Total BETI duality based solver for multidomain variational inequalities

Jiří Bouchala[1], **Zdeněk Dostál**[1], **Marie Sadowská**[1]

[1] Department of Applied Mathematics, Faculty of Electrical Engineering and Computer Science, VŠB - Technical University Ostrava, Czech Republic

Abstract

A variant of the recently proposed Total BETI (TBETI) domain decomposition algorithm for the solution of elliptic multidomain variational inequalities is presented. After simplified presentation of the BETI method with a natural decomposition for variational inequalities, we describe the algorithms for the solution of the discretized problem that combine our semimonotonic augmented Lagrangian method (SMALBE) that can treat efficiently small number domains with a modification of our MPRGP active set based algorithm that is closely related to the semismooth Newton method. Both theoretical results and numerical experiments indicate efficiency of the algorithms presented. The algorithm is a variant of the total BETI (TBETI) algorithm which has been recently proved to be optimal.
Keywords Boundary elements, variational inequality, domain decomposition, quadratic programming, rate of convergence.

1 Introduction

We are concerned with elliptic boundary variational inequalities such as those describing the equilibrium of a system of elastic bodies in mutual contact. Such problems are difficult to solve because their boundary conditions involve the inequalities which make them strongly non-linear. Since the classical Dirichlet and Neumann boundary conditions are known only after the solution has been found, the analysis should not rely on the ellipticity of the related quadratic forms. Translated into the language of mechanics, it follows that any effective solver of such problems should be able not only to identify an a priori unknown contact interface, but also to deal with the singular matrices describing the response of "floating" bodies to a given traction.

The first step in the numerical solution of variational inequalities is their discretization, which can be based either on the finite element discretization [18] or on the boundary element discretization [21, 17], each approach having its own merits. For example, our development of boundary element based methods has been motivated by possible applications in shape optimization, where the finite element method requires remeshing of the interior of the body with adverse effect on the precision of shape gradients [20].

In this paper we describe application of a variant of the recently proposed TBETI (Total Boundary Element Tearing and Interconnecting Method) domain decomposition method using only a natural decomposition which assigns each body to one subdomain. It is easy to

implement; its specific feature is implementation of the Dirichlet boundary conditions by the Lagrange multipliers, so that all the stiffness matrices are singular and their kernels can be easily found. The method was introduced for linear problems independently by Dostál, Horák, and Kučera [16] as Total FETI (TFETI) method for the problems discretized by the FETI method and by Of [27] as all floating BETI (AF BETI) method for the problems discretized by the BETI method. Though the method turned out to be efficient for the linear problems, it seems that it should be even more efficient for the variational inequalities as it treats the coercive and semicoercive problems in the same way and reduces the quadratic programming problems with linear inequality constraints to those with the bound constraints. The resulting quadratic programming problem is then solved by a variant of the special quadratic programming algorithms [19, 9] that were recently used to develop scalable methods for variational inequalities discretized by both boundary [4] and finite elements [18, 9]. When the dimension of the null space of the discretized Poncar$\acute{e}$-Steklov operator is small, it turns out that different variants of algorithms and the choice of parameters are appropriate.

The paper is organized as follows. After describing a model problem, the related variational inequality is reduced to minimization of the energy functional defined on the boundary subject to the inequality constraints. The problem is then discretized by the Galerkin method using the well-known results on representation of the Steklov–Poincaré operator. Using the duality theory, we finally reduce the problem to a rather well-conditioned, strictly convex quadratic programming problem with bound and equality constraints, so that our efficient algorithms [19, 9, 11] may be applied. The unique feature of these algorithms is the rate of convergence in terms of the spectral condition number of the Hessian of the related quadratic form. Both theoretical results and numerical experiments indicate that there are problems which may be solved efficiently by the algorithms presented.

The application of the boundary element methods to boundary variational inequalities have been studied earlier, e.g., by Spann [31], Dostál, Friedlander, Santos, and Malík [17], and Eck, Steinbach, and Wendland [21], but it seems that no results concerning the rate of convergence in matrix–vector multiplication have been reported so far.

2 A model problem

To simplify our exposition, we shall reduce our presentation to a simple model boundary variational inequality defined on two domains, but our analysis remains valid also for related multidomain problems. After a little modification, our analysis may also be adapted to the solution of more general multidomain variational inequalities such as those describing an equilibrium of a system of ellastic bodies in mutual contact.

Let us consider the domains $\Omega^1 = \left(0, \frac{1}{2}\right) \times \left(0, \frac{1}{2}\right)$ and $\Omega^2 = \left(\frac{1}{2}, 1\right) \times \left(0, \frac{1}{2}\right)$ with boundaries Γ^1 and Γ^2, respectively. Each boundary Γ^m is further decomposed into three parts Γ^m_u, Γ^m_f, and Γ^m_c. We distinguish two cases, depending on whether Γ^2_u is an empty set or not; see Figure 1a and Figure 1b. Our goal is to find a sufficiently smooth (u^1, u^2) satisfying

$$-\triangle u^m = f \quad \text{in } \Omega^m, \quad u^m = 0 \quad \text{on } \Gamma^m_u, \quad \frac{\partial u^m}{\partial n} = 0 \quad \text{on } \Gamma^m_f, \quad m = 1, 2, \tag{1}$$

