Scalable Total BETI based algorithm for 3D coercive contact problems of linear elastostatics

J. Bouchala, Z. Dostál, and M. Sadowská
Department of Applied Mathematics
VŠB – Technical University of Ostrava
Ostrava, Czech Republic

Abstract

A Total BETI (TBETI) based domain decomposition algorithm with the preconditioning by a natural coarse grid of the rigid body motions is adapted for the solution of contact problems of elasticity and proved to be scalable for the coercive problems, i.e., the cost of the solution is asymptotically proportional to the number of variables. The analysis is based on the original results by Langer and Steinbach on the scalability of BETI for linear problems and our development of optimal quadratic programming algorithms for bound and equality constrained problems. Both theoretical results and numerical experiments indicate a high efficiency of the algorithms presented.

Keywords Boundary elements, contact problems, domain decomposition, BETI, scalability.

AMS Subject Classifications: 65N38, 65N55, 65K05

Key words: domain decomposition, boundary elements, BETI, variational inequality, contact problems, scalable solvers, linear elastostatics

1 Introduction

The numerical solution of large contact problems of elasticity is a difficult task because their boundary conditions involve the inequalities which make them strongly non-linear. Observing that the classical Dirichlet and Neumann boundary conditions are known only after the solution has been found, it is natural to assume the solution of contact problems to be more costly than the solution of a related linear problem with the classical boundary conditions. In particular, since the cost of the solution of any problem increases at least linearly with the number of the unknowns, it follows that the development of a scalable algorithm for contact problems is a challenging task, which requires to identify the contact interface in a sense for free.

In spite of this, there has been a considerable effort in this direction and a number of interesting results have been obtained. Most of the results, either experimental or theoretical, were obtained for the problems discretized by the finite element method, either in the framework of the domain decomposition methods, see, e.g., Schöberl [43], Dureisseix and Farhat [25], Avery et al. [1], Dostál and Horák [19], and Dostál, Horák, and Stefanica [22], or by the multigrid methods, see, e.g., Kornhuber [33], Kornhuber and Krause [34], and Wohlmuth and Krause [48]. However, our recent results obtained for numerical solution of scalar elliptic variational inequalities discretized by the Boundary Element Method (BEM) [7] indicate that it is possible to develop scalable algorithm also for the contact problem of elasticity discretized by the BEM. The point of this paper is to show that it is indeed the case.

Let us recall that a number of researchers developed algorithms for the solution of contact problems by BEM, including problems with friction [26], problems discretized by mortars [38], or semicoercive problems [26]. The main benefit of application of BEM, as compared with the more popular Finite Element Methods (FEMs), is the formulation of the problem reduced to the boundary of the underlying domain which yields a dimension reduction. In particular, BEM is desirable, for example, when dealing with large or unbounded domains [36] or shape optimization problems. However, since BEM requires the explicit knowledge of a fundamental solution of the given partial differential operator, it is applicable only to the problems involving materials with rather simple properties.

Let us recall that there are two approaches to BEM, namely direct and indirect BEM. The indirect approach is based on the fact that single and double layer potentials solve the underlying homogeneous partial differential equation exactly for given classes of density functions. In this way we transform the boundary value problem into the problem of finding an unknown density of the potential. The direct approach reformulates the boundary value problem in terms of the Boundary Integral Equations (BIEs) and the unknown Cauchy data (trace of the solution and its corresponding conormal derivative) are found by solving these BIEs numerically. Here we prefer the letter method in combination with the Galerkin discretization; though we have to handle double boundary integrals instead of a single boundary integration that arises from the application of the collocation method, we get the stiffness matrices that are closely related to the Schur complements of the matrices arising from FEM.

Apart from our in a sense optimal quadratic programming algorithms, our main tool is the Boundary Element Tearing and Interconnecting (BETI) method – a combination of the symmetric Galerkin BEM with the duality based domain decomposition (DD) approach – as it was originally introduced by Langer and Steinbach [35]. The essential idea behind DD methods is splitting the original boundary value problem into local problems on smaller subdomains that decompose the underlying domain. The local problems are then coupled by suitable transmission conditions introduced on the artificial interfaces between subdomains. We use the "All Floating" or "Total" variant of the BETI method introduced independently by Of [39] and Dostál et al. [20], respectively. This approach enforces the Dirichlet pboundary conditions by additional Lagrange multipliers, so that the kernels of the stiffness matrices of all the subdomain are a priori known. After the application of duality, we employ preconditioning by the projectors to the so–called natural coarse grid that was originally proposed by Farhat et al. [28] for preconditioning of their FETI method. Since Langer and Steinbach show in [35] that the discrete approximate Steklov–Poincaré operators generated by the FETI and BETI methods are spectrally equivalent, we can exploit the analysis of Farhat et al. [28] to get the bounds on the spectrum of the preconditioned dual stiffness matrix independent of the discretization and decomposition parameters h and H, respectively. Let us point out that although our method is based on that introduced by Langer and Steinbach [35], we cannot use their preconditioning strategy, since their preconditioner transforms the bound constraints into more general inequalities, which prevents the application of our optimal algorithms.

In this paper, we present the basic algorithm and analysis for coercive contact problems. Our presentation is complete in sense that it starts with the equations of equilibrium, presents the variational formulation, its discretization, relevant theoretical results, the solution algorithms and their properties, and results of numerical experiments. The analysis can be extended to semicoercive problems and the performance can be further improved by application of standard BETI preconditioners [47] to the linear steps and by the applications of the Fast BEMs, such as Fast Multipole Method (FMM) [31, 40, 50] or Adaptive Cross Approximation (ACA) [4, 41]. We shall give the details elsewhere.

The paper is organized as follows. After introducing a model problem, we briefly review the BETI methodology [7] that transforms the boundary variational inequality into bound and equality constrained dual problem whose conditioning is further improved by using the projectors to the natural coarse grid. Then we review our algorithms for the solution of the resulting quadratic programming problem with bound and equality constraints whose rate of convergence can be expressed in terms of bounds on the spectrum of the preconditioned dual stiffness matrix [15, 23]. Finally, we present the main results about optimality of our method and give results of numerical experiments which are in a good agreement with the theory behind and demonstrate the scalability of the presented method.

2 Model Contact Problem

For the sake of simplicity, we shall confine ourselves to the following model coercive 3D contact problem, but our reasoning can be extended to more general problems.

Let us consider an elastic body which occupies in the reference configuration the bounded Lipschitz domain $\Omega := (0, a)^3 \subset \mathbb{R}^3$, $a > 0$, with the boundary $\Gamma := \partial\Omega$ comprising three parts

$$\Gamma_u := \{x \in \Gamma : \ x_2 = 0\}, \quad \Gamma_c := \{x \in \Gamma : \ x_3 = 0\}, \quad \Gamma_f := \Gamma \setminus \{\Gamma_u \cup \Gamma_c\}.$$

We assume that the body is fixed on Γ_u, free on Γ_f, and it is not allowed to penetrate the rigid obstacle $P_d := \{x \in \mathbb{R}^3 : \ x_3 \le d\}$, $d < 0$. Inside Ω, we assume that the body is loaded by volume forces with the

density $\underline{f}$. See also Figure 1.

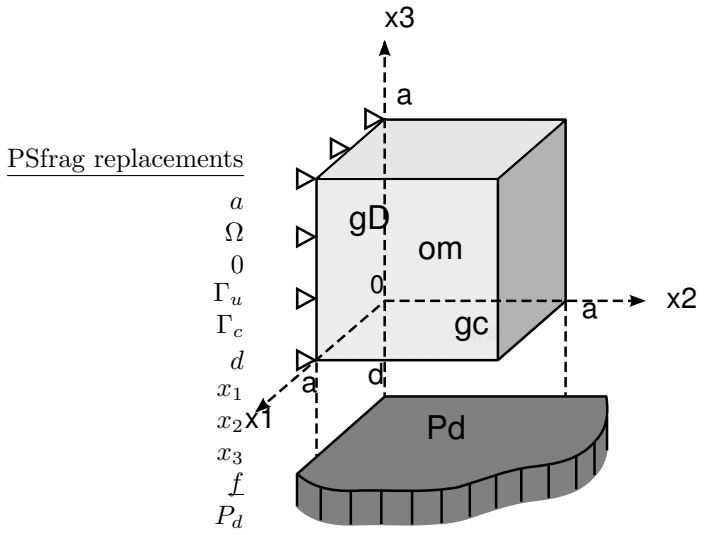

Figure 1: Geometry of the model contact problem

We focus on finding a sufficiently smooth displacement field $\underline{u}$ satisfying

$$\begin{aligned} (\mathcal{L}\underline{u})_i(x) := -\sum_{j=1}^{3} \frac{\partial}{\partial x_j}\sigma_{ij}(\underline{u},x) &= f_i(x) \qquad \text{for } x\in\Omega,\ i=1,2,3,\\ \underline{u}(x) &= \underline{0} \qquad \text{for } x\in\Gamma_u, \\ t_i(x) := \sum_{j=1}^{3} \sigma_{ij}(\underline{u},x)n_j(x) &= 0 \qquad \text{for } x\in\Gamma_f,\ i=1,2,3, \end{aligned} \tag{2.1}$$

together with the contact conditions

$$u_3(x)\geq d, \quad t_3(x)\geq 0, \quad (u_3(x)-d)\,t_3(x)=0 \quad \text{for } x\in\Gamma_c \tag{2.2}$$

with $n_j(x)$ denoting the jth component of the exterior unit normal vector $\underline{n}(x)$ of Ω that is defined for almost all $x\in\Gamma$.

We assume the body is made of homogeneous isotropic material, so that the stress tensor $\{\sigma_{ij}(\underline{u},x)\}_{i,j=1}^3$ complies with the Hook law of the form

$$\sigma_{ij}(\underline{u},x) := \frac{E\nu}{(1+\nu)(1-2\nu)}\delta_{ij}\sum_{k=1}^{3} e_{kk}(\underline{u},x) + \frac{E}{1+\nu}e_{ij}(\underline{u},x) \quad \text{for } x\in\overline{\Omega},\ i,j=1,2,3,$$

where δ_{ij} denotes the Kronecker delta, the strain tensor $\{e_{ij}(\underline{u},x)\}_{i,j=1}^3$ is given by

$$e_{ij}(\underline{u},x) := \frac{1}{2}\left(\frac{\partial}{\partial x_i}u_j(x) + \frac{\partial}{\partial x_j}u_i(x)\right) \quad \text{for } x\in\overline{\Omega},\ i,j=1,2,3,$$

and E and ν are material constants, to be specific, $E>0$ is the Young modulus and $\nu\in(0,1/2)$ is the Poisson ratio. Since we assume ν is bounded away from $1/2$, we deal here with the case of compressible elastostatics. Furthermore, we consider the density $\underline{f}$ of internal forces belonging to $[L^2(\Omega)]^3$.

