Scalable BETI for Variational Inequalities

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Summary. We briefly review our first results concerning the development of scalable BETI based domain decomposition methods adapted to the solution of variational inequalities such as those describing the equilibrium of a system of bodies in mutual contact. They exploit classical results on the FETI and BETI domain decomposition methods for elliptic partial differential equations and our recent results on quadratic programming. The results of the numerical solution of a semicoercive model problem are given that are in agreement with the theory and illustrate the numerical scalability of our algorithm.

1 Introduction

The FETI (Finite Element Tearing and Interconnecting) domain decomposition method proposed by Farhat and Roux turned out to be one of the most successful methods for a parallel solution of linear problems described by elliptic partial differential equations and discretized by the finite element method (see [11]). Its key ingredient is a decomposition of the spatial domain into non-overlapping subdomains that are "glued" by Lagrange multipliers, so that, after eliminating the primal variables, the original problem is reduced to a small, typically equality constrained, quadratic programming problem that is solved iteratively. The time that is necessary for both the elimination and iterations can be reduced nearly proportionally to the number of the subdomains, so that the algorithm enjoys parallel scalability. Since then, many preconditioning methods were developed which guarantee also numerical scalability of the FETI methods (see, e.g., [15]). Recently Steinbach and Langer (see [13]) adapted the FETI method to the solution of problems discretized by the boundary element method. They coined their new BETI (Boundary Element Tearing and Interconnecting) method and proved its numerical scalability.

The FETI based results were recently extended to the solution of elliptic boundary variational inequalities, such as those describing the equilibrium of a system of elastic bodies in mutual contact. Using the so-called "natural coarse grid" introduced by Farhat, Mandel, and Roux (see [10]) and new algorithms for the solution of special quadratic programming problems (see [9, 4, 5]), Dostál and Horák modified the basic FETI algorithm and proved its numerical scalability also for the solution of variational inequalities (see [7]).

The latter algorithms turned out to be effective also for the solution of problems discretized by boundary elements (see [8, 2, 3]). In this paper, we review our BETI based algorithm for the solution of variational inequalities and report our theoretical results that guarantee the scalability of BETI with a natural coarse grid. Theoretical results are illustrated by numerical experiments.

2 Model Problem and Domain Decomposition

Let us consider the domain $\Omega = (0,1) \times (0,1)$ and let us denote $\Gamma_c = \{(0,y) :\ y \in [0,1]\}$ and $\Gamma_f = \partial\Omega \setminus \Gamma_c$. Moreover, let $f \in L^2(\Omega)$ satisfy

$$\int_\Omega f(x)\,\mathrm{d}x < 0 \tag{1}$$

and $g \in L^2(\Gamma_c)$. We shall look for a sufficiently smooth function u satisfying

$$-\triangle u = f \quad \text{in } \Omega, \quad \frac{\partial u}{\partial n} = 0 \quad \text{on } \Gamma_f \tag{2}$$

together with the Signorini conditions

$$u - g \geq 0, \quad \frac{\partial u}{\partial n} \geq 0, \quad \frac{\partial u}{\partial n}(u-g) = 0 \quad \text{on } \Gamma_c. \tag{3}$$

Let us decompose the domain Ω into p non-overlapping subdomains,

$$\overline{\Omega} = \bigcup_{i=1}^{p} \overline{\Omega_i},\ \Omega_i \cap \Omega_j = \emptyset \quad \text{for } i \neq j,\ \Gamma_i = \partial\Omega_i,\ \Gamma_{i,j} = \Gamma_i \cap \Gamma_j,\ \Gamma_s = \bigcup_{i=1}^{p} \Gamma_i.$$