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

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

The function f is defined by

$$f(x) = \begin{cases} -1 & \text{for } x \in \left(0, \frac{1}{2}\right) \times \left[\frac{3}{8}, \frac{1}{2}\right), \\ -3 & \text{for } x \in \left(\frac{1}{2}, 1\right) \times \left(0, \frac{1}{8}\right], \\ 0 & \text{elsewhere in } \Omega^1 \cup \Omega^2 \end{cases}$$

and

$$f(x) = \begin{cases} -3 & \text{for } x \in \left(0, \frac{1}{2}\right) \times \left[\frac{3}{8}, \frac{1}{2}\right), \\ -1 & \text{for } x \in \left(\frac{1}{2}, 1\right) \times \left(0, \frac{1}{8}\right], \\ 0 & \text{elsewhere in } \Omega^1 \cup \Omega^2 \end{cases}$$

for coercive and semicoercive problem, respectively.

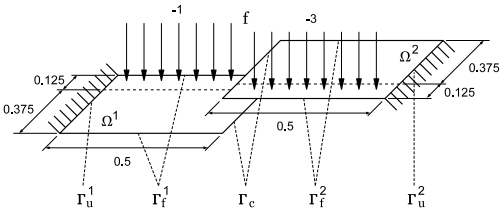

Fig. 1a: Coercive model problem.

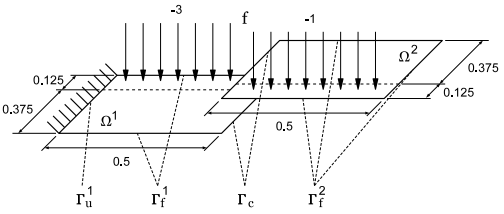

Fig. 1b: Semicoercive model problem.

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 Ω^1 is fixed on the left edge. In the coercive case the right membrane Ω^2 is fixed on the right edge whereas in the semicoercive case it floats. The left edge of Ω^2 is not allowed to penetrate below the right edge of Ω^1. By default, we shall deal with the coercive and semicoercive case together in what follows.

3 Reduction to the boundary

Let us introduce the standard boundary integral operators, in particular the single layer potential operator V^m, the double layer potential operator K^m, the adjoint double layer potential operator K'^m, and the hypersingular integral operator D^m defined for $x \in \Gamma^m$ by

$$(V^m \lambda^m)(x) = \int_{\Gamma^m} U(x,y)\lambda^m(y)\, \mathrm{d}s_y, \quad V^m : H^{-1/2}(\Gamma^m) \mapsto H^{1/2}(\Gamma^m),$$

$$(K^m u^m)(x) = \int_{\Gamma^m} \frac{\partial}{\partial n_y} U(x,y) u^m(y)\, \mathrm{d}s_y, \quad K^m :\ H^{1/2}(\Gamma^m) \mapsto H^{1/2}(\Gamma^m),$$

$$(K'^m \lambda^m)(x) = \int_{\Gamma^m} \frac{\partial}{\partial n_x} U(x,y) \lambda^m(y)\, \mathrm{d}s_y, \quad K'^m :\ H^{-1/2}(\Gamma^m) \mapsto H^{-1/2}(\Gamma^m),$$

$$(D^m u^m)(x) = -\frac{\partial}{\partial n_x} \int_{\Gamma^m} \frac{\partial}{\partial n_y} U(x,y) u^m(y)\, \mathrm{d}s_y, \quad D^m :\ H^{1/2}(\Gamma^m) \mapsto H^{-1/2}(\Gamma^m).$$

The function U is the so-called fundamental solution of the Laplace equation in $\mathbb{R}^2$ given by

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

The fact that

$$\operatorname{diam} \Omega^m < 1$$

ensures that the operator V^m is $H^{-1/2}(\Gamma^m)$-elliptic, and therefore its inversion is well-defined. It follows that for $x \in \Gamma^m$ we can define the Steklov–Poincaré operator S^m by

$$(S^m u^m)(x) = \left[D^m + \left(\frac{1}{2} I + K'^m \right) (V^m)^{-1} \left(\frac{1}{2} I + K^m \right) \right] u^m(x), \quad S^m :\ H^{1/2}(\Gamma^m) \mapsto H^{-1/2}(\Gamma^m),$$

and the Newton potential $N^m f$ by

$$(N^m f)(x) = (V^m)^{-1} (N_0^m f)(x),$$

where

$$(N_0^m f)(x) = \int_{\Omega^m} U(x,y) f(y)\, \mathrm{d}y.$$

It can be shown that the Steklov–Poincaré operator S^m is bounded and symmetric on $H^{1/2}(\Gamma^m)$ and $H^{1/2}(\Gamma^m)$-semielliptic. Moreover, if the measure of Γ_u^m is positive, then the operator S^m is $H_0^{1/2}(\Gamma^m, \Gamma_u^m)$-elliptic. Here,

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

More details concerning these properties of the Steklov–Poincaré operator may be found, e.g., in [33].