3 Domain Decomposition and Minimum of Energy

In order to develop a method suitable for parallel solution of our model problem, let us decompose the domain Ω into $p \in \mathbb{N}$ non-overlapping Lipschitz subdomains Ω_m with the boundaries $\Gamma_m := \partial\Omega_m$,

$$\overline{\Omega} = \bigcup_{m=1}^{p} \overline{\Omega_m}, \quad \Omega_m \cap \Omega_n = \emptyset \quad \text{for } m \neq n, \quad \Gamma_{mn} := \Gamma_m \cap \Gamma_n, \quad \Gamma_s := \bigcup_{m=1}^{p} \Gamma_m.$$

The set Γ_s is called a skeleton of Ω. Moreover, let $\underline{n}_m(x)$ denote the exterior unit normal vector of Ω_m defined for almost all $x \in \Gamma_m$ and $f_{m,i} := f_i|_{\Omega_m}$ for $i = 1, 2, 3$. Thus instead of (2.1), (2.2) we can consider the system of local boundary value problems

$$\begin{aligned} \mathcal{L}\underline{u}_m(x) &= \underline{f}_m(x) && \text{for } x \in \Omega_m, \\ \underline{u}_m(x) &= \underline{0} && \text{for } x \in \Gamma_u \cap \Gamma_m, \\ t_{m,i}(x) := \sum_{j=1}^{3} \sigma_{ij}(\underline{u}_m, x) n_{m,j}(x) &= 0 && \text{for } x \in \Gamma_f \cap \Gamma_m, \ i = 1, 2, 3, \end{aligned} \tag{3.1}$$

together with the local contact conditions

$$u_{m,3}(x) \geq d, \quad t_{m,3}(x) \geq 0, \quad (u_{m,3}(x) - d)\, t_{m,3}(x) = 0 \quad \text{for } x \in \Gamma_c \cap \Gamma_m \tag{3.2}$$

and with the transmission conditions

$$\underline{u}_m(x) = \underline{u}_n(x), \quad \underline{t}_m(x) + \underline{t}_n(x) = \underline{0} \quad \text{for } x \in \Gamma_{mn}, \tag{3.3}$$

which link the local problems together and ensure "smoothness" across the artificial interfaces Γ_{mn}.

The fundamental solution $\{U_{ij}(x,y)\}_{i,j=1}^{3}$ of the operator $\mathcal{L}$ corresponding to the 3D isotropic homogeneous linear elastostatics is given by Kelvin's tensor

$$U_{ij}(x,y) := \frac{1+\nu}{8\pi E(1-\nu)} \left((3-4\nu) \frac{\delta_{ij}}{\|x-y\|} + \frac{(x_i - y_i)(x_j - y_j)}{\|x-y\|^3} \right)$$

defined for $i, j = 1, 2, 3$ and $x, y \in \mathbb{R}^3$. Moreover, let us denote $\underline{U}_j := (U_{1j}, U_{2j}, U_{3j})$ and define

$$[H^1_{\mathcal{L}}(\Omega_m)]^3 := \left\{ \underline{v} \in [H^1(\Omega_m)]^3 : \ \mathcal{L}\underline{v} \in [L^2(\Omega_m)]^3 \right\}.$$

It is well-known [26, 46] that any distributional solution $\underline{u}_m \in [H^1_{\mathcal{L}}(\Omega_m)]^3$ of the first equation of (3.1) can be represented via Somigliana's identity as

$$u_{m,j}(x) = \int_{\Omega_m} \left(\underline{f}_m(y), \underline{U}_j(x,y)\right) \mathrm{d}y + \int_{\Gamma_m} \left(\gamma_1^m \underline{u}_m(y), \underline{U}_j(x,y)\right) \mathrm{d}s_y - \int_{\Gamma_m} \left(\gamma_0^m \underline{u}_m(y), \gamma_{1,y}^m \underline{U}_j(x,y)\right) \mathrm{d}s_y \tag{3.4}$$

for $x \in \Omega_m$ and $j = 1, 2, 3$, where

$$\gamma_0^m : \ [H^1(\Omega_m)]^3 \mapsto [H^{1/2}(\Gamma_m)]^3 \quad \text{and} \quad \gamma_1^m : \ [H^1_{\mathcal{L}}(\Omega_m)]^3 \mapsto [H^{-1/2}(\Gamma_m)]^3$$

are the local interior trace and boundary stress operators satisfying for all $\underline{v} \in [C^\infty(\overline{\Omega_m})]^3$ and $i = 1, 2, 3$

$$(\gamma_0^m \underline{v})_i = v_i|_{\Gamma_m} \quad \text{and} \quad (\gamma_1^m \underline{v})_i(x) = \sum_{j=1}^{3} \sigma_{ij}(\underline{v}, x) n_{m,j}(x) \quad \text{for } x \in \Gamma_m,$$

respectively, and $(\cdot, \cdot)$ denotes the Euclidean scalar product.

By applying the operators γ_0^m and γ_1^m to Somigliana's identity (3.4), we can derive the Dirichlet–Neumann map

$$\gamma_1^m \underline{u}_m(x) = (S_m \gamma_0^m \underline{u}_m)(x) - (N_m \underline{f}_m)(x) \quad \text{for } x \in \Gamma_m$$

with the local Steklov–Poincaré operator

$$S_m := (\frac{1}{2}I + K'_m)V_m^{-1}(\frac{1}{2}I + K_m) + D_m : \ [H^{1/2}(\Gamma_m)]^3 \mapsto [H^{-1/2}(\Gamma_m)]^3$$

and the local Newton operator

$$N_m \underline{f}_m := V_m^{-1} N_{m,0} \underline{f}_m \in [H^{-1/2}(\Gamma_m)]^3,$$

using the the local single layer potential operator V_m, double layer potential operator K_m, adjoint double layer potential operator K'_m, hypersingular integral operator D_m defined for $x \in \Gamma_m$ and $i = 1, 2, 3$ by

$$\begin{aligned}
(V_m \underline{t})_i(x) &:= \int_{\Gamma_m} (\underline{t}(y), \underline{U}_i(x,y)) \, \mathrm{d}s_y, && V_m : \ [H^{-1/2}(\Gamma_m)]^3 \mapsto [H^{1/2}(\Gamma_m)]^3, \\
(K_m \underline{u})_i(x) &:= \int_{\Gamma_m} \big(\underline{u}(y), \gamma^m_{1,y} \underline{U}_i(x,y)\big) \, \mathrm{d}s_y, && K_m : \ [H^{1/2}(\Gamma_m)]^3 \mapsto [H^{1/2}(\Gamma_m)]^3 \\
(K'_m \underline{t})_i(x) &:= \int_{\Gamma_m} \big(\underline{t}(y), \gamma^m_{1,x} \underline{U}_i(x,y)\big) \, \mathrm{d}s_y, && K'_m : \ [H^{-1/2}(\Gamma_m)]^3 \mapsto [H^{-1/2}(\Gamma_m)]^3 \\
(D_m \underline{u})_i(x) &:= -\gamma^m_{1,x} \int_{\Gamma_m} \big(\underline{u}(y), \gamma^m_{1,y} \underline{U}_i(x,y)\big) \, \mathrm{d}s_y, && D_m : \ [H^{1/2}(\Gamma_m)]^3 \mapsto [H^{-1/2}(\Gamma_m)]^3,
\end{aligned}$$

and the local Newton potential operator $N_{m,0}$ defined for $x \in \Gamma_m$ and $i = 1, 2, 3$ by

$$(N_{m,0} \underline{f}_m)_i(x) := \int_{\Omega_m} (\underline{f}_m(y), \underline{U}_i(x,y)) \, \mathrm{d}y, \qquad N_{m,0} : \ [L^2(\Omega_m)]^3 \mapsto [H^{1/2}(\Gamma_m)]^3.$$

The mapping properties of the above integral operators are well known [11, 46], namely, the local single layer potential operator is $[H^{-1/2}(\Gamma_m)]^3$-elliptic, so that its inversion is well-defined.

Theorem 3.1 [46] *The local Steklov–Poincaré operator S_m is linear, bounded, symmetric, and semi-elliptic on $[H^{1/2}(\Gamma_m)]^3$. Moreover, if meas$\{\Gamma_m \cap \Gamma_u\} > 0$ and $H_0^{1/2}(\Gamma_m, \Gamma_m \cap \Gamma_u) := \{v \in H^{1/2}(\Gamma_m) : \ v(x) = 0$ for $x \in \Gamma_m \cap \Gamma_u\}$, then S_m is $[H_0^{1/2}(\Gamma_m, \Gamma_m \cap \Gamma_u)]^3$-elliptic.*

Now let us define $H^{1/2}(\Gamma_s)$ as a trace space of $H^1(\Omega)$ restricted to the skeleton Γ_s equipped with the norm

$$\|v\|_{H^{1/2}(\Gamma_s)} := \left(\sum_{m=1}^{p} \big\| v|_{\Gamma_m} \big\|^2_{H^{1/2}(\Gamma_m)} \right)^{1/2}.$$

Moreover, let

$$H_0^{1/2}(\Gamma_s, \Gamma_u) := \Big\{ v \in H^{1/2}(\Gamma_s) : \ v(x) = 0 \quad \text{for } x \in \Gamma_u \Big\},$$

$$\mathcal{K} := \Big\{ \underline{v} \in [H_0^{1/2}(\Gamma_s, \Gamma_u)]^3 : \ v_3(x) \geq d \quad \text{for } x \in \Gamma_c \Big\},$$

and

$$\underline{v}_m := \underline{v}|_{\Gamma_m} \quad \text{for } \underline{v} \in [H_0^{1/2}(\Gamma_s, \Gamma_u)]^3.$$

Let us define the bilinear form

$$\mathcal{A}(\underline{u}, \underline{v}) := \sum_{m=1}^{p} \langle S_m \underline{u}_m, \underline{v}_m \rangle_{\Gamma_m} \qquad \text{for } \underline{u}, \underline{v} \in [H_0^{1/2}(\Gamma_s, \Gamma_u)]^3$$

and the linear functional

$$\mathcal{F}(\underline{v}) := \sum_{m=1}^{p} \langle N_m \underline{f}_m, \underline{v}_m \rangle_{\Gamma_m} \qquad \text{for } \underline{v} \in [H_0^{1/2}(\Gamma_s, \Gamma_u)]^3$$

with

$$\langle \underline{v},\, \underline{w}\rangle_{\Gamma_m} := \sum_{i=1}^{3} \langle v_i,\, w_i\rangle_{L^2(\Gamma_m)} \qquad \text{for } \underline{v}, \underline{w} \in [H_0^{1/2}(\Gamma_s, \Gamma_u)]^3.$$

We call a function $\underline{u} \in \mathcal{K}$ a boundary weak solution of (3.1)–(3.3) if

$$\mathcal{A}(\underline{u},\, \underline{v} - \underline{u}) \geq \mathcal{F}(\underline{v} - \underline{u}) \quad \text{for all } \underline{v} \in \mathcal{K}. \tag{3.5}$$

Theorem 3.2 [?] *There is a unique boundary weak solution $\underline{u} \in \mathcal{K}$ of (3.1)–(3.3). Moreover, variational inequality (3.5) is equivalent to the problem: find $\underline{u} \in \mathcal{K}$ such that*

$$\mathcal{J}(\underline{u}) = \min\{\mathcal{J}(\underline{v}) :\ \underline{v} \in \mathcal{K}\}, \tag{3.6}$$

where $\mathcal{J}$ is the energy functional defined as

$$\mathcal{J}(\underline{v}) := \frac{1}{2}\,\mathcal{A}(\underline{v},\, \underline{v}) - \mathcal{F}(\underline{v}) \quad \textit{for } \underline{v} \in [H_0^{1/2}(\Gamma_s,\, \Gamma_u)]^3.$$

Proof: First note that $\mathcal{K}$ is convex, closed, and non-empty set and functional $\mathcal{F}$ is bounded on $[H_0^{1/2}(\Gamma_s, \Gamma_u)]^3$. Following standard results of analysis of variational inequalities, to prove unique solvability of (3.5), it suffices to show that the bilinear form $\mathcal{A}$ is bounded and elliptic on $[H_0^{1/2}(\Gamma_s, \Gamma_u)]^3$. Let us note that the boundedness of $\mathcal{A}$ follows particularly from the boundedness of the local operators S_m on $[H^{1/2}(\Gamma_m)]^3$.

