Efficient Preconditioners for Boundary Element Methods and their Use in Domain Decomposition Methods

O. STEINBACH AND W. L. WENDLAND [1]

1 Introduction

Boundary element methods are well suited for partial differential equations with piecewise constant coefficients and for problems in infinite regions. Moreover, domain decomposition methods are a powerful technique for parallelization and coupling with other discretization methods like finite elements. The formulation of boundary element methods for mixed boundary value problems and their use in domain decomposition methods depends on the boundary integral equations used and their discretizations as e.g. collocation or Galerkin methods. We discuss a general approach to solve mixed boundary value problems by preconditioned iterative methods and we give a preconditioning technique resulting from boundary integral equations, too. Common examples are problems in potential theory or in linear elasticity.

Let us consider a selfadjoint and elliptic boundary value problem of 2nd order in a bounded domain $\Omega \subset I\!R^n$ $(n = 2,3)$ with a Lipschitz continuous boundary Γ, which is decomposed into two distinct parts Γ_D and Γ_N, where boundary conditions of Dirichlet and Neumann type, respectively, are given:

$$\begin{aligned} L(x)u(x) &= f(x) && \text{for } x \in \Omega, \\ \gamma_0 u(x) &= g(x) && \text{for } x \in \Gamma_D, \\ \gamma_1 u(x) &= h(x) && \text{for } x \in \Gamma_N. \end{aligned} \qquad (1)$$

[1] Universität Stuttgart, Mathematisches Institut A, Pfaffenwaldring 57, 70569 Stuttgart, Germany. E-Mail: wendland@mathematik.uni-stuttgart.de.
This work was partially supported by the Priority Research Programme "Boundary Element Methods" of the German Research Foundation DFG under Grant Nb. We 659/8-5.

Domain Decomposition Methods in Sciences and Engineering, edited by R. Glowinski *et al.*

For a non–overlapping domain decomposition

$$\overline{\Omega} = \bigcup_{i=1}^{p} \overline{\Omega}_i\,, \quad \Omega_i \cap \Omega_j = \emptyset\,, \quad \Gamma_{ij} = \Gamma_i \cap \Gamma_j$$

with Lipschitz continuous subdomain boundaries $\Gamma_i = \partial\Omega_i$, we suppose that we are given fundamental solutions of the differential operator in (1) locally, i.e. for all $i = 1, \ldots, p$ there exist functions $E^i(x, y)$ satisfying

$$L(x)\, E^i(x,y) \;=\; \delta(x-y) \cdot \mathbf{I}(x) \quad \text{for } x, y \in \Omega_i\,. \tag{2}$$

Setting

$$u_i(x) \;=\; \gamma_0^i u(x)\,, \quad t_i(x) \;=\; \gamma_1^i u(x) \quad \text{for } x \in \Gamma_i\,,$$

the solution $u(\cdot)$ of (1) is given by the local representation formulae

$$u(x) \;=\; \int_{\Gamma_i} t_i(y) \cdot \gamma_0^i E^i(x,y)\, ds_y \;-\; \int_{\Gamma_i} u_i(y) \cdot \gamma_1^i E^i(x,y)\, ds_y \;+\; \int_{\Omega_i} f(y) \cdot E^i(x,y)\, dy \tag{3}$$

for $x \in \Omega_i$, where the densities t_i and u_i have to satisfy transmission conditions

$$u_i(x) - u_j(x) \;=\; 0\,, \quad t_i(x) + t_j(x) \;=\; 0 \quad \text{for } x \in \Gamma_{ij} \tag{4}$$

in addition to the boundary conditions

$$t_i(x) = h(x) \quad \text{for } x \in \Gamma_i \cap \Gamma_N\,, \quad u_i(x) = g(x) \quad \text{for } x \in \Gamma_i \cap \Gamma_D\,.$$

Associated with the fundamental solutions (2), we define common boundary integral operators by

$$\begin{aligned}
(V_i t_i)(x) &= \int_{\Gamma_i} t_i(y) \cdot \gamma_0^i E^i(x,y)\, ds_y\,, \\
(K_i u_i)(x) &= \int_{\Gamma_i} u_i(y) \cdot \gamma_1^i E^i(x,y)\, ds_y\,, \\
(K_i' t_i)(x) &= \int_{\Gamma_i} t_i(y) \cdot \gamma_1^i(x) E^i(x,y)\, ds_y\,, \\
(D_i u_i)(x) &= -\gamma_1^i \int_{\Gamma_i} u_i(y) \cdot \gamma_1^i E^i(x,y)\, ds_y
\end{aligned}$$

for $x \in \Gamma_i$ and the boundary traces of the volume or Newton potentials by

$$N_j^i(x) \;=\; \gamma_j^i \int_{\Omega_i} f(y) \cdot E^i(x,y)\, dy \tag{5}$$

for $x \in \Gamma_i$ and $j = 0, 1$. By using the Calderon projector, we can write the boundary integral equations resulting from (3) as the overdetermined system

$$\begin{pmatrix} u_i(x) \\ t_i(x) \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I - K_i & V_i \\ D_i & \frac{1}{2}I + K_i' \end{pmatrix} \begin{pmatrix} u_i(x) \\ t_i(x) \end{pmatrix} - \begin{pmatrix} N_0^i \\ N_1^i \end{pmatrix} f(x) \tag{6}$$

for $x \in \Gamma_i$ and $i = 1, \ldots, p$. The boundary integral operators V_i, K_i, D_i are pseudodifferential operators of orders $-1, 0, 1$, respectively, and their mapping properties on Lipschitz domains are well known [Cos88]. The right hand side includes still volume integrals which require a discretization of Ω, too. In this case, the advantage of dimension reduction by boundary element methods is partly lost. To overcome this drawback, one can homogenize problem (1). In general, the volume integrals (5) are to be replaced by boundary integrals, too. We will discuss such methods in connection with fictitious domain methods coupled with boundary element methods in [SW].

