

# SOLUTION OF CONTACT PROBLEMS BY FETI DOMAIN DECOMPOSITION WITH NATURAL COARSE SPACE PROJECTIONS \*

Z. Dostál <sup>†</sup>    Francisco A. M. Gomes Neto <sup>‡</sup>    Sandra A. Santos <sup>§</sup>

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## Abstract

An efficient non-overlapping domain decomposition algorithm of the Neumann-Neumann type for solving both coercive and semicoercive contact problems has been presented. The discretized problem is first turned by the duality theory of convex programming to the quadratic programming problem with bound and equality constraints and the latter is further modified by means of orthogonal projectors to the natural coarse space introduced recently by Farhat and Roux in the framework of their FETI method. The resulting problem is then solved by an augmented Lagrangian type algorithm with an outer loop for the Lagrange multipliers for the equality constraints and an inner loop for the solution of the bound constrained quadratic programming problems. The projectors are shown to guarantee an optimal rate of convergence of iterative solution of auxiliary linear problems and to comply with efficient quadratic programming algorithms proposed earlier. Reported theoretical results and numerical experiments indicate high numerical and parallel scalability of the algorithm.

### Key words and phrases:

Domain decomposition, natural coarse grid, contact problem

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<sup>†</sup>Department of Applied Mathematics, VŠB-Technical University Ostrava, Ostrava, Czech Republic, on visit to Department of Applied Mathematics, IMECC – UNICAMP, University of Campinas, (zdenek.dostal@vsb.cz).

<sup>‡</sup>Department of Applied Mathematics, IMECC – UNICAMP, University of Campinas, CP 6065, 13081-970 Campinas SP, Brazil (chico@ime.unicamp.br).

<sup>§</sup>Department of Mathematics, IMECC – UNICAMP, University of Campinas, CP 6065, 13081-970 Campinas SP, Brazil (sandra@ime.unicamp.br).

# 1 Introduction

Duality based domain decomposition methods proved to be practical and efficient tools for parallel solution of large elliptic boundary value problems [23, 24, 38]. Using this approach, a body is partitioned into non-overlapping subdomains, for each subdomain is defined an elliptic problem with Neumann boundary conditions on the subdomain interfaces, and intersubdomain field continuity is enforced via Lagrange multipliers. The Lagrange multipliers are evaluated by solving a relatively well conditioned dual problem of small size that may be efficiently solved by a suitable variant of the conjugate gradient algorithm. The first practical implementations by Farhat and Roux [23, 24] exploited only the favorable distribution of the spectrum of the matrix of the smaller problem [37], known also as the dual Schur complement matrix, but such algorithm was efficient only with a small number of subdomains. Later, they introduced a “natural coarse problem” whose solution was implemented by auxiliary projectors so that the resulting algorithm became optimal [25, 38].

It has been soon observed that duality based domain decomposition methods may also be successful for the solution of variational inequalities that describe equilibrium of a system of elastic bodies in unilateral contact [35]. The first observation was that duality not only reduces the dimension and improves conditioning of the original problem, but also reduces all the inequalities to simple bounds on variables [11, 12, 17] so that the dual problem may be solved much more efficiently than the primal problem [27, 14, 16]. Recently, we have shown how to use the “natural coarse grid” to the solution of a scalar variational inequality [19].

Our goal here is to exploit the projector to the solution of the “natural coarse problem” to improve numerical scalability of our previous algorithms for numerical solution of contact problems. In particular, it turns out that application of the projectors decomposes the Hessian of the augmented Lagrangian so that it has at most one point of the spectrum outside the span of the spectrum of the dual Schur complement, and that iterative solution of auxiliary linear problems with such Hessian has an optimal rate of convergence with respect to both penalization and discretization parameters. The algorithm preserves all the plausible properties of our duality based algorithms for the solution of contact problems [11, 12, 17], in particular fast identification of a priori unknown contact interfaces and convergence of the outer loop with inexact solution of auxiliary problems.

We start our exposition in Section 2 by describing the decomposition of

a system of elastic bodies in contact into subdomains. Then we review the conditions of equilibrium of a system of elastic bodies in contact without friction. After discretization we get an indefinite quadratic programming problem with a block diagonal matrix.

In Section 3, we show that the difficulties arising from general inequality constraints and semidefiniteness of the primal problem may be essentially reduced by application of the duality theory [11, 12, 17]. The matrix of the dual quadratic form turns out to be positive definite with a spectrum that is favorably distributed for application of conjugate gradient based methods. Moreover, the inequality constraints of the dual problem are just those of non-negativity, so that we can use our recent results on application of projections and adaptive precision control [19].

The dual formulation is modified in Section 4 in order to improve conditioning of the dual Schur complement by enhancing projectors to the natural coarse space. Results on distribution of the spectrum of the augmented Lagrangian of the modified problem and on the convergence of auxiliary problems are presented.

The quadratic programming algorithms that we use are reviewed in Section 5. We describe first the algorithm for quadratic programming problems with equality constraints and simple bounds. The approximations of the Lagrange multipliers for the equalities are generated in the outer loop of the augmented Lagrangian algorithm while bound constrained problems are solved in the inner loop. We have adapted the basic scheme proposed by Conn, Gould and Toint [7] for the solution of more general problems. However, we use the special structure of our problem to improve the performance of the algorithm. The precision of the solution of the auxiliary problems in the inner loop is controlled by the norm of the feasibility residue of the current iterate and an estimate of the rate of convergence is given that has no term that accounts for the inexact solution of the auxiliary problems. We include a description of the algorithm for solving the bound constrained quadratic programming problems [27, 14, 26, 28, 4] in the inner loop. Our active set type algorithm generates search directions by conjugate gradients with optional preconditioning [3], exploits the projections to the feasible set, and uses the adaptive precision control of the solution of auxiliary problems. Theoretical results on convergence, robustness and optimality of the algorithm are reported.