We shall now prove the $[H_0^{1/2}(\Gamma_s, \Gamma_u)]^3$-ellipticity of $\mathcal{A}$. Let $\underline{u} \in [H_0^{1/2}(\Gamma_s,\, \Gamma_u)]^3$ and let $\underline{v} \in [H_0^1(\Omega,\, \Gamma_u)]^3$ be such that for $m = 1,\, 2,\, \ldots,\, p$ the function $\underline{v}_m := \underline{v}|_{\Omega_m}$ is the weak solution of

$$\begin{aligned} \mathcal{L}\underline{v}_m(x) &= \underline{0} && \text{for } x \in \Omega_m, \\ \gamma_0^m \underline{v}_m(x) &= \underline{u}_m(x) && \text{for } x \in \Gamma_m. \end{aligned}$$

It is known that

$$\langle S_m \underline{u}_m,\, \underline{u}_m\rangle_{\Gamma_m} = \int_{\Omega_m} W(\underline{v}_m(x), \underline{v}_m(x))\,\mathrm{d}x,$$

where

$$W(\underline{v}_m(x), \underline{v}_m(x)) = \frac{E\nu}{(1+\nu)(1-2\nu)} \left(\sum_{i=1}^{3} e_{ii}(\underline{v}_m, x)\right)^2 + \frac{E}{1+\nu} \sum_{i,j=1}^{3} e_{ij}^2(\underline{v}_m, x).$$

Using this result and Korn's inequality we obtain

$$\begin{aligned} \mathcal{A}(\underline{u}, \underline{u}) &= \sum_{m=1}^{p} \int_{\Omega_m} W(\underline{v}_m(x), \underline{v}_m(x))\,\mathrm{d}x = \int_{\Omega} W(\underline{v}(x), \underline{v}(x))\,\mathrm{d}x \\ &\geq k_1 \int_{\Omega} \sum_{i,j=1}^{3} e_{ij}^2(\underline{v}, x)\,\mathrm{d}x \geq k_2 \int_{\Omega} \sum_{i,j=1}^{3} \left(\frac{\partial v_i}{\partial x_j}(x)\right)^2 \mathrm{d}x = k_2 \sum_{i=1}^{3} \int_{\Omega} \|\nabla v_i(x)\|^2\,\mathrm{d}x \end{aligned}$$

with $\|\cdot\|$ denoting the Euclidean norm. Furthermore, we shall use the Friedrichs theorem and the boundedness of the local trace operator, i.e. the estimate

$$\|\gamma_0^m \underline{w}\|_{[H^{1/2}(\Gamma_m)]^3} \leq k \|\underline{w}\|_{[H^1(\Omega_m)]^3} \quad \text{for all } \underline{w} \in [H^1(\Omega_m)]^3,$$

to get

$$\begin{aligned} \sum_{i=1}^{3} \int_{\Omega} \|\nabla v_i(x)\|^2\,\mathrm{d}x &\geq k_3 \sum_{i=1}^{3} \|v_i\|^2_{H^1(\Omega)} = k_3 \|\underline{v}\|^2_{[H^1(\Omega)]^3} = k_3 \sum_{m=1}^{p} \|\underline{v}_m\|^2_{[H^1(\Omega_m)]^3} \\ &\geq k_4 \sum_{m=1}^{p} \|\underline{u}_m\|^2_{[H^{1/2}(\Gamma_m)]^3} = k_4 \|\underline{u}\|^2_{[H^{1/2}(\Gamma_s)]^3}. \end{aligned}$$

Since the operator S_m is symmetric on $[H^{1/2}(\Gamma_m)]^3$, it is straightforward that $\mathcal{A}$ is also symmetric on $[H_0^{1/2}(\Gamma_s, \Gamma_u)]^3$, and therefore problems (3.6) and (3.5) are equivalent.

□

4 Transition to Discrete Problem

Let us first define suitable approximations of the local operators S_m and $N_m \underline{f}_m$ in order to avoid their implicit representations. We shall approximate both operators by using boundary elements as it is described, e.g., in [45].

For $\underline{u} \in [H^{1/2}(\Gamma_m)]^3$ we have

$$(S_m \underline{u})(x) = (D_m \underline{u})(x) + (\frac{1}{2} I + K'_m)\underline{w}(x) \quad \text{for all } x \in \Gamma_m,$$

where $\underline{w} \in [H^{-1/2}(\Gamma_m)]^3$ is the unique solution of the problem

$$\langle V_m \underline{w}, \underline{v} \rangle_{\Gamma_m} = \left\langle (\frac{1}{2} I + K_m)\underline{u}, \underline{v} \right\rangle_{\Gamma_m} \quad \text{for all } \underline{v} \in [H^{-1/2}(\Gamma_m)]^3. \tag{4.1}$$

Let

$$Z_h := \left[\text{span}\,\{\psi_k^m\}_{k=1}^{L_m}\right]^3 \subset [H^{-1/2}(\Gamma_m)]^3$$

be a local finite-dimensional space of shape functions with piecewise constant basis functions ψ_k^m. Then the Galerkin formulation of (4.1) reads: find $\underline{w}_h \in Z_h$ such that

$$\langle V_m \underline{w}_h, \underline{v}_h \rangle_{\Gamma_m} = \left\langle (\frac{1}{2} I + K_m)\underline{u}, \underline{v}_h \right\rangle_{\Gamma_m} \quad \text{for all } \underline{v}_h \in Z_h. \tag{4.2}$$

We define the approximation $\widetilde{S}_m$ of S_m by

$$(\widetilde{S}_m \underline{u})(x) := (D_m \underline{u})(x) + (\frac{1}{2} I + K'_m)\underline{w}_h^u(x) \quad \text{for } x \in \Gamma_m, \tag{4.3}$$

where $\underline{w}_h^u$ is the unique solution of (4.2).

In the very similar way we define the approximation $\widetilde{N}_m \underline{f}_m \in Z_h$ of $N_m \underline{f}_m$ as a unique solution of

$$\left\langle V_m \widetilde{N}_m \underline{f}_m, \underline{v}_h \right\rangle_{\Gamma_m} = \langle N_{0,m} \underline{f}_m, \underline{v}_h \rangle_{\Gamma_m} \quad \text{for all } \underline{v}_h \in Z_h.$$

Theorem 4.1 *The approximation $\widetilde{S}_m$ of S_m defined by (4.3) preserves all properties of S_m mentioned in Theorem 3.1.*

PROOF: All the properties except the symmetry of $\widetilde{S}_m$ are discussed in detail in [45]. The proof of the symmetry of $\widetilde{S}_m$ proceeds as follows. Let $\underline{u}, \underline{v} \in [H^{1/2}(\Gamma_m)]^3$ be arbitrary and $\underline{w}_h^u, \underline{w}_h^v \in Z_h$ be the corresponding unique solutions of (4.2). In particular, due to the symmetry of V_m on $[H^{-1/2}(\Gamma_m)]^3$, we get

$$\begin{aligned}
\left\langle (\frac{1}{2} I + K'_m)\underline{w}_h^u, \underline{v} \right\rangle_{\Gamma_m} &= \left\langle (\frac{1}{2} I + K_m)\underline{v}, \underline{w}_h^u \right\rangle_{\Gamma_m} = \langle V_m \underline{w}_h^v, \underline{w}_h^u \rangle_{\Gamma_m} \\
&= \langle V_m \underline{w}_h^u, \underline{w}_h^v \rangle_{\Gamma_m} = \left\langle (\frac{1}{2} I + K_m)\underline{u}, \underline{w}_h^v \right\rangle_{\Gamma_m} = \left\langle (\frac{1}{2} I + K'_m)\underline{w}_h^v, \underline{u} \right\rangle_{\Gamma_m}
\end{aligned}$$

Since D_m is symmetric on on $[H^{1/2}(\Gamma_m)]^3$, we conclude that $\widetilde{S}_m$ is symmetric on $[H^{1/2}(\Gamma_m)]^3$.

□

Now let

$$W_h := \left[\text{span}\,\{\varphi_k\}_{k=1}^{M}\right]^3 \subset [H^{1/2}(\Gamma_s)]^3$$

be a global finite-dimensional trial space on the skeleton Γ_s, where φ_k are piecewise linear basis functions, and let

$$W_{m,h} := \left[\text{span}\,\{\varphi_k^m\}_{k=1}^{M_m}\right]^3$$

be the restriction of W_h onto Γ_m. Plane triangles of the corresponding boundary element mesh shall be denoted by τ_k^m, $m = 1, \ldots, p$, $k = 1, \ldots, M_m$. By application of the Ritz method to (3.6) with S_m and $N_m \underline{f}_m$ approximated by $\widetilde{S}_m$ and $\widetilde{N}_m \underline{f}_m$, respectively, we obtain the following quadratic programming problem:

$$\text{minimize} \quad J(\mathbf{v}) \quad \text{subject to} \quad \mathsf{B}_I \mathbf{v} \leq \mathbf{c}_I \quad \text{and} \quad \mathsf{B}_E \mathbf{v} = \mathbf{0}, \tag{4.4}$$

where

$$J(\mathbf{v}) := \frac{1}{2} \mathbf{v}^\top \widetilde{\mathsf{S}} \mathbf{v} - \widetilde{\mathbf{R}}^\top \mathbf{v},$$

$$\widetilde{\mathsf{S}} := \begin{pmatrix} \widetilde{\mathsf{S}}_{1,h} & \mathsf{O} & \mathsf{O} \\ \mathsf{O} & \ddots & \mathsf{O} \\ \mathsf{O} & \mathsf{O} & \widetilde{\mathsf{S}}_{p,h} \end{pmatrix}, \quad \mathbf{v} := \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_p \end{pmatrix}, \quad \mathbf{v}_m := \begin{pmatrix} \mathbf{v}_{m,1} \\ \mathbf{v}_{m,2} \\ \mathbf{v}_{m,3} \end{pmatrix}, \quad \widetilde{\mathbf{R}} := \begin{pmatrix} \widetilde{\mathbf{R}}_{1,h} \\ \vdots \\ \widetilde{\mathbf{R}}_{p,h} \end{pmatrix}, \tag{4.5}$$

and

$$\mathsf{B}_E := \begin{pmatrix} \mathsf{B}_C \\ \mathsf{B}_D \end{pmatrix}.$$

Here, $\widetilde{\mathsf{S}}_{m,h} \in \mathbb{R}^{3M_m \times 3M_m}$ is the discrete approximate local Steklov–Poincaré operator

$$\widetilde{\mathsf{S}}_{m,h} := \mathsf{D}_{m,h} + (\frac{1}{2}\mathsf{M}_{m,h} + \mathsf{K}_{m,h})^\top \mathsf{V}_{m,h}^{-1} (\frac{1}{2}\mathsf{M}_{m,h} + \mathsf{K}_{m,h})$$

and $\widetilde{\mathbf{R}}_{m,h} \in \mathbb{R}^{3M_m}$ is the discrete approximate local Newton operator

$$\widetilde{\mathbf{R}}_{m,h} := \mathsf{M}_{m,h}^\top \mathsf{V}_{m,h}^{-1} \mathbf{N}_{0,m,h}.$$

