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Inexact Fast Multipole Boundary Element Tearing and Interconnecting Methods

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Abstract

The Boundary Element Tearing and Interconnecting (BETI) methods have recently been introduced as boundary element counterparts of the well–established Finite Element Tearing and Interconnecting (FETI) methods. In this paper we present inexact data–sparse versions of the BETI methods which avoid the elimination of the primal unknowns and dense matrices. The data–sparse approximation of the matrices and the preconditioners involved is fully based on Fast Multipole Methods (FMM). This leads to robust solvers which are almost optimal with respect to the asymptotic complexity estimates.

1 Introduction

[8] have recently introduced the BETI methods as boundary element counterparts of the well–established FETI methods which were proposed by [3]. We refer the reader to the monograph by [12] for more information and references to FETI and FETI–DP methods. In particular, we mention the paper by [5] who introduced and investigated the inexact FETI technique that avoids the elimination of the primal unknowns (displacements).

In this paper we introduce inexact BETI methods for solving the inhomogeneous Dirichlet boundary value problem (BVP) for the homogeneous potential equation in 3D bounded domains, where all matrices and preconditioners involved in the BETI solver are data-sparse via FMM representations. However, instead of symmetric and positive definite systems, we finally have to solve two–fold saddle point problems. The proposed iterative solver and preconditioner result in an almost optimal solver the complexity of which is proportional to the numbers of unknowns on the skeleton up to some polylogarithmical factor. More precisely, the solver requires $\mathcal{O}((H/h)^{(d-1)}(1+\log(H/h))^4 \log \varepsilon^{-1})$ arithmetical operations in a parallel regime and $\mathcal{O}((H/h)^{(d-1)}(1+\log(H/h))^2)$ storage units per processor, where $d = 3$ in the 3D case considered here, and $\varepsilon \in (0,1)$ is the relative accuracy of the iteration error in a suitable norm. H and h denote the usual scalings of the subdomains and the boundary elements, respectively. Moreover, the solvers are robust with respect to large coefficient jumps. For the sake of simplicity, we present here only the case where all subdomains are non-floating. All results remain valid for the general case that is discussed together with some other issues including other preconditioners in the forthcoming paper by [6] where the reader can also find the proofs in detail.

The rest of the paper is organized as follows. In Section 2, we introduce the fast multipole boundary element domain decomposition (DD) method. Section 3 is devoted to the inexact BETI method. In Section 4, we describe the ingredients from which the preconditioner and the solver for the two–fold saddle point problem that we finally have to solve is built. In Section 5, we present and discuss the results of our numerical experiments. Finally, we draw some conclusions.

2 Fast Multipole Boundary Element DD Methods

Let us consider the Dirichlet BVP for the potential equation

$$-\text{div}[a(x)\nabla\hat{u}(x)] = 0 \text{ for } x \in \Omega \subset I\!\!R^3, \quad \hat{u}(x) = g(x) \text{ for } x \in \Gamma = \partial\Omega, \tag{2.1}$$

with given Dirichlet data $g \in H^{1/2}(\Gamma)$ as a typical model problem, where Ω is a bounded Lipschitz domain that is assumed to be decomposed into p non–overlapping subdomains Ω_i with Lipschitz boundaries $\Gamma_i = \partial\Omega_i$. We further assume that the coefficient function $a(\cdot)$ in the potential equation (2.1) is piecewise constant such that $a(x) = a_i > 0$ for $x \in \Omega_i$, $i = 1,\ldots,p$.
The solution $\hat{u}$ of (2.1) is obviously harmonic in all subdomains Ω_i. Using the representation formula and its normal derivative on Γ_i, we can reformulate the BVP (2.1) as a DD boundary integral variational problem living on the skeleton $\Gamma_S = \cup_{i=1}^p \Gamma_i$ of the DD, see [2] and [4]. After homogenization of the Dirichlet boundary condition via the ansatz $\hat{u} = \hat{g} + u$ with $\hat{g}_{|\Gamma} = g$ and $u_{|\Gamma} = 0$, this DD boundary integral variational problem can be written as mixed variational problem of form: find $t = (t_1, t_2, \ldots, t_p) \in T = T_1 \times T_2 \times \ldots \times T_p = H^{-1/2}(\Gamma_1) \times H^{-1/2}(\Gamma_2) \times \ldots \times H^{-1/2}(\Gamma_p)$ and $u \in U = \{v_{|\Gamma_S} : v \in H_0^1(\Omega)\}$ such that

