

# Theoretically Supported Scalable BETI Method for Variational Inequalities

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## Abstract

The Boundary Element Tearing and Interconnecting (BETI) methods were recently introduced as boundary element counterparts of the well established Finite Element Tearing and Interconnecting (FETI) methods. Here we combine the BETI method preconditioned by the projector to the “natural coarse grid” with recently proposed optimal algorithms for the solution of bound and equality constrained quadratic programming problems in order to develop a scalable solver for elliptic multidomain boundary variational inequalities such as those describing the equilibrium of a system of bodies in mutual contact. The key observation is that the “natural coarse grid” defines a subspace that contains the solution, so that the preconditioning affects also the nonlinear steps. The results are validated by numerical experiments.

**Keywords:** Domain decomposition, boundary elements, variational inequality, scalability, parallel algorithms, BETI

## 1 Introduction

The Boundary Element Tearing and Interconnecting (BETI) methods were introduced by Langer and Steinbach [29] as boundary element counterparts of the Finite Element Tearing and Interconnecting (FETI) domain decomposition methods proposed by Farhat and Roux [22, 23] for parallel solving of the linear problems described by elliptic partial differential equations. The key ingredient of both methods is 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, relatively well conditioned, 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 processors, so that the algorithm enjoys parallel scalability. Both the FETI and BETI procedures can be conveniently described in the framework of the duality theory of convex programming.

If either BETI or FETI procedure is applied to an elliptic variational inequality, the resulting quadratic programming problem has not only the equality

constraints, but also the non-negativity constraints. Even though the latter is a considerable complication as compared with linear problems, it seems that these duality based procedures should be even more powerful for the solution of variational inequalities than for the linear problems. The reason is that these methods do not only reduce the original problem to a smaller and better conditioned one, but they also replace for free all the inequalities by the bound constraints. Promising experimental results by Dureisseix and Farhat [18] in the FETI framework supported this claim and even indicated numerical scalability of their method. Recently, Dostál and Horák [12] used the FETI method with a “natural coarse grid” to develop a scalable algorithm for numerical solution of both coercive and semicoercive variational inequalities. The rate of convergence is given in terms of the effective condition number of the dual Schur complement of the stiffness matrix, which is known [21] to be bounded by  $CH/h$ , where  $C$  is a constant independent of the discretization and decomposition parameters  $h$  and  $H$ , respectively. We refer the reader to [12] for more comprehensive review of application of other FETI based approaches to variational inequalities, in particular those concerning application of the FETI–DP (Dual–Primal) method introduced by Farhat et al. [20].

In this paper, we describe a scalable BETI based algorithm for numerical solution of multidomain boundary variational inequalities discretized by symmetric Galerkin boundary element equations. Though the BETI part of our development is based on Langer and Steinbach [29], we could not use their preconditioning strategy. The reason is that their preconditioner transforms the bound constraints into more general inequality constraints which can not be treated by our in a sense optimal quadratic programming algorithms. Instead we use the preconditioning by so called “natural coarse grid” which is defined by the equality constraints which guarantee solvability of the dual problem. The key tool in our analysis is the observation by Langer and Steinbach [29] that the discretized Steklov–Poincaré operators generated by FETI and BETI are spectrally equivalent, so that we can exploit the analysis by Farhat, Mandel and Roux [21]. We exploit the “all floating” or “total” variant of BETI/FETI methods introduced independently by Of [30] and Dostál, Horák, and Kučera [13], respectively.

Since the nonlinearity of the boundary variational inequality is limited to the boundary, the idea to eliminate the interior unknowns by application of the boundary element (BE) method seems to be a natural step in the solution of these problems. This idea has been enhanced by several authors, see, e.g., Spann [32] and Eck, Steinbach, and Wendland [19]. The dual formulation in combination with BE was considered by Dostál et al. [14], Sadowská [31], and Bouchala, Dostál, and Sadowská [3, 4]. The boundary element approach is attractive also for the applications in contact shape optimization [17].

The paper is organized as follows. After describing a model problem, we briefly review the BETI methodology [3, 4] that turns the variational inequality into the well conditioned quadratic programming problem with bound and equality constraints. The conditioning of the dual problem is further improved by application of the projector to the natural coarse grid. Then we review our algorithms for solution of the resulting bound and equality constrained quadratic programming problem whose rate of convergence can be expressed in terms of bounds on the spectrum of the dual Schur complement matrix [8, 16, 7]. Finally, we present the main results about optimality of our method and give results of numerical experiments.

## 2 Model Problem

To simplify our exposition, we shall restrict our attention to a simple semi-coercive model problem, but our reasoning can be extended to more general problems. In particular, our analysis is valid also for a coercive variant of our model problem which can be obtained by enhancing additional Dirichlet conditions.

Let us consider the domains  $\Omega^1 := (0, 1) \times (0, 1)$  and  $\Omega^2 := (1, 2) \times (0, 1)$  with boundaries  $\Gamma^1$  and  $\Gamma^2$ , respectively. Each boundary  $\Gamma^m$  is decomposed into three parts  $\Gamma_u^m$ ,  $\Gamma_f^m$  and  $\Gamma_c^m$ ; see Figure 1. Note that  $\Gamma_u^2$  is empty. We shall be concerned with the following model problem of finding a sufficiently smooth  $(u^1, u^2)$  satisfying

$$-\Delta u^m = f \quad \text{in } \Omega^m, \quad u^1 = 0 \quad \text{on } \Gamma_u^1, \quad \frac{\partial u^m}{\partial n} = 0 \quad \text{on } \Gamma_f^m, \quad m = 1, 2, \quad (2.1)$$

together with the conditions given on  $\Gamma_c := \Gamma_c^1 = \Gamma_c^2$ :

$$u^2 - u^1 \geq 0, \quad \frac{\partial u^2}{\partial n} \geq 0, \quad \frac{\partial u^2}{\partial n}(u^2 - u^1) = 0, \quad \frac{\partial u^1}{\partial n} + \frac{\partial u^2}{\partial n} = 0. \quad (2.2)$$

The function  $f$  is defined by

$$f(x) := \begin{cases} -3 & \text{for } x \in (0, 1) \times [0.75, 1), \\ -1 & \text{for } x \in (1, 2) \times (0, 0.25], \\ 0 & \text{elsewhere in } \Omega^1 \cup \Omega^2. \end{cases}$$

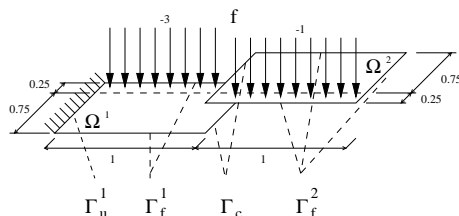


Figure 1: Model problem.

The solution  $(u^1, u^2)$  of our model problem may be interpreted as a vertical displacement of two membranes stretched by normalized horizontal forces and pressed down by forces with the density  $f$ . The left membrane  $\Omega^1$  is fixed on the left edge. The left edge of  $\Omega^2$  is not allowed to penetrate below the right edge of  $\Omega^1$ .

## 3 Domain Decomposition and Reduction to the Boundary

Let us decompose each domain  $\Omega^m$  into  $p^m$  non-overlapping Lipschitz subdomains  $\Omega_i^m$  with boundaries  $\Gamma_i^m$ ,

$$\overline{\Omega}^m = \bigcup_{i=1}^{p^m} \overline{\Omega}_i^m, \quad \Omega_i^m \cap \Omega_j^m = \emptyset \quad \text{for } i \neq j,$$

$$\Gamma_{i,j}^m := \Gamma_i^m \cap \Gamma_j^m, \quad \Gamma_s^m := \bigcup_{i=1}^{p^m} \Gamma_i^m.$$

The set  $\Gamma_s^m$  is a skeleton of  $\Omega^m$ .

Moreover, we shall assume that for each subdomain  $\Omega_i^m$  we have

$$\text{diam } \Omega_i^m < 1. \quad (3.1)$$

Now instead of the original problem (2.1), (2.2), we shall consider a system of the local subproblems

$$-\Delta u_i^m = f \quad \text{in } \Omega_i^m, \quad (3.2)$$

$$u_i^1 = 0 \quad \text{on } \Gamma_i^m \cap \Gamma_u^1, \quad \lambda_i^m := \frac{\partial u_i^m}{\partial n} = 0 \quad \text{on } \Gamma_i^m \cap \Gamma_f^m, \quad (3.3)$$

$$u_j^2 - u_i^1 \geq 0, \quad \lambda_j^2 \geq 0, \quad \lambda_j^2 (u_j^2 - u_i^1) = 0, \quad \text{and} \quad \lambda_j^2 + \lambda_i^1 = 0 \quad \text{on } \Gamma_i^1 \cap \Gamma_j^2, \quad (3.4)$$

together with the transmission conditions

$$u_i^m = u_j^m \quad \text{and} \quad \lambda_i^m + \lambda_j^m = 0 \quad \text{on } \Gamma_{i,j}^m. \quad (3.5)$$