From (6) we find two explicit representations of a Dirichlet–Neumann map, including the so–called Steklov–Poincaré operator S_i:

$$\begin{aligned} t_i &= S_i u_i + \tilde{N}^i \\ &= V_i^{-1}\left(\tfrac{1}{2}I + K_i\right) u_i \;+\; V_i^{-1} N_0^i \\ &= \left[\left(\tfrac{1}{2}I + K_i'\right) V_i^{-1}\left(\tfrac{1}{2}I + K_i\right) + D_i\right] u_i - N_1^i + \left(\tfrac{1}{2}I + K_i'\right) V_i^{-1} N_0^i, \end{aligned} \tag{7}$$

which is a selfadjoint, strongly elliptic pseudodifferential operator of order -1, corresponding to the solution of the local Dirichlet problem, where $u_i = g$ on Γ_i is given. For the inverse operation, the Neumann–Dirichlet map is described by

$$\begin{aligned} u_i - r_i &= U_i t_i + \hat{N}^i \\ &= \left(\tfrac{1}{2}I \dot{+} K_i\right)^{-1}\left(V_i t_i - N_0^i\right) \\ &= \left(\tfrac{1}{2}I - K\right) \dot{D}_i^{-1}\left[\left(\tfrac{1}{2}I - K_i'\right) t_i + N_1^i\right] + V_i t_i - N_0^i \,, \end{aligned} \tag{8}$$

where $\dot{D}_i^{-1}$ denotes the pseudoinverse of D_i with respect to the rigid motions r_i associated with the differential operator in (1). This map corresponds to the solution of a Neumann problem, where solvability conditions must be satisfied.

If we introduce the skeleton Γ_S by

$$\Gamma_S = \bigcup_{i=1}^{p} \Gamma_i \,,$$

we are able to give variational formulations of the transmission problem (4) in related Sobolev spaces $H^s(\Gamma_S)$.

Variational formulation 1. *Find $u \in H^{1/2}(\Gamma_S)$ with $u_{|\Gamma_D} = g$ such that*

$$\sum_{i=1}^{p} \int_{\Gamma_i} S_i u_{|\Gamma_i}(x) \cdot v_{|\Gamma_i}(x)\, ds_x = \int_{\Gamma_N} h(x) \cdot v(x)\, ds_x - \sum_{i=1}^{p} \int_{\Gamma_i} \tilde{N}^i(x) \cdot v(x)\, ds_x$$

holds for all $v \in H^{1/2}(\Gamma_S)$ with $v_{|\Gamma_D} = 0$.

With $u_i = u_{|\Gamma_i}$ the first transmission condition in (4) is satisfied strongly, while the second condition has to be satisfied in a weak sense with $t_i = S_i u_{|\Gamma_i}$. This formulation is equivalent to the variational formulation used in domain decomposition methods for finite element methods and is therefore well suited for coupling of finite and boundary element discretization methods [Cos87, Hsi90, Lan94, Wen88]. However, we can change the meaning of the Cauchy data to get a second formulation corresponding to nonconforming finite elements [HSW] :

Variational formulation 2. *Find* $t \in \prod_{i=1}^{p} H^{-1/2}(\Gamma_i)$ *with* $t(x) = h(x)$ *for* $x \in \Gamma_N$ *such that*

$$\sum_{i=1}^{p} \int_{\Gamma_i} U_i t_{|\Gamma_i}(x) \cdot \tau_{|\Gamma_i}(x)\, ds_x = \int_{\Gamma_D} g(x) \cdot \tau(x)\, ds_x - \sum_{i=1}^{p} \int_{\Gamma_i} \hat{N}^i(x) \cdot \tau(x)\, ds_x$$

holds for all $\tau \in \prod_{i=1}^{p} H^{-1/2}(\Gamma_i)$.

Setting $t_i = t_{|\Gamma_{ij}}, t_j = -t_{|\Gamma_{ij}}$ for $i < j$, the second transmission condition is satisfied strongly, while the first one with $u_i = T_i t_i$ has to be fulfilled in a weak sense.

The existence and uniqueness of solutions of the variational formulations above follow directly from the coerciveness of the bilinear forms involved; for the Neumann problem this is true only with respect to appopriate quotient spaces generated by the rigid motions r_i. Moreover, these variational formulations give us a large variety for using boundary element methods for the discretization. The second one is well suited for the macro–element technique using Neumann series for realizing the Poincaré–Steklov map U_i by adaptive strategies as to keep symmetry and $H^{-1/2}$–ellipticity also in the discrete form [HSW, Tür95].

To discretize the local Steklov–Poincaré operators S_i included in the variational formulation 1, we have to introduce approximate operators

$$S_i^h u_{h|\Gamma_i} := t_h^i \in H_h^{-1/2}(\Gamma_i)$$

by the solution of the local finite–dimensional variational problems

$$\langle V_i t_h^i, \tau_h^i \rangle_{\Gamma_i} = \langle (\frac{1}{2} I + K_i) u_{h|\Gamma_i}, \tau_h^i \rangle_{\Gamma_i} \quad \forall \tau_h^i \in H_h^{-1/2}(\Gamma_i)\ . \tag{9}$$

Due to the properties of the local single layer potential operators V_i we have the quasi–optimal error estimates [Wen83]

$$||S_i u_{h|\Gamma_i} - S_i^h u_{h|\Gamma_i}||_{H^{-1/2}(\Gamma_i)} \le c \inf_{\tau_h^i \in H_h^{-1/2}(\Gamma_i)} ||S_i u_{h|\Gamma_i} - \tau_h^i||_{H^{-1/2}(\Gamma_i)}\ .$$