Results of numerical experiments that demonstrate the power of our algorithms are given in Section 6. Finally, in Section 7, some comments and conclusions are presented.

To simplify our exposition, we have restricted our attention to the frictionless contact problems. However, the algorithm may be extended to the solution of contact problems with Coulomb friction [20] and adhesive friction [36].

Our exposition of the variational formulation with the basic FETI algorithm for contact problems follows [17] in agreement with the copyright policy of AMS.

## 2 Conditions of equilibrium of elastic bodies

Consider a system of  $s$  homogeneous isotropic elastic bodies, each of which occupies, in a reference configuration, a domain  $\Omega^p$  in  $\mathbb{R}^d$ ,  $d = 2, 3$  with sufficiently smooth boundary  $\Gamma^p$  as in Figure 1. Suppose that each  $\Gamma^p$  consists of three disjoint parts  $\Gamma_U^p, \Gamma_F^p$  and  $\Gamma_C^p$ ,  $\Gamma^p = \Gamma_U^p \cup \Gamma_F^p \cup \Gamma_C^p$ , and that the displacements  $\mathbf{U}^p : \Gamma_U^p \rightarrow \mathbb{R}^d$  and forces  $\mathbf{F}^p : \Gamma_F^p \rightarrow \mathbb{R}^d$  are given. The part  $\Gamma_C^p$  denotes the part of  $\Gamma^p$  that may get into contact with some other body. In particular, we shall denote by  $\Gamma_C^{pq}$  the part of  $\Gamma^p$  that can be, in the solution, in contact with the body  $\Omega^q$ .

We can also decompose each body into subdomains, as in Figure 2, to obtain optional secondary decomposition. To simplify our notation and, in particular, to avoid two indices for subdomains  $\Omega^{pi}$  of  $\Omega^p$ , we shall denote by  $s$  the total number of the subdomains, renumber all the subdomains so that they will be identified by just one index, and introduce new ‘gluing’ conditions on the artificial intersubdomain boundary  $\Gamma_G$ . For parts of  $\Gamma_G$ , we shall introduce notation in analogy to the notation of the contact boundary, so that  $\Gamma_G^{pq}$  denotes the part of  $\Gamma^p$  that is glued to  $\Omega^q$  and  $\Gamma_G^p$  denote the part of  $\Gamma^p$  that is glued to the other subdomains. Obviously  $\Gamma_G^{pq} = \Gamma_G^{qp}$ . An auxiliary decomposition of the problem of Figure 1 with renumbered subdomains and artificial intersubdomain boundaries is in Figure 3. The gluing conditions require continuity of displacements and of their normal derivatives across  $\Gamma_G$ .

Let  $c_{ijkl}^p : \Omega^p \rightarrow \mathbb{R}^d$  and  $\mathbf{g}^p : \Omega^p \rightarrow \mathbb{R}^d$  denote the entries of the elasticity tensor and a vector of body forces, respectively. For any sufficiently smooth displacement  $\mathbf{u} : \Omega^1 \times \dots \times \Omega^s \rightarrow \mathbb{R}^d$ , the total potential energy is defined by

$$J(\mathbf{u}) = \sum_{p=1}^s \left\{ \frac{1}{2} \int_{\Omega^p} a(\mathbf{u}^p, \mathbf{u}^p) d\Omega - \int_{\Omega^p} (\mathbf{g}^p)^T \mathbf{u}^p d\Omega - \int_{\Gamma_F^p} (\mathbf{F}^p)^T \mathbf{u}^p d\Gamma \right\} \quad (2.1)$$

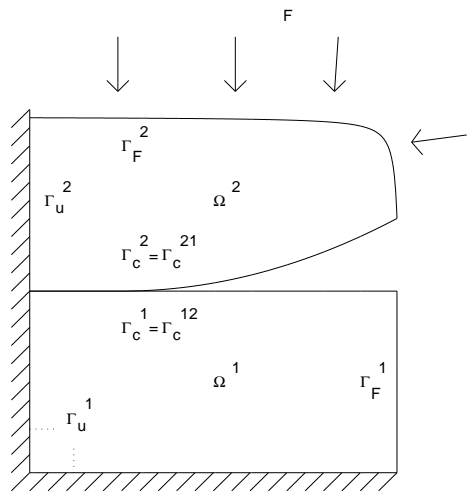


Figure 1: Contact problem

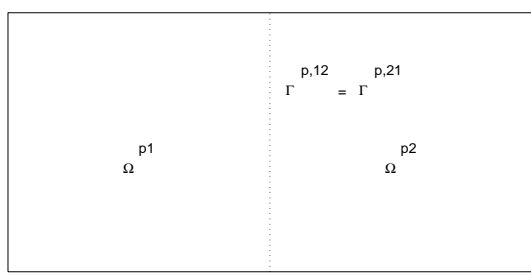


Figure 2: Secondary decomposition of  $\Omega^p$

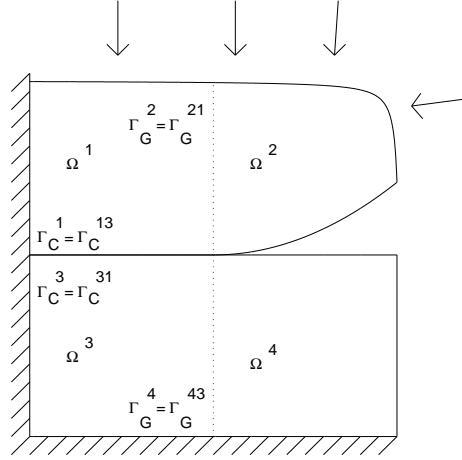


Figure 3: Contact problem with optional decomposition

where

$$a^p(\mathbf{u}^p, \mathbf{v}^p) = \frac{1}{2} \int_{\Omega^p} c_{ijkl} e_{ij}^p(\mathbf{u}^p) e_{kl}^p(\mathbf{v}^p) d\Gamma \quad (2.2)$$

$$e_{kl}^p(\mathbf{u}^p) = \frac{1}{2} \left( \frac{\partial u_k^p}{\partial x_\ell^p} + \frac{\partial u_\ell^p}{\partial x_k^p} \right). \quad (2.3)$$