Let us introduce the standard boundary integral operators, in particular the local single layer operator  $V_i^m$ , double layer operator  $K_i^m$ , adjoint double layer operator  $K_i'^m$ , and hypersingular operator  $D_i^m$  defined by

$$(V_i^m \lambda_i^m)(x) := \int_{\Gamma_i^m} U(x, y) \lambda_i^m(y) \, ds_y,$$

$$(K_i^m u_i^m)(x) := \int_{\Gamma_i^m} \frac{\partial}{\partial n_y} U(x, y) u_i^m(y) \, ds_y,$$

$$(K_i'^m \lambda_i^m)(x) := \int_{\Gamma_i^m} \frac{\partial}{\partial n_x} U(x, y) \lambda_i^m(y) \, ds_y,$$

$$(D_i^m u_i^m)(x) := -\frac{\partial}{\partial n_x} \int_{\Gamma_i^m} \frac{\partial}{\partial n_y} U(x, y) u_i^m(y) \, ds_y,$$

$x \in \Gamma_i^m$ . The mapping properties of these boundary integral operators may be found, e.g., in [34]. The function  $U$  is the so-called fundamental solution of the Laplace equation in  $\mathbb{R}^2$  given by

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

It follows from the assumptions and particularly from 3.1 that the operator  $V_i^m$  is  $H^{-1/2}(\Gamma_i^m)$ -elliptic, and therefore its inversion is well-defined. Now we can define the local Steklov–Poincaré operator  $S_i^m$  by

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

and the local Newton potential  $N_i^m f$  by

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

where

$$(N_{0,i}^m f)(x) := \int_{\Omega_i^m} U(x, y) f(y) \, dy.$$

It can be further shown that the local Steklov–Poincaré operator

$$S_i^m : H^{1/2}(\Gamma_i^m) \mapsto H^{-1/2}(\Gamma_i^m)$$

is bounded, symmetric, and semielliptic on  $H^{1/2}(\Gamma_i^m)$ . For more details on the properties of the Steklov–Poincaré operator, we refer, e.g., to [34].

Now we can introduce the weak formulation of the problem (3.2), (3.3), (3.4), and (3.5) reduced to the skeleton: find  $(u^1, u^2) \in \mathcal{K}$  such that

$$\sum_{m=1}^2 \sum_{i=1}^{p^m} \int_{\Gamma_i^m} (S_i^m u_i^m)(x) (v_i^m - u_i^m)(x) \, ds_x \geq \sum_{m=1}^2 \sum_{i=1}^{p^m} \int_{\Gamma_i^m} (N_i^m f)(x) (v_i^m - u_i^m)(x) \, ds_x \quad (3.6)$$

for all  $(v^1, v^2) \in \mathcal{K}$ , where

$$\mathcal{K} := \left\{ (v^1, v^2) \in H_0^{1/2}(\Gamma_s^1, \Gamma_u^1) \times H^{1/2}(\Gamma_s^2) : v^2 - v^1 \geq 0 \quad \text{on } \Gamma_c \right\},$$

and  $v_i^m$  denotes the restriction of  $v^m$  onto  $\Gamma_i^m$ . Here,  $H^{1/2}(\Gamma_s^m)$  is a trace space of  $H^1(\Omega^m)$  restricted to  $\Gamma_s^m$  equipped with the norm

$$\|v\|_{H^{1/2}(\Gamma_s^m)} := \left[ \sum_{i=1}^{p^m} \|v|_{\Gamma_i^m}\|_{H^{1/2}(\Gamma_i^m)}^2 \right]^{1/2},$$

and

$$H_0^{1/2}(\Gamma_s^1, \Gamma_u^1) := \left\{ v \in H^{1/2}(\Gamma_s^1) : v = 0 \quad \text{on } \Gamma_u^1 \right\}.$$

It is well-known that problem (3.6) is equivalent to the problem of minimization of the energy functional: find  $(u^1, u^2) \in \mathcal{K}$  such that

$$\mathcal{J}_0(u^1, u^2) = \min \left\{ \mathcal{J}_0(v^1, v^2) : (v^1, v^2) \in \mathcal{K} \right\}, \quad (3.7)$$

where

$$\mathcal{J}_0(v^1, v^2) := \sum_{m=1}^2 \sum_{i=1}^{p^m} \left[ \frac{1}{2} \int_{\Gamma_i^m} (S_i^m v_i^m)(x) v_i^m(x) \, ds_x - \int_{\Gamma_i^m} (N_i^m f)(x) v_i^m(x) \, ds_x \right].$$

Functional  $\mathcal{J}_0$  is coercive due to

$$\int_{\Omega^1 \cup \Omega^2} f(x) \, dx < 0.$$

This observation implies, see, e.g., [26], that problem (3.7) is uniquely solvable.

## 4 Approximation of the Local Steklov–Poincaré Operator and Newton Potential

Since the local Steklov–Poincaré operators  $S_i^m$  and Newton potentials  $N_i^m f$  are given only implicitly, for the practical computations we have to choose suitable approximations  $\tilde{S}_i^m$  and  $\tilde{N}_i^m f$ , e.g., as introduced in [34]. For  $v_i^m \in H^{1/2}(\Gamma_i^m)$  we have

$$(S_i^m v_i^m)(x) = (D_i^m v_i^m)(x) + \left(\frac{1}{2}I + K_i^m\right) w_i^m(x) \quad \text{for } x \in \Gamma_i^m,$$

where  $w_i^m \in H^{-1/2}(\Gamma_i^m)$  is the unique solution of the problem

$$\langle V_i^m w_i^m, \tau_i^m \rangle_{L^2(\Gamma_i^m)} = \left\langle \left(\frac{1}{2}I + K_i^m\right) v_i^m, \tau_i^m \right\rangle_{L^2(\Gamma_i^m)} \quad \text{for all } \tau_i^m \in H^{-1/2}(\Gamma_i^m). \quad (4.1)$$

Let

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

be a finite-dimensional space of trial functions. Then the Galerkin formulation of (4.1) reads: find  $w_{i,h}^m \in Z_{i,h}^m$  such that

$$\langle V_i^m w_{i,h}^m, \tau_{i,h}^m \rangle_{L^2(\Gamma_i^m)} = \left\langle \left(\frac{1}{2}I + K_i^m\right) v_i^m, \tau_{i,h}^m \right\rangle_{L^2(\Gamma_i^m)} \quad \text{for all } \tau_{i,h}^m \in Z_{i,h}^m.$$

Now we define an approximation of  $S_i^m$  by

$$(\tilde{S}_i^m v_i^m)(x) := (D_i^m v_i^m)(x) + \left(\frac{1}{2}I + K_i^m\right) w_{i,h}^m(x) \quad \text{for } x \in \Gamma_i^m.$$

Analogously we can derive an approximation of  $N_i^m f$  defined by

$$(\tilde{N}_i^m f)(x) := \lambda_{i,h}^m(x) \quad \text{for } x \in \Gamma_i^m,$$

where  $\lambda_{i,h}^m \in Z_{i,h}^m$  solves uniquely the Galerkin variational problem

$$\langle V_i^m \lambda_{i,h}^m, \tau_{i,h}^m \rangle_{L^2(\Gamma_i^m)} = \langle N_0 f, \tau_{i,h}^m \rangle_{L^2(\Gamma_i^m)} \quad \text{for all } \tau_{i,h}^m \in Z_{i,h}^m.$$

Thus, instead of (3.7), we shall consider the following problem: find  $(u^1, u^2) \in \mathcal{K}$  such that

$$\mathcal{J}(u^1, u^2) = \min \{ \mathcal{J}(v^1, v^2) : (v^1, v^2) \in \mathcal{K} \}, \quad (4.2)$$

where

$$\mathcal{J}(v^1, v^2) := \sum_{m=1}^2 \sum_{i=1}^{p^m} \left[ \frac{1}{2} \int_{\Gamma_i^m} (\tilde{S}_i^m v_i^m)(x) v_i^m(x) \, ds_x - \int_{\Gamma_i^m} (\tilde{N}_i^m f)(x) v_i^m(x) \, ds_x \right].$$

## 5 Discretization

Let

$$W_h^1 := \text{span} \{ \varphi_k^1 \}_{k=1}^{M^1} \subset H_0^{1/2}(\Gamma_s^1, \Gamma_u^1)$$

and

$$W_h^2 := \text{span} \{ \varphi_k^2 \}_{k=1}^{M^2} \subset H^{1/2}(\Gamma_s^2)$$

be the global finite-dimensional trial spaces on the skeletons  $\Gamma_s^1$  and  $\Gamma_s^2$ . We shall assume that the grids on  $\Gamma_s^1$  and  $\Gamma_s^2$  match across  $\Gamma_c$ . Then the Ritz formulation of (4.2) reads: find  $(u_h^1, u_h^2) \in \mathcal{K}_h$  such that

$$\mathcal{J}(u_h^1, u_h^2) = \min \{ \mathcal{J}(v_h^1, v_h^2) : (v_h^1, v_h^2) \in \mathcal{K}_h \}, \quad (5.1)$$

where

$$\mathcal{K}_h := \{ (v_h^1, v_h^2) \in W_h^1 \times W_h^2 : v_h^2(z_j^2) - v_h^1(z_i^1) \geq 0 \quad \text{for all matching nodes} \\ z_i^1, z_j^2 \text{ across } \Gamma_c \}.$$