We assume that each subdomain boundary Γ_i is Lipschitz, and that for each subdomain Ω_i we have

$$\operatorname{diam} \Omega_i < 1. \tag{4}$$

We now reformulate the problem (2), (3) as a system of local subproblems

$$-\triangle u_i = f \quad \text{in } \Omega_i, \quad \lambda_i = \frac{\partial u_i}{\partial n} = 0 \quad \text{on } \Gamma_i \cap \Gamma_f, \tag{5}$$

$$u_i - g \geq 0, \quad \lambda_i \geq 0, \quad \lambda_i(u_i - g) = 0 \quad \text{on } \Gamma_i \cap \Gamma_c \tag{6}$$

together with the so-called transmission conditions

$$u_i = u_j \quad \text{and} \quad \lambda_i + \lambda_j = 0 \quad \text{on } \Gamma_{i,j}. \tag{7}$$

We introduce the local single layer potential operator V_i, the double layer potential operator K_i, the adjoint double layer potential operator K_i', and the hypersingular boundary integral operator D_i defined by

$$\begin{aligned}
(V_i\lambda_i)(x) &= \int_{\Gamma_i} U(x,y)\lambda_i(y)\,\mathrm{d}s_y, \quad V_i: \ H^{-1/2}(\Gamma_i) \mapsto H^{1/2}(\Gamma_i),\\
(K_i u_i)(x) &= \int_{\Gamma_i} \frac{\partial}{\partial n_y} U(x,y) u_i(y)\,\mathrm{d}s_y, \quad K_i: \ H^{1/2}(\Gamma_i) \mapsto H^{1/2}(\Gamma_i),\\
(K_i'\lambda_i)(x) &= \int_{\Gamma_i} \frac{\partial}{\partial n_x} U(x,y)\lambda_i(y)\,\mathrm{d}s_y, \quad K_i': \ H^{-1/2}(\Gamma_i) \mapsto H^{-1/2}(\Gamma_i),\\
(D_i u_i)(x) &= -\frac{\partial}{\partial n_x}\int_{\Gamma_i} \frac{\partial}{\partial n_y} U(x,y) u_i(y)\,\mathrm{d}s_y, \quad D_i: \ H^{1/2}(\Gamma_i) \mapsto H^{-1/2}(\Gamma_i),
\end{aligned}$$

$x \in \Gamma_i$. The function U denotes the fundamental solution of the Laplace operator in $\mathbb{R}^2$ and it is defined by

$$U(x,y) = -\frac{1}{2\pi}\log\|x-y\| \quad \text{for } x,\, y \in \mathbb{R}^2.$$

From the assumption (4) it follows that the operator V_i is $H^{-1/2}(\Gamma_i)$-elliptic, and therefore its inversion is well-defined. Now let us define the local Dirichlet to Neumann map as

$$\lambda_i(x) = (S_i u_i)(x) - (N_i f)(x), \quad x \in \Gamma_i,$$

where S_i denotes the local Steklov-Poincaré operator given by

$$(S_i u_i)(x) = \left[D_i + (\frac{1}{2}I + K_i')V_i^{-1}(\frac{1}{2}I + K_i)\right] u_i(x), \quad x \in \Gamma_i,$$

and $N_i f$ denotes the local Newton potential given by

$$(N_i f)(x) = V_i^{-1}\left(N_{0,i} f\right)(x), \quad x \in \Gamma_i,$$

with $(N_{0,i}f)(x) = \int_{\Omega_i} U(x,y)f(y)\,\mathrm{d}y$. It can be further shown that the local Steklov-Poincaré operator $S_i: \ H^{1/2}(\Gamma_i) \mapsto H^{-1/2}(\Gamma_i)$ is bounded, symmetric, and semi-elliptic on $H^{1/2}(\Gamma_i)$. More details on the properties of the Steklov-Poincaré operator may be found, e.g., in [14].

