

Max-Planck-Institut  
für Mathematik  
in den Naturwissenschaften  
Leipzig

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by

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Preprint no.: 25

2004





# Direct Schur Complement Method by Domain Decomposition Based on $\mathcal{H}$ -Matrix Approximation

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April 28, 2004

## Abstract

The goal of this paper is the construction of a data-sparse approximation to the Schur complement on the interface corresponding to FEM and BEM approximations of an elliptic equation by domain decomposition. Using the hierarchical ( $\mathcal{H}$ -matrix) formats we elaborate the *approximate Schur complement inverse* in an explicit form. The required cost  $\mathcal{O}(N_\Gamma \log^q N_\Gamma)$  is almost linear in  $N_\Gamma$  – the number of degrees of freedom on the interface. As input, we require the Schur complement matrices corresponding to subdomains and represented in the  $\mathcal{H}$ -matrix format. In the case of piecewise constant coefficients these matrices can be computed via the BEM representation with the cost  $\mathcal{O}(N_\Gamma \log^q N_\Gamma)$ , while in the general case the FEM discretisation leads to the complexity  $\mathcal{O}(N_\Omega \log^q N_\Omega)$ , where  $N_\Omega$  is the number of degrees of freedom in the domain.

*AMS Subject Classification:* 65F30, 65F50, 65N35, 65F10

*Key words:* elliptic equations, data-sparse  $\mathcal{H}$ -matrix approximation, BEM, FEM, FETI, Schur complement, domain decomposition

## 1 Introduction

In [8], a direct domain decomposition method was described for rather general elliptic equations based on a traditional FEM. Using  $\mathcal{H}$ -matrix techniques, almost linear<sup>1</sup> cost in the number  $N_\Omega$  of degrees of freedom in the computational domain  $\Omega$  could be achieved. In this paper, we concentrate on the inversion of the Schur complement matrix associated with the *interface* that defines the domain decomposition.

We distinguish three approaches to construct and approximate the Schur complement matrix:

- (a) Methods based on a traditional FEM for rather general variable coefficients (cf. [8]);
- (b) Approximation by boundary concentrated FEM in the case of coefficients which are smooth in the subdomains (cf. [13]);
- (c) BEM/FEM based methods for piecewise constant coefficients (cf. [12, 14, 16]).

Below, we focus on the cases (a) and (c). In the latter case, which is not covered by [8], we make use of the standard advantages of BEM compared to FEM. Furthermore, besides the approximation theory (cf. Theorem 3.1), in the 2D case, we can show the approximability of the Schur complement in the  $\mathcal{H}$ -matrix format based on the weak admissibility criteria (cf. [11]). In both cases we give numerical results.

Notice that our approach can be viewed as an *approximate direct parallel solver* based on the data-sparse approximation to the Schur complement matrix in the domain decomposition method.

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<sup>1</sup>By “almost linear” we mean  $\mathcal{O}(N \log^q N)$  for a fixed  $q$ .

## 2 FEM-Galerkin Approximation

In a polygonal domain  $\Omega \subset \mathbb{R}^2$ , we consider the elliptic operator  $\mathcal{L} : V \rightarrow V'$  for  $V = H_0^1(\Omega)$  and  $V' = H^{-1}(\Omega)$ , with the corresponding  $V$ -elliptic bilinear form  $a_\Omega : V \times V \rightarrow \mathbb{R}$ ,

$$a_\Omega(u, v) = \int_\Omega \left( \sum_{i,j=1}^d a_{ij} \partial_j u \partial_i v + a_0 uv \right) dx, \quad a_0 > 0. \quad (2.1)$$

The corresponding variational equation is: Find  $u \in V$  such that

$$a_\Omega(u, v) = \langle f, v \rangle \quad \text{for all } v \in V, \quad (2.2)$$

where  $f \in H^{-1}(\Omega)$ . We suppose the domain  $\Omega$  to be composed of  $M \geq 1$  possibly matching, but non-overlapping polygonal subdomains  $\Omega_i$ ,  $\bar{\Omega} = \cup_{i=1}^M \bar{\Omega}_i$ . We denote the interface (skeleton) of the decomposition of  $\Omega$  by  $\Gamma = \cup \Gamma_i$  with  $\Gamma_i := \partial\Omega_i$ .

We may write the bilinear form  $a_\Omega(\cdot, \cdot)$  in (2.1) as a sum of local bilinear forms,

$$a_\Omega(u, v) = \sum_{i=1}^M a_{\Omega_i}(R_i u, R_i v), \quad \text{where } R_i : V \rightarrow V_i := H^1(\Omega_i)$$

is the restriction of functions onto  $\Omega_i$  and the integration in  $a_{\Omega_i} : V_i \times V_i \rightarrow \mathbb{R}$  is restricted to  $\Omega_i$ . Furthermore, we suppose that there exist  $0 < C_1 \leq C_2$  such that (for suitable constants  $\mu_i > 0$ )

$$C_1 \mu_i |u|_{H^1(\Omega_i)}^2 \leq a_{\Omega_i}(u, u) \leq C_2 \mu_i |u|_{H^1(\Omega_i)}^2 \quad \text{for all } u \in H^1(\Omega_i). \quad (2.3)$$

We introduce the space  $V_\Gamma \subset V$  of piecewise  $\mathcal{L}$ -harmonic functions by

$$V_\Gamma := \{v \in V : a_\Omega(v, z) = 0 \quad \text{for all } z \in V_0\}$$

with  $V_0 := \{v \in V : v(x) = 0 \text{ for all } x \in \Gamma\}$ . Note that  $V = V_0 + V_\Gamma$  is an orthogonal splitting with respect to scalar product  $a_\Omega(\cdot, \cdot)$ .

Because we focus on the solution of an interface equation, we suppose that the right-hand side  $f$  is supported only by the interface, i.e., with given  $\psi_i \in H^{-1/2}(\Gamma_i)$ ,  $i = 1, \dots, M$ ,

$$\langle f, v \rangle = \sum_{i=1}^M \langle \psi_i, v \rangle_{\Gamma_i}. \quad (2.4)$$

An equation with general  $f$  can be reduced to the case (2.4) by subtracting particular solutions in the subdomains which can be performed in parallel. Specifically, let  $u_{0,i} \in H_0^1(\Omega_i)$  be the solution of equation (2.2) reduced to a subdomain  $\Omega_i$ ,

$$a_{\Omega_i}(u_{0,i}, v) = \int_{\Omega_i} f(x) v dx \quad \text{for all } v \in V_i. \quad (2.5)$$

We split the solution of (2.2) into  $u = u_0 + u_H$  with  $u_0 \in V_0$ ,  $u_H \in V_H$ , where  $u_0$  solves the problem

$$a_\Omega(u_0, v) = \langle f, v \rangle \quad \text{for all } v \in V_0, \quad (2.6)$$

and thus satisfies  $R_i u_0 = u_{0,i}$  with  $u_{0,i}$  being the solution of (2.5). For the remaining piecewise  $\mathcal{L}$ -harmonic component  $u_H = u - u_0 \in V_H$ , we obtain the global equation

$$a_\Omega(u_H, v) = \langle f, v \rangle - a_\Omega(u_0, v) \quad \text{for all } v \in V_H, \quad (2.7)$$

where the right-hand side takes the form (2.4) with  $\psi_i := \gamma_{1,i} u_{0,i}$ . Here  $\gamma_{1,i} : H^{1/2}(\Gamma_i) \rightarrow H^{-1/2}(\Gamma_i)$  is the operator of conormal derivative. The bilinear form  $a_\Omega(\cdot, \cdot)$  in (2.7) is defined via the space of piecewise  $\mathcal{L}$ -harmonic functions which are uniquely determined by their traces on the skeleton  $\Gamma$ .

Next we reduce the variational equation (2.2) with  $f$  satisfying (2.4), to an *interface equation* (in fact, in this case the solution satisfies  $u \in V_\Gamma$ ). To this end, let us introduce the following *trace space* on  $\Gamma$ ,

$$Y_\Gamma := \{u = z|_\Gamma : z \in V\}, \quad \|u\|_{Y_\Gamma} = \inf_{z \in V : z|_\Gamma = u} \|z\|_V,$$

with the energy norm  $\|z\|_V = \sqrt{a_\Omega(z, z)}$ . We define the local Poincaré-Steklov operator (Dirichlet-Neumann map) on  $\Gamma_i = \partial\Omega_i$ ,

$$\mathcal{T}_i : H^{1/2}(\Gamma_i) \rightarrow H^{-1/2}(\Gamma_i)$$

by

$$\lambda \in H^{1/2}(\Gamma_i), \quad \mathcal{T}_i(\lambda) := \gamma_{1,i}u.$$

Here  $\gamma_{1,i}u$  is the conormal derivative of  $u$  on  $\Gamma_i$  and  $u$  solves (2.2) in  $\Omega_i$  such that  $u|_{\Gamma_i} = \lambda$ . The *interface problem* which is equivalent to (2.2) reads as: Find  $z = u|_\Gamma \in Y_\Gamma$  such that

$$b_\Gamma(z, v) := \sum_{i=1}^M \langle \mathcal{T}_i z_i, v_i \rangle_{\Gamma_i} = \langle \Psi_\Gamma, v \rangle := \sum_{i=1}^M \langle \psi_i, v \rangle_{\Gamma_i} \quad \text{for all } v \in Y_\Gamma, \quad (2.8)$$

where  $b_\Gamma(\cdot, \cdot) : Y_\Gamma \times Y_\Gamma \rightarrow \mathbb{R}$  is a continuous bilinear form,  $\Psi_\Gamma \in Y_\Gamma'$  and  $z_i = z|_{\Gamma_i}$ ,  $v_i = v|_{\Gamma_i}$ .