Let

$$W_{i,h}^m := \text{span} \{ \varphi_k^{m,i} \}_{k=1}^{M_i^m}$$

be the restriction of  $W_h^m$  onto  $\Gamma_i^m$ . Clearly, for any  $\varphi_k^{m,i} \in W_{i,h}^m$  there exists a unique  $\varphi_l^m \in W_h^m$  satisfying  $\varphi_k^{m,i} = \varphi_l^m|_{\Gamma_i^m}$ . For any  $v_h^m \in W_h^m$  and its restriction  $v_{i,h}^m \in W_{i,h}^m$  we can compute the so-called connectivity matrix  $\mathbf{A}_i^m \in \mathbb{R}^{M_i^m \times M^m}$  such that

$$\mathbf{v}_i^m = \mathbf{A}_i^m \mathbf{v}^m, \quad (5.2)$$

where  $\mathbf{v}_i^m$  and  $\mathbf{v}^m$  are the vectors of coordinates of  $v_{i,h}^m$  and  $v_h^m$  in the bases  $\{ \varphi_k^{m,i} \}_{k=1}^{M_i^m}$  and  $\{ \varphi_k^m \}_{k=1}^{M^m}$ , respectively. Problem (5.1) is further equivalent to the problem:

find  $(\mathbf{u}^1, \mathbf{u}^2) \in K$  such that

$$J_0(\mathbf{u}^1, \mathbf{u}^2) = \min \{ J_0(\mathbf{v}^1, \mathbf{v}^2) : (\mathbf{v}^1, \mathbf{v}^2) \in K \}, \quad (5.3)$$

where

$$J_0(\mathbf{v}^1, \mathbf{v}^2) := \sum_{m=1}^2 \sum_{i=1}^{p^m} \left[ \frac{1}{2} \left( \tilde{\mathbf{S}}_{i,h}^m \mathbf{A}_i^m \mathbf{v}^m, \mathbf{A}_i^m \mathbf{v}^m \right) - \left( \tilde{\mathbf{R}}_{i,h}^m, \mathbf{A}_i^m \mathbf{v}^m \right) \right]$$

and

$$K := \left\{ (\mathbf{v}^1, \mathbf{v}^2) \in \mathbb{R}^{M^1} \times \mathbb{R}^{M^2} : \mathbf{v}^2[j] - \mathbf{v}^1[i] \geq 0 \text{ for all indices } i, j \text{ corresponding to the matching nodes } z_i^1, z_j^2 \text{ across } \Gamma_c \right\}.$$

Here,  $\tilde{\mathbf{S}}_{i,h}^m \in \mathbb{R}^{M_i^m \times M_i^m}$  is the discrete approximate local Steklov–Poincaré operator

$$\tilde{\mathbf{S}}_{i,h}^m := \mathbf{D}_{i,h}^m + \left( \frac{1}{2} \mathbf{M}_{i,h}^m + \mathbf{K}_{i,h}^m \right)^T (\mathbf{V}_{i,h}^m)^{-1} \left( \frac{1}{2} \mathbf{M}_{i,h}^m + \mathbf{K}_{i,h}^m \right)$$

and  $\tilde{\mathbf{R}}_{i,h}^m \in \mathbb{R}^{M_i^m}$  is the discrete approximate local Newton potential

$$\tilde{\mathbf{R}}_{i,h}^m := (\mathbf{M}_{i,h}^m)^T (\mathbf{V}_{i,h}^m)^{-1} \mathbf{N}_{0,i,h}^m.$$

The boundary element matrices and vector  $\mathbf{N}_{0,i,h}^m$  are given by

$$\begin{aligned} \mathbf{V}_{i,h}^m[k, l] &:= \left\langle V_i^m \psi_l^{m,i}, \psi_k^{m,i} \right\rangle_{L^2(\Gamma_i^m)}, & \mathbf{V}_{i,h}^m &\in \mathbb{R}^{N_i^m \times N_i^m}, \\ \mathbf{M}_{i,h}^m[l, n] &:= \left\langle \varphi_n^{m,i}, \psi_l^{m,i} \right\rangle_{L^2(\Gamma_i^m)}, & \mathbf{M}_{i,h}^m &\in \mathbb{R}^{N_i^m \times M_i^m}, \\ \mathbf{K}_{i,h}^m[l, n] &:= \left\langle K_i^m \varphi_n^{m,i}, \psi_l^{m,i} \right\rangle_{L^2(\Gamma_i^m)}, & \mathbf{K}_{i,h}^m &\in \mathbb{R}^{N_i^m \times M_i^m}, \\ \mathbf{D}_{i,h}^m[q, n] &:= \left\langle D_i^m \varphi_n^{m,i}, \varphi_q^{m,i} \right\rangle_{L^2(\Gamma_i^m)}, & \mathbf{D}_{i,h}^m &\in \mathbb{R}^{M_i^m \times M_i^m}, \\ \mathbf{N}_{0,i,h}^m[l] &:= \left\langle N_{0,i,h}^m f, \psi_l^{m,i} \right\rangle_{L^2(\Gamma_i^m)}, & \mathbf{N}_{0,i,h}^m &\in \mathbb{R}^{N_i^m}. \end{aligned}$$

The local stiffness matrices  $\mathbf{V}_{i,h}^m$ ,  $\mathbf{K}_{i,h}^m$  and  $\mathbf{D}_{i,h}^m$  can be evaluated using analytical integration in combination with numerical integration schemes. All these matrices are dense. In computations, we can exploit the symmetry of  $\mathbf{V}_{i,h}^m$  and  $\mathbf{D}_{i,h}^m$  and the equations

$$\frac{1}{2} \sum_{n=1}^{M_i^m} \mathbf{M}_{i,h}^m[l, n] = - \sum_{n=1}^{M_i^m} \mathbf{K}_{i,h}^m[l, n] \quad \text{and} \quad \sum_{n=1}^{M_i^m} \mathbf{D}_{i,h}^m[q, n] = 0$$

for  $l = 1, \dots, N_i^m$ ,  $q = 1, \dots, M_i^m$ . For evaluation of the vector  $\mathbf{N}_{0,i,h}^m$  it is necessary to compute the local Newton potential  $N_{0,i,h}^m f$ . This can be done by an indirect approach using the finite element method, as introduced in [33, 34]. Now considering (5.2), we can read the minimized functional in (5.3) as the function of variables  $\mathbf{v}_1^1, \dots, \mathbf{v}_{p^1}^1, \mathbf{v}_1^2, \dots, \mathbf{v}_{p^2}^2$ . Let us denote

$$\mathbf{v} := [(\mathbf{v}_1^1)^T, \dots, (\mathbf{v}_{p^1}^1)^T, (\mathbf{v}_1^2)^T, \dots, (\mathbf{v}_{p^2}^2)^T]^T.$$



To ensure the continuity condition across all interfaces  $\Gamma_{i,j}^m$ , we define the equality constraints

$$\mathbf{B}_C \mathbf{v} = \mathbf{0},$$

and to describe the non-interpenetration condition across the interface  $\Gamma_c$ , we introduce the inequality constraints

$$\mathbf{B}_I \mathbf{v} \leq \mathbf{0}.$$

Each row of  $\mathbf{B}_C$  and  $\mathbf{B}_I$  is associated with a set of matching nodes on  $\Gamma_{i,j}^m$  and  $\Gamma_c$ , respectively; it has 1 and  $-1$  on the appropriate positions and zeros elsewhere. More details can be found in [10] and [11]. Following the recently proposed TFETI domain decomposition method [13, 30], we can enforce also the homogeneous Dirichlet condition on  $\Gamma_u^1$  by the equality constraints

$$\mathbf{B}_D \mathbf{v} = \mathbf{0}.$$

This approach is motivated by an effort to treat all the subdomains in the same way and to enrich the kernel of the stiffness matrix which we shall use in construction of our preconditioner. As a result, we shall consider also the trial functions  $\varphi_k^1$  that are nonzero on  $\Gamma_u^1$ . The rows of the matrix  $B_D$  are associated with the nodes on  $\Gamma_u^1$ ; their entries are equal to zero except the unique 1 in the position corresponding to the node with prescribed zero displacement. Now we can reformulate (5.3) as the following problem: find  $\mathbf{u}$  such that

$$J(\mathbf{u}) = \min \{J(\mathbf{v}) : \mathbf{B}_I \mathbf{v} \leq \mathbf{0}, \mathbf{B}_E \mathbf{v} = \mathbf{0}\}, \quad (5.4)$$

where

$$\begin{aligned} J(\mathbf{v}) &:= \frac{1}{2} \mathbf{v}^T \tilde{\mathbf{S}} \mathbf{v} - \tilde{\mathbf{R}}^T \mathbf{v}, \\ \mathbf{B}_E &:= \left[ \mathbf{B}_C^T, \mathbf{B}_D^T \right]^T, \\ \tilde{\mathbf{S}} &:= \text{diag} (\tilde{\mathbf{S}}_{1,h}^1, \dots, \tilde{\mathbf{S}}_{p^1,h}^1, \tilde{\mathbf{S}}_{1,h}^2, \dots, \tilde{\mathbf{S}}_{p^2,h}^2), \\ \tilde{\mathbf{R}} &:= \left[ (\tilde{\mathbf{R}}_{1,h}^1)^T, \dots, (\tilde{\mathbf{R}}_{p^1,h}^1)^T, (\tilde{\mathbf{R}}_{1,h}^2)^T, \dots, (\tilde{\mathbf{R}}_{p^2,h}^2)^T \right]^T. \end{aligned}$$

