given by

$$U^\star(x-y,t-s) = \begin{cases} \left(\dfrac{\alpha}{4\pi(t-s)}\right)^{1/2} \exp\left(\dfrac{-\alpha|x-y|^2}{4(t-s)}\right), & s<t, \\ 0\,, & \text{else.} \end{cases}$$

Hence it suffices to determine the yet unknown Cauchy datum $\partial_n u_{|\Sigma}$ to compute the solution of (1). It is well known [5] that for $u_0 \in L^2(\Omega)$ and $g \in H^{1/2,1/4}(\Sigma)$ the problem (1) has a unique solution $u \in H^{1,1/2}(Q, \alpha\partial_t - \Delta_x)$ with the anisotropic Sobolev space

$$H^{1,1/2}(Q,\alpha\partial_t - \Delta_x) := \left\{ u \in H^{1,1/2}(Q) : (\alpha\partial_t - \Delta_x)u \in L^2(Q) \right\}.$$

In the one-dimensional case the spatial component of the space–time boundary Σ collapses to the points $\{a,b\}$ and therefore we can identify the anisotropic Sobolev spaces $H^{r,s}(\Sigma)$ with $H^s(\Sigma)$. The unknown density $w := \partial_n u_{|\Sigma} \in H^{-1/4}(\Sigma)$ can be found by applying the interior Dirichlet trace operator $\gamma_0^{\text{int}} : H^{1,1/2}(Q) \to H^{1/4}(\Sigma)$ to the representation formula (2),

$$g(x,t) = (M_0 u_0)(x,t) + (Vw)(x,t) + ((\frac{1}{2}I - K)g)(x,t) \quad \text{for } (x,t) \in \Sigma.$$

The initial potential $M_0 : L^2(\Omega) \to H^{1/4}(\Sigma)$, the single layer boundary integral operator $V : H^{-1/4}(\Sigma) \to H^{1/4}(\Sigma)$, and the double layer boundary integral operator $\frac{1}{2}I - K : H^{1/4}(\Sigma) \to H^{1/4}(\Sigma)$ are obtained by composition of the potentials in (2) with the Dirichlet trace operator γ_0^{int}, see, e.g., [1, 6]. In fact, we have to solve the variational formulation to find $w \in H^{-1/4}(\Sigma)$ such that

$$\langle Vw, \tau\rangle_\Sigma = \langle (\frac{1}{2}I + K)g, \tau\rangle_\Sigma - \langle M_0 u_0, \tau\rangle_\Sigma \quad \text{for all } \tau \in H^{-1/4}(\Sigma), \tag{3}$$

where $\langle \cdot,\cdot\rangle_\Sigma$ denotes the duality pairing on $H^{1/4}(\Sigma) \times H^{-1/4}(\Sigma)$. The single layer boundary integral operator V is bounded and elliptic, i.e. there exists a constant $c_1^V > 0$ such that

$$\langle Vw, w\rangle_\Sigma \geq c_1^V \, \|w\|^2_{H^{-1/4}(\Sigma)} \quad \text{for all } w \in H^{-1/4}(\Sigma).$$

Thus, the variational formulation (3) is uniquely solvable. When applying the Neumann trace operator $\gamma_1^{\text{int}} : H^{1,1/2}(Q, \alpha\partial_t - \Delta_x) \to H^{-1/4}(\Sigma)$ to the representation formula (2) we obtain the second boundary integral equation

$$w(x,t) = (M_1 u_0)(x,t) + ((\frac{1}{2}I + K')w)(x,t) + (Dg)(x,t) \quad \text{for } (x,t) \in \Sigma$$

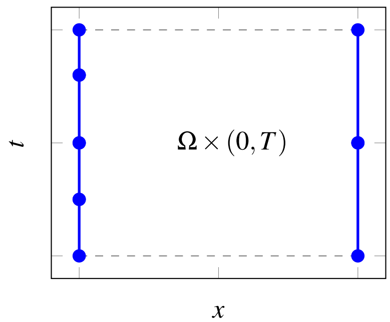

Fig. 1 Sample BE mesh. We consider an arbitrary decomposition of the space–time boundary Σ. Note that there is no time-stepping scheme involved

with the hypersingular boundary integral operator $D : H^{1/4}(\Sigma) \to H^{-1/4}(\Sigma)$, and with the adjoint double layer boundary integral operator $K' : H^{-1/4}(\Sigma) \to H^{-1/4}(\Sigma)$. Moreover, $M_1 : L^2(\Omega) \to H^{-1/4}(\Sigma)$.