To apply  $\mathcal{H}$ -matrix approximations to the discrete version of (2.8), we represent the inverse operator  $\mathcal{L}^{-1}$  using the interface map  $\mathcal{B}_\Gamma$  defined by

$$\langle \mathcal{B}_\Gamma u, v \rangle_\Gamma = b_\Gamma(u, v) \quad \text{for all } u, v \in Y_\Gamma. \quad (2.9)$$

The following statement describes the structure of the inverse  $\mathcal{L}^{-1} : Y_\Gamma' \rightarrow V$ .

**Lemma 2.1** *The representation  $\mathcal{L}^{-1} = \mathcal{E}_{\Omega \leftarrow \Gamma}^{\text{harm}} \mathcal{B}_\Gamma^{-1}$  holds, where  $\mathcal{E}_{\Omega \leftarrow \Gamma}^{\text{harm}} : Y_\Gamma \rightarrow V_\Gamma$  is the  $\mathcal{L}$ -harmonic extension from  $Y_\Gamma$  to  $V_\Gamma$ .*

*Proof.* The bilinear form  $b_\Gamma(\cdot, \cdot) : Y_\Gamma \times Y_\Gamma \rightarrow \mathbb{R}$  is symmetric, continuous and positive definite and thus the same holds for  $\mathcal{B}_\Gamma$  and  $\mathcal{B}_\Gamma^{-1} : Y_\Gamma' \rightarrow Y_\Gamma$ . Therefore the operator  $\mathcal{L}^{-1} = \mathcal{E}_{\Omega \leftarrow \Gamma}^{\text{harm}} \mathcal{B}_\Gamma^{-1}$  is well-defined. Next, we check that  $u = \mathcal{L}^{-1} \Psi_\Gamma$  solves (2.2). Green's formula yields

$$a_\Omega(u, v) = \sum_{i=1}^M a_{\Omega_i}(R_i u, R_i v) = \sum_{i=1}^M \langle \mathcal{T}_i u, v_i \rangle_{\Gamma_i} = \sum_{i=1}^M \langle \psi_i, v \rangle_{\Gamma_i} \quad \text{for all } v \in V. \quad (2.10)$$

This provides  $\mathcal{B}_\Gamma^{-1} \Psi_\Gamma = u|_\Gamma$  completing the proof.  $\blacksquare$

In the general case, we consider a conventional FEM approximation of (2.2) by piecewise linear elements on a regular triangulation that aligns with  $\Gamma$ . Let  $\mathbf{A}_\Omega \in \mathbb{R}^{I_\Omega \times I_\Omega}$  be the Galerkin-FEM stiffness matrix

$$\mathbf{A}_\Omega = \begin{pmatrix} \mathbf{A}_{II} & \mathbf{A}_{II_\Gamma} \\ \mathbf{A}_{I_\Gamma I} & \mathbf{A}_{I_\Gamma I_\Gamma} \end{pmatrix} \equiv \begin{pmatrix} \mathbf{A}_1 & \dots & 0 & \mathbf{A}_{1,\Gamma} \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathbf{A}_M & \mathbf{A}_{M,\Gamma} \\ \mathbf{A}_{\Gamma,1} & \dots & \mathbf{A}_{\Gamma,M} & \mathbf{A}_{\Gamma,\Gamma} \end{pmatrix}, \quad (2.11)$$

corresponding to the chosen FE space  $V_h \subset V$ . Here  $I_\Gamma$  is the index set corresponding to the interface degrees of freedom and  $I = I_\Omega \setminus I_\Gamma = \bigcup_{i=1}^M I_i$  is the (disjoint) union of subdomain index sets. Eliminating all interior degrees of freedom corresponding to  $I$ , we obtain the so-called *FEM Schur complement* matrix

$$\mathbf{B}_{\Gamma, \text{FEM}} := \mathbf{A}_{I_\Gamma I_\Gamma} - \mathbf{A}_{I_\Gamma I} \mathbf{A}_{II}^{-1} \mathbf{A}_{II_\Gamma} \in \mathbb{R}^{I_\Gamma \times I_\Gamma},$$

where  $\mathbf{A}_{II} = \text{blockdiag}\{\mathbf{A}_1, \dots, \mathbf{A}_M\}$  is the stiffness matrix for  $\mathcal{L}$  subject to zero Dirichlet conditions on  $\Gamma$ , hence  $\mathbf{A}_{II}^{-1} = \text{blockdiag}\{\mathbf{A}_1^{-1}, \dots, \mathbf{A}_M^{-1}\}$  can be computed in parallel. In a standard way, each of the ‘‘substructure’’ matrices  $\mathbf{A}_i^{-1}$ ,  $i = 1, \dots, M$ , can be represented by the  $\mathcal{H}$ -matrix format (cf. [8]).

Using  $\mathbf{B}_{\Gamma, \text{FEM}}$ , the original FEM system

$$\mathbf{A}_\Omega U = F, \quad U, F \in \mathbb{R}^{I_\Omega}, \quad (2.12)$$

is reduced to the interface equation

$$\mathbf{B}_{\Gamma, \text{FEM}} U_\Gamma = F_\Gamma, \quad U_\Gamma, F_\Gamma \in \mathbb{R}^{I_\Gamma}, \quad \text{where } U_\Gamma = U|_{I_\Gamma}. \quad (2.13)$$

We construct the approximate direct solver for the Schur complement system (2.13) focusing on the cases of general and of piecewise constant coefficients. In the latter case, the matrix  $\mathbf{B}_{\Gamma, \text{FEM}}$  can be computed by

BEM with cost  $\mathcal{O}(N_\Gamma \log^q N_\Gamma)$ , where  $N_\Gamma = \text{card}(I_\Gamma)$ , while for general coefficients the cost is  $\mathcal{O}(N_\Omega \log^q N_\Omega)$  (cf. [8]). Furthermore,  $\mathbf{B}_{\Gamma, FEM}$  is proved to be of almost linear cost in  $N_\Gamma$  concerning operations for storage and for the matrix-by-vector multiplication. Due to the  $\mathcal{H}$ -matrix arithmetic, our approximate inverse Schur complement matrix  $\mathbf{B}_{\Gamma, FEM}^{-1}$  again needs almost linear complexity  $\mathcal{O}(N_\Gamma \log^q N_\Gamma)$ .

Introduce the FE trace space  $Y_N := V_h|_\Gamma \subset Y_\Gamma$  with  $N = N_\Gamma = \dim Y_N$ . Based on the representation in Lemma 2.1 and using the  $\mathcal{H}$ -matrix approximation to the operators involved, we can construct an approximate direct solver of almost linear complexity in  $N_\Gamma$  that realises the action  $\mathcal{B}_\Gamma^{-1} \Psi_\Gamma$ . For this purpose we split the numerical realisation of  $\mathcal{L}^{-1} = \mathcal{E}_{\Omega \leftarrow \Gamma}^{\text{harm}} \mathcal{B}_\Gamma^{-1}$  into three independent steps:

- (i) Computation of a functional  $\Psi_{\Gamma, h} \in Y'_\Gamma$  approximating  $\Psi_\Gamma$ ;
- (ii) An  $\mathcal{H}$ -matrix approximation to the discrete interface operator  $\mathcal{B}_\Gamma^{-1}$ ;
- (iii) Implementation of a discrete  $\mathcal{L}$ -harmonic extension operator  $\mathcal{E}_{\Omega \leftarrow \Gamma}^{\text{harm}}$ .

In Step (i), we define  $\Psi_{\Gamma, h} \in Y'_N$  by  $\langle \Psi_{\Gamma, h}, v \rangle_\Gamma := \sum_{i=1}^M \langle \psi_{ih}, v \rangle_{\Gamma_i}$  for all  $v \in Y_N$ .