We suppose that the elasticity tensor satisfies natural physical restrictions so that

$$a^p(\mathbf{u}^p, \mathbf{v}^p) = a(\mathbf{v}^p, \mathbf{u}^p) \quad \text{and} \quad a(\mathbf{u}^p, \mathbf{u}^p) \geq 0. \quad (2.4)$$

To describe the linearized non-interpenetration conditions, let us define for each  $p < q$  a one-to-one continuous mapping  $\mathbf{O}^{pq} : \Gamma_C^{pq} \rightarrow \Gamma_C^{qp}$  that assigns to each  $\mathbf{x} \in \Gamma_C^{pq}$  some point of  $\Gamma_C^{qp}$  that is near to  $\mathbf{x}$ , as in Figure 4. The linearized non-interpenetration condition at  $\mathbf{x} \in \Gamma_C^{pq}$  then reads

$$(\mathbf{u}^p(\mathbf{x}) - \mathbf{u}^q(\mathbf{O}^{pq}(\mathbf{x}))) \mathbf{n}^p \leq (\mathbf{O}^{pq}(\mathbf{x}) - \mathbf{x}) \mathbf{n}^p, \quad \mathbf{x} \in \Gamma_C^{pq}, \quad p < q. \quad (2.5)$$

Now let us introduce the Sobolev space

$$\mathcal{V} = H^1(\Omega^1)^d \times \dots \times H^1(\Omega^s)^d, \quad (2.6)$$



### 3 Discretized contact problem on interface

If there is no secondary decomposition, then finite element discretization of  $\Omega = \Omega^1 \cup \dots \cup \Omega^s$  with suitable numbering of nodes results in the quadratic programming (QP) problem

$$\frac{1}{2}u^T K u - f^T u \rightarrow \min \quad \text{subject to } B_I u \leq c, \quad (3.1)$$

with a symmetric positive definite or positive semidefinite block-diagonal matrix  $K = \text{diag}(K_1, \dots, K_s)$  of order  $n$ , an  $m \times n$  full rank matrix  $B_I$ ,  $f \in \mathbb{R}^n$ , and  $c \in \mathbb{R}^m$ . The matrix  $B_I$  and the vector  $c$  describe the linearized incremental non-interpenetration conditions. The rows  $b_i$  of  $B_I$  are formed by zeros and appropriately placed coordinates of outer unit normals, so that the change of normal distance due to the displacement  $u$  is given by  $u^T b_i$ , and the entry  $c_i$  of  $c$  describes the normal distance between the  $i$ -th couple of corresponding nodes on the contact interface in the reference configuration. Some care should be taken to guarantee that  $B_I$  is a full rank matrix. The vector  $f$  describes the nodal forces arising from the volume forces and/or some other imposed tractions. Typically  $n$  is large and  $m$  is much smaller than  $n$ . The diagonal blocks  $K_p$  that correspond to subdomains  $\Omega^p$  are positive definite or semidefinite sparse matrices. Moreover, we shall assume that the nodes of the discretization are numbered in such a way that  $K_p$  are banded matrices that can be effectively decomposed, possibly after some regularization, by means of the Cholesky factorization.

If there is a secondary decomposition, then the continuity of the displacements across auxiliary interfaces requires that  $u^T b_i = 0$ , where  $b_i$  are vectors of order  $n$  with zero entries except 1 and  $-1$  at appropriate positions. If  $B_E$  is the matrix with rows  $b_i$ , then the discretization of problem (3.1) with the secondary decomposition results in the QP problem

$$\frac{1}{2}u^T K u - f^T u \rightarrow \min \quad \text{subject to } B_I u \leq c \quad \text{and} \quad B_E u = 0. \quad (3.2)$$

Some care should be taken to guarantee that  $B_E$  is a full rank matrix when corner nodes are present. An effective treatment of the corner nodes may be found in [19]. An elimination of the corner nodes that is compatible with our algorithm is described in [38].

Even though (3.1) and (3.2) are standard convex quadratic programming problems, their formulation is not suitable for numerical solution. The reasons are that  $K$  is typically ill conditioned and possibly singular and that



the feasible set is in general so complex that projections into it can hardly be effectively computed. Under these circumstances, it would be very difficult to achieve fast identification of the active set at the solution and fast solution of auxiliary linear problems.

The complications mentioned above may be essentially reduced by applying the duality theory of convex programming (e.g. Dostál et al. [11, 12, 17]). Since the dual formulation of problem (3.1) without secondary decomposition may be considered a special case of the dual formulation of problem (3.2) and has been discussed earlier [11, 12], we shall restrict our attention to dual formulation of the latter problem. Moreover, we shall assume that the matrix  $K$  has a nontrivial null space that defines the natural coarse grid. An equivalent assumption is using a decomposition of the domain of the problem that comprises floating subdomains.