Then there exists an unique solution $\tilde{u}_h$ of the perturbed variational problem

$$\sum_{i=1}^{p} \int_{\Gamma_i} S_i^h \tilde{u}_h(x) \cdot v_h(x)\, ds_x = f(v_h) \tag{10}$$

and we get the error estimate

$$\begin{aligned} ||u - \tilde{u}_h||_{H^{1/2}(\Gamma_S)} \le\ & C(h_0) \Bigg\{ \inf_{v_h \in H_h^{1/2}(\Gamma_S)} ||u - v_h||_{H^{1/2}(\Gamma_S)} \\ & + \sum_{i=1}^{p} \inf_{\tau_h^i \in H_h^{-1/2}(\Gamma_i)} ||S_i u_{h|\Gamma_i} - \tau_h^i||_{H^{-1/2}(\Gamma_i)} \Bigg\} \end{aligned}$$

for all $h < h_0$, which ensures the convergence of this approach based on the non–symmetric formulation due to the approximation property of the trial spaces used.

The discretization of the variational problem (10) leads now to the discrete system of linear equations

$$\tilde{M}_h^\top V_h^{-1}\left(\frac{1}{2}M_h + K_h\right)\underline{u} = \underline{f}\,, \tag{11}$$

where

$$V_h = \operatorname{diag}\left(V_i^h\right)_{i=1}^p$$

is block diagonal and therefore well suited for the parallel computation of V_h^{-1}. To invert the locally stored blocks V_i^h one can e.g. use direct methods like LU–decomposition. This can be done in a previous step of the iteration process. Furtheron, preconditioned iterative methods itself seems to be an efficient tool to realize the action of $V_i^{h,-1}$; in this case local preconditioners C_V^i are necessary. For the global iteration, due to the non–symmetry we have to use a generalized method of orthogonal directions like GMRES or BiCGStab, and a preconditioner for the discrete Steklov–Poincaré operator is needed, too. However, in any global iteration step we have to solve a local Dirichlet problem in Ω_i; involving the whole boundary Γ_i, which may be inefficient. Setting

$$\underline{t} = V_h^{-1}\left(\frac{1}{2}M_h + K_h\right)\underline{u}\,,$$

we get the coupled system

$$\begin{pmatrix} V_h & -\frac{1}{2}\tilde{M}_h - K_h \\ M_h^\top & 0 \end{pmatrix}\begin{pmatrix} \underline{t} \\ \underline{u} \end{pmatrix} = \begin{pmatrix} \underline{f} \\ \underline{0} \end{pmatrix}. \tag{12}$$

The first row of blocks corresponds to the local approximations in (9), which can be handled by Galerkin or collocation methods, while the coupling conditions have to be discretized by Galerkin concepts in any case. For collocation methods we get almost $\tilde{M}_h \simeq I$, whereas for Galerkin methods we have $\tilde{M}_h = M_h$. This system can be solved again by preconditioned iterative methods, where we have only three matrix multiplications per iteration step. As block preconditioners we can use the same components as above.

Before discretizing the variational problem 1 we can replace $t_i = S_i u_{|\Gamma_i}$ by the corresponding expression in the Calderon projector (6) and we arrive at the symmetric formulation [Cos87, Sir79]:

$$\begin{aligned} \sum_{i=1}^p \left\{\langle D_i u_{|\Gamma_i}, v_{|\Gamma_i}\rangle_{\Gamma_i} + \tfrac{1}{2}\langle t_i, v_{|\Gamma_i}\rangle_{\Gamma_i} + \langle t_i, K_i v_{|\Gamma_i}\rangle_{\Gamma_i}\right\} &= f_1(v) \\ \langle V_i t_i, \tau_i\rangle_{\Gamma_i} - \tfrac{1}{2}\langle u_{|\Gamma_i}, \tau_i\rangle_{\Gamma_i} - \langle K_i u_{|\Gamma_i}, \tau_i\rangle_{\Gamma_i} &= f_2(\tau_i)\,, \end{aligned}$$

whose Galerkin discretization leads to the skew–symmetric positive definite system

$$\begin{pmatrix} V_h & -K_h & -\frac{1}{2}M_h - K_h \\ K_h^\top & D_{h,NN} & D_{h,CN} \\ \frac{1}{2}M_h^\top + K_h^\top & D_{h,NC} & D_{h,CC} \end{pmatrix}\begin{pmatrix} \underline{t} \\ \underline{u}_N \\ \underline{u}_C \end{pmatrix} = \begin{pmatrix} \underline{f}_D \\ \underline{f}_N \\ \underline{f}_C \end{pmatrix}. \tag{13}$$

The vector $\underline{u}_C$ corresponds to all unknowns along the coupling interfaces, whereas $\underline{u}_N$ denotes only the unknowns at the original Neumann boundary.

2 Iterative solution methods

In this section we want to describe different possibilities to solve system (13) by iterative methods, which are well suited for parallel computations, too. We restrict ourselves to the symmetric formulation; however, to solve (12), which can be transformed into a saddle point problem, we can apply related techniques. Instead of (13) we solve the transformed system

$$\begin{pmatrix} C_V^{-1/2} & 0 \\ 0 & C_S^{-1/2} \end{pmatrix} \begin{pmatrix} V_h & -\tilde{K}_h \\ \tilde{K}_h^\top & D_h \end{pmatrix} \begin{pmatrix} C_V^{-1/2} & 0 \\ 0 & C_S^{-1/2} \end{pmatrix} \begin{pmatrix} \tilde{\underline{t}} \\ \tilde{\underline{u}} \end{pmatrix} = \begin{pmatrix} \tilde{\underline{f}} \\ \underline{0} \end{pmatrix} \tag{14}$$

with $\tilde{K}_h = (K_h|\frac{1}{2}M_h + K_h)$; where C_V and C_S are symmetric and positive definite preconditioners for V_h and $S_h = D_h + K_h^\top V_h^{-1} K_h$, respectively, i.e. we suppose the inequalities