Now we can introduce the boundary weak formulation of our model problem (1) and (2): find $(u^1, u^2) \in \mathcal{K}$ such that

$$\sum_{m=1}^{2} \int_{\Gamma^m} (S^m u^m)(x)(v^m - u^m)(x)\, \mathrm{d}s_x \geq \sum_{m=1}^{2} \int_{\Gamma^m} (N^m f)(x)(v^m - u^m)(x)\, \mathrm{d}s_x \tag{3}$$

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

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

It is well-known that problem (3) is equivalent to the following minimization problem

$$\min_{(v^1,v^2)\in\mathcal{K}} \quad \sum_{m=1}^{2} \left[\frac{1}{2} \int_{\Gamma^m} (S^m v^m)(x) v^m(x) \, \mathrm{d}s_x - \int_{\Gamma^m} (N^m f)(x) v^m(x) \, \mathrm{d}s_x \right]. \tag{4}$$

In the coercive case, the coercivity of the quadratic functional is ensured by the $H_0^{1/2}(\Gamma^1, \Gamma_u^1)$-ellipticity of S^1 and by the $H_0^{1/2}(\Gamma^2, \Gamma_u^2)$-ellipticity of S^2. In the semicoercive case the problem is coercive due to

$$\int_{\Omega^2} f(x) \, \mathrm{d}x < 0.$$

These observations imply, see, e.g., [25], that our model problem (4) is uniquely solvable in both the coercive and semicoercive case.

4 Approximation of the Steklov–Poincaré operator and Newton potential

Since the Steklov–Poincaré operators S^m and Newton potentials $N^m f$ are given only implicitly, for the practical computations we have to choose suitable approximations $\tilde{S}^m$ and $\tilde{N}^m f$, e.g., as introduced in [33]. For $v^m \in H^{1/2}(\Gamma^m)$ we have

$$(S^m v^m)(x) = (D^m v^m)(x) + (\frac{1}{2} I + K'^m) w^m(x) \quad \text{for } x \in \Gamma^m,$$

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

$$\langle V^m w^m, \tau^m \rangle_{L^2(\Gamma^m)} = \left\langle (\frac{1}{2} I + K^m) v^m, \tau^m \right\rangle_{L^2(\Gamma^m)} \quad \text{for all } \tau^m \in H^{-1/2}(\Gamma^m). \tag{5}$$

Let

$$Z_h^m = \operatorname{span} \{ \psi_k^m \}_{k=1}^{N^m} \subset H^{-1/2}(\Gamma^m)$$

be a finite-dimensional space of trial functions. Then the Galerkin formulation of (5) reads: find $w_h^m \in Z_h^m$ such that

$$\langle V^m w_h^m, \tau_h^m \rangle_{L^2(\Gamma^m)} = \left\langle (\frac{1}{2} I + K^m) v^m, \tau_h^m \right\rangle_{L^2(\Gamma^m)} \quad \text{for all } \tau_h^m \in Z_h^m.$$

Now we define an approximation of S^m by

$$(\tilde{S}^m v^m)(x) = (D^m v^m)(x) + (\frac{1}{2} I + K'^m) w_h^m(x) \quad \text{for } x \in \Gamma^m.$$

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

$$(\tilde{N}^m f)(x) = \lambda_h^m(x) \quad \text{for } x \in \Gamma^m,$$

where $\lambda_h^m \in Z_h^m$ solves uniquely the Galerkin variational problem

$$\langle V^m \lambda_h^m, \tau_h^m \rangle_{L^2(\Gamma^m)} = \langle N_0 f, \tau_h^m \rangle_{L^2(\Gamma^m)} \quad \text{for all } \tau_h^m \in Z_h^m.$$

Thus, instead of (4), we shall consider the problem to find

$$\min_{(v^1,v^2)\in\mathcal{K}} \quad \sum_{m=1}^{2} \left[\frac{1}{2} \int_{\Gamma^m} (\tilde{S}^m v^m)(x) v^m(x) \, \mathrm{d}s_x - \int_{\Gamma^m} (\tilde{N}^m f)(x) v^m(x) \, \mathrm{d}s_x \right]. \tag{6}$$

5 Discretized variational inequality

Let

$$W_h^m = \operatorname{span}\{\varphi_k^m\}_{k=1}^{M^m} \subset H_0^{1/2}(\Gamma^m, \Gamma_u^m)$$

be a finite-dimensional trial space on the boundary Γ^m. We shall assume that the corresponding grids on Γ^1 and Γ^2 match across Γ_c. Then the Ritz formulation of (6) reads:

$$\min_{(v_h^1,v_h^2)\in\mathcal{K}_h} \quad \sum_{m=1}^{2} \left[\frac{1}{2} \int_{\Gamma^m} (\tilde{S}^m v_h^m)(x) v_h^m(x) \, \mathrm{d}s_x - \int_{\Gamma^m} (\tilde{N}^m f)(x) v_h^m(x) \, \mathrm{d}s_x \right], \tag{7}$$

where

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

Problem (7) is further equivalent to

$$\min_{(v^1,v^2)\in K} \quad \sum_{m=1}^{2} \left[\frac{1}{2} \left(\tilde{S}_h^m v^m, v^m \right) - \left(\tilde{R}_h^m, v^m \right) \right], \tag{8}$$

where

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

Here, $\tilde{S}_h^m \in \mathbb{R}^{M^m \times M^m}$ is the discrete approximate Steklov–Poincaré operator

$$\tilde{S}_h^m = D_h^m + \left(\frac{1}{2} M_h^m + K_h^m \right)^{\mathrm{T}} (V_h^m)^{-1} \left(\frac{1}{2} M_h^m + K_h^m \right)$$