The Lagrangian associated with problem (3.2) is

$$L(u, \lambda_I, \lambda_E) = \frac{1}{2}u^T K u - f^T u + \lambda_I^T (B_I u - c) + \lambda_E^T B_E u, \quad (3.3)$$

where  $\lambda_I$  and  $\lambda_E$  are the Lagrange multipliers associated with the inequalities and equalities, respectively. Introducing notation

$$\lambda = \begin{bmatrix} \lambda_I \\ \lambda_E \end{bmatrix}, \quad B = \begin{bmatrix} B_I \\ B_E \end{bmatrix}, \quad \text{and} \quad \hat{c} = \begin{bmatrix} c \\ 0 \end{bmatrix},$$

we can write the Lagrangian briefly as

$$L(u, \lambda) = \frac{1}{2}u^T K u - f^T u + \lambda^T (B u - \hat{c}).$$

It is well known [6] that (3.2) is equivalent to the saddle point problem

$$\text{Find } (\hat{u}, \hat{\lambda}) \text{ s.t. } L(\hat{u}, \hat{\lambda}) = \sup_{\lambda_I \geq 0} \inf_u L(u, \lambda). \quad (3.4)$$

For fixed  $\lambda$ , the Lagrange function  $L(\cdot, \lambda)$  is convex in the first variable and the minimizer  $u$  of  $L(\cdot, \lambda)$  satisfies

$$K u - f + B^T \lambda = 0. \quad (3.5)$$

Equation (3.5) has a solution iff

$$f - B^T \lambda \in \text{Im}K, \quad (3.6)$$

which can be expressed more conveniently by means of a matrix  $R$  whose columns span the null space of  $K$  as

$$R^T(f - B^T \lambda) = 0. \quad (3.7)$$

The matrix  $R$  may be formed directly so that each floating subdomain is assigned to a row of  $R$  with ones in positions of the nodal variables that belong to the subdomain and zeros elsewhere. We shall assume that  $B$  is formed properly so that  $R^T B^T$  is a full rank matrix. The matrix  $R$  may be also extracted from  $K$  [22].

Now assume that  $\lambda$  satisfies (3.6) and denote by  $K^\dagger$  any matrix that satisfies

$$K K^\dagger K = K. \quad (3.8)$$

It may be verified directly that if  $u$  solves (3.5), then there is a vector  $\alpha$  such that

$$u = K^\dagger(f - B^T \lambda) + R\alpha. \quad (3.9)$$

After substituting expression (3.9) into problem (3.4) and a change of signs, we shall get the minimization problem

$$\min \Theta(\lambda) \quad \text{s.t.} \quad \lambda_I \geq 0 \quad \text{and} \quad R^T(f - B^T \lambda) = 0, \quad (3.10)$$

where

$$\Theta(\lambda) = \frac{1}{2} \lambda^T B K^\dagger B^T \lambda - \lambda^T (B K^\dagger f - \hat{c}). \quad (3.11)$$

Though any matrix  $K^\dagger$  that satisfies (3.8) such as the Moore-Penrose pseudo-inverse may be used to get (3.9), we must be more cautious when we consider effective solving of our problem. Farhat and Roux [23, 24] proposed to use for  $K^\dagger$  the left generalized inverse that satisfies (3.8),  $K_p^\dagger = K_p^{-1}$  whenever  $K_p$  is non-singular, and

$$K^\dagger = \text{diag}(K_1^\dagger, \dots, K_s^\dagger)$$

but does not necessarily satisfy the other identities that define the Moore-Penrose or other pseudoinverse. If  $K_p$  is singular then it is easy to check that there is a permutation matrix  $P_p$  and a non-singular matrix  $T_p$  such that

$$P_p^T K_p P_p = \begin{pmatrix} T_p & S_p \\ S_p^T & S_p^T T_p^{-1} S_p \end{pmatrix}$$

and that

$$K_p^\dagger = P_p^T \begin{pmatrix} T_p^{-1} & 0 \\ 0 & 0 \end{pmatrix} P_p$$

satisfies (3.8).

Once the solution  $\hat{\lambda}$  of (3.10) is obtained, the vector  $u$  that solves (3.4) can be evaluated provided the vector  $\alpha$  of (3.9) is known. To find a formula for  $\alpha$ , notice that the solution of (3.2) satisfies

$$\tilde{B}_I u = \tilde{c} \quad \text{and} \quad B_E u = 0, \quad (3.12)$$

where  $[\tilde{B}_I, \tilde{c}]$  is the matrix formed by the rows of  $B_I$  and  $c$  that correspond to active constraints, the latter being characterized by  $\hat{\lambda}_i = 0$ . After multiplying (3.9) on the left by

$$\tilde{B} = \begin{bmatrix} \tilde{B}_I \\ \tilde{B}_E \end{bmatrix}$$

and substituting by (3.12), we get equation

$$\tilde{c} = \tilde{B} K^\dagger (f - B^T \hat{\lambda}) + \tilde{B} R \alpha \quad (3.13)$$

that determines  $\alpha$ . Solving the normal equation [32] to (3.13) for  $\alpha$  then yields

$$\alpha = (R^T \tilde{B}^T \tilde{B} R)^{-1} R^T \tilde{B}^T (\tilde{c} - \tilde{B} K^\dagger (f - B^T \hat{\lambda})) \quad (3.14)$$

which can be substituted into (3.9) to get  $u$ .

The matrix  $R^T B^T$  is, under our assumptions, a full rank matrix, so that the Hessian of  $\Theta$  is positive definite. Moreover, the Hessian is closely related to that of the basic FETI method by Farhat and Roux [23, 24], so that its spectrum is relatively favorably distributed for application of the conjugate gradient method [37].

## 4 Modifications

Even though problem (3.10) is much more suitable for computations than (3.2) and was used for efficient solution of contact problems [17], further improvement may be achieved by adapting some simple observations and the results of Farhat, Mandel and Roux [25]. We shall formulate a problem that is equivalent to (3.10) but its augmented Lagrangian has such a spectral distribution that the rate of convergence of unconstrained minimization by

the conjugate gradient method does not depend on either penalisation or discretization parameters.