## 6 Dual Formulation

Now we shall eliminate the primal variables using the duality theory in order to improve conditioning and simplify the structure of our problem. In particular, this step shall replace the general inequality constraints in the primal formulation (5.4) by the bound constraints in the dual formulation. First, the matrices  $\tilde{\mathbf{S}}_{i,h}^m$  are positive semidefinite due to the lack of the Dirichlet boundary condition, and therefore they are singular. Let us denote by  $\tilde{\mathbf{S}}_i^{m,+}$  any symmetric matrix that satisfies

$$\tilde{\mathbf{S}}_{i,h}^m = \tilde{\mathbf{S}}_{i,h}^m \tilde{\mathbf{S}}_i^{m,+} \tilde{\mathbf{S}}_{i,h}^m,$$

so that the matrix  $\tilde{\mathbf{S}}^+ := \text{diag} (\tilde{\mathbf{S}}_1^{1,+}, \dots, \tilde{\mathbf{S}}_{p^1}^{1,+}, \tilde{\mathbf{S}}_1^{2,+}, \dots, \tilde{\mathbf{S}}_{p^2}^{2,+})$  satisfies

$$\tilde{\mathbf{S}} = \tilde{\mathbf{S}}\tilde{\mathbf{S}}^+ \tilde{\mathbf{S}}.$$

Let us also denote by  $\mathbf{R}$  a matrix whose columns span the null space of  $\tilde{\mathbf{S}}$ . We shall assume that

$$\mathbf{R} := \text{diag}(\mathbf{R}_1^1, \dots, \mathbf{R}_{p^1}^1, \mathbf{R}_1^2, \dots, \mathbf{R}_{p^2}^2),$$

where  $\mathbf{R}_i^m$  corresponds to the kernel of  $\mathbf{S}_i^m$ . Thus matrix  $\mathbf{R}$  has  $p := p^1 + p^2$  columns, each subdomain being associated with a column of  $\mathbf{R}$  with ones in the positions corresponding to the indices of the nodes belonging to the subdomain and zeros elsewhere. By introducing the Lagrange multipliers  $\boldsymbol{\lambda}_I$  and  $\boldsymbol{\lambda}_E$  associated with the inequalities and equalities, respectively, and denoting

$$\boldsymbol{\lambda} := \begin{bmatrix} \boldsymbol{\lambda}_I \\ \boldsymbol{\lambda}_E \end{bmatrix} \quad \text{and} \quad \mathbf{B} := \begin{bmatrix} \mathbf{B}_I \\ \mathbf{B}_E \end{bmatrix},$$

we may equivalently replace problem (5.4) by the problem: find  $\bar{\boldsymbol{\lambda}}$  such that

$$\Theta(\bar{\boldsymbol{\lambda}}) = \min \left\{ \Theta(\boldsymbol{\lambda}) : \boldsymbol{\lambda}_I \geq \mathbf{0}, \tilde{\mathbf{G}}\boldsymbol{\lambda} = \tilde{\mathbf{e}} \right\}, \quad (6.1)$$

where

$$\Theta(\boldsymbol{\lambda}) := \frac{1}{2} \boldsymbol{\lambda}^T \mathbf{F} \boldsymbol{\lambda} - \boldsymbol{\lambda}^T \tilde{\mathbf{d}}$$

and

$$\mathbf{F} := \mathbf{B}\tilde{\mathbf{S}}^+ \mathbf{B}^T, \quad \tilde{\mathbf{d}} := \mathbf{B}\tilde{\mathbf{S}}^+ \tilde{\mathbf{R}}, \quad \tilde{\mathbf{G}} := \mathbf{R}^T \mathbf{B}^T, \quad \tilde{\mathbf{e}} := \mathbf{R}^T \tilde{\mathbf{R}}.$$

Once the solution  $\bar{\boldsymbol{\lambda}}$  of (6.1) is known, the solution  $\mathbf{u}$  of (5.4) may be evaluated by

$$\mathbf{u} = \tilde{\mathbf{S}}^+ (\tilde{\mathbf{R}} - \mathbf{B}^T \bar{\boldsymbol{\lambda}}) + \mathbf{R}\boldsymbol{\alpha}$$

and the formula

$$\boldsymbol{\alpha} = -(\mathbf{R}^T \tilde{\mathbf{B}}^T \tilde{\mathbf{B}} \mathbf{R})^{-1} \mathbf{R}^T \tilde{\mathbf{B}}^T \tilde{\mathbf{B}} \tilde{\mathbf{S}}^+ (\tilde{\mathbf{R}} - \mathbf{B}^T \bar{\boldsymbol{\lambda}}),$$

where  $\tilde{\mathbf{B}} := \begin{bmatrix} \tilde{\mathbf{B}}_I^T & \mathbf{B}_E^T \end{bmatrix}^T$ , and the matrix  $\tilde{\mathbf{B}}_I$  is formed by the rows of  $\mathbf{B}_I$  corresponding to the positive entries of  $\bar{\boldsymbol{\lambda}}_I$ . The procedure is similar to that described in [15].

## 7 Natural Coarse Grid

Even though problem (6.1) is much more suitable for computations than (5.4), further improvement may be achieved. As we shall give only a sketch here, we note that the details may be found, e.g., in [11].

Let us introduce a nonsingular matrix  $\mathbf{T}$  defining orthonormalization of the rows of  $\tilde{\mathbf{G}}$  so that the matrix

$$\mathbf{G} := \mathbf{T}\tilde{\mathbf{G}}$$

has orthonormal rows. After denoting

$$\mathbf{e} := \mathbf{T}\tilde{\mathbf{e}},$$

problem (6.1) reads: find  $\bar{\boldsymbol{\lambda}}$  such that

$$\Theta(\bar{\boldsymbol{\lambda}}) = \min \{ \Theta(\boldsymbol{\lambda}) : \boldsymbol{\lambda}_I \geq \mathbf{0}, \mathbf{G}\boldsymbol{\lambda} = \mathbf{e} \}. \quad (7.1)$$

Our next step is to look for the solution of (7.1) in the form  $\bar{\boldsymbol{\lambda}} = \boldsymbol{\mu} + \tilde{\boldsymbol{\lambda}}$ , where  $\mathbf{G}\tilde{\boldsymbol{\lambda}} = \mathbf{e}$ . The following lemma shows that we can even find  $\tilde{\boldsymbol{\lambda}}$  such that  $\tilde{\boldsymbol{\lambda}}_I \geq \mathbf{0}$ .

**Lemma 7.1.** *Let  $\mathbf{B}$  be such that the negative entries of  $\mathbf{B}_I$  are in the columns that correspond to the nodes in the floating domain  $\Omega^2$ . Then there is a  $\tilde{\boldsymbol{\lambda}}$  such that  $\tilde{\boldsymbol{\lambda}}_I \geq \mathbf{0}$  and  $\mathbf{G}\tilde{\boldsymbol{\lambda}} = \mathbf{e}$ .*

**Proof:** See [11].  $\square$

Since

$$\frac{1}{2}\bar{\boldsymbol{\lambda}}^T \mathbf{F}\bar{\boldsymbol{\lambda}} - \bar{\boldsymbol{\lambda}}^T \tilde{\mathbf{d}} = \frac{1}{2}\boldsymbol{\mu}^T \mathbf{F}\boldsymbol{\mu} - \boldsymbol{\mu}^T (\tilde{\mathbf{d}} - \mathbf{F}\tilde{\boldsymbol{\lambda}}) + \frac{1}{2}\tilde{\boldsymbol{\lambda}}^T \mathbf{F}\tilde{\boldsymbol{\lambda}} - \tilde{\boldsymbol{\lambda}}^T \tilde{\mathbf{d}},$$

problem (7.1) is, after returning to the old notation, equivalent to the problem: find  $\bar{\boldsymbol{\lambda}}$  such that

$$\Lambda_0(\bar{\boldsymbol{\lambda}}) = \min \left\{ \Lambda_0(\boldsymbol{\lambda}) : \boldsymbol{\lambda}_I \geq -\tilde{\boldsymbol{\lambda}}_I, \mathbf{G}\boldsymbol{\lambda} = \mathbf{0} \right\}, \quad (7.2)$$

where

$$\Lambda_0(\boldsymbol{\lambda}) := \frac{1}{2}\boldsymbol{\lambda}^T \mathbf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T \tilde{\mathbf{d}}$$

and  $\tilde{\mathbf{d}} := \tilde{\mathbf{d}} - \mathbf{F}\tilde{\boldsymbol{\lambda}}$ . We can further observe that problem (7.2) is equivalent to the problem: find  $\bar{\boldsymbol{\lambda}}$  such that

$$\Lambda(\bar{\boldsymbol{\lambda}}) = \min \left\{ \Lambda(\boldsymbol{\lambda}) : \boldsymbol{\lambda}_I \geq -\tilde{\boldsymbol{\lambda}}_I, \mathbf{G}\boldsymbol{\lambda} = \mathbf{0} \right\}, \quad (7.3)$$

where

$$\Lambda(\boldsymbol{\lambda}) := \frac{1}{2}\boldsymbol{\lambda}^T \mathbf{P}\mathbf{F}\mathbf{P}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T \mathbf{P}\tilde{\mathbf{d}}$$

and

$$\mathbf{P} := \mathbf{I} - \mathbf{Q} \quad \text{and} \quad \mathbf{Q} := \mathbf{G}^T \mathbf{G}$$

are the orthogonal projectors on the kernel of  $\mathbf{G}$  and on the image space of  $\mathbf{G}^T$ , respectively. The projectors  $\mathbf{P}$  and  $\mathbf{Q}$  define the so-called natural coarse grid. Finally, we introduce an augmented Lagrangian associated with problem (7.3)

$$L(\boldsymbol{\lambda}, \boldsymbol{\mu}, \rho) = \frac{1}{2}\boldsymbol{\lambda}^T (\mathbf{P}\mathbf{F}\mathbf{P} + \rho\mathbf{Q})\boldsymbol{\lambda} - \boldsymbol{\lambda}^T \mathbf{P}\tilde{\mathbf{d}} + \boldsymbol{\mu}^T \mathbf{G}\boldsymbol{\lambda}. \quad (7.4)$$

Let us note that if  $[a, b]$  is an interval containing nonzero elements of the spectrum  $\sigma\{\mathbf{P}\mathbf{F}\mathbf{P}\}$  of  $\mathbf{P}\mathbf{F}\mathbf{P}$ ,  $0 < a$ , then  $\sigma\{\mathbf{P}\mathbf{F}\mathbf{P} + \rho\mathbf{Q}\} \subseteq [a, b] \cup \{\rho\}$ , so that  $\mathbf{P}\mathbf{F}\mathbf{P} + \rho\mathbf{Q}$  is nonsingular, and there is a bound on the rate of convergence of the conjugate gradient method applied to the linear problem with the matrix  $\mathbf{P}\mathbf{F}\mathbf{P} + \rho\mathbf{Q}$  that is independent of the penalization term  $\rho$  [6].