$$\left. \begin{aligned} c_1^V\,(C_V\underline{t},\underline{t}) \;\le\; (V_h\underline{t},\underline{t}) \;\le\; c_2^V\,(C_V\underline{t},\underline{t}) \\ c_1^S\,(C_S\underline{u},\underline{u}) \;\le\; ((D_h + K_h^\top V_h^{-1}K_h)\underline{u},\underline{u}) \;\le\; c_2^S\,(C_S\underline{u},\underline{u}) \end{aligned} \right\} \tag{15}$$

for all $\underline{t}$ and $\underline{u}$. We remark that the new system matrix in (14),

$$H = \begin{pmatrix} C_V^{-1/2} V_h C_V^{-1/2} & -C_V^{-1/2}\tilde{K}_h C_D^{-1/2} \\ C_D^{-1/2}\tilde{K}_h^\top C_V^{-1/2} & C_D^{-1/2} D_h C_D^{-1/2} \end{pmatrix},$$

is of the same structure as the original one in (13).

To solve the skew–symmetric and positive definite system

$$\begin{pmatrix} A & -B \\ B^\top & D \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \end{pmatrix} = \begin{pmatrix} \underline{f}_1 \\ \underline{f}_2 \end{pmatrix}, \tag{16}$$

which corresponds to (13) as well as to (14), we introduce a regular transformation matrix T and solve the transformed system

$$T \cdot H\,\underline{x} = T \cdot \underline{f}\,.$$

Moreover, we suppose the spectral equivalence inequalities

$$\left. \begin{aligned} c_1^A\,(\underline{x}_1,\underline{x}_1) \;\le\; (A\underline{x}_1,\underline{x}_1) \;\le\; c_2^A\,(\underline{x}_1,\underline{x}_1) \\ c_1^S\,(\underline{x}_2,\underline{x}_2) \;\le\; ((D + B^\top A^{-1}B)\underline{x}_2,\underline{x}_2) \;\le\; c_2^S\,(\underline{x}_2,\underline{x}_2) \end{aligned} \right\} \tag{17}$$

corresponding to (15), where we require $c_1^A > 1$ by scaling the preconditioner C_V.

For $T = I$ we still have the original preconditioned system, which can be solved by generalized methods of conjugate directions, such as GMRES or methods of biorthogonal directions [Bea92, Stec] . Taking $T = H^\top$ we arrive at the system of normal equations with a symmetric and positive definite matrix $H^\top H$, for which we can use the standard conjugate gradient iteration; but here the spectral condition number is squared, and therefore this variant may be inefficient.

Following [BP88], the transformed matrix

$$\tilde{M} = \begin{pmatrix} I & 0 \\ -B^\top & I \end{pmatrix} \begin{pmatrix} A & -B \\ B^\top & D \end{pmatrix} = \begin{pmatrix} A & -B \\ B^\top(I-A) & D+B^\top B \end{pmatrix}$$

is selfadjoint with respect to the specially chosen inner product

$$[\underline{x}, \underline{x}] := ((A-I)\underline{x}_1, \underline{x}_1) + (\underline{x}_2, \underline{x}_2) \tag{18}$$

due to $c_1^A > 1$ in (17). Moreover, there hold spectral equivalence inequalities

$$c_1^R \cdot \min\{1, c_1^S\} \cdot [\underline{x}, \underline{x}] \leq [\tilde{M}\underline{x}, \underline{x}] \leq c_2^R \cdot \max\{1, c_2^S\} \cdot [\underline{x}, \underline{x}]$$

with the constants [BP88]

$$c_1^R = \left(1 + \frac{\alpha}{2} + \sqrt{\frac{\alpha^2}{4} + \alpha}\right)^{-1}, \; c_2^R = \frac{1+\sqrt{\alpha}}{1-\alpha}, \; \alpha = 1 - \frac{1}{c_2^A}.$$

Therefore, a scaling of the preconditioner C_S is necessary, too.

Obviously, this method requires the symmetry of A to define the inner product (18). We are interested in an approach, which allows a generalization to unsymmetric perturbations of symmetric matrices as in (12). Therefore we consider the second transformed matrix

$$\hat{M} = \begin{pmatrix} A-I & 0 \\ -B^\top & I \end{pmatrix} \begin{pmatrix} A & -B \\ B^\top & D \end{pmatrix} = \begin{pmatrix} A^2 - A & (I-A)B \\ B^\top(I-A) & D+B^\top B \end{pmatrix},$$

which is symmetric and positive definite. However, the constants in the related spectral equivalence inequalities are no longer asymptotically optimal for $A \to I$ as in the approach proposed by [BP88]. So we have to find an appropriate preconditioning technique for $\hat{M}$. To this end we follow [HLM92] and consider the symmetric and positive definite Matrix

$$\bar{M} = \begin{pmatrix} \bar{A} & \bar{B} \\ \bar{B}^\top & \bar{D} \end{pmatrix}$$

with the factorization

$$\bar{M} = \begin{pmatrix} I & 0 \\ \bar{B}^\top \bar{A}^{-1} & I \end{pmatrix} \begin{pmatrix} \bar{A} & 0 \\ 0 & \bar{D} - \bar{B}^\top \bar{A}^{-1} \bar{B} \end{pmatrix} \begin{pmatrix} I & \bar{A}^{-1}\bar{B} \\ 0 & I \end{pmatrix}.$$