Given  $\Psi_{\Gamma, h} \in Y'_N$ , we consider the Schur complement system approximating the interface equation (2.8). Let us define the local Schur complement operator  $\mathcal{T}_{i, N}$  corresponding to the discrete  $\mathcal{L}_i$ -harmonic extension based on the FEM Galerkin space  $V_{ih} := V_h|_{\Omega_i}$ , by

$$\lambda, v \in Y_N|_{\Gamma_i} : \quad \langle \mathcal{T}_{i, N} \lambda, v \rangle_{\Gamma_i} = A_{\Omega_i}(\bar{u}_i, \bar{v}), \quad (2.14)$$

where

$$\bar{u}_i \in V_{ih}, \quad A_{\Omega_i}(\bar{u}_i, z) = 0 \quad \text{for all } z \in V_{ih} \cap H_0^1(\Omega_i)$$

and with an arbitrary  $\bar{v} \in V_{ih}$  such that  $\bar{v}|_{\Gamma_i} = v$ . With the aid of the local FEM-Galerkin discretisations  $\mathcal{T}_{i, N}$  of the Poincaré-Steklov maps  $\mathcal{T}_i$ , the discrete operator  $\mathcal{B}_{\Gamma, N}$  and the corresponding interface equation are given by

$$z \in Y_N : \quad \langle \mathcal{B}_{\Gamma, N} z, v \rangle_\Gamma := \sum_{i=1}^M \langle \mathcal{T}_{i, N} z_i, v_i \rangle_{\Gamma_i} = \langle \Psi_{\Gamma, h}, v \rangle_\Gamma \quad \text{for all } v \in Y_N,$$

where  $v_i := v|_{\Gamma_i}$  and  $z$  is a desired approximation to the trace  $u|_\Gamma$ .

Let  $\mathbf{A}_{\Omega_i}$  be the local stiffness matrix corresponding to  $a_{\Omega_i}(\cdot, \cdot)$ ,

$$\mathbf{A}_{\Omega_i} = \begin{pmatrix} \mathbf{A}_{\mathbf{i}\mathbf{i}} & \mathbf{A}_{\mathbf{i}\Gamma_i} \\ \mathbf{A}_{\Gamma_i\mathbf{i}} & \mathbf{A}_{\Gamma_i\Gamma_i} \end{pmatrix},$$

where  $\mathbf{i}$  and  $\Gamma_i$  correspond to the interior and boundary index sets in  $\Omega_i$ , respectively. Then we obtain the FEM Schur complement matrix

$$\mathbf{T}_{i, FEM} := \mathbf{A}_{\Gamma_i\Gamma_i} - \mathbf{A}_{\Gamma_i\mathbf{i}} \mathbf{A}_{\mathbf{i}\mathbf{i}}^{-1} \mathbf{A}_{\mathbf{i}\Gamma_i}, \quad (2.15)$$

where  $\mathbf{A}_{\mathbf{i}\mathbf{i}}$  is the stiffness matrix for  $\mathcal{L}_i$  subject to zero Dirichlet conditions on  $\Gamma_i$ . Thus,  $\mathbf{A}_{\mathbf{i}\mathbf{i}}^{-1}$  can be represented in the  $\mathcal{H}$ -matrix format (cf. [8]). Now, the corresponding matrix representation to the interface operator  $\mathcal{B}_{\Gamma, N}$  reads as

$$\langle \mathbf{B}_{\Gamma, FEM} U, Z \rangle_{I_\Gamma} = \sum_{i=1}^M \langle \mathbf{T}_{i, FEM} U_i, Z_i \rangle_{I_{\Gamma_i}} := \langle \mathcal{B}_{\Gamma, N} \mathcal{J}U, \mathcal{J}Z \rangle_\Gamma, \quad \mathbf{B}_{\Gamma, FEM} \in \mathbb{R}^{I_\Gamma \times I_\Gamma}, \quad (2.16)$$

where  $\mathcal{J} : \mathbb{R}^{I_\Gamma} \rightarrow Y_N$  is the natural bijection from the coefficient vectors into the FE functions. Here  $U_i, Z_i \in \mathbb{R}^{I_{\Gamma_i}}$ ,  $i = 1, \dots, M$ , are the local vector components defined by  $U_i = \mathbf{R}_{\Gamma_i} U$ ,  $Z_i = \mathbf{R}_{\Gamma_i} Z$ , where the connectivity matrix  $\mathbf{R}_{\Gamma_i} \in \mathbb{R}^{I_{\Gamma_i} \times I_\Gamma}$  provides the restriction of the vector  $Z \in \mathbb{R}^{I_\Gamma}$  onto the index set  $I_{\Gamma_i}$ . Finally, we obtain the interface matrix in the following explicit form

$$\mathbf{B}_{\Gamma, FEM} = \sum_{i=1}^M \mathbf{R}_{\Gamma_i}^\top \mathbf{T}_{i, FEM} \mathbf{R}_{\Gamma_i}. \quad (2.17)$$

Note that using the block Gauss elimination applied to the matrix (2.11), we obtain the following representation to  $\mathbf{A}_\Omega^{-1}$ ,

$$\mathbf{A}_\Omega^{-1} = \begin{pmatrix} \mathbf{A}_{II}^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \begin{bmatrix} \mathbf{A}_{II}^{-1} \mathbf{A}_{II\Gamma} \\ -I \end{bmatrix} \mathbf{B}_{\Gamma, FEM}^{-1} [\mathbf{A}_{I\Gamma} \mathbf{A}_{II}^{-1} - I],$$

or in explicit form

$$\mathbf{A}_\Omega^{-1} = \begin{pmatrix} \mathbf{A}_1^{-1} & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathbf{A}_M^{-1} & 0 \\ 0 & \dots & 0 & 0 \end{pmatrix} + \begin{bmatrix} \mathbf{A}_1^{-1} \mathbf{A}_{1,\Gamma} \\ \vdots \\ \mathbf{A}_M^{-1} \mathbf{A}_{M,\Gamma} \\ -I \end{bmatrix} \mathbf{B}_{\Gamma,FEM}^{-1} [\mathbf{A}_{\Gamma,1} \mathbf{A}_1^{-1} \dots \mathbf{A}_{\Gamma,M} \mathbf{A}_M^{-1} - I]. \quad (2.18)$$

If we solve the class of equations (2.12) with the right-hand side supported only by the interface index set, i.e.,  $F = (0, \dots, 0, F_\Gamma)^\top$ , then the first term in (2.18) is omitted and we arrive at the representation

$$\mathbf{A}_\Omega^{-1} = - \begin{bmatrix} \mathbf{A}_1^{-1} \mathbf{A}_{1,\Gamma} \\ \vdots \\ \mathbf{A}_M^{-1} \mathbf{A}_{M,\Gamma} \\ -I \end{bmatrix} \mathbf{B}_{\Gamma,FEM}^{-1}. \quad (2.19)$$

In this case we shall focus on the  $\mathcal{H}$ -matrix approximation to the Schur complement inverse  $\mathbf{B}_{\Gamma,FEM}^{-1}$ .

### 3 Discrete Interface Equation by the Galerkin BEM

Next we focus on the explicit matrix representation  $\mathbf{B}_{\Gamma,BEM}$  to the interface map  $\mathcal{B}_\Gamma$  in (2.9) using the BEM-Galerkin approximation with Lagrange multipliers (cf. [12, 14]).

Consider the classical boundary integral representations involving weakly singular, hypersingular and double layer potential operators  $\mathcal{V}_i$ ,  $\mathcal{D}_i$  and  $\mathcal{K}_i$ , respectively, defined by

$$\begin{aligned} (\mathcal{V}_i u)(x) &= \int_{\Gamma_i} g(x,y) u(y) dy, & (\mathcal{K}_i u)(x) &= \int_{\Gamma_i} \frac{\partial}{\partial n_y} g(x,y) u(y) dy, \\ (\mathcal{K}'_i u)(x) &= \int_{\Gamma_i} \frac{\partial}{\partial n_x} g(x,y) u(y) dy, & (\mathcal{D}_i u)(x) &= -\frac{\partial}{\partial n_x} \int_{\Gamma_i} \frac{\partial}{\partial n_y} g(x,y) u(y) dy, \end{aligned} \quad (3.1)$$

where  $g(x,y)$  is the corresponding singularity function (cf. [6]). In the following, we consider the model case

$$a_{\Omega_i}(u,v) := \mu_i \int_{\Omega_i} \nabla u \nabla v dx, \quad \mu_i > 0. \quad (3.2)$$

In particular, the singularity function of the Laplace operator  $\mathcal{L} = -\Delta$  in  $\mathbb{R}^d$  is given by  $g(x,y) = -\frac{1}{2\pi} \log|x-y|$  for  $d=2$  and by  $g(x,y) = \frac{1}{4\pi}|x-y|^{-1}$  for  $d=3$ , where  $|x-y|$  is the Euclidean distance.

We start from the familiar identity for the Calderon projection applied to the Cauchy data on  $\Gamma_i$ , which is a consequence of classical representation formulae in BEM (see, e.g., [2, 6, 19]),

$$\begin{pmatrix} \frac{1}{2}I - K_i & V_i \\ D_i & \frac{1}{2}I + K'_i \end{pmatrix} \begin{pmatrix} u_i \\ \delta_i \end{pmatrix} = \begin{pmatrix} u_i \\ \delta_i \end{pmatrix}, \quad (3.3)$$

where  $\delta_i = \partial \bar{u} / \partial n$  is the conormal derivative of the harmonic function  $\bar{u}$  satisfying  $-\Delta \bar{u} = 0$  in  $\Omega_i$  and  $\bar{u}|_{\Gamma_i} = u_i$ .