2 Boundary element methods

For the Galerkin boundary element discretization of the variational formulation (3) we consider a family $\{\Sigma_N\}_{N\in\mathbb{N}}$ of arbitrary decompositions of the space–time boundary Σ into boundary elements σ_l, i.e. we have

$$\overline{\Sigma}_N = \bigcup_{\ell=1}^{N} \overline{\sigma}_\ell \,.$$

In the one-dimensional case the boundary elements σ_ℓ are line segments in temporal direction with fixed spatial coordinate $x_\ell \in \{a,b\}$ as shown in Fig. 1. Let (x_ℓ, t_{ℓ_1}) and (x_ℓ, t_{ℓ_2}) be the nodes of the boundary element σ_ℓ. The local mesh size is then given as $h_\ell := |t_{\ell_2} - t_{\ell_1}|$ while $h := \max_{\ell=1,\ldots,N} h_\ell$ is the global mesh size.
For the approximation of the unknown Cauchy datum $w = \gamma_1^{\text{int}} u \in H^{-1/4}(\Sigma)$ we consider the space $S_h^0(\Sigma) := \text{span}\left\{\varphi_\ell^0\right\}_{\ell=1}^{N}$ of piecewise constant basis functions φ_ℓ^0, which is defined with respect to the decomposition Σ_N. The Galerkin-Bubnov variational formulation of (3) is to find $w_h \in S_h^0(\Sigma)$ such that

$$\langle V w_h, \tau_h \rangle_\Sigma = \langle (\frac{1}{2} I + K) g, \tau_h \rangle_\Sigma - \langle M_0 u_0, \tau_h \rangle_\Sigma \quad \text{for all } \tau_h \in S_h^0(\Sigma)\,. \tag{4}$$

This is equivalent to the system of linear equations $V_h \mathbf{w} = \mathbf{f}$ where

$$V_h[\ell,k] = \langle V \varphi_k^0, \varphi_\ell^0 \rangle_\Sigma, \quad \mathbf{f}[\ell] = \langle (\frac{1}{2} I + K) g, \varphi_\ell^0 \rangle_\Sigma - \langle M_0 u_0, \varphi_\ell^0 \rangle_\Sigma, \quad k,\ell = 1,\ldots,N.$$

Due to the ellipticity of the single layer operator V the matrix V_h is positive definite and therefore the variational formulation (4) is uniquely solvable as well. Moreover, when assuming $w \in H^s(\Sigma)$ for some $s \in [0,1]$, there holds the error estimate

$$\|w - w_h\|_{H^{-1/4}(\Sigma)} \leq c h^{1/4+s} |w|_{H^s(\Sigma)} .$$

Using standard arguments we also conclude the error estimate

$$\|w - w_h\|_{L^2(\Sigma)} \leq c h^s |w|_{H^s(\Sigma)}$$

which implies linear convergence of the $L^2(\Sigma)$–error of the Galerkin approximation w_h if $w \in H^1(\Sigma)$ is satisfied.