and $\tilde{R}_h^m \in \mathbb{R}^{M^m}$ is the discrete approximate Newton potential

$$\tilde{R}_h^m = (M_h^m)^{\mathrm{T}} (V_h^m)^{-1} N_{0,h}^m.$$

The boundary element matrices and vector $N_{0,h}^m$ are given by

$$\begin{aligned}
V_h^m[k,l] &= \left\langle V^m \psi_l^m, \psi_k^m \right\rangle_{L^2(\Gamma^m)}, & V_h^m &\in \mathbb{R}^{N^m \times N^m}, \\
M_h^m[l,n] &= \left\langle \varphi_n^m, \psi_l^m \right\rangle_{L^2(\Gamma^m)}, & M_h^m &\in \mathbb{R}^{N^m \times M^m}, \\
K_h^m[l,n] &= \left\langle K^m \varphi_n^m, \psi_l^m \right\rangle_{L^2(\Gamma^m)}, & K_h^m &\in \mathbb{R}^{N^m \times M^m}, \\
D_h^m[q,n] &= \left\langle D^m \varphi_n^m, \varphi_q^m \right\rangle_{L^2(\Gamma^m)}, & D_h^m &\in \mathbb{R}^{M^m \times M^m}, \\
N_{0,h}^m[l] &= \left\langle N_0^m f, \psi_l^m \right\rangle_{L^2(\Gamma^m)}, & N_{0,h}^m &\in \mathbb{R}^{N^m}.
\end{aligned}$$

The stiffness matrices V_h^m, K_h^m, and D_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 V_h^m and D_h^m and equations

$$\frac{1}{2} \sum_{n=1}^{M^m} M_h^m[l,n] = -\sum_{n=1}^{M^m} K_h^m[l,n] \quad \text{and} \quad \sum_{n=1}^{M^m} D_h^m[q,n] = 0$$

for $l = 1, \ldots, N^m$, $q = 1, \ldots, M^m$.

For evaluation of the vector $N_{0,h}^m$ it is necessary to compute the Newton potential $N_0^m f$. This can be done, e.g., by an indirect approach using the finite element method, as introduced in [32, 33].

Now let us denote

$$v = \begin{bmatrix} v^1 \\ v^2 \end{bmatrix},$$

and let us describe the non-interpenetration condition across the interface Γ_c by the inequality constraints

$$B_I v \leq 0.$$

Each row of the matrix B_I is associated with a pair of matching nodes on Γ_c; it has 1 and -1 in the appropriate positions and zeros elsewhere. Following the recently proposed TFETI domain decomposition method [16, 27], we can enforce also the homogeneous Dirichlet conditions on Γ_u^1 and Γ_u^2 by the equality constraints

$$B_E v = 0.$$

This approach is motivated here 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 φ_k^m that are nonzero on Γ_u^m. The rows of the matrix B_E are associated with the nodes on $\Gamma_u^1 \cup \Gamma_u^2$; 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 problem (8) as

$$\min_{v \in \mathbb{R}^{M^1+M^2}} \left[\frac{1}{2} v^{\mathrm{T}} \tilde{S} v - \tilde{R}^{\mathrm{T}} v \right] \quad \text{subject to} \quad B_I v \leq 0 \quad \text{and} \quad B_E v = 0, \tag{9}$$

where

$$\tilde{S} = \mathrm{diag}\left(\tilde{S}_h^1, \tilde{S}_h^2\right)$$

is the the block diagonal matrix and

$$\tilde{R} = \begin{bmatrix} \tilde{R}_h^1 \\ \tilde{R}_h^2 \end{bmatrix}.$$

6 Dual formulation

Now we shall eliminate the primal variables using the duality theory in order to improve the conditioning and simplify the structure of our problem. In particular, this step shall replace the general inequality constraints in the primal formulation (9) by the bound constraints in the dual formulation. First, the matrices $\tilde{S}_h^m$ are positive semidefinite due to the lack of the Dirichlet boundary conditions, and therefore they are singular. Let us denote by $\tilde{S}^{m,+}$ any symmetric matrix that satisfies

$$\tilde{S}_h^m = \tilde{S}_h^m \tilde{S}^{m,+} \tilde{S}_h^m,$$

so that the matrix $\tilde{S}^+ = \mathrm{diag}(\tilde{S}^{1,+}, \tilde{S}^{2,+})$ satisfies

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

Let us also denote by R a matrix whose columns span the null space of $\tilde{S}$. Matrix R may be formed so that it has two columns; each domain being associated with a column of R with ones in the positions corresponding to the indices of the nodes belonging to the domain and zeros elsewhere. By introducing the Lagrange multipliers λ_I and λ_E associated with the inequalities and equalities, respectively, and denoting

$$\lambda = \begin{bmatrix} \lambda_I \\ \lambda_E \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} B_I \\ B_E \end{bmatrix},$$

we may equivalently replace problem (9) by

$$\min \left[\frac{1}{2}\lambda^{\mathrm{T}} F \lambda - \lambda^{\mathrm{T}} \tilde{d}\right] \quad \text{subject to} \quad \lambda_I \geq 0 \quad \text{and} \quad \tilde{G}\lambda = \tilde{e} \tag{10}$$

with

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

Once the solution λ of (10) is known, the solution v of (9) may be evaluated by

$$v = \tilde{S}^+(\tilde{R} - B^{\mathrm{T}}\lambda) + R\alpha$$

and the formula

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

where $\tilde{B} = \left[\tilde{B}_I^{\mathrm{T}},\ B_E^{\mathrm{T}}\right]^{\mathrm{T}}$, and the matrix $\tilde{B}_I$ is formed by the rows of B_I corresponding to the positive entries of λ_I. The procedure is similar to that described in [18].