3 Boundary Variational Formulation and Discretization

The boundary weak formulation of the problem (5), (6), (7) may be equivalently rewritten as the problem of finding $u \in \mathcal{K} = \left\{v \in H^{1/2}(\Gamma_s): \ v - g \geq 0 \text{ on } \Gamma_c\right\}$ such that

$$\mathcal{J}(u) = \min\{\mathcal{J}(v) : \ v \in \mathcal{K}\}, \tag{8}$$
$$\mathcal{J}(v) = \sum_{i=1}^{p} \left[\frac{1}{2} \int_{\Gamma_i} (S_i v|_{\Gamma_i})(x) v|_{\Gamma_i}(x) \, \mathrm{d}s_x - \int_{\Gamma_i} (N_i f)(x) v|_{\Gamma_i}(x) \, \mathrm{d}s_x \right].$$

The coercivity of the functional $\mathcal{J}$ follows (see [12]) from the condition (1). We shall now follow the technique of Langer and Steinbach (see [13]). Let us define the local boundary element space

$$Z_{i,h} = \mathrm{span}\ \left\{\psi_k^i\right\}_{k=1}^{N_i} \subset H^{-1/2}(\Gamma_i)$$

to get suitable approximations $\widetilde{S}_i$ and $\widetilde{N}_i f$ of S_i and $N_i f$. The exact definitions and results on stability can be found, e.g., in [14]. Let us further define the boundary element space on the skeleton Γ_s and its restriction on Γ_i as

$$W_h = \mathrm{span}\ \{\varphi_m\}_{m=1}^{M_0} \subset H^{1/2}(\Gamma_s) \ \text{ and } \ W_{i,h} = \mathrm{span}\ \left\{\varphi_m^i\right\}_{m=1}^{M_i} \subset H^{1/2}(\Gamma_i),$$

respectively. After the discretization of problem (8) by the Ritz method, we get the minimization problem

$$J(\mathbf{u}) = \min\{J(\mathbf{v}) : \ \mathbf{v} \in \mathbb{R}^M, \ \mathsf{B}_I \mathbf{v} \le \mathbf{c}_I, \ \mathsf{B}_E \mathbf{v} = \mathbf{o}\}, \tag{9}$$
$$J(\mathbf{v}) = \frac{1}{2}\mathbf{v}^T \widetilde{\mathsf{S}} \mathbf{v} - \mathbf{v}^T \widetilde{\mathbf{R}}$$

with $M = \sum_{i=1}^{p} M_i$ and with a positive semidefinite block diagonal stiffness matrix $\widetilde{\mathsf{S}}$. The blocks of $\widetilde{\mathsf{S}}$ and the relevant blocks of $\widetilde{\mathbf{R}}$ are given by

$$\widetilde{\mathsf{S}}_{i,h} = \mathsf{D}_{i,h} + (\frac{1}{2}\mathsf{M}_{i,h} + \mathsf{K}_{i,h})^T \mathsf{V}_{i,h}^{-1} (\frac{1}{2}\mathsf{M}_{i,h} + \mathsf{K}_{i,h}) \quad \text{and}$$
$$\widetilde{\mathbf{R}}_{i,h} = \mathsf{M}_{i,h}^T \mathsf{V}_{i,h}^{-1} \mathbf{N}_{0,i,h},$$

respectively. The boundary element matrices and the vector $\mathbf{N}_{0,i,h}$ are defined by

$$\mathsf{V}_{i,h}[l,k] = \left\langle V_i \psi_k^i, \psi_l^i \right\rangle_{L^2(\Gamma_i)}, \qquad \mathsf{M}_{i,h}[l,n] = \left\langle \varphi_n^i, \psi_l^i \right\rangle_{L^2(\Gamma_i)},$$
$$\mathsf{K}_{i,h}[l,n] = \left\langle K_i \varphi_n^i, \psi_l^i \right\rangle_{L^2(\Gamma_i)}, \qquad \mathsf{D}_{i,h}[m,n] = \left\langle D_i \varphi_n^i, \varphi_m^i \right\rangle_{L^2(\Gamma_i)},$$
$$\mathbf{N}_{0,i,h}[l] = \left\langle N_{0,i} f, \psi_l^i \right\rangle_{L^2(\Gamma_i)}$$

for $k,\, l = 1, \ldots, N_i$; $m,\, n = 1, \ldots, M_i$ and $i = 1, \ldots, p$. The inequality constraints are associated with the non-penetration condition across $\Gamma_i \cap \Gamma_c$, while the equality constraints arise from the continuity condition across the auxiliary interfaces $\Gamma_{i,j}$.