First, we introduce the *modified Calderon projection*  $\mathcal{C}_{\Gamma_i}$  defined by

$$\mathcal{C}_{\Gamma_i} \begin{pmatrix} u_i \\ \delta_i \end{pmatrix} := \begin{pmatrix} \mu_i \mathcal{D} & \frac{1}{2}I + \mathcal{K}'_i \\ -\frac{1}{2}I - \mathcal{K}_i & \mu_i^{-1} \mathcal{V}_i \end{pmatrix} \begin{pmatrix} u_i \\ \delta_i \end{pmatrix} = \begin{pmatrix} \delta_i \\ 0 \end{pmatrix} \quad (3.4)$$

(cf. [14]), applied to the  $\mathcal{L}_i$ -harmonic function with  $\delta_i = \mu_i \partial \bar{u} / \partial n$  and  $\bar{u}$  as above. The relation (3.4) provides a base for the explicit construction of saddle-point boundary variational equations for the Dirichlet, Neumann and mixed boundary conditions as well. The key point is that the Schur complement equation corresponding to (3.4) reads as

$$\mathcal{T}_i u_i := \mu_i \left( \mathcal{D}_i + \left( \frac{1}{2}I + \mathcal{K}'_i \right) \mathcal{V}_i^{-1} \left( \frac{1}{2}I + \mathcal{K}_i \right) \right) u_i = \delta_i, \quad (3.5)$$

providing an explicit symmetric representation to the Poincaré-Steklov map in terms of boundary integral operators. As a by-product, we shall obtain a symmetric positive definite discretisation of the Poincaré-Steklov operator  $\mathcal{T}_i$  using the corresponding BEM-Galerkin approximations to the classical boundary integral operators  $\mathcal{K}_i$ ,  $\mathcal{V}_i$  and  $\mathcal{D}_i$ .

As a simple example, consider the Neumann boundary value problem in  $\Omega_i$ , i.e., given  $\delta_i \in L_i := H^{-1/2}(\Gamma_i)$ , we search for  $u_i \in X_i := H^{1/2}(\Gamma_i)$  being the trace of the corresponding  $\mathcal{L}_i$ -harmonic function. Then the pair  $(u_i, \delta_i) \in \Sigma_i := X_i \times L_i$  satisfies the skew-symmetric system of equations

$$\mathcal{C}_{\Gamma_i} \begin{pmatrix} u \\ \lambda \end{pmatrix} = \begin{pmatrix} \delta_i \\ 0 \end{pmatrix},$$

where  $\lambda$  plays the role of a Lagrange multiplier (in fact,  $\lambda = \delta_i$ ). Introducing the associated bilinear form  $c_{\Gamma_i} : \Sigma_i \times \Sigma_i \rightarrow \mathbb{R}$ , the above system can be transformed to the uniquely solvable variational formulation (cf. [12])

$$\begin{aligned} c_{\Gamma_i}(u, \lambda; v, \eta) &:= \mu_i(\mathcal{D}_i u, v) + ((\tfrac{1}{2}I + \mathcal{K}'_i)\lambda, v) - ((\tfrac{1}{2}I + \mathcal{K}_i)u, \eta) + \mu_i^{-1}(\mathcal{V}_i \lambda, \eta) \\ &= (\delta_i, v) \quad \text{for all } (v, \eta) \in X_i \times L_i. \end{aligned} \quad (3.6)$$

In fact, it is easy to show that  $c_{\Gamma_i}(\cdot, \cdot)$  is  $X_i \times L_i$ -elliptic on the subspace  $X_{i,1} := \{u \in X_i : \langle u, 1 \rangle = 0\} \subset X_i$ , which implies the unique solvability of (3.6) due to the Lax-Milgram Lemma.

Let  $X_{ih} \times L_{ih} \subset X_i \times L_i$  be the FE space of piecewise linear functions with respect to a quasi-uniform mesh on  $\Gamma$  that aligns with the skeleton  $\Gamma = \cup \Gamma_i$ . The variational Galerkin equation corresponding to (3.6) reads as:

Find  $(u, \lambda) \in X_{ih} \times L_{ih}$  such that

$$c_{\Gamma_i}(u, \lambda; v, \eta) = (\delta_i, v) \quad \text{for all } (v, \eta) \in X_{ih} \times L_{ih}. \quad (3.7)$$

Transforming (3.7) to the matrix form and taking the Schur complement with respect to the Lagrange multiplier  $\lambda$ , we are led to the symmetric representation

$$\mathbf{T}_{i,BEM} := \mu_i (\mathbf{D}_{ih} + (\tfrac{1}{2}\mathbf{I}_{ih}^T + \mathbf{K}_{ih}^T) \mathbf{V}_{ih}^{-1} (\tfrac{1}{2}\mathbf{I}_{ih} + \mathbf{K}_{ih})), \quad (3.8)$$

where  $\mathbf{D}_{ih}$ ,  $\mathbf{K}_{ih}$  and  $\mathbf{V}_{ih}$  are the Galerkin stiffness matrices of the boundary integral operators and  $\mathbf{I}_{ih}$  is the corresponding mass matrix.

Similar to the single-domain equation (3.6), we consider a skew-symmetric interface problem for  $M > 1$  (see equation (3.9) below). Let us introduce the trace space  $\Sigma_\Gamma := Y_\Gamma \times \Lambda_\Gamma$  with  $\Lambda_\Gamma := \prod_{i=1}^M H^{-1/2}(\Gamma_i)$  and equipped with the weighted norm

$$\|P\|_{\Sigma_\Gamma}^2 = \|u\|_{Y_\Gamma}^2 + \sum_{j=1}^M \mu_j^{-1} \|\lambda_j\|_{H^{-1/2}(\Gamma_j)}^2, \quad \text{where } P = (u, \lambda) \in \Sigma_\Gamma, \lambda = (\lambda_1, \dots, \lambda_M).$$

We define the interface bilinear form  $c_\Gamma : \Sigma_\Gamma \times \Sigma_\Gamma \rightarrow \mathbb{R}$  by

$$c_\Gamma(P, Q) := \sum_{i=1}^M \langle \mathcal{C}_{\Gamma_i} P_i, Q_i \rangle_{\Gamma_i} \equiv \sum_{i=1}^M c_{\Gamma_i}(P_i, Q_i) \quad \text{for all } P = (u, \lambda), Q = (v, \eta) \in \Sigma_\Gamma$$

with  $\mathcal{C}_{\Gamma_i}$  given by (3.4). Here  $P_i = (R_i u, \lambda_i)$  is the corresponding restriction of  $P$  onto  $\Gamma_i$ . Using the representation (3.6) in each subdomain, the original interface problem (cf. (2.8)) will be reduced to the following skew-symmetric variational interface equation:

$$\begin{aligned} &\text{Given } \Psi_\Gamma \in Y'_\Gamma, \text{ find } P = (u, \lambda) \in \Sigma_\Gamma \text{ such that} \\ c_\Gamma(P, Q) &= \langle \Psi_\Gamma, v \rangle_\Gamma \quad \text{for all } Q = (v, \eta) \in \Sigma_\Gamma. \end{aligned} \quad (3.9)$$

Introducing the FE Galerkin ansatz space  $\Sigma_h := Y_N \times \Lambda_h$  with  $\Lambda_h := \prod_{i=1}^M L_{ih}$ , we arrive at the corresponding BEM-Galerkin saddle-point system of equations:

$$\begin{aligned} &\text{Given } \Psi_\Gamma \in Y'_\Gamma, \text{ find } P_h = (u_h, \lambda_h) \in Y_N \times \Lambda_h \text{ such that} \\ c_\Gamma(P_h, Q) &= \langle \Psi_\Gamma, v \rangle_\Gamma \quad \text{for all } Q = (v, \eta) \in Y_N \times \Lambda_h. \end{aligned} \quad (3.10)$$

We further assume  $\mathcal{V}_i$ ,  $i = 1, \dots, M$ , to be positive definite. For  $d = 3$  this is no restriction, while for  $d = 2$  it will be satisfied in the case  $\text{diam } \Omega_i < 1$  (in practice the above condition can be achieved by scaling the computational domain  $\Omega$ ).

Items (i), (ii) in the next statement are the refined version of Theorems 2, 3 in [12].

**Theorem 3.1** (i) *The bilinear form  $c_\Gamma : \Sigma_\Gamma \times \Sigma_\Gamma \rightarrow \mathbb{R}$  is continuous and  $\Sigma_\Gamma$ -elliptic uniformly in  $h$  and  $\mu_i$ ,  $i = 1, \dots, M$ .*

(ii) *The optimal error estimate*

$$\|P_h - P\|_{\Sigma_\Gamma}^2 \leq C \inf_{(w, \mu) \in \Sigma_h} \sum_{i=1}^M \left[ \mu_i |u_i - w_i|_{H^{1/2}(\Gamma_i)}^2 + \mu_i^{-1} \|\lambda_i - \mu_i\|_{H^{-1/2}(\Gamma_i)}^2 \right] \quad (3.11)$$

holds, where  $P_h$  solves (3.10) and  $C$  does not depend on  $h$  and  $\mu_i$ .