Let us denote

$$\begin{aligned} F &= BK^\dagger B^T, & \tilde{d} &= BK^\dagger f, \\ \tilde{G} &= R^T B^T, & \tilde{e} &= R^T f \end{aligned}$$

and let  $T$  denote a regular matrix that defines the orthonormalization of the rows of  $\tilde{G}$  so that the matrix

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

has orthogonal rows. After denoting

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

problem (3.10) reads

$$\min \frac{1}{2}\lambda^T F\lambda - \lambda^T \tilde{d} \quad \text{s.t.} \quad \lambda_I \geq 0 \quad \text{and} \quad G\lambda = e. \quad (4.1)$$

Next we shall transform the problem of minimization on the subset of the affine space to that on the subset of the vector space by means of arbitrary  $\bar{\lambda}$  that satisfies

$$G\bar{\lambda} = e.$$

To this purpose, we shall look for the solution of (4.1) in the form  $\lambda = \mu + \bar{\lambda}$ . Since

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

problem (4.1) is, after returning to the old notation, equivalent to

$$\min \frac{1}{2}\lambda^T F\lambda - d^T \lambda \quad \text{s.t.} \quad G\lambda = 0 \quad \text{and} \quad \lambda_I \geq -\bar{\lambda}_I. \quad (4.2)$$

with  $d = \tilde{d} - F\bar{\lambda}$ .

To assess our progress, let us compare the distribution of the spectrum of the Hessians  $H_1 = F + \rho\tilde{G}^T\tilde{G}$  and  $H_2 = F + \rho G^T G$  of the augmented Lagrangians for problems (3.10) and (4.2), respectively. Let us assume that the eigenvalues of  $F$  are in the interval  $[a, b]$  and that the nonzero eigenvalues of  $\tilde{G}^T\tilde{G}$  are in  $[\gamma, \delta]$  and, for each square matrix  $A$ , let  $\sigma(A)$  denote its spectrum. Using the analysis of [16, 15], it follows that

$$\sigma(H_1) \subseteq [a, b] \cup [a + \rho\gamma, b + \rho\delta] \quad \text{and} \quad \sigma(H_2) \subseteq [a, b] \cup [a + \rho, b + \rho].$$

If  $\rho$  is sufficiently large and  $\gamma < \delta$ , then the spectrum of  $H_1$  is distributed in two intervals with the larger one on the right. In this case, the analysis of Axelsson [1] shows that the rate of convergence of the conjugate gradient method for minimization of the quadratic function with Hessian  $H_1$  depends on the penalization parameter  $\rho$ . However, the situation is much more favorable for minimization of the quadratic function with the Hessian  $H_2$  since, in this case, the spectrum is always distributed in two intervals of the same length. It follows, by analysis of Axelsson, [1] that the rate of convergence is governed by the effective condition number  $\bar{\kappa}(H_2) = 4b/a$  so that the number  $k$  of conjugate gradient iterations that are necessary to reduce the gradient of the augmented Lagrangian for (4.2) by  $\epsilon$  satisfies

$$k \leq \frac{1}{2} \text{int} \left( \sqrt{4 \frac{b}{a} \ln \left( \frac{2}{\epsilon} \right) + 1} \right). \quad (4.3)$$

The bound is only twice the bound on minimization with  $F$  and does not depend on the penalization parameter  $\rho$ .

Our final step is based on observation that the augmented Lagrangian for problem(4.2) may be decomposed by the orthogonal projectors

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

on the image space of  $G^T$  and on the kernel of  $G$ , respectively. Indeed, problem (4.2) is equivalent to

$$\min \frac{1}{2} \lambda^T P F P \lambda - \lambda^T P d \quad \text{s.t.} \quad G \lambda = 0 \quad \text{and} \quad \lambda_I \geq -\bar{\lambda}_I. \quad (4.4)$$

and the Hessian  $H_3 = P F P + \rho Q$  of the augmented Lagrangian

$$L(\lambda, \mu, \rho) = \frac{1}{2} \lambda^T (P F P + \rho Q) \lambda - \lambda^T P d + \mu^T G \lambda \quad (4.5)$$

is decomposed by projectors  $P$  and  $Q$  whose image spaces are invariant subspaces of  $H_3$ . If  $[a_P, b_P]$  denotes the interval that contains the non-zero eigenvalues of  $P F P$ , it follows that the eigenvalues of  $H_3$  satisfy

$$\sigma(H_3) \subseteq [a_P, b_P] \cup \{\rho\} \quad \text{and} \quad [a_P, b_P] \subseteq [a, b] \quad (4.6)$$

so that, by the analysis of Axelsson [2], the number  $k$  of conjugate gradient iterations that are necessary to reduce the gradient of the augmented Lagrangian (4.5) for (4.4) by  $\epsilon$  satisfies

$$k \leq \frac{1}{2} \text{int} \left( \sqrt{\frac{b_P}{a_P} \ln \left( \frac{2}{\epsilon} \right) + 3} \right). \quad (4.7)$$

Moreover, analysis of the FETI method by Farhat, Mandel and Roux [25] implies that, for the regular decomposition,

$$\frac{b_P}{a_P} \leq \text{const} \frac{H}{h}, \quad (4.8)$$

where  $h$  and  $H$  are the mesh and subdomain diameters, respectively. Examining (4.7) and (4.8), we conclude that the rate of convergence for unconstrained minimization of the augmented Lagrangian (4.5) does not depend on either the penalization parameter  $\rho$  or the discretization parameter  $h$  provided the aspect ratios of both discretization and decomposition are close to one and the ratio  $H/h$  is kept bounded by a constant. More discussion of the conjugate gradient method applied to systems with augmented Lagrangian including numerical experiments may be found in [15]. More detailed derivation of (4.8) may be found in [25].