3 Preconditioning strategies

Since the boundary element discretization is done with respect to the whole space–time boundary Σ we need to have an efficient iterative solution technique. In fact, the linear system $V_h \mathbf{w} = \mathbf{f}$ with the positive definite but nonsymmetric matrix V_h can be solved by using a preconditioned GMRES method. Here we will apply a preconditioning technique based on boundary integral operators of opposite order [10], also known as operator or Calderon preconditioning [3]. Since the single layer integral operator $V : H^{-1/4}(\Sigma) \to H^{1/4}(\Sigma)$ and the hypersingular integral operator $D : H^{1/4}(\Sigma) \to H^{-1/4}(\Sigma)$ are both elliptic, the operator $DV : H^{-1/4}(\Sigma) \to H^{-1/4}(\Sigma)$ behaves like the identity. Hence we can use the Galerkin discretization of D as a preconditioner for V_h. But for the Galerkin discretization D_h of the hypersingular integral operator $D : H^{1/4}(\Sigma) \to H^{-1/4}(\Sigma)$ we need to use a conforming ansatz space $Y_h = \operatorname{span}\{\psi_i\}_{i=1}^N \subset H^{1/4}(\Sigma)$ while the discretization of the single layer integral operator V is done with respect to $S_h^0(\Sigma)$. Since the boundary element space $S_h^0(\Sigma)$ of piecewise constant basis functions φ_k^0 also satisfies $S_h^0(\Sigma) \subset H^{1/4}(\Sigma)$ we can choose $Y_h = S_h^0(\Sigma)$. The inverse hypersingular operator D^{-1} is spectrally equivalent to the single layer operator V, therefore the approximation of the preconditioning operator corresponds to a mixed approximation scheme, and hence we need to assume a discrete stability condition to be satisfied.

Theorem 1 ([3, 10]). *Assume the discrete stability condition*

$$\sup_{0 \neq v_h \in Y_h} \frac{\langle \tau_h, v_h \rangle_{L^2(\Sigma)}}{\|v_h\|_{H^{1/4}(\Sigma)}} \geq c_1^M \|\tau_h\|_{H^{-1/4}(\Sigma)} \quad \text{for all } \tau_h \in S_h^0(\Sigma). \tag{5}$$

Then there exists a constant $c_\kappa > 1$ such that

$$\kappa \left(M_h^{-1} D_h M_h^{-\top} V_h \right) \leq c_\kappa$$

where, for $k, \ell = 1, \ldots, N$,

$$V_h[\ell,k] = \langle V \varphi_k^0, \varphi_\ell^0 \rangle_\Sigma , \quad D_h[\ell,k] = \langle D \psi_k, \psi_\ell \rangle_\Sigma , \quad M_h[\ell,k] = \langle \varphi_k^0, \psi_\ell \rangle_{L^2(\Sigma)} .$$

Thus we can use $C_V^{-1} = M_h^{-1} D_h M_h^{-\top}$ as a preconditioner for V_h. Since M_h is sparse and spectrally equivalent to a diagonal matrix, the inverse M_h^{-1} can be computed efficiently. It remains to define, for given $S_h^0(\Sigma)$, a suitable boundary element space Y_h such that the stability condition (5) is satisfied. In what follows we will discuss a possible choice.

If we choose $Y_h = S_h^0(\Sigma)$ for the discretization of the hypersingular operator D, then M_h becomes diagonal and is therefore easily invertible. In order to prove the stability condition (5) we need to establish the $H^{1/4}(\Sigma)$–stability of the $L^2(\Sigma)$–projection $Q_h^0 : L^2(\Sigma) \to S_h^0(\Sigma) \subset L^2(\Sigma)$ which is defined as

$$\langle Q_h^0 v, \tau_h \rangle_{L^2(\Sigma)} = \langle v, \tau_h \rangle_{L^2(\Sigma)} \quad \text{for all } \tau_h \in S_h^0(\Sigma).$$

Following [7], and when assuming local quasi-uniformity of the boundary element mesh Σ_N we are able to establish the stability of $Q_h^0 : H^{1/4}(\Sigma) \to H^{1/4}(\Sigma)$, see [2] for a more detailed discussion: For $\ell = 1, ..., N$ we define $I(\ell)$ to be the index set of the boundary element σ_ℓ and all its adjacent elements. We assume the boundary element mesh Σ_N to be locally quasi-uniform, i.e. there exists a constant $c_L \geq 1$ such that

$$\frac{1}{c_L} \leq \frac{h_\ell}{h_k} \leq c_L \quad \text{for all } k \in I(\ell) \text{ and } \ell = 1, ..., N.$$