## 8 Bounds on Spectrum

Now we shall examine the spectrum of the Hessian  $F$  of  $\Lambda_0$ . Our main tool will be the observation of Langer and Steinbach [29] that the local boundary element stiffness matrix  $\tilde{S}_{i,h}^m$  is spectrally equivalent to some Schur complement of the related local finite element stiffness matrix  $K_{i,h}^m$ . We shall use this observation to translate the classical estimate concerning the dual Schur complement matrices arising from application of the FETI method into bounds on the spectrum of the nonsingular part of  $F_{\text{BEM}} := F$ .

To describe this result and its consequences in more detail, let us assume that  $h$  is fixed, so that we can skip it. Let us also identify each subdomain  $\Omega_i^m$  with the single index  $j := (m-1)p^1 + i$  and denote  $S_{\text{BEM},j} := \tilde{S}_{i,h}^m$ ,  $R_j := R_i^m$ . Thus  $S_{\text{BEM},j}$  is defined for  $j \in \{1, \dots, p\}$  and

$$S_{\text{BEM}} := \text{diag}(S_{\text{BEM},1}, S_{\text{BEM},2}, \dots, S_{\text{BEM},p}).$$

Finally, observing that the number of columns of  $B$  is the same as the number of columns of  $S_{\text{BEM}}$ , we can impose the block structure of  $S_{\text{BEM}}$  on the columns of  $B$ , so that

$$B = [B_1, B_2, \dots, B_p]$$

and

$$F_{\text{BEM}} = BS_{\text{BEM}}^+ B^T = \sum_{j=1}^p B_j S_{\text{BEM},j}^+ B_j^T.$$

Let us now specify the FETI counterpart of  $F_{\text{BEM}}$ . In each subdomain, let us consider the regular grid which generates the same boundary mesh as that used to form  $F_{\text{BEM}}$ , and let us denote by  $K_{\text{FEM},j}$  the local finite element stiffness matrix arising from the application of linear triangular elements. Numbering the unknowns in the interior of the subdomain  $\Omega_j$  first, we can write

$$K_{\text{FEM},j} = \begin{bmatrix} K_{\text{ii},j} & K_{\text{ib},j} \\ K_{\text{bi},j} & K_{\text{bb},j} \end{bmatrix},$$

where the subscripts b and i refer to the subdomain boundary and the interior unknowns, respectively. The finite element Schur complement matrix arising from elimination of the interior variables can be represented in the form

$$S_{\text{FEM},j} = K_{\text{bb},j} - K_{\text{bi},j} K_{\text{ii},j}^{-1} K_{\text{ib},j}.$$

Notice that the diagonal block  $K_{\text{ii},j}$  is invertible as it can be interpreted as the stiffness matrix of a membrane fixed on the boundary, but  $S_{\text{FEM},j}$  is singular with the same kernel as  $S_{\text{BEM},j}$ . The FETI counterparts of  $S_{\text{BEM}}$  and  $F_{\text{BEM}}$  are defined [21] by

$$S_{\text{FEM}} := \text{diag}(S_{\text{FEM},1}, S_{\text{FEM},2}, \dots, S_{\text{FEM},p})$$

and

$$\mathbf{F}_{\text{FEM}} := \mathbf{B}\mathbf{S}_{\text{FEM}}^+\mathbf{B}^T = \sum_{j=1}^p \mathbf{B}_j \mathbf{S}_{\text{FEM},j}^+ \mathbf{B}_j^T.$$

The bounds on the spectrum of  $\mathbf{F}_{\text{FEM}}$  were established in Farhat, Mandel, and Roux [21]. To formulate them, let us denote by  $\lambda_{\min}(\mathbf{A})$  and  $\lambda_{\max}(\mathbf{A})$  the smallest and the largest eigenvalue of a given symmetric matrix  $\mathbf{A}$ , respectively.

**Theorem 8.1.** *There are constants  $C_1 > 0$  and  $C_2 > 0$  independent of the discretization parameter  $h$  and the decomposition parameter  $H$  such that*

$$\lambda_{\min}(\mathbf{P}\mathbf{F}_{\text{FEM}}\mathbf{P} \mid \text{Im } \mathbf{P}) \geq C_1 \quad \text{and} \quad \|\mathbf{P}\mathbf{F}_{\text{FEM}}\mathbf{P}\| \leq C_2 \frac{H}{h}. \quad (8.1)$$

**Proof:** See Theorem 3.2 of Farhat, Mandel, and Roux [21].  $\square$

The statement of Theorem 3.2 of Farhat, Mandel, and Roux [21] gives only an upper bound on the spectral condition number  $\kappa(\mathbf{P}\mathbf{F}_{\text{FEM}}\mathbf{P} \mid \text{Im } \mathbf{P})$ . However, the reasoning that precedes and substantiates their estimate proves both bounds of (8.1).

The following lemma allows us to carry over the above mentioned bounds on the spectrum of  $\mathbf{F}_{\text{FEM}}$  to those on  $\mathbf{F}_{\text{BEM}}$ .

**Lemma 8.2.** *There are constants  $c > 0$  and  $C > 0$  independent of the discretization parameter  $h$  and the decomposition parameter  $H$  such that*

$$c(\mathbf{S}_{\text{FEM},j}^+ \mathbf{B}_j^T \boldsymbol{\lambda}, \mathbf{B}_j^T \boldsymbol{\lambda}) \leq (\mathbf{S}_{\text{BEM},j}^+ \mathbf{B}_j^T \boldsymbol{\lambda}, \mathbf{B}_j^T \boldsymbol{\lambda}) \leq C(\mathbf{S}_{\text{FEM},j}^+ \mathbf{B}_j^T \boldsymbol{\lambda}, \mathbf{B}_j^T \boldsymbol{\lambda}) \quad (8.2)$$

for any  $\boldsymbol{\lambda}$  such that  $\mathbf{R}_j^T \mathbf{B}_j^T \boldsymbol{\lambda} = \mathbf{0}$ .

**Proof:** See Lemma 3.3 by Langer and Steinbach [29].  $\square$

Langer and Steinbach consider in their proof only the Moore–Penrose generalized inverse  $\mathbf{S}_{\text{BEM},j}^\#$ . However, observing that  $\mathbf{R}_j^T \mathbf{B}_j^T \boldsymbol{\lambda} = \mathbf{0}$  is equivalent to  $\mathbf{B}_j^T \boldsymbol{\lambda} \in \text{Im } \mathbf{S}_{\text{BEM},j}$ , we get that there is a  $\mathbf{y}$  so that  $\mathbf{B}_j^T \boldsymbol{\lambda} = \mathbf{S}_{\text{BEM},j} \mathbf{y}$  and

$$\begin{aligned} (\mathbf{S}_{\text{BEM},j}^+ \mathbf{B}_j^T \boldsymbol{\lambda}, \mathbf{B}_j^T \boldsymbol{\lambda}) &= \mathbf{y}^T \mathbf{S}_{\text{BEM},j} \mathbf{S}_{\text{BEM},j}^+ \mathbf{S}_{\text{BEM},j} \mathbf{y} \\ &= \mathbf{y}^T \mathbf{S}_{\text{BEM},j} \mathbf{y} \\ &= \mathbf{y}^T \mathbf{S}_{\text{BEM},j} \mathbf{S}_{\text{BEM},j}^\# \mathbf{S}_{\text{BEM},j} \mathbf{y} \\ &= (\mathbf{S}_{\text{BEM},j}^\# \mathbf{B}_j^T \boldsymbol{\lambda}, \mathbf{B}_j^T \boldsymbol{\lambda}), \end{aligned}$$

so that Lemma 8.2 holds for any generalized inverse.

Now we are able to formulate the BETI counterpart to Theorem 8.1.