The idea of using projectors in preconditioning is near to the older idea of preconditioning by projector [8], but only the discovery of the role of the natural coarse space [25] revealed its full power.

## 5 Solution of Bound and Equality Constrained Quadratic Programming Problems

Our development of an efficient algorithm for the solution of (4.4) is based on the observation that the solution of such problems may be reduced, by the augmented Lagrangian technique [7, 16], to the solution of a sequence of quadratic programming (QP) problems with simple bounds, and that the latter can be solved much more efficiently than more general QP problems due to the possibility of using projections and results on adaptive precision control in the active set strategy [27, 26, 28, 4, 14]. Here we shall briefly review these results.

To simplify our notation, let us denote  $F_P = PFP$  so that the augmented Lagrangian for problem (4.4) and its gradient are given by

$$L(\lambda, \mu, \rho) = \frac{1}{2} \lambda^T F_P \lambda - \lambda^T P d + \mu^T G \lambda + \frac{1}{2} \rho \|Q \lambda\|^2$$

and

$$g(\lambda, \mu, \rho) = F_P \lambda - P d + G^T (\mu + \rho G \lambda),$$

respectively. The *projected gradient*  $g^P = g^P(\lambda, \mu, \rho)$  of  $L$  at  $\lambda$  is then given entrywise by

$$g_i^P = g_i \text{ for } \lambda_i > -\bar{\lambda}_i \text{ or } i \notin I \text{ and } g_i^P = g_i^- \text{ for } \lambda_i = -\bar{\lambda}_i \text{ and } i \in I$$

with  $g_i^- = \min(g_i, 0)$ , where  $I$  is the set of indices of constrained entries of  $\lambda$ .

The algorithm that we propose here may be considered a variant of the algorithm proposed by Conn, Gould and Toint [7] for identification of stationary points of more general problems. However, our algorithm is modified in order to exploit the specific structure of our problem to get improved performance. The most important of such modifications consists in including the adaptive precision control of auxiliary problems in Step 1.

All of the parameters that must be defined prior to the application of the algorithm are listed in Step 0. Typical values of these parameters for our problems are given in brackets.

**Algorithm 5.1.** (Simple bound and equality constraints)

*Step 0.* { Initialization of parameters }

Set  $0 < \alpha < 1$  [ $\alpha = 0.1$ ] for equality precision update,  $1 < \beta$  [ $\beta = 10$ ] for penalty update,  $\rho_0 > 0$  [ $\rho_0 = 10^4$ ] for initial penalty parameter,  $\eta_0 > 0$  [ $\eta_0 = 0.1$ ] for initial equality precision,  $M > 0$  [ $M = 10^4$ ] for balancing ratio,  $\mu^0$  [ $\mu^0 = 0$ ] and  $k = 0$ .

*Step 1.* Find  $\lambda^k$  so that  $\|g^P(\lambda^k, \mu^k, \rho_k)\| \leq M\|G\lambda^k\|$ .

*Step 2.* If  $\|g^P(\lambda^k, \mu^k, \rho_k)\|$  and  $\|G\lambda^k\|$  are sufficiently small, then  $\lambda^k$  is the solution.

*Step 3.* If  $\|G\lambda^k\| \leq \eta_k$

*Step 3a.* then  $\mu^{k+1} = \mu^k + \rho_k G\lambda^k$ ,  $\rho_{k+1} = \rho_k$ ,  $\eta_{k+1} = \alpha\eta_k$

*Step 3b.* else  $\rho_{k+1} = \beta\rho_k$ ,  $\eta_{k+1} = \eta_k$

end if.

*Step 4.* Increase  $k$  and return to Step 1.

An implementation of Step 1 is carried out by the minimization of the augmented Lagrangian  $L$  subject to  $\lambda_I \geq 0$  by means of the algorithm that we shall describe later. The unique solution  $\hat{\lambda} = \hat{\lambda}(\mu, \rho)$  of this auxiliary problem satisfies the Karush-Kuhn-Tucker conditions

$$g^P(\hat{\lambda}, \mu, \rho) = 0. \quad (5.1)$$

Even though there are many parameters in Algorithm 5.1, only  $\rho_0$  and  $M$  seem to be essentially problem dependent. Theoretical results of [18, Corollary 2.7] suggest that the rate of convergence of the Lagrange multipliers increases very little with  $M$  considerable less than  $\|(GF^{-1}G^T)^{-1}\| \leq \|F\|$  and that  $\rho_0$  should be larger than  $M$ . The algorithm is designed so that  $\rho$  adjusts to the other parameters including  $M$ . Let us recall here that a large penalty parameter does not necessarily slow down the convergence of the conjugate gradient iterations [15].

The salient feature of this algorithm is that it deals completely separately with each type of constraint and that it accepts inexact solutions of the auxiliary box constrained problems in Step 1. For parallel implementation, it is necessary to keep the factors that form  $F_P$  since the latter is just used in the matrix-vector products. The action of  $K^\dagger$  may be evaluated by means of a Cholesky decomposition. Besides, the matrix  $G$  of problem (4.4) that is used to compute the projections  $Q$  and  $P$  may be generated by means of the QR decomposition of  $\tilde{G}$ . We shall present more details on implementation elsewhere.

It was recognized earlier that the augmented Lagrangian method may be useful for the solution of contact problems [39]. However, most of these applications are based on the original scheme proposed by Powel and Hestenes that looks for the Lagrange multipliers for equality constraints [30]. We believe that the results presented here give sufficient evidence that the variant of the augmented Lagrangian method that we proposed is more than competitive to this older approach.