The local boundary element matrices $\mathsf{V}_{m,h}$, $\mathsf{K}_{m,h}$, and $\mathsf{D}_{m,h}$ are all fully populated. Matrices $\mathsf{V}_{m,h}$ and $\mathsf{D}_{m,h}$ are symmetric positive definite and semi-definite, respectively.

For the discrete local single layer potential operator we have the representation [41, 46]

$$\mathsf{V}_{m,h} = \frac{1+\nu}{2E(1-\nu)} \left((3-4\nu) \begin{pmatrix} \mathsf{V}_{m,h}^{\triangle} & \mathsf{O} & \mathsf{O} \\ \mathsf{O} & \mathsf{V}_{m,h}^{\triangle} & \mathsf{O} \\ \mathsf{O} & \mathsf{O} & \mathsf{V}_{m,h}^{\triangle} \end{pmatrix} + \begin{pmatrix} \mathsf{V}_{11,m,h} & \mathsf{V}_{12,m,h} & \mathsf{V}_{13,m,h} \\ \mathsf{V}_{12,m,h} & \mathsf{V}_{22,m,h} & \mathsf{V}_{23,m,h} \\ \mathsf{V}_{13,m,h} & \mathsf{V}_{23,m,h} & \mathsf{V}_{33,m,h} \end{pmatrix} \right)$$

with the discrete local single layer potential operator $\mathsf{V}_{m,h}^{\triangle} \in \mathbb{R}^{L_m \times L_m}$ for the 3D Laplace operator defined by

$$\mathsf{V}_{m,h}^{\triangle}[k,l] := \frac{1}{4\pi} \int_{\tau_k^m} \int_{\tau_l^m} \frac{1}{\|x-y\|} \, \mathrm{d}s_y \, \mathrm{d}s_x$$

and the matrices $\mathsf{V}_{ij,m,h} \in \mathbb{R}^{L_m \times L_m}$ defined by

$$\mathsf{V}_{ij,m,h}[k,l] := \frac{1}{4\pi} \int_{\tau_k^m} \int_{\tau_l^m} \frac{(x_i - y_i)(x_j - y_j)}{\|x-y\|^3} \, \mathrm{d}s_y \, \mathrm{d}s_x$$

for $k, l = 1, \ldots, L_m$, $i, j = 1, 2, 3$, $i \leq j$.

For the discrete local double layer potential operator we have the representation [41, 46]

$$\mathsf{K}_{m,h} = \begin{pmatrix} \mathsf{K}_{m,h}^{\triangle} & \mathsf{O} & \mathsf{O} \\ \mathsf{O} & \mathsf{K}_{m,h}^{\triangle} & \mathsf{O} \\ \mathsf{O} & \mathsf{O} & \mathsf{K}_{m,h}^{\triangle} \end{pmatrix} - \begin{pmatrix} \mathsf{V}_{m,h}^{\triangle} & \mathsf{O} & \mathsf{O} \\ \mathsf{O} & \mathsf{V}_{m,h}^{\triangle} & \mathsf{O} \\ \mathsf{O} & \mathsf{O} & \mathsf{V}_{m,h}^{\triangle} \end{pmatrix} \mathsf{T}_m + \frac{E}{1+\nu} \mathsf{V}_{m,h} \, \mathsf{T}_m$$

with the discrete local double layer potential operator $\mathsf{K}_{m,h}^{\triangle} \in \mathbb{R}^{L_m \times M_m}$ for the 3D Laplace operator defined by

$$\mathsf{K}_{m,h}^{\triangle}[k,n] := \frac{1}{4\pi} \int_{\tau_k^m} \int_{\Gamma_m} \frac{(x-y, \, \underline{n}_m(y))}{\|x-y\|^3} \varphi_n^m(y) \, \mathrm{d}s_y \, \mathrm{d}s_x$$

and the sparse local transformation matrix

$$\mathsf{T}_m := \begin{pmatrix} \mathsf{O} & \mathsf{T}_{12,m} & \mathsf{T}_{13,m} \\ -\mathsf{T}_{12,m} & \mathsf{O} & \mathsf{T}_{23,m} \\ -\mathsf{T}_{13,m} & -\mathsf{T}_{23,m} & \mathsf{O} \end{pmatrix},$$

where the blocks $\mathsf{T}_{ij,m} \in \mathbb{R}^{L_m \times M_m}$ are given by

$$\mathsf{T}_{ij,m}[k,n] := n_j(x)\frac{\partial \varphi_n^m}{\partial x_i}(x) - n_i(x)\frac{\partial \varphi_n^m}{\partial x_j}(x), \quad x \in \tau_k^m,$$

for $k = 1, \ldots, L_m$, $n = 1, \ldots, M_m$, $i, j = 1, 2, 3$, $i < j$.

In computations, we exploit the symmetry of $\mathsf{V}_{m,h}^{\triangle}$ and $\mathsf{V}_{ij,m,h}$. Entries of the matrices $\mathsf{V}_{m,h}^{\triangle}$, $\mathsf{V}_{ij,m,h}$, and $\mathsf{K}_{m,h}^{\triangle}$ may be calculated so that the inner integral is evaluated analytically and the outer one is approximated by using suitable numerical scheme. The detailed description of this procedure may be found in [41].

For the discrete local hypersingular integral operator $\mathsf{D}_{m,h}$ we can find a representation which is based on the local transformation matrix T_m and the matrices $\mathsf{V}_{m,h}^{\triangle}$ and $\mathsf{V}_{m,h}$, see [41, **?**].

The mass matrix $\mathsf{M}_{m,h}$ has the form

$$\mathsf{M}_{m,h} = \begin{pmatrix} \mathsf{M}_{m,h}^{\triangle} & \mathsf{O} & \mathsf{O} \\ \mathsf{O} & \mathsf{M}_{m,h}^{\triangle} & \mathsf{O} \\ \mathsf{O} & \mathsf{O} & \mathsf{M}_{m,h}^{\triangle} \end{pmatrix}$$

with the local mass matrix $\mathsf{M}_{m,h}^{\triangle} \in \mathbb{R}^{L_m \times M_m}$ defined by

$$\mathsf{M}_{m,h}^{\triangle}[k,n] := \int_{\tau_k^m} \varphi_n^m(x)\,\mathrm{d}s_x$$

for $k = 1, \ldots, L_m$ and $n = 1, \ldots, M_m$.

The vector $\mathbf{N}_{0,m,h} \in \mathbb{R}^{3L_m}$ is given by

$$\mathbf{N}_{0,m,h}[(i-1)L_m + k] := \langle (N_{0,m}\underline{f}_m)_i,\, \psi_k^m \rangle_{L^2(\Gamma_m)}$$

for $k = 1, \ldots, L_m$ and $i = 1, 2, 3$. Evaluation of $N_{0,m}\underline{f}_m$ can be done by using an indirect approach, as it is introduced in [44, 45].

Finally, it remains to describe the constraining matrices arising in (4.4). "Gluing" across the interfaces Γ_{mn} and "fixation" along the part Γ_u are enforced by the equality constraints

$$\mathsf{B}_C\mathbf{v} = \mathbf{0} \quad \text{and} \quad \mathsf{B}_D\mathbf{v} = \mathbf{0},$$

respectively. Every row of B_C consists of a single 1 and single -1 at the positions corresponding to the pair of matching nodes across Γ_{mn} and zeros elsewhere, while every row of B_D consists of a single 1 at the position corresponding to the node with prescribed zero displacement and zeros elsewhere. When constructing the matrices B_C and B_D, we constrain all three coordinate directions. Note that since we define additional equality constraints to satisfy the Dirichlet boundary condition, we use the "Total/All floating" variant of BETI [20, 39]. To avoid the penetration into obstacle, we introduce the inequality constraints

$$\mathsf{B}_I\mathbf{v} \leq \mathbf{c}_I,$$

where we constrain only the corresponding parts of the third blocks of the corresponding vectors $\mathbf{v}_m$. Every row of B_I consists of a single -1 at the appropriate position and zeros elsewhere, while every entry of $\mathbf{c}_I$ equals to $-d$.

5 Dual Formulation

Now the intention is to reduce the dimension, simplify the structure, and improve the conditioning of our problem. We shall use the duality theory, so that we shall eliminate primal variables and replace the general inequality constraints in the primal formulation (4.4) by the bound constraints in the dual formulation.

First, the blocks $\widetilde{\mathsf{S}}_{m,h}$ of $\widetilde{\mathsf{S}}$ are only positive semi-definite, so that they are singular. If we denote by $\widetilde{\mathsf{S}}^{+}_{m,h}$ a symmetric left generalized inverse of $\widetilde{\mathsf{S}}_{m,h}$, then the matrix

$$\widetilde{\mathsf{S}}^{+} := \begin{pmatrix} \widetilde{\mathsf{S}}^{+}_{1,h} & \mathsf{O} & \mathsf{O} \\ \mathsf{O} & \ddots & \mathsf{O} \\ \mathsf{O} & \mathsf{O} & \widetilde{\mathsf{S}}^{+}_{p,h} \end{pmatrix}$$

is a symmetric left generalized inverse of $\widetilde{\mathsf{S}}$, i.e. it satisfies

$$\widetilde{\mathsf{S}} = \widetilde{\mathsf{S}}\widetilde{\mathsf{S}}^{+}\widetilde{\mathsf{S}}.$$

Let R denote a full column rank matrix whose columns span the null space of $\widetilde{\mathsf{S}}$. Examining the null space of the Steklov–Poincaré operator S_m [41, 46], we put

$$\mathsf{R} := \begin{pmatrix} \mathsf{R}_1 & \mathsf{O} & \mathsf{O} \\ \mathsf{O} & \ddots & \mathsf{O} \\ \mathsf{O} & \mathsf{O} & \mathsf{R}_p \end{pmatrix}, \quad \text{where} \quad \mathsf{R}_m := \begin{pmatrix} \mathbf{1} & \mathbf{0} & \mathbf{0} & -\mathbf{x}^m_2 & \mathbf{0} & \mathbf{x}^m_3 \\ \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{x}^m_1 & -\mathbf{x}^m_3 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{x}^m_2 & -\mathbf{x}^m_1 \end{pmatrix},$$

and $\mathbf{x}^m_i$ is a vector of the ith coordinates of all nodes located on Γ_m.