(iii) *Let  $\mathbf{T}_{i,BEM}$  be the local BEM Schur complement given by (3.8). Then the BEM Schur complement matrix (representing  $\mathbf{B}_\Gamma$  by making use of (3.10)) takes the form*

$$\langle \mathbf{B}_{\Gamma,BEM} Z, V \rangle_{I_\Gamma} = \sum_{i=1}^M \langle \mathbf{T}_{i,BEM} Z_i, V_i \rangle_{I_{\Gamma_i}} = \sum_{i=1}^M \langle \mathbf{R}_{\Gamma_i}^\top \mathbf{T}_{i,BEM} \mathbf{R}_{\Gamma_i} Z, V \rangle_{I_\Gamma}, \quad (3.12)$$

which implies the explicit representation  $\mathbf{B}_{\Gamma,BEM} = \sum_{i=1}^M \mathbf{R}_{\Gamma_i}^\top \mathbf{T}_{i,BEM} \mathbf{R}_{\Gamma_i}$  with  $\mathbf{B}_{\Gamma,BEM} \in \mathbb{R}^{I_\Gamma \times I_\Gamma}$ .

*Proof.* Continuity of  $c_\Gamma$  follows by

$$c_\Gamma(u, \lambda; v, \eta) = \sum_{i=1}^M \mu_i (\mathcal{D}_i u_i, v_i) + ((\frac{1}{2}I + \mathcal{K}'_i) \lambda_i, v_i) - ((\frac{1}{2}I + \mathcal{K}_i) u_i, \eta_i) + \mu_i^{-1} (\mathcal{V}_i \lambda_i, \eta_i),$$

due to the continuity of the boundary integral operators involved. First, we note that due to the trace lemma (for seminorms) applied in each subdomain

$$\inf_{z \in V_i: z|_{\Gamma_i} = u} a_{\Omega_i}(u, u) \leq C \mu_i |u|_{H^{1/2}(\Gamma_i)}^2,$$

the norm equivalence

$$C_1 \sum_{i=1}^M \mu_i |u_i|_{1/2}^2 \leq \|u\|_{Y_\Gamma}^2 \leq C_2 \sum_{i=1}^M \mu_i |u_i|_{1/2}^2 \quad \text{for all } u \in Y_\Gamma \quad (3.13)$$

holds, uniformly in  $h$  and  $\mu_i$ . Now, for the pairs  $z = (u, \lambda) \in X_i \times L_i$ , let us define the quadratic form  $b_i(z; z) := \mu_i |u|_{1/2}^2 + \frac{1}{\mu_i} \|\lambda\|_{-1/2}^2 + 2|u|_{1/2} \|\lambda\|_{-1/2}$ . Then the continuity of  $c_\Gamma$  follows by the Cauchy-Schwarz inequality

$$\begin{aligned} c_\Gamma(P; Q) &\leq C \sum_{i=1}^M \left[ \mu_i |u_i|_{1/2} |v_i|_{1/2} + \frac{1}{\mu_i} \|\lambda_i\|_{-1/2} \|\eta_i\|_{-1/2} + \|\lambda_i\|_{-1/2} |v_i|_{1/2} + \|\eta_i\|_{-1/2} |u_i|_{1/2} \right] \\ &\leq C \left( \sum_{i=1}^M b_i(u_i, \lambda_i; u_i, \lambda_i) \right)^{1/2} \left( \sum_{i=1}^M b_i(v_i, \eta_i; v_i, \eta_i) \right)^{1/2} \\ &\leq 4C \left( \sum_{i=1}^M \mu_i |u_i|_{1/2}^2 + \frac{1}{\mu_i} \|\lambda_i\|_{-1/2}^2 \right)^{1/2} \left( \sum_{i=1}^M \mu_i |v_i|_{1/2}^2 + \frac{1}{\mu_i} \|\eta_i\|_{-1/2}^2 \right)^{1/2} \\ &\leq C \|P\| \|Q\|, \quad (P = (u, \lambda), Q = (v, \eta)) \end{aligned}$$

using the simple bound  $2ab \leq \mu_i a^2 + \frac{1}{\mu_i} b^2$ ,  $a, b \in \mathbb{R}_+$ . Furthermore, the norm equivalence (3.13) then implies  $\Sigma_\Gamma$ -ellipticity due to the representation

$$c_\Gamma(u, \lambda; u, \lambda) = \sum_{i=1}^M \mu_i (\mathcal{D}_i u_i, u_i) + \mu_i^{-1} (\mathcal{V}_i \lambda_i, \lambda_i),$$

together with the positive definiteness of  $\mathcal{D}_i$  and  $\mathcal{V}_i$ , i.e.,

$$(\mathcal{D}_i u, u) \geq c_{\mathcal{D}} |u|_{H^{1/2}(\Gamma_i)}^2, \quad (\mathcal{V}_i u, u) \geq c_{\mathcal{V}} \|u\|_{H^{-1/2}(\Gamma_i)}^2 \quad \text{for some } c_{\mathcal{D}}, c_{\mathcal{V}} > 0.$$

Now item (ii) follows by Céa's Lemma. Assertion (iii) is due to the BEM-Galerkin structure of the discrete saddle-point system (3.10). In fact, making use of (3.10) in the matrix form and eliminating the vector components corresponding to  $\lambda_h$  leads to the matrix representation (3.12) of  $\mathbf{B}_{\Gamma}$ .  $\blacksquare$

One can see that the accuracy of our BEM-Galerkin approximation is proved to be of optimal order with respect to the weighted energy norm  $\|\cdot\|_{\Sigma_{\Gamma}}$  for a class of functions in  $H^{1/2+s}(\Gamma) \times \prod_{i=1}^M H^{-1/2+s}(\Gamma_i)$ ,  $s > 0$ , characterised by a certain Sobolev regularity (cf. Theorem 3.1).

**Remark 3.2** *The results above remain valid if  $L_{ih}$  is the space of piecewise constant finite elements.*

**Remark 3.3** *The corresponding non-symmetric representation is given by*

$$\mathcal{T}_i := \mu_i \mathcal{V}_i^{-1} \left( \frac{1}{2} I + \mathcal{K}_i \right). \quad (3.14)$$

Using the Galerkin ansatz space  $X_{ih} \times L_{ih}$  as above, we consider the approximation  $\mathcal{T}_{i,BEM} := \mu_i \mathcal{V}_{ih}^{-1} \left( \frac{1}{2} I + \mathcal{K}_{ih} \right)$  of  $\mathcal{T}_i$  by substituting the corresponding BEM-Galerkin operators in (3.14). Then one obtains the non-symmetric matrix representation

$$\mathbf{T}_{i,BEM} := \mu_i \mathbf{V}_{ih}^{-1} \left( \frac{1}{2} \mathbf{I}_{ih} + \mathbf{K}_{ih} \right),$$

which is simpler to implement than the symmetric one (cf. (3.8)). However, in the present paper this representation will not be analysed.

For general discussions, we skip the subscripts *FEM* and *BEM* and just use the notation  $\mathbf{B}_{\Gamma}$ . In the next section, we consider the  $\mathcal{H}$ -matrix approximation to  $\mathbf{B}_{\Gamma}$  using the corresponding local approximations to  $\mathbf{T}_{i,FEM}$  and  $\mathbf{T}_{i,BEM}$ , and then we construct the hierarchical data-sparse representation to the interface matrix inverse  $\mathbf{B}_{\Gamma}^{-1}$ .

## 4 $\mathcal{H}$ -Matrix Approximation to $\mathbf{B}_{\Gamma}$ and $\mathbf{B}_{\Gamma}^{-1}$

For the FEM-Galerkin approximations (cf. (2.17)), first, we represent  $\mathbf{A}_{II}^{-1}$  in the hierarchical format, then we perform the formatted multiplications  $\mathbf{A}_{\Gamma_i I} \mathbf{A}_{II}^{-1} \mathbf{A}_{I \Gamma_i}$  and addition with  $\mathbf{A}_{\Gamma_i \Gamma_i}$ . Hence, in the case of generic variable coefficients, the computation of  $\mathbf{T}_{i,FEM}$  amounts to the cost  $\mathcal{O}(N_{\Omega_i} \log^q N_{\Omega_i})$ .

Using the BEM-Galerkin representation, our goal is an algorithm of almost linear complexity in  $N_{\Gamma} := \dim Y_N$  to compute the  $\mathcal{H}$ -matrix representation of both  $\mathbf{B}_{\Gamma}$  and  $\mathbf{B}_{\Gamma}^{-1}$ . It is based on the observation that each BEM-Galerkin matrix involved in the representation for  $\mathbf{T}_{i,BEM}$  (cf. (3.8)) can be computed with  $\mathcal{O}(N_{i,\Gamma} \log^q N_{i,\Gamma})$  complexity. Using the  $\mathcal{H}$ -matrix arithmetics, one can then compute the corresponding  $\mathcal{H}$ -matrix representation of  $\mathbf{T}_{i,BEM}$ .