4 Dual Formulation and Natural Coarse Grid

We shall now use the duality theory to replace the general inequality constraints by the bound constraints. Let $\widetilde{\mathsf{S}}^+$ be a generalized inverse of $\widetilde{\mathsf{S}}$ satisfying $\widetilde{\mathsf{S}} = \widetilde{\mathsf{S}}\widetilde{\mathsf{S}}^+\widetilde{\mathsf{S}}$ and let R be a matrix whose columns span the kernel of

$\widetilde{\mathsf{S}}$. By introducing the Lagrange multipliers $\boldsymbol{\lambda}_I$ and $\boldsymbol{\lambda}_E$ associated with the inequalities and equalities, respectively, and denoting

$$\boldsymbol{\lambda} = \left[\boldsymbol{\lambda}_I^T,\ \boldsymbol{\lambda}_E^T\right]^T, \quad \mathsf{B} = \left[\mathsf{B}_I^T,\ \mathsf{B}_E^T\right]^T, \quad \text{and} \quad \mathbf{c} = \left[\mathbf{c}_I^T, \mathbf{o}^T\right]^T,$$

we can equivalently replace problem (9) by

$$\begin{aligned} &\Theta(\overline{\boldsymbol{\lambda}}) = \min\{\Theta(\boldsymbol{\lambda}) :\ \boldsymbol{\lambda}_I \geq \mathbf{o} \quad \text{and} \quad \widetilde{\mathsf{G}}\boldsymbol{\lambda} = \widetilde{\mathbf{e}}\}, \\ &\Theta(\boldsymbol{\lambda}) = \frac{1}{2}\boldsymbol{\lambda}^T\mathsf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T\widetilde{\mathbf{d}}, \quad \mathsf{F} = \mathsf{B}\widetilde{\mathsf{S}}^+\mathsf{B}^T, \quad \widetilde{\mathbf{d}} = \mathsf{B}\widetilde{\mathsf{S}}^+\widetilde{\mathbf{R}} - \mathbf{c}, \\ &\widetilde{\mathsf{G}} = \mathsf{R}^T\mathsf{B}^T, \quad \widetilde{\mathbf{e}} = \mathsf{R}^T\widetilde{\mathbf{R}}. \end{aligned} \tag{10}$$

The solution $\mathbf{u}$ of (9) then may be evaluated by

$$\mathbf{u} = \widetilde{\mathsf{S}}^+(\widetilde{\mathbf{R}} - \mathsf{B}^T\overline{\boldsymbol{\lambda}}) + \mathsf{R}\boldsymbol{\alpha} \quad \text{and} \quad \boldsymbol{\alpha} = (\mathsf{R}^T\widetilde{\mathsf{B}}^T\widetilde{\mathsf{B}}\mathsf{R})^{-1}\mathsf{R}^T\widetilde{\mathsf{B}}^T(\widetilde{\mathbf{c}} - \widetilde{\mathsf{B}}\widetilde{\mathsf{S}}^+(\widetilde{\mathbf{R}} - \mathsf{B}^T\overline{\boldsymbol{\lambda}})),$$

where $\widetilde{\mathsf{B}} = [\widetilde{\mathsf{B}}_I^T,\ \mathsf{B}_E^T]^T$ and $\widetilde{\mathbf{c}} = [\widetilde{\mathbf{c}}_I^T, \mathbf{o}^T]^T$, and the matrix $[\widetilde{\mathsf{B}}_I, \widetilde{\mathbf{c}}_I]$ is formed by the rows of $[\mathsf{B}_I, \mathbf{c}_I]$ corresponding to the positive entries of $\boldsymbol{\lambda}_I$. Now let us denote by T a regular matrix such that the matrix $\mathsf{G} = \mathsf{T}\widetilde{\mathsf{G}}$ has orthonormal rows. Then (see, e.g., [6]) problem (10) is equivalent to the following problem