The algorithm has been proved [16] to converge for any set of parameters that satisfy the prescribed relations. Moreover, it has been proved that the asymptotic rate of convergence is the same as for the algorithm with exact solution of auxiliary quadratic programming problems (i.e.  $M = 0$ ) and that the penalty parameter is uniformly bounded. These results, with the above discussion on elimination of the negative effect of penalization, give theoretical support to Algorithm 5.1.

In the rest of this section we shall describe, in more detail, the implementation of Step 1 of Algorithm 5.1, assuming that  $\mu$  and  $\rho$  are fixed and denoting

$$\theta(\lambda) = L(\lambda, \mu, \rho).$$

Let us recall that the set of indices of the dual variables  $\lambda_i$  is decomposed into two disjoint sets  $I$  and  $E$  with  $I$  denoting the indices of the constrained entries of  $\lambda$ , and let us denote by  $\mathcal{A}(\lambda)$  and  $\mathcal{F}(\lambda)$  the *active set* and *free set*



of indices of  $\lambda$ , respectively, i.e.

$$\mathcal{A}(\lambda) = \{i \in I : \lambda_i = -\bar{\lambda}_i\} \quad \text{and} \quad \mathcal{F}(\lambda) = \{i : \lambda_i > -\bar{\lambda}_i \text{ or } i \in E\}. \quad (5.2)$$

The *chopped gradient*  $g^C$  and the *inner gradient*  $g^I$  of  $\theta(\lambda)$  are defined by

$$g_i^I = g_i \text{ for } i \in \mathcal{F}(\lambda) \text{ and } g_i^I = 0 \text{ for } i \in \mathcal{A}(\lambda) \quad (5.3)$$

$$g_i^C = 0 \text{ for } i \in \mathcal{F}(\lambda) \text{ and } g_i^C = g_i^- \text{ for } i \in \mathcal{A}(\lambda). \quad (5.4)$$

Hence the Karush-Kuhn-Tucker conditions for the solution of the problem to find

$$\min \theta(\lambda) \quad \text{s.t.} \quad \lambda_I \geq -\bar{\lambda}_I \quad (5.5)$$

are satisfied iff the projected gradient  $g^P = g^I + g^C$  vanishes.

An efficient algorithm for the solution of convex QP problems with simple bounds has been proposed independently by Friedlander and Martínez [27, 26, 28, 4] and Dostál [14]. The algorithm may be considered a modification of the Polyak algorithm that uses projections and controls the precision of the solution of auxiliary problems by the norm of  $g^C$  in each inner iterate  $y^i$ .

If the inequality

$$\|g^C(y^i)\| \leq \Gamma \|g^I(y^i)\|$$

holds for  $\Gamma > 0$ , then we call  $y^i$  *proportional* [14]. The algorithm explores the face

$$W_J = \{y : y_i = -\bar{\lambda}_i \text{ for } i \in J\}$$

with a given active set  $J \subseteq I$  as long as the iterates are proportional. If  $y^i$  is not proportional, we generate  $y^{i+1}$  by means of the descent direction  $d^i = -g^C(y^i)$  in a step that we call *proportioning*, and then we continue exploring the new face defined by  $J = \mathcal{A}(y^{i+1})$ . The class of algorithms driven by proportioning may be defined as follows.

**Algorithm 5.2 (General Proportioning Scheme - GPS)**

Let a feasible  $\lambda^0$  and  $\Gamma > 0$  [ $\Gamma = 1$ ] be given. For  $i > 0$ , choose  $\lambda^{i+1}$  by the following rules:

- (i) If  $\lambda^i$  is not proportional, define  $\lambda^{i+1}$  by proportioning.
- (ii) If  $\lambda^i$  is proportional, choose  $\lambda^{i+1}$  feasible so that

$$\theta(\lambda^{i+1}) \leq \theta(\lambda^i)$$

and  $\lambda^{i+1}$  satisfies at least one of the conditions:  $\mathcal{A}(\lambda^i) \subset \mathcal{A}(\lambda^{i+1})$ ,  $\lambda^{i+1}$  is not proportional, or  $\lambda^{i+1}$  minimizes  $\theta$  subject to  $\lambda \in W_J$ ,  $J = \mathcal{A}(\lambda^i)$ .

The set relation  $\subset$  is used in the strict sense so that it is satisfied if the set on the left is a proper subset of the set on the right. Basic theoretical results have been proved in [27, 14, 26, 28, 4].

**Theorem 5.3.** *Let  $\lambda^k$  denote an infinite sequence generated by Algorithm GPS with given  $\lambda^0$  and  $\Gamma > 0$ . Let  $\theta(\lambda)$  be a strictly convex quadratic function. Then the following statements are true:*

- (i)  $\lambda^k$  converges to the solution  $\lambda^*$  of (5.5).
- (ii) If problem (5.5) is not dual degenerate, then there is  $k$  such that  $\lambda^* = \lambda^k$ .
- (iii) If  $\Gamma \geq \kappa(\theta_{\lambda\lambda})^{1/2}$ , where  $\kappa$  denotes the spectral condition number, then there is  $k$  such that  $\lambda^* = \lambda^k$ .

Step (ii) of Algorithm GPS may be implemented by means of the conjugate gradient method. The most simple implementation of this step starts from  $y^0 = \lambda^k$  and generates the conjugate gradient iterations  $y^1, y^2, \dots$  for  $\min\{\theta(y) : y \in \mathcal{W}_J, J = \mathcal{A}(y^0)\}$  until  $y^i$  is found that is not feasible or not proportional or minimizes  $\theta(\lambda)$  subject to  $\lambda_I \geq -\bar{\lambda}_I$ . If  $y^i$  is feasible, then we put  $\lambda^{k+1} = y^i$ , otherwise  $y^i = y^{i-1} - \alpha^i p^i$  is not feasible and we can find  $\tilde{\alpha}^i$  so that  $\lambda^{k+1} = y^i - \tilde{\alpha}^i p^i$  is feasible and  $\mathcal{A}(\lambda^k) \not\subseteq \mathcal{A}(\lambda^{k+1})$ . We shall call the resulting algorithm *feasible proportioning* [14].