If the spectral equivalence inequalities

$$c_1^{\bar{A}} \cdot (\underline{x}_1, \underline{x}_1) \leq (\bar{A}\underline{x}_1, \underline{x}_1) \leq c_2^{\bar{A}} \cdot (\underline{x}_1, \underline{x}_1)$$

and

$$c_1^{\bar{S}} \cdot (\underline{x}_2, \underline{x}_2) \leq ((\bar{D} - \bar{B}^\top \bar{A}^{-1} \bar{B})\underline{x}_2, \underline{x}_2) \leq c_2^{\bar{S}} \cdot (\underline{x}_2, \underline{x}_2)$$

both are satisfied, then the matrix

$$C_{\bar{M}} = \begin{pmatrix} I & 0 \\ \bar{B}^\top & I \end{pmatrix} \begin{pmatrix} I & \bar{B} \\ 0 & I \end{pmatrix}$$

is spectrally equivalent to $\bar{M}$, i.e. we have the inequalities

$$\gamma_1 \, (C_{\bar{M}}\underline{x}, \underline{x}) \; \leq \; (\bar{M}\underline{x}, \underline{x}) \; \leq \; \gamma_2 \, (C_{\bar{M}}\underline{x}, \underline{x})$$

with the positive constants [HLM92]

$$\gamma_1 = \min\{c_1^{\bar{A}}, c_1^{\bar{S}}\} \left[1 + \frac{1}{2}\left(\mu - \sqrt{\mu^2 + 4\mu}\right)\right],$$

$$\gamma_2 = \max\{c_2^{\bar{A}}, c_2^{\bar{S}}\} \left[1 + \frac{1}{2}\left(\mu + \sqrt{\mu^2 + 4\mu}\right)\right]$$

and the spectral condition number

$$\mu \; = \; \rho\left(\left[\bar{D} - \bar{B}^\top \bar{A}^{-1}\bar{B}\right]^{-1}\left[\bar{B}^\top(\bar{A}^{-1} - I)\bar{A}(\bar{A}^{-1} - I)\bar{B}\right]\right) \; .$$

With $\bar{A} = A^2 - A$, from (17) there follows directly

$$(c_1^A - 1)c_1^A \, (\underline{x}_1, \underline{x}_1) \, ((A^2 - A)\underline{x}_1, \underline{x}_1) \; \leq \; (c_2^A - 1)c_2^A \, (\underline{x}_1, \underline{x}_2) \; ,$$

and a straightforward computation gives

$$\bar{S} \; = \; \bar{D} - \bar{B}^\top \bar{A}^{-1}\bar{B} \; = \; D + B^\top A^{-1} B \; ;$$

and therefore $c_1^{\bar{S}} = c_1^S, c_2^{\bar{S}} = c_2^S$. From

$$\begin{aligned} T &= \bar{B}^\top(\bar{A}^{-1} - I)\bar{A}(\bar{A}^{-1} - I)\bar{B} \\ &= B^\top(I - A)((A - I)^{-1}A^{-1} - I)(A^2 - A)(A^{-1}(A - I)^{-1} - I)(I - A)B \\ &= B^\top(A^{-1} - A + I)(A^2 - A)(A^{-1} - A + I)B \end{aligned}$$

we conclude, that T tends to zero for $A \to I$. Because of the stability of the discrete Steklov–Poincaré operator S we have then asymptotically $\mu \to 0$ for $A \to I$. We will discuss this approach in more details in [Steb]. Finally we remark, that we can generalize this method to the non–symmetric case (12) by choosing the transformation

$$\hat{M} \; = \; \begin{pmatrix} A^\top - I & 0 \\ -C & I \end{pmatrix} \begin{pmatrix} A & -B \\ C & 0 \end{pmatrix} \; = \; \begin{pmatrix} A^\top A - A & (I - A)B \\ C(I - A) & CB \end{pmatrix} \; ;$$

the related system of linear equations can be solved by any preconditioned iterative method discussed above. Due to the (non–symmetric) discretization of self–adjoint operators involved, the block matrices $A \sim A^\top$ and $B^\top \sim C$, respectively, are perturbations of symmetric matrices, such that the BiCGStab algorithm behaves asymptotically like the classical conjugate gradient method.

3 The construction of optimal preconditioners

The iterative methods described above are based on preconditioners with respect to the discrete single layer potential V_h, the hypersingular integral operator D_h

and the discrete Steklov–Poincaré operator S_h, respectively. Here these operators are pseudodifferential operators of order ± 1. Efficient algebraic preconditioners are multigrid methods, which in a generalized form can also used for operators of negative order [Bra93]. In general, if preconditioners are constructed from equivalence relations of bilinear forms and their matrix representations, then one has to invert spectral equivalent matrices, where the work for doing this job should be in the same order as a matrix multiplication. In two–dimensional boundary element methods one can use periodic Sobolev spaces to construct efficient preconditioners [HKW80, Rja90, Wen80]. For uniform meshes, this approach leads to circulant matrices, which can be handled by the Fast Fourier Transformation. There are generalizations to adaptive meshes and to three–dimensional problems [KW92]; in the case of axially–symmetric surfaces, the discretization leads to block circulant matrices [MR90]. However, generalizations to three–dimensional problems are restricted to structered surface meshes in a corresponding ordering. Here we want to give a general concept to construct efficient preconditioners independent of geometrical properties.