**Theorem 8.3.** *There are constants  $C_3 > 0$  and  $C_4 > 0$  independent of the discretization parameter  $h$  and the decomposition parameter  $H$  such that*

$$\lambda_{\min}(\mathbf{P}\mathbf{F}_{\text{BEM}}\mathbf{P} \mid \text{Im } \mathbf{P}) \geq C_3 \quad \text{and} \quad \|\mathbf{P}\mathbf{F}_{\text{BEM}}\mathbf{P}\| \leq C_4 \frac{H}{h}. \quad (8.3)$$

**Proof:** Let us assume that  $\boldsymbol{\lambda} \in \text{Im } \mathbf{P}$  which means

$$\mathbf{R}_j^T \mathbf{B}_j^T \boldsymbol{\lambda} = \mathbf{0} \quad \text{for } j = 1, \dots, p,$$

and  $\|\boldsymbol{\lambda}\| = 1$ . Using Theorem 8.1 and Lemma 8.2, we get that there are constants  $c, C, C_1$ , and  $C_2$  such that

$$\begin{aligned} C_1 &\leq \boldsymbol{\lambda}^T \mathbf{F}_{\text{FEM}} \boldsymbol{\lambda} = \sum_{j=1}^p (\mathbf{S}_{\text{FEM},j}^+ \mathbf{B}_j^T \boldsymbol{\lambda}, \mathbf{B}_j^T \boldsymbol{\lambda}) \\ &\leq \frac{1}{c} \sum_{j=1}^p (\mathbf{S}_{\text{BEM},j}^+ \mathbf{B}_j^T \boldsymbol{\lambda}, \mathbf{B}_j^T \boldsymbol{\lambda}) \leq \frac{C}{c} \sum_{j=1}^p (\mathbf{S}_{\text{FEM},j}^+ \mathbf{B}_j^T \boldsymbol{\lambda}, \mathbf{B}_j^T \boldsymbol{\lambda}) \\ &= \frac{C}{c} \boldsymbol{\lambda}^T \mathbf{F}_{\text{FEM}} \boldsymbol{\lambda} \leq \frac{C}{c} C_2 \frac{H}{h}. \end{aligned}$$

Since

$$\boldsymbol{\lambda}^T \mathbf{F}_{\text{BEM}} \boldsymbol{\lambda} = \sum_{j=1}^p (\mathbf{S}_{\text{BEM},j}^+ \mathbf{B}_j^T \boldsymbol{\lambda}, \mathbf{B}_j^T \boldsymbol{\lambda}),$$

we have thus proved that

$$cC_1 \leq \boldsymbol{\lambda}^T \mathbf{F}_{\text{BEM}} \boldsymbol{\lambda} \leq CC_2 \frac{H}{h}.$$

To finish the proof, it is enough to set  $C_3 := cC_1$  and  $C_4 := CC_2$ .  $\square$

Langer and Steinbach [29] give stronger polylogarithmic bounds for the preconditioned  $\mathbf{F}$ . We cannot use this result since such preconditioning transforms the bound constraints to more general ones.

## 9 Algorithms

We shall now briefly review our algorithms for the solution of the bound and equality constrained problem (7.3). They combine our semimonotonic augmented Lagrangian method [7] which generates approximations for the Lagrange multipliers for the equality constraints in the outer loop with the working set algorithm for the bound constrained auxiliary problems in the inner loop [16]. The gradient of the augmented Lagrangian (7.4) is given by

$$\mathbf{g}(\boldsymbol{\lambda}, \boldsymbol{\mu}, \rho) = \mathbf{P}\mathbf{F}\mathbf{P}\boldsymbol{\lambda} - \mathbf{P}\mathbf{d} + \mathbf{G}^T(\boldsymbol{\mu} + \rho\mathbf{G}\boldsymbol{\lambda}).$$

Let  $\mathcal{I}$  denote the set of the indices of the bound constrained entries of  $\boldsymbol{\lambda}$ . The *projected gradient*  $\mathbf{g}^P = \mathbf{g}^P(\boldsymbol{\lambda}, \boldsymbol{\mu}, \rho)$  of  $L$  at  $\boldsymbol{\lambda}$  is then given component-wise by

$$\mathbf{g}_i^P := \begin{cases} \mathbf{g}_i & \text{for } \lambda_i > -\tilde{\lambda}_i \text{ or } i \notin \mathcal{I}, \\ \mathbf{g}_i^- & \text{for } \lambda_i = -\tilde{\lambda}_i \text{ and } i \in \mathcal{I}, \end{cases}$$

where  $\mathbf{g}_i^- = \min\{\mathbf{g}_i, 0\}$ . Our algorithm is a variant of that proposed by Conn, Gould and Toint [5] for identifying stationary points of more general problems. Its modification by Dostál, Friedlander, and Santos [9] was used by Dostál and Horák to develop a scalable FETI based algorithm, as shown experimentally in

[11]. All the necessary parameters are listed in *Step 0*, and typical values of these parameters for our model problem are given in brackets.

**Algorithm 9.1.** *Semi-monotonic Augmented Lagrangian Method for Bound and Equality Constrained Problems (SMALBE).*

*Step 0.* {Initialization of parameters.}

Given  $\eta > 0$  [ $\eta := \|\mathbf{Pd}\|$ ],  $\beta > 1$  [ $\beta := 10$ ],  $M > 0$  [ $M := 1$ ],  
 $\rho_0 > 0$  [ $\rho_0 := 100$ ], and  $\boldsymbol{\mu}^0$  [ $\boldsymbol{\mu}^0 := \mathbf{0}$ ], set  $k := 0$ .

*Step 1.* {Inner iteration with adaptive precision control.}

Find  $\boldsymbol{\lambda}^k$  such that  $\boldsymbol{\lambda}_{\mathcal{I}}^k \geq -\tilde{\boldsymbol{\lambda}}_{\mathcal{I}}$  and  
 $\|\mathbf{g}^P(\boldsymbol{\lambda}^k, \boldsymbol{\mu}^k, \rho_k)\| \leq \min\{M\|\mathbf{G}\boldsymbol{\lambda}^k\|, \eta\}$ .

*Step 2.* {Stopping criterion.}

If  $\|\mathbf{g}^P(\boldsymbol{\lambda}^k, \boldsymbol{\mu}^k, \rho_k)\|$  and  $\|\mathbf{G}\boldsymbol{\lambda}^k\|$  are sufficiently small, then  
 $\boldsymbol{\lambda}^k$  is the solution.

*Step 3.* {Update of the Lagrange multipliers.}

$\boldsymbol{\mu}^{k+1} := \boldsymbol{\mu}^k + \rho_k \mathbf{G}\boldsymbol{\lambda}^k$

*Step 4.* {Update the penalty parameter.}

If  $k > 0$  and  $L(\boldsymbol{\lambda}^k, \boldsymbol{\mu}^k, \rho_k) < L(\boldsymbol{\lambda}^{k-1}, \boldsymbol{\mu}^{k-1}, \rho_{k-1}) + \frac{\rho_k}{2}\|\mathbf{G}\boldsymbol{\lambda}^k\|^2$ ,  
then

$\rho_{k+1} := \beta\rho_k$ ,

else

$\rho_{k+1} := \rho_k$ .

*Step 5.* Increase  $k$  and return to *Step 1*.

*Step 1* may be implemented by any algorithm for minimization of the augmented Lagrangian  $L$  with respect to  $\boldsymbol{\lambda}$  subject to  $\boldsymbol{\lambda}_{\mathcal{I}} \geq -\tilde{\boldsymbol{\lambda}}_{\mathcal{I}}$  which guarantees convergence of the projected gradient to zero. More about the properties and implementation of the SMALBE algorithm may be found in [7].

The unique feature of the SMALBE algorithm is its capability to find an approximate solution of problem (7.3) in a number of steps which is bounded in terms of bounds on the spectrum of  $\mathbf{PFP} + \rho\mathbf{Q}$  [7]. To get a bound on the number of matrix multiplication, it is necessary to have algorithm which can solve the problem

$$L(\boldsymbol{\lambda}, \boldsymbol{\mu}, \rho) \longrightarrow \min \quad \text{subject to} \quad \boldsymbol{\lambda}_{\mathcal{I}} \geq -\tilde{\boldsymbol{\lambda}}_{\mathcal{I}} \quad (9.1)$$

with the rate of convergence in terms of the bounds on the spectrum of the Hessian matrix of  $L$ .

To describe such algorithm, let us recall that the unique solution  $\bar{\boldsymbol{\lambda}} = \bar{\boldsymbol{\lambda}}(\boldsymbol{\mu}, \rho)$  of (9.1) satisfies the Karush–Kuhn–Tucker (KKT) conditions

$$\bar{\boldsymbol{\lambda}}_i = -\tilde{\boldsymbol{\lambda}}_i \quad \text{and} \quad i \in \mathcal{I} \quad \text{implies} \quad \mathbf{g}_i(\bar{\boldsymbol{\lambda}}) \geq 0$$

and

$$\bar{\boldsymbol{\lambda}}_i > -\tilde{\boldsymbol{\lambda}}_i \quad \text{or} \quad i \notin \mathcal{I} \quad \text{implies} \quad \mathbf{g}_i(\bar{\boldsymbol{\lambda}}) = 0.$$

Let  $\mathcal{A}(\boldsymbol{\lambda})$  and  $\mathcal{F}(\boldsymbol{\lambda})$  denote the *active set* and *free set* of indices of  $\boldsymbol{\lambda}$ , respectively, i.e.,

$$\mathcal{A}(\boldsymbol{\lambda}) := \{i \in \mathcal{I} : \lambda_i = -\tilde{\lambda}_i\} \quad \text{and} \quad \mathcal{F}(\boldsymbol{\lambda}) := \{i : \lambda_i > -\tilde{\lambda}_i \text{ or } i \notin \mathcal{I}\}.$$