$$a_i \left[\langle \tau_i, V_i t_i \rangle_{\Gamma_i} - \langle \tau_i, (\frac{1}{2}I + K_i) u_{|\Gamma_i} \rangle_{\Gamma_i} \right] = a_i \langle \tau_i, (\frac{1}{2}I + K_i)\hat{g}_{|\Gamma_i} \rangle_{\Gamma_i} \tag{2.2}$$

for all $\tau_i \in T_i$, $i = 1, 2, \ldots, p$, and

$$\sum_{i=1}^p a_i \left[-\langle (\frac{1}{2}I + K_i')t_i, v_{|\Gamma_i} \rangle_{\Gamma_i} - \langle D_i u_{|\Gamma_i}, v_{|\Gamma_i} \rangle_{\Gamma_i} \right] = \sum_{i=1}^p a_i \langle D_i \hat{g}_{|\Gamma_i}, v_{|\Gamma_i} \rangle_{\Gamma_i} \tag{2.3}$$

for all $v \in U$, where V_i, K_i, K_i', and D_i denote the local single layer potential operator, the local double layer potential operator, its adjoint, and the local hypersingular boundary integral operator, respectively.
Let us now introduce the boundary element trial spaces $U_h = S_h^1(\Gamma_S) = \text{span}\{\varphi_m\}_{m=1}^M \subset U$ and $T_{i,h} = S_h^0(\Gamma_i) = \text{span}\{\psi_k^i\}_{k=1}^{N_i} \subset T_i$ spanned by continuous piecewise linear basis functions φ_m and by piecewise constant basis functions ψ_k^i with respect to a regular globally quasi–uniform boundary element mesh with the average mesh size h on Γ_S and Γ_i, respectively. The Galerkin discretization finally leads to a large–scale symmetric and indefinite system of form

$$\begin{pmatrix} a_1\widetilde{V}_{1,h} & & & -a_1\widetilde{K}_{1,h}R_{1,h} \\ & \ddots & & \vdots \\ & & a_p\widetilde{V}_{p,h} & -a_p\widetilde{K}_{p,h}R_{p,h} \\ -a_1R_{1,h}^\top\widetilde{K}_{1,h}^\top & \ldots & -a_pR_{p,h}^\top\widetilde{K}_{p,h}^\top & -\widetilde{D}_h \end{pmatrix} \begin{pmatrix} \underline{\widetilde{t}}_1 \\ \vdots \\ \underline{\widetilde{t}}_p \\ \underline{\widetilde{u}} \end{pmatrix} = \begin{pmatrix} a_1\underline{\widetilde{g}}_1 \\ \vdots \\ a_p\underline{\widetilde{g}}_p \\ \underline{\widetilde{f}} \end{pmatrix} \tag{2.4}$$

for defining the coefficient vectors $\underline{\widetilde{t}}_i \in I\!\!R^{N_i}$ and $\underline{\widetilde{u}} \in I\!\!R^M$. The matrices $\widetilde{V}_{i,h}$, $\widetilde{K}_{i,h}$ and $\widetilde{D}_h$ are data–sparse FMM approximations to the originally dense Galerkin matrices $V_{i,h}$, $K_{i,h}$ and $D_h = \sum_{i=1}^p a_i R_{i,h}^\top D_{i,h} R_{i,h}$, respectively. The use of the FMM is indicated by the "tilde" on the matrices and vectors. The FMM approximation of these matrices reduces the quadratic complexity with respect to the number of unknowns to an almost linear one, but without disturbing the accuracy. The restriction operator $R_{i,h}$ maps some global coefficient vector $\underline{v} \in I\!\!R^M$ to the local vector $\underline{v}_i \in I\!\!R^{M_i}$ containing those components of $\underline{v}$ which correspond to Γ_i only, $i = 1, 2, \ldots, p$. The matrices $R_{i,h}$ are Boolean matrices which are sometimes also called subdomain connectivity matrices.