By introducing vectors of the Lagrange multipliers $\boldsymbol{\lambda}_I$ and $\boldsymbol{\lambda}_E$ associated with the inequalities and equalities, respectively, and denoting

$$\boldsymbol{\lambda} := \begin{pmatrix} \boldsymbol{\lambda}_I \\ \boldsymbol{\lambda}_E \end{pmatrix}, \quad \mathsf{B} := \begin{pmatrix} \mathsf{B}_I \\ \mathsf{B}_E \end{pmatrix}, \quad \text{and} \quad \mathbf{c} := \begin{pmatrix} \mathbf{c}_I \\ \mathbf{0} \end{pmatrix},$$

we can equivalently replace problem (4.4) by the modified dual problem:

$$\text{minimize} \quad \Theta(\boldsymbol{\lambda}) \quad \text{subject to} \quad \boldsymbol{\lambda}_I \geq \mathbf{0} \quad \text{and} \quad \widetilde{\mathsf{G}}\boldsymbol{\lambda} = \widetilde{\mathbf{e}}, \tag{5.1}$$

where

$$\Theta(\boldsymbol{\lambda}) := \frac{1}{2}\boldsymbol{\lambda}^{\top}\mathsf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^{\top}\widetilde{\mathbf{d}}$$

and

$$\mathsf{F} := \mathsf{B}\widetilde{\mathsf{S}}^{+}\mathsf{B}^{\top}, \quad \widetilde{\mathbf{d}} := \mathsf{B}\widetilde{\mathsf{S}}^{+}\widetilde{\mathbf{R}} - \mathbf{c}, \quad \widetilde{\mathsf{G}} := \mathsf{R}^{\top}\mathsf{B}^{\top}, \quad \widetilde{\mathbf{e}} := \mathsf{R}^{\top}\widetilde{\mathbf{R}}.$$

Furthermore, once the solution $\overline{\boldsymbol{\lambda}}$ of (5.1) is known, the solution $\mathbf{u}$ of (4.4) may be evaluated by

$$\mathbf{u} = \widetilde{\mathsf{S}}^{+}(\widetilde{\mathbf{R}} - \mathsf{B}^{\top}\overline{\boldsymbol{\lambda}}) + \mathsf{R}\boldsymbol{\alpha}$$

and the formula [17]

$$\boldsymbol{\alpha} = (\mathsf{R}^{\top}\widetilde{\mathsf{B}}^{\top}\widetilde{\mathsf{B}}\mathsf{R})^{-1}\mathsf{R}^{\top}\widetilde{\mathsf{B}}^{\top}\left(\widetilde{\mathbf{c}} - \widetilde{\mathsf{B}}\widetilde{\mathsf{S}}^{+}(\widetilde{\mathbf{R}} - \mathsf{B}^{\top}\overline{\boldsymbol{\lambda}})\right),$$

where

$$\widetilde{\mathsf{B}} := \begin{pmatrix} \widetilde{\mathsf{B}}_I \\ \mathsf{B}_E \end{pmatrix} \quad \text{and} \quad \widetilde{\mathbf{c}} := \begin{pmatrix} \widetilde{\mathbf{c}}_I \\ \mathbf{0} \end{pmatrix}$$

with the matrix $(\widetilde{\mathsf{B}}_I, \widetilde{\mathbf{c}}_I)$ formed by the rows of $(\mathsf{B}_I, \mathbf{c}_I)$ corresponding to the positive entries of $\overline{\boldsymbol{\lambda}}_I$.

6 Natural Coarse Grid and Bounds on Spectrum

Here we introduce preconditoning by the natural coarse grid of the rigid body motions that was originally proposed by Farhat, Mandel, and Roux [28]. A unique feature of this preconditioning is that if applied to the MPRGP algorithm for (5.1), it improves not only the performance of the linear steps, but also the nonlinear steps. Thus we shall get a constrained quadratic programming problem equivalent to (5.1) with the spectrum of the Hessian of the augmented Lagrangian confined to the positive interval independent of h.

Let us introduce a non-singular matrix T defining orthonormalization of the rows of $\widetilde{\mathsf{G}}$, so that the matrix

$$\mathsf{G} := \mathsf{T}\widetilde{\mathsf{G}}$$

satisfies $\mathsf{G}\mathsf{G}^\top = \mathsf{I}$. By using the notation

$$\mathbf{e} := \mathsf{T}\widetilde{\mathbf{e}},$$

we can rewrite our dual problem (5.1) as:

$$\text{minimize} \quad \Theta(\boldsymbol{\lambda}) \quad \text{subject to} \quad \boldsymbol{\lambda}_I \geq \mathbf{0} \quad \text{and} \quad \mathsf{G}\boldsymbol{\lambda} = \mathbf{e}. \tag{6.1}$$

In order to homogenize the equality constraints, we shall look for the solution of (6.1) in the form

$$\boldsymbol{\lambda} = \boldsymbol{\mu} + \widetilde{\boldsymbol{\lambda}},$$

where $\widetilde{\boldsymbol{\lambda}}$ is a vector satisfying $\mathsf{G}\widetilde{\boldsymbol{\lambda}} = \mathbf{e}$. The following lemma enables us to define an initial approximation which is feasible with respect to the modified inequality constraints and is in a sense not far from the solution.

Lemma 6.1 *Let $G = [G_I, G_E]$. Then G_R is a full rank matrix and*

$$\widetilde{\boldsymbol{\lambda}} = \begin{pmatrix} \boldsymbol{o}_I \\ G_E^\top (G_E G_E^\top)^{-1} \boldsymbol{e} \end{pmatrix} \tag{6.2}$$

satisfies $\widetilde{\boldsymbol{\lambda}}_I = \boldsymbol{o}_I$ and $G\widetilde{\boldsymbol{\lambda}} = \boldsymbol{e}$.

Proof: First observe that

$$\mathsf{G} = [\mathsf{T}\widetilde{\mathsf{G}}_I, \mathsf{T}\widetilde{\mathsf{G}}_E],$$

so it is enough to prove that $\widetilde{\mathsf{G}}_E^\top \boldsymbol{\xi} = \mathsf{B}_E \mathsf{R}\boldsymbol{\xi} = \boldsymbol{o}$ implies $\boldsymbol{\xi} = \boldsymbol{o}$. Since $\mathsf{B}_E\mathsf{R}\boldsymbol{\xi}$ denotes the jumps of the vector $\mathsf{R}\boldsymbol{\xi}$ across the auxiliary interfaces and violations of the prescribed Dirichlet boundary conditions, it follows that the vector $\boldsymbol{u} = \mathsf{R}\boldsymbol{\xi}$ satisfies both the discretized Dirichlet conditions and the "gluing" conditions, but belongs to the kernel of S. Since the problem (2.1) is coercive, it follows that $\mathsf{R}\boldsymbol{\xi} = \boldsymbol{o}$, and, since the columns of R are independent, $\boldsymbol{\xi} = \boldsymbol{o}$. □

Lemma 6.1 is a key ingredient in the proof of the numerical scalability of our algorithm. Let us point out that its proof exploits the assumption that our model problem (2.1) is coercive, i.e., that the prescribed displacements prevent the body from floating.

Since

$$\Theta(\boldsymbol{\lambda}) = \frac{1}{2}\boldsymbol{\lambda}^\top \mathsf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top \widetilde{\mathbf{d}} = \frac{1}{2}\boldsymbol{\mu}^\top \mathsf{F}\boldsymbol{\mu} - \boldsymbol{\mu}^\top(\widetilde{\mathbf{d}} - \mathsf{F}\widetilde{\boldsymbol{\lambda}}) + \frac{1}{2}\widetilde{\boldsymbol{\lambda}}^\top \mathsf{F}\widetilde{\boldsymbol{\lambda}} - \widetilde{\boldsymbol{\lambda}}^\top \widetilde{\mathbf{d}},$$

we can consider (in minimization) the dual function Θ without the last two constant terms. Now we can return to the old notation and reformulate equivalently problem (6.1) as:

$$\text{minimize} \quad \Lambda_0(\boldsymbol{\lambda}) \quad \text{subject to} \quad \boldsymbol{\lambda}_I \geq -\widetilde{\boldsymbol{\lambda}}_I \quad \text{and} \quad \mathsf{G}\boldsymbol{\lambda} = \mathbf{0}, \tag{6.3}$$

where

$$\Lambda_0(\boldsymbol{\lambda}) := \frac{1}{2}\boldsymbol{\lambda}^\top \mathsf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top \mathbf{d} \tag{6.4}$$

and $\mathbf{d} := \widetilde{\mathbf{d}} - \mathsf{F}\widetilde{\boldsymbol{\lambda}}$.