7 Natural coarse grid

Even though problem (10) is much more suitable for computations than (9), further improvement may be achieved. As we shall give only a sketch here, we note that the details may be found, e.g., in [14].
Let us introduce a regular matrix T defining orthonormalization of the rows of $\tilde{G}$ so that the matrix

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

has orthonormal rows. After denoting

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

problem (10) reads

$$\min\left[\frac{1}{2}\lambda^{\mathrm{T}}F\lambda - \lambda^{\mathrm{T}}\tilde{d}\right] \quad \text{subject to} \quad \lambda_I \geq 0 \quad \text{and} \quad G\lambda = e. \tag{11}$$

Our next step is to look for the solution of (11) in the form $\lambda = \mu + \tilde{\lambda}$, where $G\tilde{\lambda} = e$. Since

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

problem (11) is, after returning to the old notation, equivalent to

$$\min\left[\frac{1}{2}\lambda^{\mathrm{T}}F\lambda - \lambda^{\mathrm{T}}d\right] \quad \text{subject to} \quad \lambda_I \geq -\tilde{\lambda}_I \quad \text{and} \quad G\lambda = 0 \tag{12}$$

with $d = \tilde{d} - F\tilde{\lambda}$.
We can further observe that problem (12) is equivalent to the problem

$$\min\left[\frac{1}{2}\lambda^{\mathrm{T}}PFP\lambda - \lambda^{\mathrm{T}}Pd\right] \quad \text{subject to} \quad \lambda_I \geq -\tilde{\lambda}_I \quad \text{and} \quad G\lambda = 0, \tag{13}$$

where

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

denote the orthogonal projectors on the kernel of G and on the image space of G^{T}, respectively. The projectors P and Q define the so-called natural coarse grid.
Finally, we introduce an augmented Lagrangian associated with problem (13)

$$L(\lambda, \mu, \rho) = \frac{1}{2}\lambda^{\mathrm{T}}(PFP + \rho Q)\lambda - \lambda^{\mathrm{T}}Pd + \mu^{\mathrm{T}}G\lambda. \tag{14}$$

Let us note that if $[a,b]$ is an interval containing nonzero elements of the spectrum $\sigma\{PFP\}$ of PFP, $0 < a$, then $\sigma\{PFP + \rho Q\} \subseteq [a,b] \cup \{\rho\}$, so that $PFP + \rho Q$ is nonsingular, and the rate of convergence of the conjugate gradient method applied to the linear problem with the matrix $PFP + \rho Q$ is independent of the penalization [8].

8 Algorithms

We shall now briefly review our algorithms for the solution of the bound and equality constrained problem (13). They combine our semimonotonic augmented Lagrangian method [9] 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 [19]. The gradient of the augmented Lagrangian (14) is given by

$$g(\lambda,\mu,\rho) = PFP\lambda - Pd + G^{\mathrm{T}}\left(\mu + \rho G\lambda\right).$$

Let I denote the set of the indices of the bound constrained entries of λ. The *projected gradient* $g^P = g^P(\lambda,\mu,\rho)$ of L at λ is then given componentwise by

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

where $g_i^- = \min\{g_i, 0\}$. 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 [13] was used by Dostál and Horák to develop a scalable FETI based algorithm, as shown experimentally in [14]. All the necessary parameters are listed in *Step 0*, and typical values of these parameters for our model problem are given in brackets.

Algorithm 1. Semi-monotonic augmented Lagrangian method for bound and equality constrained problems (**SMALBE**).

Step 0. {*Initialization of parameters*}

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

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

Find λ^k such that $\lambda_I^k \geq -\tilde{\lambda}_I$ and
$\left\|g^P(\lambda^k,\mu^k,\rho_k)\right\| \leq \min\{M\left\|G\lambda^k\right\|, \eta\}$.

Step 2. {*Stopping criterion.*}

If $\left\|g^P(\lambda^k,\mu^k,\rho_k)\right\|$ and $\left\|G\lambda^k\right\|$ are sufficiently small, then
λ^k is the solution.

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

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

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

If $k > 0$ and $L(\lambda^k,\mu^k,\rho^k) < L(\lambda^{k-1},\mu^{k-1},\rho_{k-1}) + \frac{\rho_k}{2}\left\|G\lambda^k\right\|^2$, 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 λ subject to $\lambda_I \geq -\tilde{\lambda}_I$ which guarantees convergence of the projected gradient to zero. More about the properties and implementation of the SMALBE algorithm may be found in [9].

The unique feature of the SMALBE algorithm is its capability to find an approximate solution of problem (13) in a number of steps which is bounded in terms of bounds on the spectrum of $PFP + \rho_0 Q$ [9]. To get a bound on the number of matrix multiplication, it is necessary to have algorithm which can solve the problem

$$\min L(\lambda, \mu, \rho) \quad \text{subject to} \quad \lambda_I \geq -\tilde{\lambda}_I \tag{15}$$

with the rate of convergence in terms of the bounds on the spectrum of the Hessian matrix of L. When the dimension of the null space of $\tilde{S}$ is small (it is one in our model problem), then it is possible to use larger regularization parameter ρ_0 as this causes only small increase in the rate of convergence of the conjugate gradient iterations [8].