$$\begin{aligned} &\Lambda(\overline{\boldsymbol{\lambda}}) = \min\{\Lambda(\boldsymbol{\lambda}) :\ \boldsymbol{\lambda}_I \geq -\widetilde{\boldsymbol{\lambda}}_I \quad \text{and} \quad \mathsf{G}\boldsymbol{\lambda} = \mathbf{o}\}, \\ &\Lambda(\boldsymbol{\lambda}) = \frac{1}{2}\boldsymbol{\lambda}^T\mathsf{PFP}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T\mathsf{P}\mathbf{d}, \quad \mathsf{P} = \mathsf{I} - \mathsf{Q}, \quad \mathsf{Q} = \mathsf{G}^T\mathsf{G}, \\ &\mathbf{d} = \widetilde{\mathbf{d}} - \mathsf{F}\widetilde{\boldsymbol{\lambda}}, \quad \widetilde{\boldsymbol{\lambda}} = \mathsf{G}^T\mathbf{e}, \quad \mathbf{e} = \mathsf{T}\widetilde{\mathbf{e}}. \end{aligned} \tag{11}$$

The matrices P and Q are orthogonal projectors on the kernel of G and the image of G^T, respectively, and they define the so-called natural coarse grid.

The key ingredient in the next development is the observation that there are positive constants C_1, C_2 such that

$$C_1\|\mathsf{P}\boldsymbol{\lambda}\|^2 \leq \boldsymbol{\lambda}^T\mathsf{PFP}\boldsymbol{\lambda} \leq C_2 H/h. \tag{12}$$

This nontrivial estimate is a corollary of two well-known results. The first one is the classical estimate of Farhat, Mandel, and Roux (see [10]) which gives that if F_{FETI} and P_{FETI} denote the matrices arising by an application of the above procedures to the problem discretized by sufficiently regular finite element grid with the discretization and decomposition parameters h and H, respectively, then there are positive constants C_3, C_4 such that the spectrum $\sigma(\mathsf{F}_{FETI}|\mathrm{Im}\mathsf{P}_{FETI})$ of the restriction of F_{FETI} to $\mathrm{Im}\mathsf{P}_{FETI}$ satisfies

$$\sigma(\mathsf{F}_{FETI}|\mathrm{Im}\mathsf{P}_{FETI}) \subseteq [C_3,\ C_4 H/h].$$

The second result is due to Langer and Steinbach, in particular, Lemma 3.3 of [13] which guarantees that $\mathsf{F}|\mathrm{Im}\mathsf{P}$ is spectrally equivalent to $\mathsf{F}_{FETI}|\mathrm{Im}\mathsf{P}_{FETI}$. Combining these two results, it is possible to prove (12). We shall give more details elsewhere.

5 Algorithms and Optimality

To solve the bound and equality constrained problem (11), we use our recently proposed algorithms MPRGP by Dostál and Schöberl (see [9]) and SMALBE (see [4, 5]). The SMALBE, a variant of the augmented Lagrangian method with adaptive precision control, enforces the equality constraints by the Lagrange multipliers generated in the outer loop, while auxiliary bound constrained problems are solved approximately in the inner loop by MPRGP, an active set based algorithm which uses the conjugate gradient method to explore the current face, the fixed steplength gradient projection to expand the active set, the adaptive precision control of auxiliary linear problems, and the reduced gradient with the optimal steplength to reduce the active set. The unique feature of SMALBE with the inner loop implemented by MPRGP when used to (11) is the rate of convergence in bounds on spectrum of the regular part of the Hessian of Λ (see [5]). Combining this result with the estimate (12), we get that if H/h is bounded, then there is a bound on the number of multiplications by the Hessian of Λ that are necessary to find an approximate solution $\overline{\boldsymbol{\lambda}}_{h,H}$ of (11) discretized with the decomposition parameter H and the discretization parameter h which satisfies