Final step is the definition of the following matrices

$$\mathsf{Q} := \mathsf{G}^\top \mathsf{G} \quad \text{and} \quad \mathsf{P} := \mathsf{I} - \mathsf{Q}.$$

It is easy to check that Q and P are orthogonal projectors on $\operatorname{Im} \mathsf{G}^\top$ and $\operatorname{Ker} \mathsf{G}$, respectively. Problem (6.3) is then equivalent to the problem:

$$\text{minimize} \quad \Lambda(\boldsymbol{\lambda}) \quad \text{subject to} \quad \boldsymbol{\lambda}_I \geq -\widetilde{\boldsymbol{\lambda}}_I \quad \text{and} \quad \mathsf{G}\boldsymbol{\lambda} = \mathbf{0}, \tag{6.5}$$

where

$$\Lambda(\boldsymbol{\lambda}) := \frac{1}{2}\boldsymbol{\lambda}^\top \mathsf{PFP}\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top \mathsf{P}\mathbf{d}.$$

Let us introduce the augmented Lagrangian associated with problem (6.5)

$$L(\boldsymbol{\lambda}, \boldsymbol{\mu}, \rho) := \frac{1}{2}\boldsymbol{\lambda}^\top (\mathsf{PFP} + \rho\mathsf{Q})\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top \mathsf{P}\mathbf{d} + \boldsymbol{\mu}^\top \mathsf{G}\boldsymbol{\lambda} \tag{6.6}$$

with some penalty factor $\rho > 0$. Let us note that the Hessian $\mathcal{H} := \mathsf{PFP} + \rho\mathsf{Q}$ of (6.6) is decomposed by the projectors Q and P whose image spaces are invariant subspaces of $\mathcal{H}$. Now let $[a,\, b] \subset \mathbb{R}_+$ be an interval containing non-zero elements of the spectrum $\sigma\{\mathsf{PFP}\}$ of PFP. Then $\sigma\{\mathcal{H}\} \subset [a,\, b] \cup \{\rho\}$, so that $\mathcal{H}$ is non-singular, and, by the analysis of Axelsson [2], there is an upper bound on the number of the conjugate gradient iterations n_{CG} that is needed for reduction of the gradient of the augmented Lagrangian (6.6) by a tolerance $\varepsilon > 0$:

$$n_{CG} \leq \frac{1}{2} \operatorname{int}\left(\sqrt{\frac{b}{a}} \log\left(\frac{2}{\varepsilon}\right) + 3\right).$$

Now we can employ the reasoning used in Section 8 of [7] to obtain the following important result:

Theorem 6.1 *There are constants $c, C > 0$ independent of the discretization parameter h and the decomposition parameter H such that*

$$\lambda_{\min}(\mathsf{PFP} \,|\, \operatorname{Im} \mathsf{P}) \;\geq\; c \quad \textit{and} \quad \|\mathsf{PFP}\| \;\leq\; C\frac{H}{h}. \tag{6.7}$$

Proof: The proof is the same as the proof of Theorem 8.3 of Bouchala, Dostál, and Sadowská [7]. The proof is based on the similar bounds on spectrum formulated for the FETI case by Farhat, Mandel, and Roux [28] and on the observation of Langer and Steinbach [35] that the local boundary element stiffness matrix $\widetilde{\mathsf{S}}_h^m$ is spectrally equivalent to some Schur complement of the corresponding local finite element stiffness matrix. □

Thus if we refine the mesh and increase the number of subdomains so that the ratio H/h is kept constant, we have still the same upper bound on the spectral condition number of $\mathsf{PFP} \,|\, \operatorname{Im} \mathsf{P}$. Langer and Steinbach [35] give stronger polylogarithmic bounds for the preconditioned F, but we cannot use this result since such preconditioning transforms the bound constraints to more general ones.

7 Optimal Algorithms

We shall now briefly review our algorithms for the efficient solution of the bound and equality constrained problem (6.5). They combine our semimonotonic augmented Lagrangian method [15] 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 [23]. The gradient of the augmented Lagrangian (6.6) with respect to the first variable is given by

$$\mathbf{g}(\boldsymbol{\lambda}, \boldsymbol{\mu}, \rho) := \nabla_{\boldsymbol{\lambda}} L(\boldsymbol{\lambda}, \boldsymbol{\mu}, \rho) = \mathsf{PFP}\boldsymbol{\lambda} - \mathsf{P}\mathbf{d} + \mathsf{G}^\top \left(\boldsymbol{\mu} + \rho\mathsf{G}\boldsymbol{\lambda}\right).$$

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

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

where $\mathbf{g}_i^- = \min\{\mathbf{g}_i, 0\}$. Our algorithm is a variant of the SMALBE algorithm introduced by Dostál [14, 15]. The original SMALBE algorithm is based on that proposed by Conn, Gould, and Toint [10] for identifying stationary points of more general problems. Its modification by Dostál, Friedlander, and Santos [16] was used by Dostál and Horák to develop a scalable FETI based algorithm, as shown experimentally in [18]. Our algorithm differs from SMALBE in that it keeps the penalty factor constant and, instead, it decrease the parameter M which controls the precision of the inner loop solution.

Algorithm 9.1. Semimonotonic Augmented Lagrangian Method for Bound and Equality Constrained Problems with Modification of M (SMALBE-M).

Step 0: {*Initialization.*}
Choose $\eta > 0,\ \beta < 1,\ M_0 > 0,\ \rho > 0,\ \boldsymbol{\mu}^0$, set $k := 0$.

Step 1: {*Inner iteration with adaptive precision control.*}
Find $\boldsymbol{\lambda}^k$ such that $\boldsymbol{\lambda}_{\mathcal{I}}^k \geq -\widetilde{\boldsymbol{\lambda}}_{\mathcal{I}}$ and
$\|\mathbf{g}^P(\boldsymbol{\lambda}^k, \boldsymbol{\mu}^k, \rho)\| \leq \min\{M_k \|\mathsf{G}\boldsymbol{\lambda}^k\|, \eta\}$.

Step 2: {*Stopping criterion.*}
If $\|\mathbf{g}^P(\boldsymbol{\lambda}^k, \boldsymbol{\mu}^k, \rho)\|$ and $\|\mathsf{G}\boldsymbol{\lambda}^k\|$ are sufficiently small, then
$\boldsymbol{\lambda}^k$ is the solution.

Step 3: {*Update of the Lagrange multipliers.*}
$\boldsymbol{\mu}^{k+1} := \boldsymbol{\mu}^k + \rho\mathsf{G}\boldsymbol{\lambda}^k$

Step 4: {*Update of the parameter M provided the increase of the Lagrangian is insufficient.*}
If $k > 0$ and $L(\boldsymbol{\lambda}^k, \boldsymbol{\mu}^k, \rho) < L(\boldsymbol{\lambda}^{k-1}, \boldsymbol{\mu}^{k-1}, \rho) + \frac{\rho}{2}\|\mathsf{G}\boldsymbol{\lambda}^k\|^2$,
then
$M_{k+1} := \beta\, M_k$,
else
$M_{k+1} := M_k$.

Step 5: Set $k := k + 1$ and return to *Step 1*.

Note that all the necessary parameters are listed in *Step 0*. *Step 1* may be implemented by any algorithm for minimization of the augmented Lagrangian L with respect to $\boldsymbol{\lambda}$ subject to $\boldsymbol{\lambda}_{\mathcal{I}} \geq -\widetilde{\boldsymbol{\lambda}}_{\mathcal{I}}$ which guarantees convergence of the projected gradient to zero.

The SMALBE-M algorithm has similar properties as the original SMALBE algorithm. In particular, if we choose ρ_0 and M for the algorithm SMALBE and ρ and M_0 for the algorithm SMALBE-M such that $\rho_0 = \rho$, $M = M_0$, and

$$\rho_0 \geq \frac{M^2}{\lambda_{\min}(\mathcal{H})},$$

then SMALBE and SMALBE-M will generate $\rho_k = \rho$ and $M_k = M$, respectively [13]. Thus if the other parameters of the both algorithms are initiated by the same values, the algorithms will generate exactly the same iterates. The unique feature of the SMALBE algorithm is its capability to find an approximate solution of problem (6.5) in a number of steps which is bounded in terms of bounds on the spectrum of the Hessian $\mathcal{H}$ of L [15]. To get a bound on the number of matrix multiplication, it is necessary to have algorithm which can solve the problem

$$\text{minimize} \quad L(\boldsymbol{\lambda}, \boldsymbol{\mu}, \rho) \quad \text{subject to} \quad \boldsymbol{\lambda}_{\mathcal{I}} \geq -\widetilde{\boldsymbol{\lambda}}_{\mathcal{I}} \tag{7.1}$$

with the rate of convergence in terms of the bounds on the spectrum of $\mathcal{H}$.

To describe such an algorithm, let us recall that the unique solution $\overline{\boldsymbol{\lambda}} = \overline{\boldsymbol{\lambda}}(\boldsymbol{\mu}, \rho)$ of (7.1) satisfies the Karush–Kuhn–Tucker (KKT) conditions

$$\overline{\boldsymbol{\lambda}}_i = -\widetilde{\boldsymbol{\lambda}}_i \quad \text{and} \quad i \in \mathcal{I} \quad \text{imply} \quad \mathbf{g}_i(\overline{\boldsymbol{\lambda}}) \geq 0$$

and

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

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.

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

To enable an alternative reference to the KKT conditions [3], let us define the `free gradient` $\boldsymbol{\varphi}(\boldsymbol{\lambda})$ and the `chopped gradient` $\boldsymbol{\beta}(\boldsymbol{\lambda})$ by

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

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 $\boldsymbol{\lambda}_i \geq -\widetilde{\boldsymbol{\lambda}}_i$ for $i \in \mathcal{I}$. The projection P to the set of feasible vectors is defined for any $\boldsymbol{\lambda}$ by

$$P(\boldsymbol{\lambda})_i := \begin{cases} \max\{\boldsymbol{\lambda}_i, -\widetilde{\boldsymbol{\lambda}}_i\} & \text{for } i \in \mathcal{I}, \\ \boldsymbol{\lambda}_i & \text{for } i \notin \mathcal{I}. \end{cases}$$

Let us recall that $\mathcal{H}$ denotes the Hessian of L with respect to $\boldsymbol{\lambda}$. The `expansion step` is defined by

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

with the steplength $\overline{\alpha} \in (0, \, 2\,\|\mathcal{H}\|^{-1}]$. This step may expand the current active set. To describe it without P, let $\widetilde{\boldsymbol{\varphi}}(\boldsymbol{\lambda})$ be the `reduced free gradient` for any feasible $\boldsymbol{\lambda}$, with entries

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

such that

$$P\left(\boldsymbol{\lambda} - \overline{\alpha}\boldsymbol{\varphi}(\boldsymbol{\lambda})\right) = \boldsymbol{\lambda} - \overline{\alpha}\widetilde{\boldsymbol{\varphi}}(\boldsymbol{\lambda}).$$

If the inequality

$$\|\boldsymbol{\beta}(\boldsymbol{\lambda}^k)\|^2 \leq \Gamma^2 \widetilde{\boldsymbol{\varphi}}(\boldsymbol{\lambda}^k)^\top \boldsymbol{\varphi}(\boldsymbol{\lambda}^k) \tag{7.2}$$

holds, then we call the iterate $\boldsymbol{\lambda}^k$ `strictly proportional`. The test (7.2) 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 α_{CG} is chosen to minimize $L(\boldsymbol{\lambda}^k - \alpha\boldsymbol{\beta}(\boldsymbol{\lambda}^k), \boldsymbol{\mu}^k, \rho_k)$ with respect to α, i.e.

$$\alpha_{CG} := \frac{\boldsymbol{\beta}(\boldsymbol{\lambda}^k)^\top \mathbf{g}(\boldsymbol{\lambda}^k)}{\boldsymbol{\beta}(\boldsymbol{\lambda}^k)^\top \mathcal{H}\boldsymbol{\beta}(\boldsymbol{\lambda}^k)}.$$

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 [2] which is constructed recurrently. The recurrence starts (or restarts) with $\boldsymbol{p}^s := \boldsymbol{\varphi}(\boldsymbol{\lambda}^s)$ 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 formulas [2]

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

The conjugate gradient steps are used to carry out the minimization in the face

$$\mathcal{W}_\mathcal{J} := \{\boldsymbol{\lambda} : \ \boldsymbol{\lambda}_i = -\widetilde{\boldsymbol{\lambda}}_i \quad \text{for } i \in \mathcal{J}\}, \quad \mathcal{J} := \mathcal{A}(\boldsymbol{\lambda}^s),$$

efficiently. The algorithm that we use may now be described as follows.