In this case the operator $Q_h^0 : H^{1/4}(\Sigma) \to H^{1/4}(\Sigma)$ is bounded, i.e. there exists a constant $c_S^0 > 0$ such that

$$\left\| Q_h^0 v \right\|_{H^{1/4}(\Sigma)} \leq c_S^0 \left\| v \right\|_{H^{1/4}(\Sigma)} \quad \text{for all } v \in H^{1/4}(\Sigma). \tag{6}$$

By using the stability estimate (6) we can conclude

$$\frac{1}{c_S^0} \left\| \tau_h \right\|_{H^{-1/4}(\Sigma)} \leq \sup_{0 \neq v_h \in S_h^0(\Sigma)} \frac{\langle \tau_h, v_h \rangle_{L^2(\Sigma)}}{\left\| v_h \right\|_{H^{1/4}(\Sigma)}} \quad \text{for all } \tau_h \in S_h^0(\Sigma).$$

Hence the stability condition (5) holds and we can use $C_V^{-1} = M_h^{-1} D_h M_h^{-\top}$ as a preconditioner for V_h.

4 Numerical results

For the numerical experiments we choose $\Omega = (0,1)$, $T = 1$, and we consider the model problem (1) with homogeneous Dirichlet conditions $g = 0$, and some given initial datum u_0 satisfying the compatibility conditions $u_0(0) = u_0(1) = 0$. The Galerkin boundary element discretization of the variational formulation (3) is done by piecewise constant basis functions. The resulting system of linear equations $V_h \mathbf{w} = \mathbf{f}$ is solved by using the GMRES method. As a preconditioner we use the discretization $C_V^{-1} = M_h^{-1} D_h M_h^{-\top}$ of the hypersingular operator D with piecewise constant basis functions.

Uniform refinement

The first example corresponds to the initial datum $u_0(x) = \sin 2\pi x$ and a globally uniform boundary element mesh of mesh size $h = 2^{-L}$. Table 1 shows the $L^2(\Sigma)$–error $\|w - w_h\|_{L_2(\Sigma)}$ and the estimated order of convergence (eoc), which is linear as expected. Moreover, the condition numbers of the stiffness matrix V_h and of the preconditioned matrix $C_V^{-1} V_h$ as well as the number of iterations to reach a relative accuracy of 10^{-8} are given which confirm the theoretical estimates.

Table 1 Error, condition and iteration numbers in the case of uniform refinement

L	N	$\|w - w_h\|_{L_2(\Sigma)}$	eoc	$\kappa(V_h)$	It.	$\kappa(C_V^{-1} V_h)$	It.
0	2	2.249	-	1.001	1	1.002	1
1	4	1.311	0.778	2.808	2	1.279	2
2	8	0.658	0.996	4.905	4	1.422	4
3	16	0.324	1.021	7.548	8	1.486	8
4	32	0.160	1.017	11.140	16	1.541	14
5	64	0.079	1.010	16.724	31	1.563	13
6	128	0.040	1.006	13.470	41	1.590	13
7	256	0.020	1.003	22.053	50	1.615	12
8	512	0.010	1.001	32.043	59	1.636	12
9	1024	0.005	1.001	60.957	70	1.777	11
10	2048	0.002	1.000	88.488	82	1.762	11
11	4096	0.001	1.000	125.957	96	1.765	10

Adaptive refinement

For the second example we consider the initial datum $u_0(x) = 5e^{-10x} \sin \pi x$ which motivates the use of a locally quasi-uniform boundary element mesh resulting from some adaptive refinement strategy. The numerical results as given in Table 2 again confirm the theoretical findings, in particular the robustness of the proposed preconditioning strategy in the case of an adaptive refinement which is not the case when using none or only diagonal preconditioning $\widetilde{C}_V = \mathrm{diag} V_h$.