Let us consider strongly elliptic and self–adjoint pseudodifferential operators of orders $\pm 2\alpha$ in the Sobolev spaces on Γ,

$$A \,:\, H^s(\Gamma) \to H^{s-2\alpha}(\Gamma)\,, \quad B \,:\, H^{s-2\alpha}(\Gamma) \to H^s(\Gamma)$$

satisfying the coerciveness inequalities

$$\begin{aligned} c_1^A \|t\|^2_{H^s(\Gamma)} \,\le\, \langle At, t\rangle_{H^{s-\alpha}} \,\le\, c_2^A \|t\|^2_{H^s(\Gamma)} \qquad & \forall\, t \in V = H^s(\Gamma)_{/\mathrm{ker}A} \\ c_1^B \|u\|^2_{H^{s-2\alpha}(\Gamma)} \,\le\, \langle Bu, u\rangle_{H^{s-\alpha}} \,\le\, c_2^B \|u\|^2_{H^{s-2\alpha}(\Gamma)} \qquad & \forall\, u \in W = H^{s-2\alpha}(\Gamma)_{/\mathrm{ker}B}\,. \end{aligned} \tag{19}$$

For the finite–dimensional $\mathrm{ker}B$ we use an orthonormal basis representation

$$\mathrm{ker}B \,=\, \left\{ v \in H^{s-2\alpha}(\Gamma) \,:\, Bv = 0 \right\} \,=\, \mathrm{span}\, \{v_k\}_{k=1}^m$$

with

$$\langle v_k, v_\ell\rangle_{H^{s-2\alpha}(\Gamma)} \,=\, \delta_{k\ell} \quad \text{for all } k, \ell = 1, \ldots, m\,.$$

If we introduce the factor space $V^0(B)$ by

$$V^0(B) \,=\, \left\{ t \in H^s(\Gamma) \,:\, \langle t, v_k\rangle_{H^{s-\alpha}(\Gamma)} = 0 \;\text{ for all } v_k \in \mathrm{ker}B \right\}$$

we can define the pseudoinverse operator to B,

$$\dot{B}^{-1} \,:\, V^0(B) \to W\,,$$

which is a selfadjoint operator satisfying the inequalities

$$\frac{1}{c_2^B}\, \|t\|^2_{H^s(\Gamma)} \,\le\, \langle \dot{B}^{-1} t, t\rangle_{H^{s-\alpha}(\Gamma)} \,\le\, \frac{1}{c_1^B}\, \|t\|^2_{H^s(\Gamma)}$$

for all $t \in V^0(B)$. Then from the assumptions there follows immediately

Lemma 1. *For all $t \in V \cap V^0(B)$ there hold the inequalities*

$$\tilde{\gamma}_1 \cdot \langle \dot{B}^{-1} t, t\rangle_{H^{s-\alpha}(\Gamma)} \,\le\, \langle At, t\rangle_{H^{s-\alpha}(\Gamma)} \,\le\, \tilde{\gamma}_2 \cdot \langle \dot{B}^{-1} t, t\rangle_{H^{s-\alpha}(\Gamma)}\,.$$

with positive constants $\tilde{\gamma}_1 = c_1^A \cdot c_1^B$ and $\tilde{\gamma}_2 = c_2^A \cdot c_2^B$.

To construct a preconditioner for all $u \in V$ we have to split the space V into an orthogonal sum

$$V = V^0(B) \oplus \left[V^0(B)\right]^\perp .$$

If we define the Bessel potential operator

$$J : H^{s-2\alpha}(\Gamma) \to H^s(\Gamma)$$

such that the relation

$$\langle Ju, v\rangle_{H^{s-\alpha}(\Gamma)} = \langle u, v\rangle_{H^{s-2\alpha}(\Gamma)}$$

holds for all $v \in H^{s-2\alpha}(\Gamma)$, we can formulate the basic result [Stea]:

Theorem 2. *The operator defined by the bilinear form*

$$c(t,\tau) = \langle \dot{B}^{-1}t_0, \tau_0\rangle_{H^{s-\alpha}(\Gamma)} + \sum_{k=1}^{m} \langle t, v_k\rangle_{H^{s-\alpha}(\Gamma)} \langle \tau, v_k\rangle_{H^{s-\alpha}(\Gamma)} \tag{20}$$

with

$$t_0(x) = t(x) - \sum_{j=1}^{m} \langle t, v_j\rangle_{H^{s-\alpha}(\Gamma)} (Jv_j)(x) \in V^0(B)$$

is spectrally equivalent to A, i.e. there hold the inequalities

$$\gamma_1 \cdot c(t,t) \le \langle At, t\rangle_{H^{s-\alpha}(\Gamma)} \le \gamma_2 \cdot c(t,t) .$$

with positive constants $\gamma_1 = c_1^A \cdot \min\{1, c_1^B\}$ and $\gamma_2 = c_2^A \cdot \max\{1, c_2^B\}$.

Let a finite approximation space $V_h \subset V$ be given by

$$V_h = \operatorname{span} \{\varphi_k^\nu(\cdot)\}_{k=1}^N$$

with the trial functions φ_k^ν, e.g. smoothest splines of polynomial degree ν, and the discretization parameter N. Then it follows directly from Theorem 2, that the matrices A_h and C_h defined by their elements

$$A_h[\ell,k] = \langle A\varphi_k^\nu, \varphi_\ell^\nu\rangle_{H^{s-\alpha}(\Gamma)} , \quad C_h[\ell,k] = c(\varphi_k^\nu, \varphi_\ell^\nu)$$

are spectrally equivalent, i.e. the spectral condition number of the preconditioned system is bounded by

$$\kappa(C_h^{-1}A_h) \le \frac{c_2^A \cdot \max\{1, c_2^B\}}{c_1^A \cdot \min\{1, c_1^B\}}$$

and therefore independent of all bad parameters like mesh adaptivity or the degree of trial functions. Moreover, there are no restrictions to the space dimension of the problem considered. However, to use the proposed preconditioner, one has to realize the action of C_h^{-1} in a very efficient way.