Algorithm 9.2. Modified proportioning with reduced gradient projections (MPRGP).

Choose $\boldsymbol{\lambda}^0$ such that $\boldsymbol{\lambda}^0_i \geq -\widetilde{\boldsymbol{\lambda}}_i$ for $i \in \mathcal{I}$, $\overline{\alpha} \in (0, 2\|\mathcal{H}\|^{-1}]$, and $\Gamma > 0$, set $k := 0$.
For $k \geq 0$ and $\boldsymbol{\lambda}^k$ known, choose $\boldsymbol{\lambda}^{k+1}$ by the following rules:

i) If $\mathbf{g}^P(\boldsymbol{\lambda}^k) = \mathbf{0}$, then set $\boldsymbol{\lambda}^{k+1} := \boldsymbol{\lambda}^k$.

ii) 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 $\boldsymbol{\lambda}^{k+1}_i \geq -\widetilde{\boldsymbol{\lambda}}_i$ for $i \in \mathcal{I}$, then accept it, else generate $\boldsymbol{\lambda}^{k+1}$ by the expansion step.

iii) 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 $\mathcal{H}$ of L [12, 13]. The proof of this rate of convergence for $\overline{\alpha} \in (0, \|\mathcal{H}\|^{-1}]$ may be also found in [23]. For more details about the properties and implementation of the MPRGP algorithm, we refer to [13, 23].

8 Optimality

Let us first review our optimality result achieved for the original SMALBE algorithm [14, 15].

In order to show that the SMALBE algorithm with the inner loop implemented by Algorithm 9.2 is optimal for the solution of problem (6.5), let us introduce a new notation that coincides with that used in [14]. We shall use

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

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

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

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

$$\begin{array}{ll} \mathsf{A}_t := \mathcal{H} = \mathsf{PFP} + \rho \mathsf{Q}, & \mathbf{b}_t := \mathsf{P}\mathbf{d}, \\ \mathsf{C}_t := \mathsf{G}, & \boldsymbol{\ell}_{t,\mathcal{I}} := -\widetilde{\boldsymbol{\lambda}}_\mathcal{I}, \qquad \boldsymbol{\ell}_{t,\mathcal{E}} := -\infty \end{array}$$

by the vectors and matrices generated with the discretization and decomposition parameters H and h, respectively, so that problem (6.5) is equivalent to the problem

$$\text{minimize} \quad \Lambda_t(\boldsymbol{\lambda}_t) \quad \text{subject to} \quad \mathsf{C}_t \boldsymbol{\lambda}_t = \mathbf{0} \quad \text{and} \quad \boldsymbol{\lambda}_t \geq \boldsymbol{\ell}_t \tag{8.1}$$

with

$$\Lambda_t(\boldsymbol{\lambda}_t) := \frac{1}{2} \boldsymbol{\lambda}_t^\top \mathsf{A}_t \boldsymbol{\lambda}_t - \mathbf{b}_t^\top \boldsymbol{\lambda}_t.$$

By using these definitions, Lemma 6.1, and $\mathsf{G}\mathsf{G}^\top = \mathsf{I}$, we get

$$\|\mathsf{C}_t\| \leq 1 \quad \text{and} \quad \|\boldsymbol{\ell}_t^+\| = 0, \tag{8.2}$$

where for any vector $\mathbf{v}$ with the entries $\mathbf{v}_i$ we define a vector $\mathbf{v}^+$ by $\mathbf{v}_i^+ := \max\{\mathbf{v}_i, 0\}$. Moreover, it follows by Theorem 6.1 that for any $C \geq 2$ there are constants $a_{\max}^C \geq a_{\min}^C > 0$ such that

$$a_{\min}^C \leq \lambda_{\min}(\mathsf{A}_t) \leq \lambda_{\max}(\mathsf{A}_t) \leq a_{\max}^C \tag{8.3}$$

for any $t \in \mathcal{T}_C$. Furthermore, 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 in (8.2) and (8.3)) of [14] are satisfied for any set of indices $\mathcal{T}_C,\ C \geq 2$, so that we have the following result:

Theorem 8.1 [14] *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 the SMALBE algorithm for* (8.1) *with*

$$\|\mathbf{b}_t\| \geq \eta_t > 0,\ \beta > 1,\ M > 0,\ \rho_{t,0} := \rho_0 > 0,\ \text{and } \boldsymbol{\mu}_t^0 := \mathbf{0}.$$

Let $s \geq 0$ denote the smallest integer such that

$$\beta^s \rho_0 \geq \frac{M^2}{a_{\min}^C}$$

and assume that Step 1 of the SMALBE algorithm is implemented by means of Algorithm 9.2 (MPRGP) with parameters $\Gamma > 0$ and $\overline{\alpha} \in (0, (a_{\max}^C + \beta^s \rho_0)^{-1}]$, so that it generates the iterates $\boldsymbol{\lambda}_t^{k,0}$, $\boldsymbol{\lambda}_t^{k,1}$, …, $\boldsymbol{\lambda}_t^{k,l} =: \boldsymbol{\lambda}_t^k$ for the solution of (8.1) *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*

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

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 (8.1), SMALBE generates an approximate solution $\boldsymbol{\lambda}_t^{k_t}$ which satisfies

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

at $O(1)$ matrix–vector multiplications by the Hessian of the augmented Lagrangian L_t for (8.1) and $\rho_{t,k_t} \leq \beta^s \rho_0$.

The same statement may be proved also for the SMALBE-M algorithm, which is the variant of SMALBE with constant penalty and updated M. To see the reason, notice that the inequality

$$\rho_{t,k} \geq \frac{M^2}{\lambda_{\min}(\mathsf{A}_t)}, \tag{8.4}$$

which guarantees

$$L(\boldsymbol{\lambda}^{t,k+1}, \boldsymbol{\mu}^{t,k+1}, \rho_{k+1}) \geq L(\boldsymbol{\lambda}^{t,k}, \boldsymbol{\mu}^{t,k}, \rho_{t,k}) + \frac{\rho_{t,k+1}}{2} \|\mathsf{C}_t \boldsymbol{\lambda}^{t,k+1}\|^2,$$

can be achieved either by increasing the regularization parameter $\rho_{t,k}$, or by decreasing the balancing parameter M. Thus if the algorithm keeps the regularization factor fixed, we have the left hand side of (8.4) constant and we can achieve (8.4) by decreasing the value of parameter M. Further analysis of the optimality then follows that of the original SMALBE. In particular, if we choose M and $\rho_{t,0}$ so that (8.4) is satisfied, then the two variants of SMALBE are identical.

9 Numerical Experiments

The elastic body is represented by the cube $\Omega := (0,10)^3$ with the sizes given in millimeters. The material constants are defined by the following values: Young's modulus $E := 1.14 \cdot 10^5$ [MPa] and Poisson's ratio $\nu := 0.24$. This choice of the material parameters corresponds to steel. The body is fixed in all directions along the Dirichlet part of the boundary $\Gamma_u := [0,10] \times \{0\} \times [0,10]$. The body may touch the rigid plane

PSfrag replacements

x_1
x_2
x_3

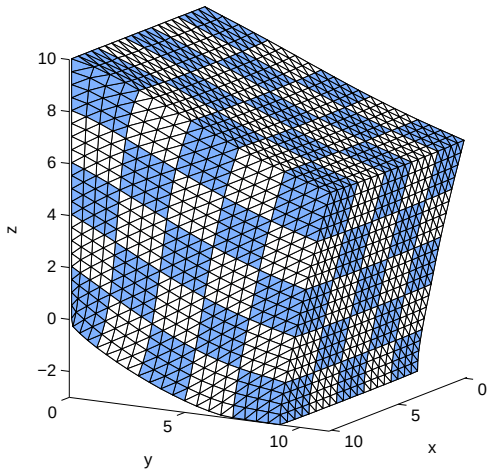

Figure 2: Body after deformation

obstacle along the contact part of the boundary $\Gamma_c := [0,10] \times [0,10] \times \{0\}$. The initial distance $|d|$ between the cube and the rigid obstacle is set to 3 [mm]. The remaining part of the boundary of the cube is free, i.e. it is neither loaded by any boundary forces nor fixed in any direction. The density of the internal forces is defined for any $x \in \Omega$ by $\underline{f}(x) := (0, 0, -2.1 \cdot 10^3)$ [N/mm^3].

The body was decomposed into identical cubic subdomains with the edge length H. We gradually chose decompositions into 2^3, 3^3, ..., 6^3 cubes which correspond to $H := 10/2,\ 10/3,\ \ldots,\ 10/6$. All subdomain boundaries were further discretized by the same triangular uniform meshes characterized by the discretization parameter h. The deformed body for the choice of parameters $h := 1/2$ and $H := 10/5$ is depicted in Figure 2. Splitting into subdomains is indicated by the chess–board on the surface.

We used the following SMALBE-M parameters:

$$\rho := \|\mathsf{FPF}\|, \quad M_0 := 1, \quad \beta := \frac{1}{10}, \quad \eta := \|\mathsf{Pd}\|, \quad \boldsymbol{\mu}^0 := \mathbf{0}.$$

The initial approximation $\boldsymbol{\lambda}^0$ was set to $\max\{-\widetilde{\boldsymbol{\lambda}}, 0.5\mathsf{B}\widetilde{\mathbf{R}}_h\}$. The stopping criterion was chosen as

$$\max\{\|\mathbf{g}^P(\boldsymbol{\lambda}^k, \boldsymbol{\mu}^k, \rho)\|,\ \|\mathsf{G}\boldsymbol{\lambda}^k\|\} \leq 10^{-4}\|\mathsf{Pd}\|.$$

The MPRGP algorithm used the parameters

$$\overline{\alpha} := \frac{2}{\rho}, \quad \Gamma := 1.$$

The numerical scalability of the discussed pair of algorithms is shown in Table 1. The upper row of each cell of the table shows the corresponding primal dimension / dual dimension / number of the outer iterations. The lower row gives the number of the CG 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 caused by the non–linearity of our problem. Furthermore, the graph illustrating the numerical scalability is depicted in Figure 3.

10 Comments and Conclusions

In this paper, we have extended the scalability results related to the application of BETI preconditioned by the "natural coarse grid" to the solution of variational inequalities presented in [7] to the 3D Lamé case.