3 Inexact BETI Methods

Introducing the local unknowns $\underline{\widetilde{u}}_i = R_{i,h}\underline{\widetilde{u}}$ as individual variables and enforcing again the global continuity of the potentials by the constraints

$$\sum_{i=1}^{p} B_i \underline{\widetilde{u}}_i = \underline{0}, \tag{3.5}$$

we immediately arrive at the two–fold saddle point problem

$$\begin{pmatrix} V & K & 0 \\ K^\top & -D & B^\top \\ 0 & B & 0 \end{pmatrix} \begin{pmatrix} \underline{t} \\ \underline{u} \\ \underline{\lambda} \end{pmatrix} = \begin{pmatrix} \underline{g} \\ \underline{f} \\ \underline{0} \end{pmatrix} \tag{3.6}$$

that is obviously equivalent to (2.4), where $\underline{t} = (\underline{\widetilde{t}}_1, \ldots, \underline{\widetilde{t}}_p)^\top$, $\underline{u} = (\underline{\widetilde{u}}_1, \ldots, \underline{\widetilde{u}}_p)^\top$, and $\underline{\lambda} \in I\!R^L$ is the vector of the Lagrange multipliers. The matrices $V = \mathrm{diag}(a_i \widetilde{V}_{i,h})$, $K = \mathrm{diag}(-a_i \widetilde{K}_{i,h})$ and $D = \mathrm{diag}(a_i \widetilde{D}_{i,h})$ are block–diagonal whereas $B = (B_1, \ldots, B_p)$. As in the FETI method each row of the matrix B is connected with a pair of matching nodes across the subdomain boundaries. The entries of such a row are 1 and -1 for the indices corresponding to the matching nodes on the interface (coupling boundaries) $\Gamma_C = \Gamma_S \setminus \Gamma$ and 0 otherwise. We assume here that the number of constraints at some matching node is equal to the number of matching subdomains minus one. This method of a minimal number of constraints respectively multipliers is called non–redundant (see, e.g., [12]). The matrices $\widetilde{V}_{i,h}$ are symmetric and positive definite (SPD). For non–floating subdomains assumed in this paper the matrices $\widetilde{D}_{i,h}$ are SPD as well. In the more complicated case of floating subdomains, the matrices $\widetilde{D}_{i,h}$ must be modified due to the non-trivial kernel $\ker(\widetilde{D}_{i,h}) = \mathrm{span}\{\underline{1}_i\}$, where $\{\underline{1}_i\} = (1, \ldots, 1)^\top$, see [8] or [6].

4 Solvers and Preconditioners

Following [13], who extended the special conjugate gradient (CG) method proposed by [1] for solving one–fold saddle point problems, to n–fold saddle point problems, we are able to construct a very efficient saddle point conjugate gradient (SPCG) solver for our two–fold saddle point problem (3.6) provided that appropriate precondtioners for the single layer potential matrices $\widetilde{V}_{i,h}$, the local boundary element Schur complements $\widetilde{S}_{i,h} = \widetilde{D}_{i,h} + \widetilde{K}_{i,h}^\top \widetilde{V}_{i,h}^{-1} \widetilde{K}_{i,h}$ and the BETI Schur complement $\widetilde{F} = \sum_{i=q+1}^{p} a_i^{-1} B_i \widetilde{S}_{i,h}^{-1} B_i^\top$ are available. We propose the following data–sparse preconditioners which are also used in our numerical experiments:

1. *Data–sparse algebraic or geometric multigrid preconditoners $\widetilde{\mathcal{V}}_{i,h}$ for the matrices $\widetilde{V}_{i,h}$:* For the geometric multigrid method, [7] proved the spectral equivalence inequalities

   $$\underline{c}_V \widetilde{\mathcal{V}}_{i,h} \le \widetilde{V}_{i,h} \le \overline{c}_V \widetilde{\mathcal{V}}_{i,h} \tag{4.7}$$

   where the spectral equivalence constants $\underline{c}_V$ and $\overline{c}_V$ are positive and independent of h and H.

2. *Data–sparse opposite order preconditioners $\widetilde{\mathcal{S}}_{i,h}$ for the local boundary element Schur complements $\widetilde{S}_{i,h}$:* In order to construct efficient preconditioners $\widetilde{\mathcal{S}}_{i,h}$, we apply the concept of boundary integral operators of the opposite order proposed by [11]. Based on the local trial space $U_{i,h} = S_h^1(\Gamma_i)$ of piecewise linear basis functions φ_m^i, as used for the Galerkin discretization of the local hypersingular boundary integral operators D_i, we define the Galerkin matrices $\bar{V}_{i,h}$ and $\bar{M}_{i,h}$ by

   $$\bar{V}_{i,h}[n,m] = \langle \varphi_n^i, V\varphi_m^i \rangle_{\Gamma_i}, \quad \bar{M}_{i,h}[n,m] = \langle \varphi_n^i, \varphi_m^i \rangle_{\Gamma_i}$$