Since the index set  $I_{\Gamma}$  corresponds to a quasi-uniform grid on  $\Gamma$ , one can represent  $\mathbf{B}_{\Gamma}$  in the  $\mathcal{H}$ -matrix format with the partitioning  $P_2(I_{\Gamma} \times I_{\Gamma})$  based on the standard admissibility condition and then compute the approximate  $\mathcal{H}$ -matrix inverse with almost linear cost  $\mathcal{O}(N_{\Gamma_i} \log^q N_{\Gamma_i})$ . As an alternative, the so-called weakly admissible partitioning (cf. [11]) can be also applied.

We compute an approximate inverse matrix in three steps as follows:

**Algorithm DII** (direct interface inverse)

- Evaluate all the local Schur complements (cf. (2.15), (3.8)) in the  $\mathcal{H}$ -matrix format.
- Construct an admissible block partitioning of the product index set  $I_{\Gamma} \times I_{\Gamma}$  and fill the corresponding blocks of  $\mathbf{B}_{\Gamma}$  by low-rank matrices<sup>2</sup> using the local Schur complements  $\mathbf{T}_{i,BEM}$  or  $\mathbf{T}_{i,FEM}$  as the input data.
- Compute the inverse matrix  $\mathbf{B}_{\Gamma}^{-1}$  by using the  $\mathcal{H}$ -matrix arithmetic.

<sup>2</sup>We make use of the easy approach to calculate a low-rank approximation of blocks in the hierarchical partitioning  $P_2(I_{\Gamma} \times I_{\Gamma})$ . The approach is based on a SVD recompression of blocks  $b \in P_2(I_{\Gamma} \times I_{\Gamma})$  obtained as a sum of a fixed number of subblocks extracted as rank- $k$  submatrices in the local Schur complements  $\mathbf{T}_{i,BEM}$  or  $\mathbf{T}_{i,FEM}$ , represented by  $\mathcal{H}$ -matrices.

At the first stage of our inversion algorithm (cf. Algorithm DII), having available all the local  $\mathcal{H}$ -matrices  $\mathbf{T}_{i,BEM}$  or  $\mathbf{T}_{i,FEM}$ , we compute the  $\mathcal{H}$ -matrix representation of  $\mathbf{B}_\Gamma$ . Note that we require no compatibility between the partitioning  $P_2(I_\Gamma \times I_\Gamma)$  and the corresponding ones  $P_2(I_{\Gamma_i} \times I_{\Gamma_i})$  used for the representation of the local  $\mathcal{H}$ -matrices  $\mathbf{T}_{i,BEM}$  or  $\mathbf{T}_{i,FEM}$ ,  $i = 1, \dots, M$ .

Now, we explain the construction of an admissible partitioning  $P_2(I_\Gamma \times I_\Gamma)$  of the “interface” index set  $I_\Gamma$ . First, the cluster tree  $T_{I_\Gamma}$  corresponding to the skeleton  $\Gamma$  has to be constructed. This is done by using a cardinality balanced *binary-space partitioning* (BSP) algorithm (cf. [4]). The basic idea of BSP is to divide a given part of  $\Gamma$  into two disjoint sets  $\Gamma_0$  and  $\Gamma_1$  by determining the vector  $v_{\max}$  of the dimension of  $N_\Gamma$  and ordering all indices of  $I_\Gamma$  with respect to  $v_{\max}$ . The sons  $\Gamma_0$  and  $\Gamma_1$  of  $\Gamma$  are afterwards defined as the first and second half of this ordered set, ensuring  $||\Gamma_0| - |\Gamma_1|| \leq 1$ . An example of this procedure is shown in Figure 1.

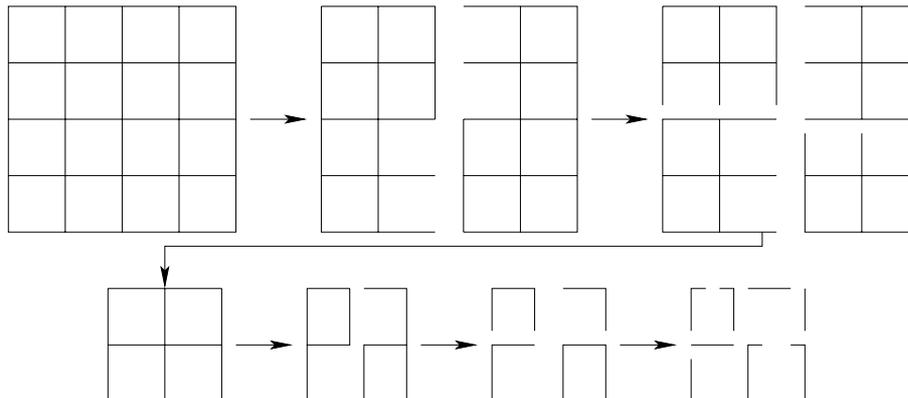


Figure 1: Construction of the clustertree  $T_{I_\Gamma}$ .

The structure of the cluster tree inherits the typical features of the corresponding constructions for 1D and 2D problems. In fact, on the first levels  $\ell = 0, \dots, L_0$  with  $L_0 = \mathcal{O}(\log M)$ , the index partitioning is similar to those for the index set corresponding to the coarse mesh FE space associated with our domain decomposition (geometric partitioning). Applying the standard admissibility condition, all admissible blocks contain only zero submatrices (as in the case with the FE stiffness matrices). The corresponding sparsity constant  $c_{sp}$  (see [5, 10]) would correspond to that one arising in FEM approximations.

On the second stage, corresponding to levels  $\ell = L_0 + 1, \dots, L$ , the leaves of the final cluster tree are sets of degrees of freedom corresponding to one-dimensional manifolds, therefore the further partitionings can be simplified. Since usually  $\log M \ll L = \mathcal{O}(N_\Omega)$ , we can see that the block structure of an admissible partitioning is rather similar to that arising for one-dimensional surfaces. Since a lower spatial dimension leads to a better sparsity constant, this property makes the algorithm faster. Note that nonzero blocks arise only in the second stage of our algorithm, i.e., for levels  $\ell = L_0 + 1, \dots, L$ .

## 5 Possible Application in FETI Methods

In this section we discuss the iterative version of our Schur complement method applied in the framework of the so-called Finite Element Tearing and Interconnecting (FETI) methods (cf. [3, 1, 15, 17]). The BEM based version of the FETI methods, the so-called BETI approach was described in [16]. The FETI/BETI method is recognised as one of the most powerful versions of modern *parallel iterative domain decomposition techniques*. The FETI system of equations to be solved is algebraically equivalent to the Schur complement equation

$$\mathbf{T}_\Gamma U = F := \sum_{i=1}^M \mathbf{R}_{\Gamma_i}^T F_i, \quad U, F \in \mathbb{R}^{I_\Gamma}, \quad (5.1)$$

where  $F_i = \{\langle \psi_i, \phi_j \rangle\}_{j \in I_{\Gamma_i}}$ , and the matrix  $\mathbf{T}_\Gamma = \sum_{i=1}^M \mathbf{R}_{\Gamma_i}^T \mathbf{T}_i \mathbf{R}_{\Gamma_i}$  can be derived by any of the approaches described above (it may be  $\mathbf{T}_i = \mathbf{T}_{i,FEM}$  or  $\mathbf{T}_i = \mathbf{T}_{i,BEM}$ ). In contrast to the situation with our approximate direct solver, now the vector components are given on each subdomain boundary  $\Gamma_i$  separately. The global continuity is then enforced by Lagrange multipliers leading to a saddle point problem that can be solved

by a preconditioned iterative method via its dual formulation. Both fast calculation of the residual and an implementation of the corresponding interface preconditioner, are based on the  $\mathcal{H}$ -matrix approximation to  $\mathbf{T}_i$  and  $\mathbf{T}_i^{-1}$ .

In the traditional way, we derive the FETI/BETI formulation starting from the equivalent minimisation problem. Due to  $a_0 > 0$  in (2.1), all local matrices  $\mathbf{T}_i$ ,  $i = 1, \dots, M$  are invertible (otherwise, one has to apply the corresponding pseudo-inverse  $\mathbf{T}_i^+$ ). Define a functional

$$\Phi(V) := \sum_{i=1}^M \left[ \frac{1}{2} \langle \mathbf{T}_i V_i, V_i \rangle_{I_{\Gamma_i}} - \langle F_i, V_i \rangle_{I_{\Gamma_i}} \right], \quad V = \bigoplus_{i=1}^M V_i, \quad V_i \in \mathbb{R}^{I_{\Gamma_i}},$$

and introduce matching matrices  $\mathbf{B}_i \in \mathbb{R}^{I_{\Gamma} \times I_{\Gamma_i}}$ , where each row is related with a pair of matching nodes. Each row has the entries 1 and  $-1$  for the indices corresponding to the matching nodes and 0 otherwise.