To enable an alternative reference to the KKT conditions [2], let us define the *free gradient*  $\boldsymbol{\varphi}(\boldsymbol{\lambda})$  and the *chopped gradient*  $\boldsymbol{\beta}(\boldsymbol{\lambda})$  by

$$\boldsymbol{\varphi}_i(\boldsymbol{\lambda}) := \begin{cases} \mathbf{g}_i(\boldsymbol{\lambda}) & \text{for } i \in \mathcal{F}(\boldsymbol{\lambda}), \\ 0 & \text{for } i \in \mathcal{A}(\boldsymbol{\lambda}), \end{cases} \quad \text{and} \quad \boldsymbol{\beta}_i(\boldsymbol{\lambda}) := \begin{cases} 0 & \text{for } i \in \mathcal{F}(\boldsymbol{\lambda}), \\ \mathbf{g}_i^-(\boldsymbol{\lambda}) & \text{for } i \in \mathcal{A}(\boldsymbol{\lambda}), \end{cases}$$

so that the KKT conditions are satisfied if and only if the *projected gradient*

$$\mathbf{g}^P(\boldsymbol{\lambda}) := \boldsymbol{\varphi}(\boldsymbol{\lambda}) + \boldsymbol{\beta}(\boldsymbol{\lambda})$$

is equal to zero. We call  $\boldsymbol{\lambda}$  *feasible* if  $\lambda_i \geq -\tilde{\lambda}_i$  for  $i \in \mathcal{I}$ . The projector  $P$  to the set of feasible vectors is defined for any  $\boldsymbol{\lambda}$  by

$$P(\boldsymbol{\lambda})_i := \max\{\lambda_i, -\tilde{\lambda}_i\} \quad \text{for } i \in \mathcal{I}, \quad P(\boldsymbol{\lambda})_i := \lambda_i \quad \text{for } i \notin \mathcal{I}.$$

Let  $\mathbf{A}$  denote the Hessian of  $L$  with respect to  $\boldsymbol{\lambda}$ . The *expansion step* is defined by

$$\boldsymbol{\lambda}^{k+1} := P\left(\boldsymbol{\lambda}^k - \bar{\alpha}\boldsymbol{\varphi}(\boldsymbol{\lambda}^k)\right)$$

with the steplength  $\bar{\alpha} \in (0, \|\mathbf{A}\|^{-1}]$ . This step may expand the current active set. To describe it without  $P$ , let  $\tilde{\boldsymbol{\varphi}}(\boldsymbol{\lambda})$  be the *reduced free gradient* for any feasible  $\boldsymbol{\lambda}$ , with entries

$$\tilde{\boldsymbol{\varphi}}_i = \tilde{\boldsymbol{\varphi}}_i(\boldsymbol{\lambda}) := \min\left\{\frac{\lambda_i + \tilde{\lambda}_i}{\bar{\alpha}}, \boldsymbol{\varphi}_i\right\} \quad \text{for } i \in \mathcal{I}, \quad \tilde{\boldsymbol{\varphi}}_i := \boldsymbol{\varphi}_i \quad \text{for } i \notin \mathcal{I}$$

such that

$$P(\boldsymbol{\lambda} - \bar{\alpha}\boldsymbol{\varphi}(\boldsymbol{\lambda})) = \boldsymbol{\lambda} - \bar{\alpha}\tilde{\boldsymbol{\varphi}}(\boldsymbol{\lambda}).$$

If the inequality

$$\|\boldsymbol{\beta}(\boldsymbol{\lambda}^k)\|^2 \leq \Gamma^2 \tilde{\boldsymbol{\varphi}}(\boldsymbol{\lambda}^k)^T \boldsymbol{\varphi}(\boldsymbol{\lambda}^k) \tag{9.2}$$

holds, then we call the iterate  $\boldsymbol{\lambda}^k$  *strictly proportional*. The test (9.2) is used to decide which component of the projected gradient  $\mathbf{g}^P(\boldsymbol{\lambda}^k)$  will be reduced in the next step.

The *proportioning step* is defined by

$$\boldsymbol{\lambda}^{k+1} := \boldsymbol{\lambda}^k - \alpha_{cg}\boldsymbol{\beta}(\boldsymbol{\lambda}^k).$$

The steplength  $\alpha_{cg}$  is chosen to minimize  $L(\boldsymbol{\lambda}^k - \alpha\boldsymbol{\beta}(\boldsymbol{\lambda}^k), \boldsymbol{\mu}^k, \rho_k)$  with respect to  $\alpha$ , i.e.,

$$\alpha_{cg} := \frac{\boldsymbol{\beta}(\boldsymbol{\lambda}^k)^T \mathbf{g}(\boldsymbol{\lambda}^k)}{\boldsymbol{\beta}(\boldsymbol{\lambda}^k)^T \mathbf{A} \boldsymbol{\beta}(\boldsymbol{\lambda}^k)}.$$



The purpose of the proportioning step is to remove indices from the active set. The *conjugate gradient step* is defined by

$$\boldsymbol{\lambda}^{k+1} := \boldsymbol{\lambda}^k - \alpha_{cg} \mathbf{p}^k,$$

where  $\mathbf{p}^k$  is the conjugate gradient direction [1] which is constructed recurrently. The recurrence starts (or restarts) with  $\mathbf{p}^s := \boldsymbol{\varphi}(\boldsymbol{\lambda}^s)$  whenever  $\boldsymbol{\lambda}^s$  is generated by the expansion step or the proportioning step. If  $\mathbf{p}^k$  is known, then  $\mathbf{p}^{k+1}$  is given by the formulae [1]

$$\mathbf{p}^{k+1} := \boldsymbol{\varphi}(\boldsymbol{\lambda}^{k+1}) - \gamma \mathbf{p}^k, \quad \gamma := \frac{\boldsymbol{\varphi}(\boldsymbol{\lambda}^{k+1})^T \mathbf{A} \mathbf{p}^k}{(\mathbf{p}^k)^T \mathbf{A} \mathbf{p}^k}.$$

The conjugate gradient steps are used to carry out the minimization in the face  $\mathcal{W}_{\mathcal{J}} := \{\boldsymbol{\lambda} : \lambda_i = -\tilde{\lambda}_i \text{ for } i \in \mathcal{J}\}$  given by  $\mathcal{J} := \mathcal{A}(\boldsymbol{\lambda}^s)$  efficiently. The algorithm that we use may now be described as follows.

**Algorithm 9.2.** *Modified Proportioning with Reduced Gradient Projections (MPRGP).*

Let  $\boldsymbol{\lambda}^0$  be a vector such that  $\lambda_i^0 \geq -\tilde{\lambda}_i$  for  $i \in \mathcal{I}$ ,  $\bar{\alpha} \in (0, \|\mathbf{A}\|^{-1}]$ , and  $\Gamma > 0$  be given. For  $k \geq 0$  and  $\boldsymbol{\lambda}^k$  known, choose  $\boldsymbol{\lambda}^{k+1}$  by the following rules:

- Step 1.* If  $\mathbf{g}^P(\boldsymbol{\lambda}^k) = 0$ , then set  $\boldsymbol{\lambda}^{k+1} := \boldsymbol{\lambda}^k$ .
- Step 2.* If  $\boldsymbol{\lambda}^k$  is strictly proportional and  $\mathbf{g}^P(\boldsymbol{\lambda}^k) \neq \mathbf{0}$ , then try to generate  $\boldsymbol{\lambda}^{k+1}$  by the conjugate gradient step.  
If  $\lambda_i^{k+1} \geq -\tilde{\lambda}_i$  for  $i \in \mathcal{I}$ , then accept it, else generate  $\boldsymbol{\lambda}^{k+1}$  by the expansion step.
- Step 3.* If  $\boldsymbol{\lambda}^k$  is not strictly proportional, define  $\boldsymbol{\lambda}^{k+1}$  by proportioning.

The MPRGP algorithm has an R-linear rate of convergence in terms of the spectral condition number of the Hessian  $\mathbf{A}$  of  $L$  [16]. More about the properties and implementation of the SMALBE algorithm may be found in [16, 8].