for $m, n = 1, \ldots, M_i$. The inverse preconditioners are now defined by

$$\widetilde{\mathcal{S}}_{i,h}^{-1} \;=\; \bar{M}_{i,h}^{-1}\widetilde{\widetilde{V}}_{i,h}\bar{M}_{i,h}^{-1} \quad \text{for } i = 1, \ldots, p, \tag{4.8}$$

where the tilde on the top of $\widetilde{\widetilde{V}}_{i,h}$ again indicates that the application of the discrete single layer potential $\bar{V}_{i,h}$ is realized by using the FMM. In [6] we prove the spectral equivalence inequalities

$$\underline{c}_S(1+\log(H/h))^{-2}\widetilde{\mathcal{S}}_{i,h} \le \widetilde{S}_{i,h} \le \overline{c}_S\widetilde{\mathcal{S}}_{i,h}, \tag{4.9}$$

where the spectral equivalence constants $\underline{c}_S$ and $\overline{c}_S$ are positive and independent of h and H. The log–term disappears in the case of floating subdomains.

3. *Data–sparse BETI preconditioner $\widetilde{\mathcal{F}}$ for the BETI Schur complements $\widetilde{F}$*: Following [8], we define the inverse BETI preconditioner

$$\widetilde{\mathcal{F}}_{i,h}^{-1} \;=\; (BC_a^{-1}B^T)^{-1}\sum_{i=1}^{p} B_i C_\alpha^{-1}\widetilde{D}_{i,h}C_{a,i}^{-1}B_i^\top(BC_a^{-1}B^\top)^{-1}. \tag{4.10}$$

with the help of the local data–sparse discrete hypersingular operators $\widetilde{D}_{i,h}$ and the scaling matrix $C_a = \operatorname{diag}(C_{a,i})$. The definition of the diagonal matrices $C_{a,i}$ can be found in [12]. In [6], the spectral equivalence inequalities

$$\underline{c}_F\widetilde{\mathcal{F}} \le \widetilde{F} \le \overline{c}_F(1+\log(H/h))^2\widetilde{\mathcal{F}} \tag{4.11}$$

were proved, where the spectral equivalence constants $\underline{c}_S$ and $\overline{c}_S$ are positive and independent of h, H and the a_i's (coefficients jumps). In the general case where non–floating as well as floating subdomains are present in the DD, the spectral equivalence inequalities (4.11) remain valid on an appropriate subspace.

Combining these spectral equivalence estimates with the results obtained by [13] and taking into account the complexity estimate for the FMM, we can easily prove the following theorem.

Theorem 4.1 *If the two–fold saddle point problem (3.6) is solved by the SPCG method where the preconditioner is build from the block preconditioners $\widetilde{\mathcal{V}}_{i,h}$, $\widetilde{\mathcal{S}}_{i,h}$, and $\widetilde{\mathcal{F}}$, then not more than $I(\varepsilon) = \mathcal{O}((1+\log(H/h))^2\log\varepsilon^{-1})$ iterations and $ops(\varepsilon) = \mathcal{O}((H/h)^2(1+\log(H/h))^4\log\varepsilon^{-1})$ arithmetical operations are required in order to reduce the initial error by the factor $\varepsilon \in (0,1)$ in a parallel regime. The number of iterations $I(\varepsilon)$ is robust with respect to the jumps in the coefficients. Moreover, not more than $\mathcal{O}((H/h)^2(1+\log(H/h))^2)$ storage units are needed per processor.*

The results of the theorem remain valid also in the general case where also floating subdomains are present in the domain decomposition (see [6]). The proposed SPCG solver is asymptotically almost optimal with respect to the complexity in arithmetic and storage as well as very efficient on a parallel computer with distributed memory.