	H				
H/h	10/2	10/3	10/4	10/5	10/6
9	11,712/5,023/17 130	39,528/18,744/13 139	93,696/43,441/12 137	183,000/92,992/13 115	316,224/163,275/17 133
8	9,264/4,053/15 124	31,266/15,090/13 134	74,112/37,341/12 137	144,750/74,712/15 140	250,128/131,109/15 180
7	7,104/3,187/15 88	23,976/11,832/14 145	56,832/29,233/11 120	111,000/58,432/15 156	191,808/102,471/14 182
6	5,232/2,425/15 93	17,658/8,970/16 101	41,856/22,117/13 145	81,750/44,152/13 140	141,264/77,361/14 163
5	3,648/1,767/16 95	12,312/6,504/13 94	29,184/15,993/14 131	57,000/31,872/15 138	98,496/55,779/15 147
4	2,352/1,213/15 102	7,938/4,434/14 120	18,816/10,861/14 101	36,750/21,592/15 147	63,504/37,725/14 145
3	1,344/763/15 93	4,536/2,760/18 83	10,752/6,720/17 92	21,000/13,312/17 131	36,288/23,199/22 157
2	624/417/16 111	2,106/1,482/19 94	4,992/3,573/17 140	9,750/7,032/16 75	16,848/12,201/24 130

Table 1: Performance for varying decomposition and discretization

In particular, we have shown that our algorithms are optimal also for the case of 3D contact problems of linear elastostatics solved by BETI, so that the solution of 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. The solution of auxiliary linear problems in the inner loop can be further improved by standard preconditioners [35]. The algorithms presented in our paper can be further adapted to mortar discretization [48, 49] and to 2D problems with Coulomb model of friction.

Acknowledgements

This research has been financially 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] Avery, P., Rebel, G., Lesoinne, M., Farhat, C.: A numerically scalable dual–primal substructuring method for the solution of contact problems – part I: the frictionless case. Comput. Methods Appl. Mech. Eng. **193**, 2403–2426 (2004)

[2] Axelsson, O.: Iterative Solution Methods. Cambridge University Press, Cambridge, 1994.

[3] Bertsekas, D. P.: Nonlinear Optimization. Athena Scientific, Belmont, 1999.

[4] Bebendorf, M., Rjasanow. S.: Adaptive lowrank approximation of collocation matrices. Computing **70**, 1–24 (2003).

[5] Bouchala, J., Dostál, Z., Sadowská, M.: 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, 221–228 (2005).

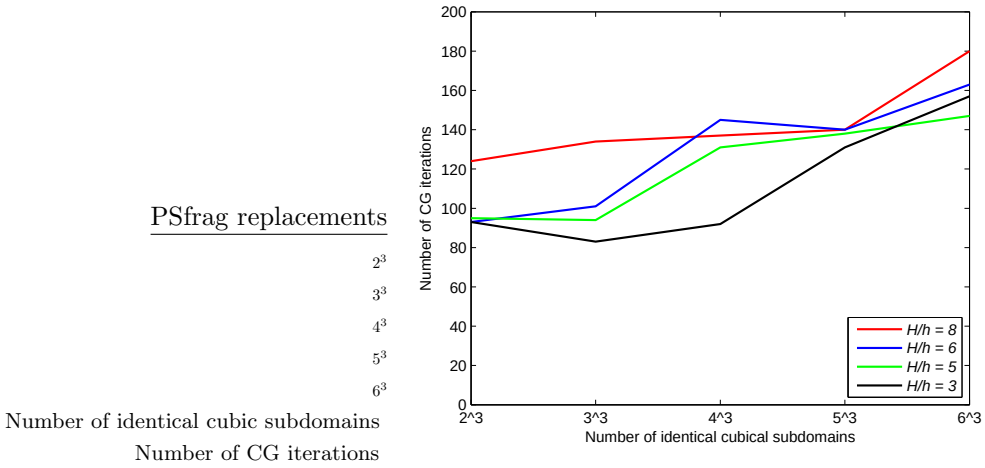

Figure 3: Graph of numerical scalability for the model contact problem

[6] Bouchala, J., Dostál, Z., Sadowská, M.: Solving 2D Contact Problem by Boundary Element Tearing and Interconnecting Method. Advances in Boundary Integral Methods - Proceedings of the Sixth UK Conference on Boundary Integral Methods, Durham University, 63–70 (2007).

[7] Bouchala, J., Dostál, Z., Sadowská, M.: Theoretically supported scalable BETI method for variational inequalities. Computing **82**, 53–75 (2008).

[8] Bouchala, J., Dostál, Z., Sadowská, M.: Scalable BETI for Variational Inequalities. Lecture Notes in Computational Science and Engineering – selection of 71 refereed papers presented at the 17th International Conference on Domain Decomposition Methods, Springer – Verlag Berlin Heidelberg, 167–174 (2008).

[9] Börm, S., Grasedyck, L., Hackbusch, W.: Hierarchical Matrices. Max Planck Institute for Mathematics in the Sciences, Leipzig, 2003.

[10] Conn, A. R., Gould, N. I. M., Toint, Ph. L.: A globally convergent augmented Lagrangian algorithm for optimization with general constraints and simple bounds. SIAM J Numer Anal **28**, 545–572 (1991).

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

[12] Domorádová, M., Dostál, Z., Sadowská, M.: Superrelaxation in minimizing quadratic functions subject to bound constraints (submitted).

[13] Dostál, Z.: Optimal Quadratic Programming Algorithms with Applications to Variational Inequalities. Springer Monograph, in print.

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

[15] Dostál, Z.: Inexact semimonotonic Augmented Lagrangians with optimal feasibility convergence for quadratic programming with simple bounds and equality constraints. SIAM J Numer Anal **45**, 500–513 (2007).

[16] Dostál, Z., Friedlander, A., Santos, S. A.: Augmented Lagrangians with adaptive precision control for quadratic programming with simple bounds and equality constraints. SIAM J Optim **13**, 1120–1140 (2003).

[17] Dostál, Z., Gomes, F. A. M., Santos, S. A.: Duality based domain decomposition with natural coarse space for variational inequalities. J Comput Appl Math **126**, 397–415 (2000).

[18] Dostál, Z., Horák, D.: Scalability and FETI based algorithm for large discretized variational inequalities. Math Comput Sim **61**, 347–357 (2003).

[19] Dostál, Z., Horák, D.: Theoretically supported scalable FETI for numerical solution of variational inequalities. SIAM J Numer Anal **45**, 500–513 (2007).

[20] Dostál, Z., Horák, D., Kučera, R.: Total FETI – an easier implementable variant of the FETI method for numerical solution of elliptic PDE. Commun Numer Meth Eng **22**, 1155–1162 (2006).

[21] Dostál, Z., Malík, J., Friedlander, A., Santos, S. A.: Analysis of semicoercive contact problems using symmetric BEM and augmented Lagrangians. Eng Anal Bound El **18**, 195–201 (1996).

[22] Dostál, Z., Horák, D., Stefanica, D.: A scalable FETI–DP algorithm for coercive variational inequalities. IMACS J Appl Numer Math **54**, 378–390 (2005).

[23] Dostál, Z., Schöberl, J.: Minimizing Quadratic Functions Subject to Bound Constraints with the Rate of Convergence and Finite Termination. Comput Opt Appl **30**, 23–43 (2005).

[24] Dostál, Z., Vondrák, V., Rasmussen, J.: 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**, 98–106 (2001).

[25] Dureisseix, D., Farhat, C.: A numerically scalable domain decomposition method for solution of frictionless contact problems. Int J Numer Meth Eng **50**, 2643–2666 (2001).

[26] Eck, C., Steinbach, 0., Wendland, W. L.: A symmetric boundary element method for contact problems with friction. Math Comput Simul **50**, 43–61 (1999).

[27] Farhat, C., Lesoinne, M., LeTallec, P., Pierson, K., Rixen, D.: FETI–DP: A dual–prime unified FETI method - part I: A faster alternative to the two–level FETI method. Int J Numer Meth Eng **50**, 1523–1544 (2001).

[28] Farhat, C., Mandel, J., Roux, F.-X.: Optimal convergence properties of the FETI domain decomposition method. Comput Meth Appl Mech Eng **115**, 365–385 (1994).

[29] Farhat, C., Roux, F.-X.: A method of finite element tearing and interconnecting and its parallel solution algorithm. Int J Numer Meth Eng **32**, 1205–1227 (1991).

[30] Farhat, C., Roux, F.-X.: An unconventional domain decomposition method for an efficient parallel solution of large–scale finite element systems. SIAM J Sci Comput **13**, 379–396 (1992).

[31] Greengard, L., Rokhlin, V.: A new version of the fast multipole method for the Laplace equation in three dimensions. Acta numerica, Cambridge University Press, 229–269 (1997).

[32] Hlaváček, I., Haslinger, J., Nečas, J., Lovíšek, J.: Solution of Variational Inequalities in Mechanics. Springer - Verlag Berlin, 1988.

[33] Kornhuber, R.: Adaptive monotone multigrid methods for nonlinear variational problems. Teubner - Verlag: Stuttgart, 1997.

[34] Kornhuber, R., Krause, R.: Adaptive multigrid methods for Signorini's problem in linear elasticity. Computer Visualization in Science **4**, 9–20 (2001).

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

[36] U. Langer, C. Pechstein: Coupled FETI/BETI solvers for nonlinear potential problems in (un)bounded domains. In Proceedings of the SCEE 2006 (ed. by Gabriela CIUPRINA and Daniel IOAN), Mathematics in Industry, vol. 11, Springer-Verlag, Heidelberg, pp. 371-377, 2007.

[37] McLean, W.: Strongly Elliptic Systems and Boundary Integral Equations. Cambridge University Press (2000).

[38] Maischak, M., Stephan, E.P.: Adaptive hp-versions of BEM for Signorini problems. Applied Numerical Mathematics archive **54, 3-4** 425 - 449 (2005).

[39] Of, G.: BETI - Gebietszerlegungsmethoden mit schnellen Randelementverfahren und Anwendungen. Ph.D. Thesis, University of Stuttgart, 2006. In German.

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

[41] Rjasanow, S., Steinbach, O.: The Fast Solution of Boundary Integral Equations. Mathematical and Analytical Techniques with Applications to Engineering, Springer - New York, 2007.

[42] Sadowská, M.: Scalable Total BETI for 2D and 3D Contact Problems. Ph.D. Thesis, VŠB - Technical University of Ostrava, http://www.am.vsb.cz/sadowska/publikace, 2008.

[43] Schöberl, J.: Solving the Signorini problem on the basis of domain decomposition techniques. Computing **60**, 4, 323–344 (1998)

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

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

[46] Steinbach, O.: Numerical Approximation Methods for Elliptic Boundary Value Problems. Finite and Boundary Elements. Springer – New York (2008).

[47] Toselli, A., Widlund, O. B.: Domain Decomposition Methods - Algorithms and Theory. Springer - Verlag Berlin Heidelberg, 2005.

[48] Wohlmuth, B. I., Krause, R.: Monotone methods on nonmatching grids for nonlinear contact problems. SIAM J Sci Comput **25**, 324–347 (2003).

[49] Wohlmuth, B. I.: Discretization Methods and Iterative Solvers Based on Domain Decomposition. Springer - Verlag, 2001.

[50] Yoshida, K.: Applications of Fast Multipole Method to Boundary Integral Equation Method. Ph.D. Thesis, Kyoto University, Japan, 2001.