To describe such algorithm, let us recall that the unique solution $\overline{\lambda} = \overline{\lambda}(\mu, \rho)$ of (15) satisfies the Karush-Kuhn-Tucker (KKT) conditions

$$\overline{\lambda}_i = -\tilde{\lambda}_i \quad \text{and} \quad i \in I \quad \text{implies} \quad g_i(\overline{\lambda}) \geq 0$$

and

$$\overline{\lambda}_i > -\tilde{\lambda}_i \quad \text{or} \quad i \notin I \quad \text{implies} \quad g_i(\overline{\lambda}) = 0.$$

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

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

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

$$\varphi_i(\lambda) = \begin{cases} g_i(\lambda) & \text{for} \quad i \in \mathcal{F}(\lambda), \\ 0 & \text{for} \quad i \in \mathcal{A}(\lambda), \end{cases} \quad \text{and} \quad \beta_i(\lambda) = \begin{cases} 0 & \text{for} \quad i \in \mathcal{F}(\lambda), \\ g_i^-(\lambda) & \text{for} \quad i \in \mathcal{A}(\lambda), \end{cases}$$

so that the KKT conditions are satisfied if and only if the *projected gradient* $g^P(\lambda) = \varphi(\lambda) + \beta(\lambda)$ is equal to zero. We call λ *feasible* if $\lambda_i \geq -\tilde{\lambda}_i$ for $i \in I$. The projector P to the set of feasible vectors is defined for any λ by

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

Let A denote the Hessian of L with respect to λ. The *expansion step* is defined by

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

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

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

such that

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

If the inequality

$$\left\|\beta(\lambda^k)\right\|^2 \leq \Gamma^2 \tilde{\varphi}(\lambda^k)^{\mathrm{T}} \varphi(\lambda^k) \tag{16}$$

holds, then we call the iterate λ^k *strictly proportional*. The test (16) is used to decide which component of the projected gradient $g^P(\lambda^k)$ will be reduced in the next step.

The *proportioning step* is defined by

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

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

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

The purpose of the proportioning step is to remove indices from the active set.

The *conjugate gradient step* is defined by

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

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

$$p^{k+1} = \varphi(\lambda^{k+1}) - \gamma p^k, \;\; \gamma = \frac{\varphi(\lambda^{k+1})^{\mathrm{T}} A p^k}{(p^k)^{\mathrm{T}} A p^k}.$$

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

Algorithm 2. Modified proportioning with reduced gradient projections (**MPRGP**).
Let λ^0 be a vector such that $\lambda_i^0 \geq -\tilde{\lambda}_i$ for $i \in I$, $\overline{\alpha} \in (0, 2\|A\|^{-1}]$, and $\Gamma > 0$ be given. For $k \geq 0$ and λ^k known, choose λ^{k+1} by the following rules:
Step 1. If $g^P(\lambda^k) = 0$, then set $\lambda^{k+1} = \lambda^k$.
Step 2. If λ^k is strictly proportional and $g^P(\lambda^k) \neq 0$, then try to generate λ^{k+1} by the conjugate gradient step. If $\lambda_i^{k+1} \geq -\tilde{\lambda}_i$ for $i \in I$, then accept it, else generate λ^{k+1} by the expansion step.
Step 3. If λ^k is not strictly proportional, define λ^{k+1} by proportioning.

The MPRGP algorithm has an R-linear rate of convergence in terms of the spectral condition number of the Hessian A of L [19, 12]. If the inner loop of SMALBE is implemented with MPRGP, then there it is possible to get an upper bound on the number of iterations that are necessary to achieve the prescribed relative precision [19, 10]. More about the properties and implementation of the SMALBE algorithm may be found in [19, 10].

9 Numerical experiments

In this section we shall present the performance of the above-described SMALBE algorithm with the inner loop implemented by a modification of MPRGP called Monotonic MPRGP to the solution of our model problems. If applied to the minimization of $L(\lambda,\mu,\rho)$ with respect to λ subject to $\lambda_I \geq \tilde{\lambda}_I$, the Monotonic MPRGP differs from the standard MPRGP in the second step which then reads:

Step 2. If $P(\lambda^k)$ is strictly proportional and $g^P\big(P(\lambda^k)\big) \neq 0$, then try to generate λ^{k+1} by the conjugate gradient step. If $L\big(P(\lambda^{k+1}),\mu,\rho\big) \leq L\big(P(\lambda^k),\mu,\rho\big)$, then accept it, else generate λ^{k+1} by the expansion step.

Our modification of MPRGP is closely related to the semismooth Newton methods [24]. See also Dostál [11, 7]. If the number of consecutive unfeasible iterations is bounded, then the algorithm preserves its linear rate of convergence bounded in terms of bounds of the Hessian matrix of the cost function. We implemented our algorithms in Matlab.

The both domain boundaries Γ^m were discretized by the same regular grid with the mesh size h. The spaces W_h^m and Z_h^m were formed by the piecewise linear and constant trial functions with respect to the discretization, respectively.