Now equation (5.1) is equivalent to the solution of a constraint minimisation problem

$$\Phi(U) = \min_{V_1, \dots, V_M: \sum_{i=1}^M \mathbf{B}_i V_i = 0} \Phi(V). \quad (5.2)$$

Introducing the Lagrange multiplier  $\Lambda$ , problem (5.2) is reduced to the saddle point problem

$$\begin{pmatrix} \mathbf{T}_1 & \dots & 0 & \mathbf{B}_1^T \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathbf{T}_M & \mathbf{B}_M^T \\ \mathbf{B}_1 & \dots & \mathbf{B}_M & 0 \end{pmatrix} \begin{pmatrix} U_1 \\ \vdots \\ U_M \\ \Lambda \end{pmatrix} = \begin{pmatrix} F_1 \\ \vdots \\ F_M \\ 0 \end{pmatrix}. \quad (5.3)$$

With  $\mathbf{T}_D := \text{blockdiag}\{\mathbf{T}_1, \dots, \mathbf{T}_M\}$ ,  $\mathbf{B} := \{\mathbf{B}_1, \dots, \mathbf{B}_M\}$  and  $F := \{F_1, \dots, F_M\}$ , we obtain the dual formulation

$$\mathbf{B} \mathbf{T}_D^{-1} \mathbf{B}^T \Lambda = -\mathbf{T}_D^{-1} \mathbf{B}^T F$$

which can be solved by an iterative PCG method with a spectrally close preconditioner  $\mathbf{C}$  of the form

$$\mathbf{C}^{-1} = \mathbf{G}^T \mathbf{T}_D \mathbf{G}.$$

Different proposals for the choice of a matrix  $\mathbf{G}$  can be found in the literature on the FETI methods (cf. [1, 15, 17] and references therein). The important observation is that both matrices  $\mathbf{T}_D$  and  $\mathbf{T}_D^{-1} = \text{blockdiag}\{\mathbf{T}_1^{-1}, \dots, \mathbf{T}_M^{-1}\}$  can be computed in parallel and then stored in the  $\mathcal{H}$ -matrix format with almost linear cost in  $N_{\Gamma}$ . Hence, the same is true for the corresponding matrix-by-vector multiplication with  $\mathbf{B} \mathbf{T}_D^{-1} \mathbf{B}^T$  and  $\mathbf{G}^T \mathbf{T}_D \mathbf{G}$ , provided that a matrix  $\mathbf{G}$  can be implemented with linear expense in  $N_{\Gamma}$ . Hence, our approach can be directly incorporated into the FETI (resp. BETI) iterative domain decomposition methods leading to a linear-logarithmic cost in  $N_{\Omega}$  (resp. in  $N_{\Gamma}$ ) in the case of generic variable (resp. piecewise constant) coefficients.

## 6 Numerical Results

### 6.1 FEM-Galerkin Approximation

In the first numerical example, we simplify the situation and apply *Algorithm DII* to all blocks using the SVD compression of the corresponding admissible matrix blocks in  $\mathbf{B}_{\Gamma, FEM}$ , considered in the full format. This algorithm leads to a polynomial cost on the preprocessing step, however, in this calculation we only investigate the  $\mathcal{H}$ -matrix approximability of  $\mathbf{B}_{\Gamma, FEM}$  and its inverse. Our fast direct algorithm (of almost linear cost) also exploits the hierarchical format of the local matrices  $\mathbf{T}_{i, FEM}$  (same for  $\mathbf{T}_{i, BEM}$ ).

The following tables show numerical results for the scaled Laplacian in  $\Omega_i$  with randomly chosen coefficients  $\mu_i \in (0, 1]$  (cf. (3.2)). Presented are the times for computing  $\mathbf{T}_{i, FEM}$ , for the  $\mathcal{H}$ -matrix inversion of  $B = \mathbf{B}_{\Gamma, FEM}$ ,  $\mathbf{B}_{\Gamma, FEM}^{-1}$  and for its matrix-by-vector multiplication (MV) as well as for the accuracy of this inversion (computed on a SunFire 6800 (900 MHz)).

Here  $\|I - B \mathbf{B}_{\mathcal{H}}^{-1}\|_2$  denotes the spectral norm. The results in the first table correspond to a decomposition of a square into  $6 \times 6$  subsquares. In the second table,  $8 \times 8$  subdomains were used. Note that the computing

times  $\mathbf{T}_{i,BEM}$  for  $N_\Omega \approx 4 \cdot 10^6$  and  $N_\Omega \approx 16 \cdot 10^6$  are about 30 *sec* and 100 *sec*, respectively<sup>3</sup>. One can see the almost linear complexity of the inversion algorithm. The moderate growth of the relative error is due to the choice of a *fixed*  $k$  (in the theory,  $k$  should grow logarithmically in  $N_{\Gamma_i}$ , see Fig. 2).

6 × 6 domains ( $k = 9$ )					
$N_\Omega$	$N_\Gamma$	$t(\mathbf{T}_{i,FEM})$	$t(\mathbf{B}_{\Gamma,FEM}^{-1})$	$t(MV)$	$\ I - BB_{\mathcal{H}}^{-1}\ _2$
16 641	1 245	0.6 <i>sec</i>	10.7 <i>sec</i>	1.36 <sub>10-2</sub> <i>sec</i>	7.7 <sub>10-6</sub>
66 049	2 525	12.2 <i>sec</i>	30.3 <i>sec</i>	3.98 <sub>10-2</sub> <i>sec</i>	8.0 <sub>10-6</sub>
263 169	5 085	105.1 <i>sec</i>	94.2 <i>sec</i>	9.43 <sub>10-2</sub> <i>sec</i>	4.6 <sub>10-5</sub>
1 050 625	10 205	696.2 <i>sec</i>	218.1 <i>sec</i>	1.85 <sub>10-1</sub> <i>sec</i>	7.1 <sub>10-5</sub>

8 × 8 domains ( $k = 9$ )					
$N_\Omega$	$N_\Gamma$	$t(\mathbf{T}_{i,FEM})$	$t(\mathbf{B}_{\Gamma,FEM}^{-1})$	$t(MV)$	$\ I - BB_{\mathcal{H}}^{-1}\ _2$
16 641	1 729	0.1 <i>sec</i>	13.9 <i>sec</i>	2.26 <sub>10-2</sub> <i>sec</i>	6.9 <sub>10-6</sub>
66 049	3 521	3.8 <i>sec</i>	41.2 <i>sec</i>	5.38 <sub>10-2</sub> <i>sec</i>	2.3 <sub>10-5</sub>
263 169	7 105	43.3 <i>sec</i>	126.8 <i>sec</i>	1.27 <sub>10-1</sub> <i>sec</i>	3.9 <sub>10-5</sub>
1 050 625	14 273	180.7 <i>sec</i>	326.7 <i>sec</i>	2.66 <sub>10-1</sub> <i>sec</i>	4.4 <sub>10-5</sub>

If we are interested in an efficient preconditioning, the local rank  $k$  can be chosen adaptively to achieve the required accuracy  $\varepsilon$  (see Fig. 2 showing  $\varepsilon$  depending on the rank  $k$ ).

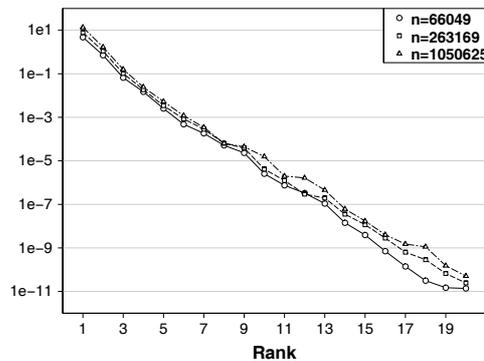


Figure 2: Preconditioning with low local ranks.

## 6.2 BEM-Galerkin Approximation

The numerical results below are based on the BEM-representation (3.8) for the local Schur complement with piecewise constant FE for the Galerkin space  $L_{ih}$  (cf. Remark 3.2). To compute the matrix entries of the corresponding stiffness matrices we use the OSTBEM code (cf. [18]). In general, we construct the  $\mathcal{H}$ -matrix representation of all four matrices involved based on the block structure via standard admissibility criteria. However, in this particular numerical example, we have a relatively small subdomain problem size  $N_{\Gamma_i}$  so that the matrix  $\mathbf{T}_{i,BEM}$  can be easily computed in the full matrix format ( $t(\mathbf{T}_{i,BEM})$  is the corresponding computational time). For comparison, in the case of  $N_\Omega = 1\,050\,625$ ,  $4\,198\,401$  and  $16\,785\,409$  the corresponding cost of the  $\mathcal{H}$ -matrix arithmetics is about 10, 30 and 100 *sec*, respectively (compared with 6.6, 62, 7, 555.4 *sec* in the following table).

<sup>3</sup> $t(\mathbf{T}_{i,BEM})$  includes only the dominating cost of two matrix-matrix multiplications and one matrix inversion in the  $\mathcal{H}$ -matrix format (cf. (3.8)).