For the map Jv_k of the functions $v_k \in \ker B$ we have to suppose a representation in terms of the basis of V_h, i.e.

$$(Jv_k)(x) = \sum_{j=1}^{N} v_k^j \cdot \varphi_j^\nu(x) ,$$

then we find by partial Gram–Schmidt orthogonalization the transformed basis

$$V_h = \operatorname{span}\{\varphi_1^\nu, \dots, \varphi_N^\nu\} = \operatorname{span}\{\varphi_1^{\nu,0}, \dots, \varphi_{N-m}^{\nu,0}, Jv_1, \dots, Jv_m\}$$

with

$$\varphi_k^{\nu,0}(x) = \varphi_k^\nu(x) - \sum_{j=1}^m \langle \varphi_k^\nu, v_j \rangle_{H^{s-\alpha}(\Gamma)} \cdot (Jv_j)(x) \in V^0(B) .$$

For a given function $t_h(x) \in V_h$ we find the basis transformation by

$$t_h(x) = \sum_{k=1}^N t_k \cdot \varphi_k^\nu(x) = \sum_{k=1}^{N-m} \tilde{t}_k \cdot \varphi_k^{\nu,0}(x) + \sum_{k=1}^m \tilde{t}_{N-m+k} \cdot (Jv_k)(x)$$

with the relations

$$t_k = \begin{cases} \tilde{t}_k + \sum\limits_{\ell=1}^m v_\ell^k \left(\tilde{t}_{N-m+\ell} - \sum\limits_{j=1}^{N-m} \langle \varphi_j^\nu, v_\ell \rangle_{H^{s-\alpha}(\Gamma)} \tilde{t}_j \right), & k = 1, \dots, N-m, \\ \sum\limits_{\ell=1}^m v_\ell^k \left(\tilde{t}_{N-m+\ell} - \sum\limits_{j=1}^{N-m} \langle \varphi_j^\nu, v_\ell \rangle_{H^{s-\alpha}(\Gamma)} \tilde{t}_j \right), & k = N-m+1, \dots, N \end{cases}$$

or in matrix representation

$$\underline{t} = T^\top \underline{\tilde{t}} .$$

If we denote by $\underline{f}$ the vector of the right hand side generated by

$$f_k = f(\varphi_k^\nu)$$

corresponding to the linear form of the original variational problem, we find for the discretization with respect to the transformed basis, i.e. for

$$\tilde{f}_k = f(\varphi_k^{\nu,0}) \ \text{ for } k = 1, \dots, N-m$$

and

$$\tilde{f}_{N-m+k} = f(Jv_k) \ \text{ for } k = 1, \dots, m$$

the matrix representation

$$\underline{\tilde{f}} = T \underline{f} ,$$

which ensures the symmetry of the proposed preconditioner.

Due to the orthonormal basis representation of V_h, discretization leads now to the decoupled stiffness matrix

$$\tilde{C}_h = \begin{pmatrix} C_0 & 0 \\ 0 & I \end{pmatrix} \tag{21}$$

with the block

$$C_0[\ell, k] = \langle \dot{B}^{-1} \varphi_k^{\nu,0}, \varphi_\ell^{\nu,0} \rangle_{H^{s-\alpha}(\Gamma)}$$

for all $k, \ell = 1, \dots, N-m$. We still have to discretize the pseudoinverse operator $\dot{B}^{-1}$, which is in general not given in explicit form. Hence we have to find an approximation

u_0^h of the exact function $u_0 = \dot{B}^{-1}t_0 \in W$ for any function $t_0 \in V^0(B)$. This can be done by solving the finite–dimensional variational problem

$$\langle Bu_0^h, v_0^h\rangle_{H^{s-\alpha}(\Gamma)} = \langle t_0, v_0^h\rangle_{H^{s-\alpha}(\Gamma)}$$

for all test functions $v_h^0 \in W$. From the assumptions for B there follows, that this problem has an unique solution and that we have the quasioptimal error estimate

$$||u_0 - u_0^h||_{H^{s-2\alpha}(\Gamma)} \leq c(B) \inf_{v_0^h \in W} ||u_0 - v_0^h||_{H^{s-2\alpha}(\Gamma)} .$$

This estimate implies

$$\left|\langle \dot{B}^{-1}t_0, t_0\rangle_{H^{s-\alpha}(\Gamma)} - \langle u_h^0, t_0\rangle_{H^{s-\alpha}(\Gamma)}\right| \leq c(B) \inf_{v_0^h \in W} ||\dot{B}^{-1}t_0 - v_0^h||_{H^{s-2\alpha}(\Gamma)}||t_0||^2_{H^s(\Gamma)}$$

and therefore we have the spectral equivalence inequalities

$$c_1(B,h_0)\cdot\langle \dot{B}_h^{-1}t_0, t_0\rangle_{H^{s-\alpha}(\Gamma)} \leq \langle \dot{B}^{-1}t_0, t_0\rangle_{H^{s-\alpha}(\Gamma)} \leq c_2(B,h_0)\cdot\langle \dot{B}_h^{-1}t_0, t_0\rangle_{H^{s-\alpha}(\Gamma)}$$

for all mesh parameters $h \leq h_0$, where h_0 is determined only by constants depending on B. Hence we can replace the block matrix C_0 in (21) by the spectrally equivalent discretization based on the approximation u_0^h. This leads to the discrete representation

$$C_0^h = \tilde{M}_h B_h^{-1} \tilde{M}_h^\top .$$

For this discretization we have to use a subspace

$$W_h = \operatorname{span}\{\varphi_1^{\mu,0}, \ldots, \varphi_{N-m}^{\mu,0}\} \subset W$$

with the transformed trial functions

$$\varphi_k^{\mu,0}(x) = \varphi_k^\mu(x) - \sum_{j=1}^m \langle \varphi_k^\mu, v_j\rangle_{H^s(\Gamma)} \cdot v_j(x) \in W$$

for $k = 1, \ldots, N-m$. Then we get the discrete representation of the operator B by

$$B_h[\ell,k] = \langle B\varphi_k^{\mu,0}, \varphi_\ell^{\mu,0}\rangle_{H^{s-\alpha}(\Gamma)} = \langle B\varphi_k^\mu, \varphi_\ell^\mu\rangle_{H^{s-\alpha}(\Gamma)}$$

using the original trial functions $\varphi_k^\mu(\cdot)$. For the modified mass matrix we find

$$\tilde{M}_h[\ell,k] = \langle \varphi_k^\nu, \varphi_\ell^\mu\rangle_{H^{s-\alpha}(\Gamma)} - \sum_{j=1}^m \langle \varphi_\ell^\mu, v_j\rangle_{H^s(\Gamma)} \cdot \langle \varphi_k^\nu, v_j\rangle_{H^{s-\alpha}(\Gamma)} ,$$

i.e. a rank–m pertubation of the original mass matrix M_h. Since we can choose the trial functions $\varphi_k^\mu(\cdot)$ in an appropriate way, we may assume, that the inverse matrix $\tilde{M}_h^{-1}$ exists. Algorithms to compute this inverse are based on Sherman–Morrison–Woodbury formulae [OR70] using the inverse matrix M_h^{-1}, which is more suitable, because M_h is almost sparse and diagonally dominant.