For the SMALBE algorithm we used parameters $\eta = \|Pd\|$, $\beta = 10$, and $M = 1$. The penalty parameter ρ_0 and the Lagrange multipliers μ^0 for the equality constraints were set to $\|PFP\|$ and 0, respectively. For the MPRGP algorithm we used parameters $\overline{\alpha} = \|PFP + \rho_k Q\|^{-1}$ and $\Gamma = 1$. Our initial approximation λ^0 was set to $\max\{-\tilde{\lambda}, 0.5B\tilde{R}\}$. The stopping criterion of the outer loop was chosen as

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

We use a variant of MPRGP which continues the conjugate gradient iterations as long as

The numbers of the outer iterations and the conjugate gradient iterations for varying mesh size h are shown in Table 1a and Table 1b. The solutions for $h = 1/256$ are shown in Figure 2a and Figure 2b.

h	primal dimension	dual dimension	outer iterations	CG iterations
1/32	256	99	4	25
1/64	512	195	4	35
1/128	1024	387	4	49
1/256	2048	771	4	70

Table 1a: Performance for varying discretization (coercive problem).

h	primal dimension	dual dimension	outer iterations	CG iterations
1/32	256	66	2	19
1/64	512	130	3	36
1/128	1024	258	2	32
1/256	2048	514	2	43

Table 1b: Performance for varying discretization (semicoercive problem).

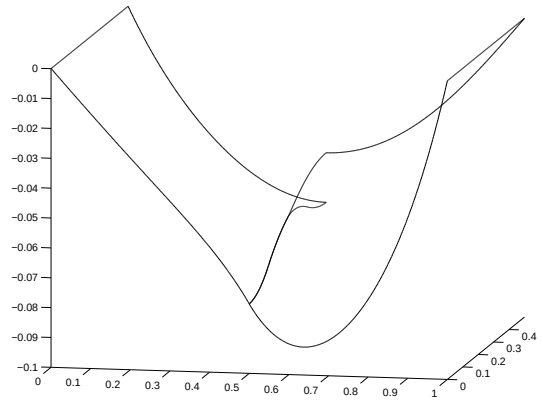

Fig. 2a: Solution of coercive problem.

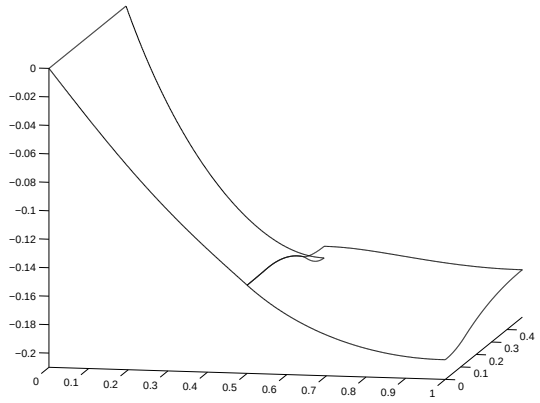

Fig. 2b: Solution of semicoercive problem.

In both cases, the number of iterations can be essentially reduced by using the BETI domain decomposition method of Langer and Steinbach [26] adapted to the solution of variational inequalities. We shall discuss this point elsewhere.

10 Comments and conclusions

The boundary element discretization of elliptic boundary variational inequality has been described which complies with recently proposed algorithms for bound (and equality) constrained quadratic programming. If applied to a multidomain problem, our algorithms may also be classified as a duality based domain decomposition method closely related to FETI [18]. Moreover, using the technique developed in domain decomposition methods [26, 4], it is even possible to prove a kind of optimality results, namely that a system of similar bodies may be solved to a given relative precision in a number of iterations which is independent of the number of subdomains. The algorithms may be useful also for the solution of problems that are discretized partly by the finite element method and partly by the boundary element method. The algorithm is a variant of our scalable BETI algorithm for the solution of elliptic variational inequalities [4]. The algorithm treats each domain separately and is suitable for parallel implementation. Application to the contact problems of elasticity is straightforward. We shall give the details elsewhere.

Acknowledgements

This research has been supported by the grants GA CR 201/07/0294, AS CR 1ET400300415, and the Ministry of Education of the Czech Republic No. MSM6198910027.

References

[1] O. Axelsson, *Iterative Solution Methods*, Cambridge University Press, Cambridge, 1994.

[2] D. P. Bertsekas, *Nonlinear Optimization*, Athena Scientific, Belmont, 1999.

[3] J. Bouchala, Z. Dostál, M. Sadowská, *Solution of boundary variational inequalities by combining fast quadratic programming algorithms with symmetric BEM*, Advances in Boundary Integral Methods - Proceedings of the Fifth UK Conference on Boundary Integral Methods, University of Liverpool (2005) 221-228.

[4] J. Bouchala, Z. Dostál, M. Sadowská, *Theoretically Supported Scalable BETI Method for Variational Inequalities*, Computing 82(2008)53-75.

[5] A. R. Conn, N. I. M. Gould, Ph. L. Toint, *A globally convergent augmented Lagrangian algorithm for optimization with general constraints and simple bounds*, SIAM Journal on Numerical Analysis 28 (1991) 545-572.

[6] M. Costabel, *Boundary integral operators on Lipschitz domains: Elementary results*, SIAM J. Math. Anal. 19 (1988) 613-626.