Remark 4.1 *If we would use optimal preconditioners $\widetilde{\mathcal{S}}_{i,h}$ for the local boundary element Schur complements $\widetilde{S}_{i,h}$, then the number of iteration $I(\varepsilon)$ of our SPCG solver would behave like $\mathcal{O}((1+\log(H/h))\log\varepsilon^{-1})$, whereas the arithmetical complexity would decrease from $\mathcal{O}((H/h)^2(1+\log(H/h))^4\log\varepsilon^{-1})$ to $\mathcal{O}((H/h)^2(1+\log(H/h))^3\log\varepsilon^{-1})$. Such preconditioners are available. If we convert the non–floating subdomains having a Dirichlet boundary part to floating subdomains by including the Dirichlet boundary condition into the constraints, then the data–sparse opposite order preconditioners $\widetilde{\mathcal{S}}_{i,h}$ given above is optimal.*

5 Numerical Results

Let us consider the unit cube which is subdivided into eight similar subdomains. In order to check the behavior of the discretization error, we take the Dirichlet data $g = \hat{u}_{|\Gamma}$ as the trace of a regular solution $\hat{u}$ of the boundary value problem (2.1) on the boundary Γ. We perform numerical experiments for the Laplace equation ($a_i = 1$ for all $i = 1, \ldots, 8$) and for the potential equation with large jumps in the coefficients ($a_i \in \{1, 10^5\}$) (chequerboard distribution).
Starting from the coarsest grid level $L = 0$ with 192 triangles on $\cup \partial\Omega_i$, we successively refine the mesh by subdividing each triangle into four smaller similar triangles. N and M denote the total numbers of triangles and nodes, respectively. M_c is the total number of coupling nodes. The numbers of local triangles and nodes on $\partial\Omega_i$ are given by N_i and M_i, respectively. If the boundary mesh of one subdomain Ω_i on level $L = 6$ with 98.304 triangles is uniformly extended to the interior of the subdomain, then the corresponding finite element mesh would consist of 4.448.731 tetrahedrals resulting in almost 36 millions tetrahedrals for the whole computational domain. In Table 1, together with the mesh features L, N, M, M_c, N_i and M_i, the time t_1 [sec] for generating the system (3.6) and for setting up the preconditioner, the time t_2 [sec] spent by the SPCG solver, the number of iterations $I(\varepsilon)$ and the absolute $L_2(\Gamma_i)$ discretization error $\|\hat{u} - \hat{u}_h\|_{L_2(\Gamma_i)}$ are displayed. The relative accuracy ε of the iteration error is chosen to be 10^{-8}. The first line in each row for the columns t_1, t_2, $I(\varepsilon)$ and $L_2(\Gamma_i)$–error corresponds to the Laplace case whereas the second line corresponds to the case of jumping coefficients. Table 1 shows that the growth in the number of iterations and in the CPU times is in good agreement with the complexity estimates given in Theorem 4.1. The efficiency of our SPCG solver is not affected by large jumps in the coefficients of the potential equations (2.1). Moreover, the number of iterations are less than in the Laplace case. In addition, the CPU time for the finest level $L = 6$ is half of the time needed for a primal preconditioned Schur complement solver in the case of jumping coefficients. All numerical experiments were performed on standard PCs with 3.06 Mhz Intel processors and 1 GB of RAM.

L	N	M	M_c	N_i	M_i	t_1	t_2	$I(\varepsilon)$	L_2-error
0	192	63	13	24	14	0	0	6	2,8527E–03
						1	0	6	2,8527E–08
1	768	261	67	96	50	1	1	33	7,1318E–04
						1	1	29	7,1318E–09
2	3072	1089	319	384	194	5	6	36	1,7830E–04
						5	6	34	1,7830E–09
3	12288	4473	1399	1536	770	16	30	38	4,4574E–05
						15	30	36	4,4577E–10
4	49152	18153	5863	6144	3074	81	186	41	1,1143E–05
						79	172	38	1,1144E–10
5	196608	73161	24007	24576	12290	316	1469	46	2,7859E–06
						310	1346	44	2,7859E–11
6	786432	293769	97159	98304	49154	1314	7250	55	6,9647E–07
						1319	7034	49	6,9651E–12

Table 1: Numerical features for the SPCG solver.

6 Conclusions

Inexact data–sparse BETI methods introduced in this paper show an almost optimal behavior with respect to the number of iterations, the arithmetical costs and the memory consumption. Moreover, the methods are robust with respect to large jumps in the coefficients of (2.1). These results were rigorously proved and were also confirmed by our numerical experiments. The treatment of the outer Dirichlet problem as well as other boundary conditions is straightforward. Inexact data–sparse BETI methods can naturally be generalized to linear elasticity BVP including elasticity problems for almost incompressible materials (cf. [10]). Combining the results of this paper with the results on inexact FETI methods obtained by [5], we can develop inexact BETI–FETI solvers for coupled boundary and finite element equations (cf. [9] for the exact version).

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