5 Conclusions and outlook

In this note we have described a space–time boundary element discretization of the spatially one-dimensional heat equation and an efficient and robust preconditioning strategy which is based on the use of boundary integral operators of opposite orders, but which requires a suitable stability condition for the boundary element spaces used for the discretization. In the particular case of the spatially one-dimensional

Table 2 Error, condition and iteration numbers in the case of adaptive refinement

L	N	$\|w-w_h\|_{L_2(\Sigma)}$	$\kappa(V_h)$	It.	$\kappa(\widetilde{C}_V^{-1}V_h)$	It.	$\kappa(C_V^{-1}V_h)$	It.
0	2	1.886	1.00	2	1.001	2	1.002	2
1	3	1.637	3.97	3	2.553	3	1.16	3
2	5	1.272	12.23	5	4.055	4	1.166	4
3	7	0.914	34.21	7	3.611	6	1.156	6
4	9	0.615	92.08	9	3.164	8	1.149	8
5	11	0.401	118.59	11	2.945	10	1.224	10
6	13	0.267	338.26	13	2.803	12	1.21	12
7	20	0.166	621.77	20	3.524	18	1.197	13
8	31	0.101	1608.08	31	4.457	27	1.252	12
9	47	0.063	2344.90	47	5.779	32	1.574	11
10	74	0.039	6141.47	74	8.348	37	1.692	11
11	114	0.024	8409.92	114	10.950	42	1.561	10
12	177	0.015	23007.60	173	14.324	47	1.716	10
13	278	0.010	27528.30	200	21.094	53	1.677	10

heat equation we can use the space $S_h^0(\Sigma)$ of piecewise constant basis functions to discretize both the single layer and the hypersingular boundary integral operator V and D, respectively. This is due to the inclusion $S_h^0(\Sigma) \subset H^{1/4}(\Sigma)$ where the latter is the Dirichlet trace space of the anisotropic Sobolev space $H^{1,1/2}(Q)$. In the case of a spatially two- or three-dimensional domain Ω a conformal approximation of the Dirichlet trace space $H^{1/2,1/4}(\Sigma)$ and therefore the discretization of the hypersingular integral operator D requires the use of continuous basis functions. Hence, to ensure the stability condition (5) we may use the space $S_h^1(\Sigma)$ of piecewise linear and continuous basis functions for the discretization of V and D, respectively, see [7, Theorem 3.2], and when assuming some appropriate mesh conditions locally [7, Section 4]. However, due to the approximation properties of $S_h^1(\Sigma)$ such an approach is restricted to spatial domains Ω with smooth boundary where the unknown flux is continuous.

When using the discontinuous boundary element space $S_h^0(\Sigma)$ for the approximation of the unknown flux we need to choose an appropriate boundary element space Y_h to ensure the stability condition (5). A possible approach is the use of a dual mesh using piecewise constant basis functions for the approximation of V, and piecewise linear and continuous basis functions for the approximation of D, see Fig. 2 for the situation in 1D. For a more detailed analysis of the proposed preconditioning strategy and suitable choices of stable boundary element spaces we refer to [2].

An efficient solution of local Dirichlet boundary value problems is an important tool when considering domain decomposition methods for the heat equation, see e.g. [9] in the case of the Laplace equation. Moreover, the preconditioning strategy of using operators of opposite order can also be used when considering related Schur complement systems on the skeleton, as they also appear in tearing and interconnecting domain decomposition methods, see, e.g., [4]. This also covers the coupling

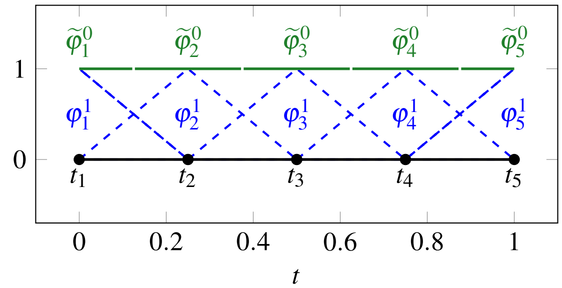

Fig. 2 Sample dual mesh. The piecewise linear and continuous functions φ_i^1 are used for the discretization of D. The piecewise constant basis functions $\tilde{\varphi}_i^0$ are used for the discretization of V

of space–time finite and boundary element methods. Related results on the stability and error analysis as well as on efficient solution strategies for space–time domain decomposition methods will be published elsewhere.

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