## 10 Optimality

To show that Algorithm 9.1 with the inner loop implemented by Algorithm 9.2 is optimal for the solution of problem (or a class of problems) (7.3), we shall introduce a new notation that complies with that used in [8]. We shall use

$$\mathcal{T} := \{(H, h) \in \mathbb{R}^2 : H \leq 1, 2h \leq H \text{ and } H/h \in \mathbb{N}\}$$

as the set of indices. Given a constant  $C \geq 2$ , we shall define a subset  $\mathcal{T}_C$  of  $\mathcal{T}$  by

$$\mathcal{T}_C := \{(H, h) \in \mathbb{R}^2 : H \leq 1, 2h \leq H, H/h \in \mathbb{N} \text{ and } H/h \leq C\}.$$

For any  $t \in \mathcal{T}$ , we shall define

$$\begin{aligned} \mathbf{A}_t &:= \text{PFP} + \rho \mathbf{Q}, & \mathbf{b}_t &:= \text{Pd}, \\ \mathbf{B}_t &:= \mathbf{G}, & \ell_{t,\mathcal{I}} &:= -\tilde{\lambda}_{\mathcal{I}}, \text{ and } \ell_{t,\mathcal{E}} := -\infty \end{aligned}$$

by the vectors and matrices generated with the discretization and decomposition parameters  $H$  and  $h$ , respectively, so that the problem (7.3) is equivalent to the problem

$$\Theta_t(\boldsymbol{\lambda}_t) \longrightarrow \min \quad \text{subject to} \quad \mathbf{B}_t \boldsymbol{\lambda}_t = \mathbf{0} \quad \text{and} \quad \boldsymbol{\lambda}_t \geq \boldsymbol{\ell}_t \quad (10.1)$$

with  $\Theta_t(\boldsymbol{\lambda}_t) := \frac{1}{2} \boldsymbol{\lambda}_t^T \mathbf{A}_t \boldsymbol{\lambda}_t - \mathbf{b}_t^T \boldsymbol{\lambda}_t$ . Using these definitions, Lemma 7.1, and  $\mathbf{G}\mathbf{G}^T = \mathbf{I}$ , we obtain

$$\|\mathbf{B}_t\| \leq 1 \quad \text{and} \quad \|\boldsymbol{\ell}_t^+\| = 0, \quad (10.2)$$

where for any vector  $\mathbf{v}$  with the entries  $\mathbf{v}_i$ ,  $\mathbf{v}^+$  denotes the vector with the entries  $\mathbf{v}_i^+ := \max\{\mathbf{v}_i, 0\}$ . Moreover, it follows by Theorem 8.3 that for any  $C \geq 2$  there are constants  $a_{\max}^C \geq a_{\min}^C > 0$  such that

$$a_{\min}^C \leq \lambda_{\min}(\mathbf{A}_t) \leq \lambda_{\max}(\mathbf{A}_t) \leq a_{\max}^C \quad (10.3)$$

for any  $t \in \mathcal{T}_C$ . Moreover, there are positive constants  $C_1$  and  $C_2$  such that  $a_{\min}^C \geq C_1$  and  $a_{\max}^C \leq C_2 C$ . In particular, it follows that the assumptions of Theorem 5 (i.e. the inequalities (10.2) and (10.3)) of [8] are satisfied for any set of indices  $\mathcal{T}_C$ ,  $C \geq 2$ , so that we have the following result:

**Theorem 10.1** *Let  $C \geq 2$  and  $\varepsilon > 0$  denote given constants, let  $\{\boldsymbol{\lambda}_t^k\}$ ,  $\{\boldsymbol{\mu}_t^k\}$ , and  $\{\rho_{t,k}\}$  be generated by Algorithm 9.1 (SMALBE) for (10.1) with  $\|\mathbf{b}_t\| \geq \eta_t > 0$ ,  $\beta > 1$ ,  $M > 0$ ,  $\rho_{t,0} := \rho_0 > 0$ , and  $\boldsymbol{\mu}_t^0 := \mathbf{0}$ . Let  $s \geq 0$  denote the smallest integer such that  $\beta^s \rho_0 \geq M^2/a_{\min}^C$  and assume that Step 1 of Algorithm 9.1 is implemented by means of Algorithm 9.2 (MPRGP) with parameters  $\Gamma > 0$  and  $\bar{\alpha} \in (0, (a_{\max}^C + \beta^s \rho_0)^{-1}]$ , so that it generates the iterates  $\boldsymbol{\lambda}_t^{k,0}, \boldsymbol{\lambda}_t^{k,1}, \dots, \boldsymbol{\lambda}_t^{k,l} =: \boldsymbol{\lambda}_t^k$  for the solution of (10.1) starting from  $\boldsymbol{\lambda}_t^{k,0} := \boldsymbol{\lambda}_t^{k-1}$  with  $\boldsymbol{\lambda}_t^{-1} := \mathbf{0}$ , where  $l = l_{t,k}$  is the first index satisfying*

$$\|\mathbf{g}^P(\boldsymbol{\lambda}_t^{k,l}, \boldsymbol{\mu}_t^k, \rho_{t,k})\| \leq M \|\mathbf{B}_t \boldsymbol{\lambda}_t^{k,l}\|$$

or

$$\|\mathbf{g}^P(\boldsymbol{\lambda}_t^{k,l}, \boldsymbol{\mu}_t^k, \rho_{t,k})\| \leq \varepsilon \|\mathbf{b}_t\| \min\{1, M^{-1}\}.$$

Then for any  $t \in \mathcal{T}_C$  and problem (10.1), Algorithm 9.1 generates an approximate solution  $\boldsymbol{\lambda}_t^{k_t}$  which satisfies

$$M^{-1} \|\mathbf{g}^P(\boldsymbol{\lambda}_t^{k_t}, \boldsymbol{\mu}_t^{k_t}, \rho_{t,k_t})\| \leq \|\mathbf{B}_t \boldsymbol{\lambda}_t^{k_t}\| \leq \varepsilon \|\mathbf{b}_t\|$$

at  $O(1)$  matrix–vector multiplications by the Hessian of the augmented Lagrangian  $L_t$  for (10.1) and  $\rho_{t,k} \leq \beta^s \rho_0$ .

## 11 Numerical Experiments

In this section, we shall present the performance of the above–described SMALBE algorithm with the inner loop implemented by the MPRGP algorithm to the solution of our model problem. We implemented our algorithms in Matlab.

We decomposed the domains  $\Omega^1$  and  $\Omega^2$  into identical square subdomains with the side length  $H$ . All subdomain boundaries were further discretized by the same regular grid with the element size  $h$ . The spaces  $W_{i,h}^m$  and  $Z_{i,h}^m$  were formed by the piecewise linear and constant trial functions with respect to the discretization, respectively. The solution for  $h := 1/512$  and  $H := 1/8$  is shown in Figure 2.

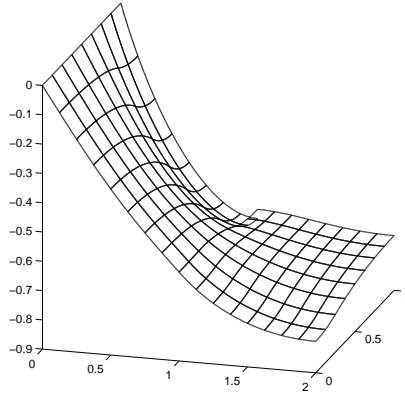


Figure 2: Solution of the model problem.

For the SMALBE algorithm, we used parameters  $\eta := \|\mathbf{Pd}\|$ ,  $\beta := 10$ , and  $M := 1$ . The penalty parameter  $\rho_0$  and the Lagrange multipliers  $\boldsymbol{\mu}^0$  for the equality constraints were set to  $25\|\mathbf{PFP}\|$  and  $\mathbf{0}$ , respectively. For the MPRGP algorithm we used parameters  $\bar{\alpha} := \rho_k^{-1}$  and  $\Gamma := 1$ . Our initial approximation  $\boldsymbol{\lambda}^0$  was set to  $\max\{-\tilde{\boldsymbol{\lambda}}, \frac{1}{2}\mathbf{B}\tilde{\mathbf{R}}_h\}$ . The stopping criterion of the outer loop was chosen as

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

The performance of our algorithms is shown in Table 1. The upper row of each field of the table shows the corresponding primal dimension / dual dimension / number of the outer iterations. The lower row gives a number of the conjugate gradient iterations. Examining the numbers of iterations in the rows, which correspond to the fixed ratio  $H/h$ , we conclude that the number of iterations is constant up to the oscillations that are due to the nonlinearity of our problem, in agreement with the theory. We conclude that the qualitative results proved in our paper can be observed at least for some problems.

## 12 Comments and Conclusions

We have presented the scalability results related to application of the BETI based domain decomposition with the “natural coarse grid” to the solution of variational inequalities. In particular, we have shown that the solution of

$H/h$	$H$			
	1/2	1/4	1/8	1/16
64	2048/778/1 35	8192/3622/2 105	32768/15502/2 111	131072/64030/2 106
32	1024/394/1 28	4096/1830/2 71	16384/7822/2 78	65536/32286/2 73
16	512/202/2 52	2048/934/2 56	8192/3982/2 51	32768/16414/2 59
8	256/106/2 42	1024/486/2 44	4096/2062/2 40	16384/8478/2 48
4	128/58/2 37	512/262/2 39	2048/1102/2 42	8192/4510/2 36

Table 1: Performance for varying decomposition and discretization.

the discretized elliptic variational inequality to a prescribed precision may be found in a number of matrix–vector multiplications bounded independently of the discretization parameter provided the ratio of the decomposition and the discretization parameters is kept bounded. Numerical experiments with the model variational inequality are in agreement with the theory and indicate that the algorithm can be efficient. The results remain valid also for the solution of frictionless coercive and semicoercive multibody 2D and 3D contact problems of elasticity and can be adapted to the solution of 2D problems with Coulomb friction. It is an interesting corollary of our theory that if we apply our algorithm to the solution of a multidomain contact problem which involves similar bodies discretized by quasiregular grids, then it is possible to give a bound on the number iterations that is independent of the number of bodies. The solution of auxiliary linear problems in the inner loop can be improved by standard preconditioners [29]. We shall discuss these topics elsewhere.

The preconditioning by the natural coarse grid may be considered as a variant of the multigrid methods. A unique feature of the natural coarse grid is that it covers also the contact interface and its complement contains the solution. This enables us to avoid difficulties related with application of multigrid [25] to variational inequalities, in particular with the proof of optimality. See, for example, Kornhuber [27], Kornhuber and Krause [28], and Wohlmuth and Krause [36], who gave an experimental evidence of numerical scalability of the algorithm based on monotone multigrid.

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