$$\|\mathbf{g}^P(\overline{\boldsymbol{\lambda}}_{h,H})\| \leq \varepsilon_1 \|\mathsf{P}_{h,H}\mathbf{d}_{h,H}\| \quad \text{and} \quad \|\mathsf{G}_{h,H}\overline{\boldsymbol{\lambda}}_{h,H}\| \leq \varepsilon_2 \|\mathsf{P}_{h,H}\mathbf{d}_{h,H}\|, \qquad (13)$$

where $\mathbf{g}^P$ denotes the projected gradient, whose nonzero components are those violating the KKT conditions for (11) (see, e.g., [1]).

6 Numerical Experiment

Let $f(x,y) = -1$ for $(x,y) \in \Omega$ and $g(0,y) = \sqrt{1/4 - (y-1/2)^2} - 1$ for $y \in [0,1]$. We decompose Ω into identical square subdomains with the side length H. All subdomain boundaries Γ_i were further discretized by the same regular grid with the element size h. The spaces $W_{i,h}$ and $Z_{i,h}$ were formed by piecewise linear and piecewise constant functions, respectively. For the SMALBE algorithm we used the parameters $\eta = ||\mathsf{P}\mathbf{d}||$, $\beta = 10$, and $M = 1$. The penalty parameter ρ_0 and the Lagrange multipliers $\boldsymbol{\mu}^0$ for the equality constraints were set to $10\,\|\mathsf{PFP}\|$ and $\mathbf{o}$, respectively. For the MPRGP algorithm we used parameters $\overline{\alpha} = \|\mathsf{PFP} + \rho_k \mathsf{Q}\|^{-1}$ and $\Gamma = 1$. Our initial approximation $\boldsymbol{\lambda}^0$ was set to $-\widetilde{\boldsymbol{\lambda}}$. The stopping criterion of the outer loop was chosen as

$$\left\|\mathbf{g}^P(\boldsymbol{\lambda}^k, \boldsymbol{\mu}^k, \rho_k)\right\| \leq 10^{-4}\,\|\mathsf{P}\mathbf{d}\| \quad \text{and} \quad \left\|\mathsf{G}\boldsymbol{\lambda}^k\right\| \leq 10^{-4}\,\|\mathsf{P}\mathbf{d}\|\,.$$

The results of our numerical experiments are given in Table 1. We conclude that the scalability may be observed in the solution of realistic problems.

7 Comments and Conclusions

We combined the BETI methodology with preconditioning by the "natural coarse grid" to develop a scalable algorithm for the numerical solution of

Table 1. Performance with the constant ratio $H/h = 32$.

h	H	primal dim.	dual dim.	outer iter.	CG iter.
1/64	1/2	512	197	2	48
1/128	1/4	2048	915	2	58
1/256	1/8	8192	3911	2	52
1/512	1/16	32768	16143	2	45

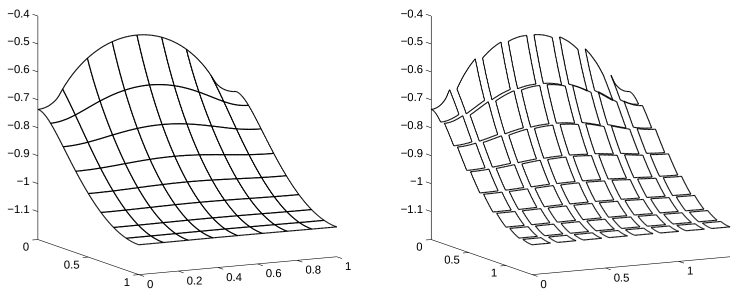

Fig. 1. Solution of the model problem with $h = 1/256$ and $H = 1/8$. On the right we emphasize the particular local solutions.

variational inequalities. The algorithm may be used for the solution of both coercive and semicoercive contact problems. Though we have restricted our exposition to a model variational inequality, our arguments are valid also for 2D and 3D contact problems of elasticity.

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