[7] Z. Dostál, *Box Constrained Quadratic Programming with Proportioning and Projections.* SIAM J. Optimization 7,3 (1997) 871-887.

[8] Z. Dostál, *On preconditioning and penalized matrices*, Num. Lin. Alg. Appl. 6 (1999) 109-114.

[9] Z. Dostál, *Inexact semimonotonic augmented Lagrangians with optimal feasibility convergence for convex bound and equality constrained quadratic programming*, SIAM J. Numer. Anal. 43,1 (2005) 96-115.

[10] Z. Dostál, *An optimal algorithm for bound and equality constrained quadratic programming problems with bounded spectrum*, Computing 78 (2006) 311-328.

[11] Z. Dostál, *Optimal Quadratic Programming Algorithms*, Springer, New York, in print.

[12] Z. Dostál, M. Domorádová, M. Sadowská, *Superrelaxation in minimizing quadratic functions subject to bound constraints*, submitted to Computational Optimization and Applications

[13] Z. Dostál, A. Friedlander, S. A. Santos, *Augmented Lagrangians with adaptive precision control for quadratic programming with simple bounds and equality constraints*, SIAM Journal on Optimization 13,4 (2003) 1120-1140.

[14] Z. Dostál, D. Horák, *Scalability and FETI based algorithm for large discretized variational inequalities*, Mathematics and Computers in Simulation 61 (2003) 347-357.

[15] Z. Dostál, D. Horák, *Theoretically supported scalable FETI for numerical solution of variational inequalities*, SIAM Journal on Numerical Analysis (2006) 45,2 (2007) 500-513.

[16] Z. Dostál, D. Horák, R. Kučera, *Total FETI - an easier implementable variant of the FETI method for numerical solution of elliptic PDE*, Communications in Numerical Methods in Engineering 22 (2006) 1155-1162.

[17] Z. Dostál, J. Malík, A. Friedlander, S. A. Santos, *Analysis of semicoercive contact problems using symmetric BEM and augmented Lagrangians*, Engineering Analysis with Boundary Elements 18 (1996) 195-201.

[18] Z. Dostál, D. Horák, D. Stefanica, *A scalable FETI-DP algorithm for coercive variational inequalities*, IMACS Journal Applied Numerical Mathematics 54,3-4 (2005) 378-390.

[19] Z. Dostál, J. Schöberl, *Minimizing Quadratic Functions Subject to Bound Constraints with the Rate of Convergence and Finite Termination*, Computational Optimization and Applications 30 (2005) 23-43.

[20] Z. Dostál, V. Vondrák, J. Rasmussen, *FETI based semianalytic sensitivity analysis in contact shape optimization*, Fast Solution of Discretized Optimization Problems, eds. K. H. Hoffmann, R. H. W. Hoppe and V. Schulz, Birkhäuser, International Series of Numerical Mathematics 138, Basel 2001, pages 98-106.

[21] C. Eck, O. Steinbach, W. L. Wendland, *A symmetric boundary element method for contact problems with friction*, Mathematics and Computers in Simulation 50 (1999) 43-61.

[22] C. Farhat, F.-X. Roux, *An unconventional domain decomposition method for an efficient parallel solution of large-scale finite element systems*, SIAM Journal on Scientific Computing 13 (1992) 379-396.

[23] L. J. Gray, *Evaluation of singular and hypersingular Galerkin integrals: direct limits and symbolic computation*, Chapter 2, Singular Integrals in Boundary Element Method, Edited by V. Sladek and J. Sladek, Comp. Mech. Publ., 1998.

[24] Hintermüller, M., Ito, K., Kunisch, K.: The primal–dual active set strategy as a semismooth Newton method. SIAM J. Optim. **13**, 865–888 (2003)

[25] I. Hlaváček, J. Haslinger, J. Nečas, J. Lovíšek, *Solution of Variational Inequalities in Mechanics*, Springer - Verlag Berlin (1988).

[26] U. Langer, O. Steinbach, *Boundary element tearing and interconnecting methods*, Computing 71 (2003) 205-228.

[27] G. Of, *BETI - Gebietszerlegungsmethoden mit schnellen Randelementverfahren und Anwendungen*, Ph.D. Thesis, University of Stuttgart, 2006.

[28] G. Of, O. Steinbach, W. L. Wendland, *The fast multipole method for the symmetric boundary integral formulation*, IMA J. Numer. Anal. 26 (2006) 272-296.

[29] S. Rjasanow, O. Steinbach, *The Fast Solution of Boundary Integral Equations. Mathematical and Analytical Techniques with Applications to Engineering*, Springer, 2007.

[30] M. Sadowská, *Solution of variational inequalities by the boundary integral equations*, M.Sc. Thesis, VŠB Technical University of Ostrava, Faculty of Electrical Engineering and Computer Science, Department of Applied Mathematics, May 2005. (In Czech)

[31] W. Spann, *On the boundary element method for the Signorini problem of the Laplacian*, Numerische Mathematik 65 (1993) 337-356.

[32] O. Steinbach, *Fast evaluation of Newton potentials in boundary element methods*, East-West J. Numer. Math. 7 (1999) 211-222.

[33] O. Steinbach, *Stability Estimates for Hybrid Coupled Domain Decomposition Methods*, Lecture Notes in Mathematics, vol. 1809, Springer - Verlag Berlin Heidelberg, 2003.