Now we are in the position to present the proposed preconditioner in a compact form, where the action to realize C_h^{-1} is given by

$$C_h^{-1} = T^\top \begin{pmatrix} \tilde{M}_h^{-1} B_h \tilde{M}_h^{-1} & 0 \\ 0 & I \end{pmatrix} T . \tag{22}$$

In the next section we give an example, which is important for applications in potential theory as well as in linear elasticity. Using the symmetric formulation to handle mixed boundary value problems or domain decomposition methods numerically with boundary elements, we will see, that this approach is optimal for an efficient preconditioning, since we can choose the operators A and B in such a way, that the additional work for the realization of the proposed preconditioner is neglicable.

4 Examples

We want to demonstrate the proposed preconditioning technique for the potential problem with the differential operator

$$L(x)u(x) = -\operatorname{div} \alpha(x) \nabla u(x) ,$$

where we suppose piecewise constant coefficients

$$\alpha(x) = \alpha_i \quad \text{for } x \in \Omega_i .$$

Therefore, the local fundamental solution for the Laplacian is given by

$$E^i(x,y) = \frac{1}{2(n-1)\pi} \cdot \begin{cases} -\log|x-y| & \text{for } n=2 , \\ |x-y|^{-1} & \text{for } n=3 . \end{cases}$$

The local single layer potential operators

$$(V_i t_i)(x) = \int_{\Gamma_i} E^i(x,y) \cdot t_i(y)\, ds_y$$

and the hypersingular operators

$$(D_i u_i)(x) = -\frac{\partial}{\partial n_x} \int_{\Gamma_i} \frac{\partial}{\partial n_y} E^i(x,y) \cdot u_i(y)\, ds_y$$

for $x \in \Gamma_i$ satisfy all assumptions of the previous sections with $A = V, B = D$ and $s = -1/2, 2\alpha = -1$. Moreover, the ratios of the constants in the inequalities (19) are independent of the local material parameter α_i.

Further we have $\ker V = \{0\}$ and $\ker D = \{1\}$. From

$$v_1(x) = 1 = \sum_{k=1}^{N} \varphi_k^\nu(x)$$

we find the basis transformation T by

$$u_h(x) = \sum_{k=1}^{N} u_k \varphi_k^\nu(x) = \sum_{k=1}^{N-1} \tilde{u}_k \, \varphi_k^{\nu,0}(x) + \omega \cdot v_1(x)$$

with

$$\varphi_k^{\nu,0}(x) = \varphi_k^\nu(x) - \frac{m_k^\nu}{|\Gamma|} \cdot v_1(x) \text{ and } m_k^\nu = \int_\Gamma \varphi_k^\nu(x) \, ds_x \, .$$

Therefore we have the representation

$$\tilde{M}_h = M_h - \frac{1}{|\Gamma|} \underline{m}^\nu (\underline{m}^\mu)^\top$$

for the modified mass matrix, where the inverse is given by the Shermann–Morrison formula

$$\tilde{M}_h^{-1} = M_h^{-1} - \frac{1}{\alpha - |\Gamma|} M_h^{-1} \underline{m}^\nu (\underline{m}^\mu)^\top M_h^{-1} \, , \; \alpha = (\underline{m}^\mu)^\top M_h^{-1} \underline{m}^\nu \, .$$

Note that there are situations, where M_h^{-1} and therefore $\tilde{M}_h^{-1}$ does not exist; e.g. in three dimensions, if we choose for the flux piecewise constant trial functions, which are defined with respect to elements, and for the potential piecewise linear trial functions defined with respect to nodes, and in general, if the numbers of elements and nodes differ, then the mass matrix will be rectangular. Therefore, one has to be very careful to select the exact trials to discretize B. If we choose piecewise linear trial functions with $\nu = \mu = 1$, M_h will be a strongly diagonally dominant sparse matrix, where the inverse M_h^{-1} can be computed very efficiently. In the two–dimensional case, M_h is tridiagonal, where we can use a Cholesky factorization with $O(N)$ multiplications. In general, this preconditioner needs $O(N^2)$ multiplications to apply B_h to a vector and some operations of lower order to realize the basis transformations T and the computation of $\tilde{M}_h^{-1}$.

Because the hypersingular operator D is positive definite with respect to the $|\cdot|_{H^{1/2}(\Gamma)}$ semi–norm, i.e.

$$\langle Du, u \rangle_{L_2(\Gamma)} \geq c_1^D \, |u|^2_{H^{1/2}(\Gamma)} \, ,$$

there follows immediately

$$\langle (c_1^D \cdot I + D)u, u \rangle_{L_2(\Gamma)} \geq c_1^D \, ||u||^2_{H^{1/2}(\Gamma)}$$

with the modified pseudodifferential operator $c_1^D \cdot I + D$, where a basis transformation is no longer required. This seems to be quite useful for applications in linear elasticity.

For the multiplication of the discrete operator D_h one should use fast multiplication algorithms like the panel clustering [HN89, Sau92] for developping more efficient algorithms.

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