6 × 6 domains ( $k = 9$ )

$N_\Omega$	$N_\Gamma$	$t(\mathbf{T}_{i,BEM})$	$t(\mathbf{B}_{\Gamma,BEM}^{-1})$	$t(MV)$	$\ I - BB_{\mathcal{H}}^{-1}\ _2$
16 641	1 245	0.04 sec	6.0 sec	$5.1_{10^{-3}}$ sec	$3.3_{10^{-5}}$
66 049	2 525	0.2 sec	20.9 sec	$2.6_{10^{-2}}$ sec	$1.4_{10^{-5}}$
263 169	5 085	1.0 sec	64.8 sec	$6.7_{10^{-2}}$ sec	$4.4_{10^{-5}}$
1 050 625	10 205	6.6 sec	167.3 sec	$1.4_{10^{-1}}$ sec	$4.4_{10^{-5}}$
4 198 401	20 445	62.7 sec	453.2 sec	$3.1_{10^{-1}}$ sec	$5.7_{10^{-5}}$
16 785 409	40 925	555.4 sec	1075.6 sec	$6.3_{10^{-1}}$ sec	$7.7_{10^{-5}}$

Extrapolating these results by making use of the  $\mathcal{H}$ -matrix format for all matrices, problem sizes of about 250 million unknowns should be reachable.

### 6.3 Multilevel Evaluation of Local Schur complement

We present numerical results illustrating the potential efficiency of a *direct multilevel domain-decomposition method* by the recursive Schur complement evaluation (see §5.2 in [8]). To compute the local Schur complement matrix  $\mathbf{T}_{i,FEM}$  in each subdomain  $\Omega_i$ , we apply the same domain decomposition algorithm as in §2, by making use of the decomposition  $\Omega_i = \bigcup_{j=1}^M \Omega_{ij}$ , that now does not require to compute the local inverse  $\mathbf{A}_{\Omega_i}^{-1}$ . Instead, we have to compute  $M$  times an  $\mathcal{H}$ -matrix inverse of the size  $N_i/M$  plus inversion of the “small” interface matrix. We benefit from:

- (a) A reduction of the computational time and relaxed requirements on the memory;
- (b) good scalability of the corresponding parallel algorithm for large number of processors (cf. [8]).

The effect in item (a) is related to the observation that we have only linear-logarithmic scaling for the complexity of the  $\mathcal{H}$ -matrix inverse, so that the logarithmic factor is really visible (see the table below). Hence we can see that  $M \cdot W(A_{\Omega_{ij}}^{-1}) \leq \sigma W(A_{\Omega_i}^{-1})$  (with  $\sigma \approx 1/3$  observed in the table below). Here and in the following  $W(\cdot)$  denotes the cost of the corresponding matrix operation. If we perform  $L \geq 1$  levels of recursion then the relation  $N_{L+1} = M^L N_1$  holds, where  $N_{L+1}$  and  $N_1$  mean the problem size for the initial (level  $\ell = L + 1$ ) and the smallest refined (level  $\ell = 1$ ) domains, respectively. Now the total work on level  $L + 1$  can be estimated by

$$W_{L+1} = M^L \mathcal{O}(N_1 \log^q N_1) = \mathcal{O}(N_{L+1} \log^q N_1)$$

(we ignore the asymptotically lower cost to handle the interface matrices), which indicates that the logarithmic factor in the complexity estimate can be relaxed since one can assume  $\log^q N_1 = \mathcal{O}(1)$ .

Fig. 3 below represents examples of multilevel decomposition of  $\Omega$ . The multilevel parallel algorithm

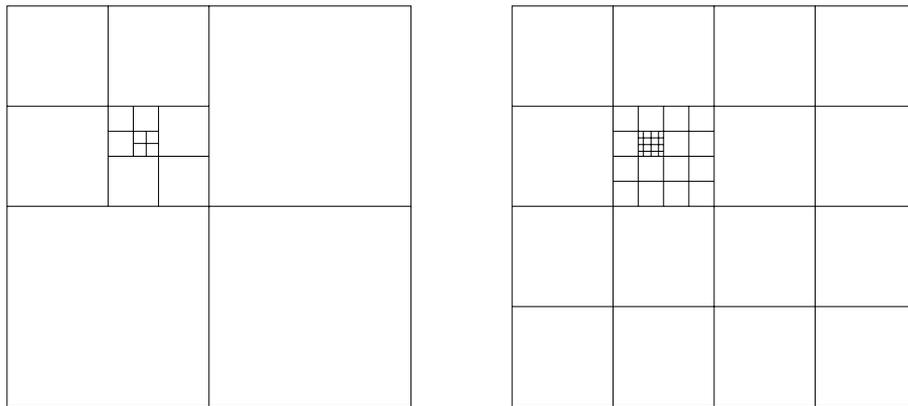


Figure 3: Multilevel  $2 \times 2$  (left) and  $4 \times 4$  decompositions.

based on  $2 \times 2$  decomposition is illustrated by Fig. 4, where subdomains on different levels are associated with different processors.

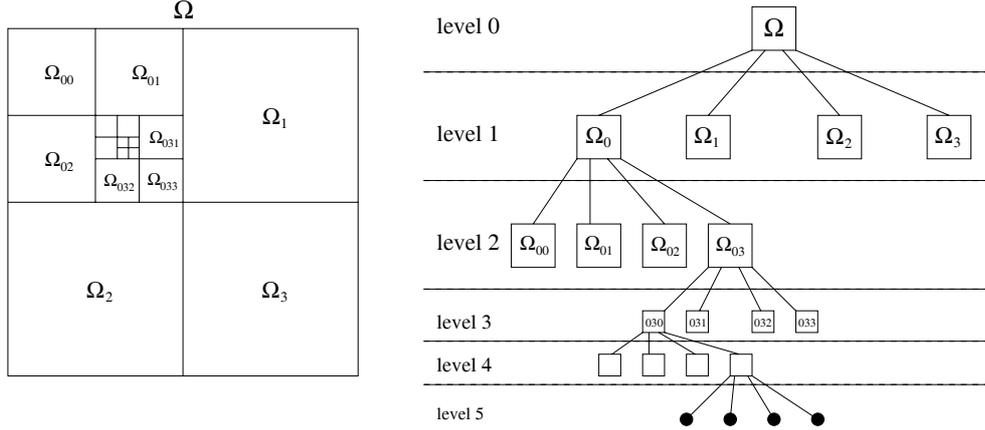


Figure 4: Multilevel parallel algorithm based on  $2 \times 2$  decomposition.

In the following we use a  $4 \times 4$  decomposition. We introduce  $L \geq 1$  levels of recursion,  $\ell = 1, \dots, L + 1$  with  $L = 4$ . We start from level  $\ell = 5$  with the problem size  $N_5 = 1\,050\,625$ . Now the degrees of freedom and the four subdomains on level  $\ell = 4$  will be further decomposed into four parts and so on until we reach level  $\ell = 1$ . The problem size on level  $\ell = i$  is  $N_i = N_1 4^{i-1}$ ,  $N_1 = 4225$  for  $i = 1, \dots, L + 1$ . On each subdomain of level  $\ell = 3, \dots, L + 1$  one has the matrix size  $N_{\ell-2}$ , thus we recursively apply the algorithm on level  $\ell - 2$  to compute the local inverse matrix  $A_{i,\ell}^{-1}$  on level  $\ell$ . This leads to the following recursion for the complexity bound:

$$W(A_{i,\ell}^{-1}) = 16W(A_{i,\ell-2}^{-1}) + W(B_{\Gamma,\ell-2}^{-1}).$$

Based on the table below, the simple calculation

$$W^{ML}(A_{4,\ell}^{-1}) = 16(16 \times 0.1 \text{ sec} + 0.8 \text{ sec}) + 16.9 \text{ sec} \approx 1 \text{ min},$$

shows that we gain a factor about 33 compared with 2020 sec depicted in the last line of our table. Similarly, an extrapolation using the two smaller grids exhibits that our direct solver applied to the problems with  $N_\Omega = 4 \cdot 10^6$ ,  $N_\Omega = 16 \cdot 10^6$ , would take about 113 sec, 1080 sec, respectively, for each subdomain.

4  $\times$  4 domains ( $k = 9$ )

$N_\Omega$	$N_\Gamma$	$t(\mathbf{T}_{i,FEM})$	$t(\mathbf{B}_{\Gamma,FEM}^{-1})$	$t(MV)$	$\ I - AA_{\mathcal{H}}^{-1}\ _2$
4225	369	0.1 sec	0.8 sec	$1.20_{10^{-3}}$ sec	$3.2_{10^{-6}}$
16641	753	3.8 sec	3.7 sec	$3.20_{10^{-3}}$ sec	$4.2_{10^{-6}}$
66049	1521	43.2 sec	16.9 sec	$9.10_{10^{-3}}$ sec	$7.7_{10^{-6}}$
263169	3057	317.4 sec	48.3 sec	$4.18_{10^{-2}}$ sec	$1.3_{10^{-5}}$
1050625	6129	2020.1 sec	118.8 sec	$8.92_{10^{-1}}$ sec	$2.1_{10^{-5}}$

Concerning the parallelisation issue, suppose that we have a multiprocessor system with

$$p = M^L,$$

processors with shared memory, where  $M$  is the number of subdomains on each level of decomposition. Then distributing properly all  $p$  processors between  $L$  levels using the tree structure (we put  $M$  processors on level  $L$ , then associate with each of them  $M$  processors on the next level and so on), we naturally enjoy the good scalability with respect to a large number of processors.

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