An obvious drawback of the feasible proportioning algorithm is that it is usually unable to add more than one index to the active set in one iteration. A simple but efficient alternative is to replace the feasibility condition by  $\theta(Py^{i+1}) \leq \theta(Py^i)$ , where  $Py$  denotes the projection on the set  $\Omega = \{y : y_i \geq -\bar{\lambda}_i \text{ for } i \in I\}$ . If the conjugate gradient iterations are interrupted by condition  $\theta(Py^{i+1}) > \theta(Py^i)$ , then a new iteration is defined by  $\lambda^{k+1} = Py^i$ . This modification of the feasible proportioning algorithm is called *monotone proportioning* [14].

The algorithm uses the single parameter  $\Gamma$ . We believe that a good choice is  $\Gamma \approx 1$ , as it seems reasonable to change the face when the error in the chopped gradient dominates that in the free gradient and the conjugate gradient method typically reduces only the latter.

The performance of the algorithm depends essentially on the rate of convergence of the conjugate gradient method that minimizes  $\theta$  in faces. In our case, the optimality results (4.7) and (4.8) suggest that the examination of faces can be carried out efficiently.

## 6 Numerical experiments

In this section, we illustrate the practical behavior of various implementations of our algorithm on the solution of a scalar model problem and on the solution of a semicoercive contact problem of elasticity arising in mining engineering. We have implemented Algorithm 5.1 to solve the basic dual problem (3.10) so that we can plug in the orthonormalization of the constraints (4.1) or the projectors to the natural coarse space (4.4). We have implemented our algorithm also with the modified lumped preconditioner

$$C^{-1} = PBKB^T P + (1/\rho)Q \quad (6.1)$$

that is expected to decrease the effective condition number of the Hessian reduced to the face that keeps the penalisation term untouched. An untransformed version of the preconditioned conjugate gradient algorithm [2, 3] is used for minimizing inside faces after the proportioning step.

**Problem 1.** This model problem results from the finite difference discretization of the following continuous problem:

$$\begin{aligned} \text{Minimize} \quad & q(u_1, u_2) = \sum_{i=1}^2 \left( \int_{\Omega^i} |\nabla u_i|^2 d\Omega - \int_{\Omega^i} f u_i d\Omega \right) \\ \text{subject to} \quad & u_1(0, y) \equiv 0 \text{ and } u_1(1, y) \leq u_2(1, y) \text{ for } y \in [0, 1], \end{aligned}$$

where  $\Omega^1 = (0, 1) \times (0, 1)$ ,  $\Omega^2 = (1, 2) \times (0, 1)$ ,  $f(x, y) = -5$  for  $(x, y) \in (0, 1) \times [0.75, 1)$ ,  $f(x, y) = 0$  for  $(x, y) \in (0, 1) \times (0, 0.75)$ ,  $f(x, y) = -1$  for  $(x, y) \in (1, 2) \times (0, 0.25)$  and  $f(x, y) = 0$  for  $(x, y) \in (1, 2) \times (0.25, 1)$ . This problem is semicoercive due to the lack of Dirichlet data on the boundary of  $\Omega^2$ .

The solution of the model problem may be interpreted as the displacement of two membranes under the traction  $f$ . The left membrane is fixed on the left and the left edge of the right membrane is not allowed to penetrate below the edge of the left membrane. The solution is unique because the right membrane is pressed down. More details about this model problem including some other results may be found in [19].

The model problem was discretized by regular grids defined by the step-size  $h = 1/n$  with  $n + 1$  nodes in each direction per subdomain  $\Omega^i$ ,  $i = 1, 2$ . Each subdomain  $\Omega^i$  was decomposed into  $n_x \times n_y$  identical rectangles with dimensions  $H_x = 1/n_x$  and  $H_y = 1/n_y$ . The solution of the model problem

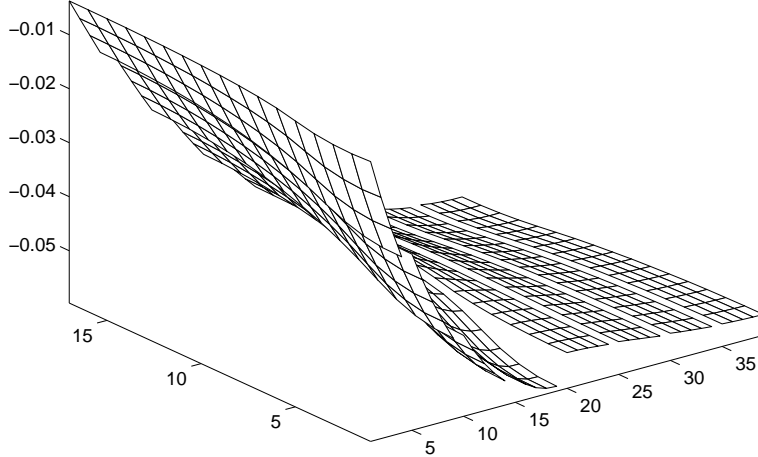


Figure 5: Solution of the model problem with  $h = 1/16$ ,  $H_x = 1/4$ ,  $H_y = 1$

with the decomposition into strips defined by  $H_x = 1/4$  and  $H_y = 1$  can be seen in Figure 5.

The model problem was solved for  $h \in \{1/64, 1/128, 1/256, 1/512\}$  with a secondary decomposition in order to test experimentally the dependence of the rate of convergence on the discretization, decomposition and penalization parameters. In all cases, we use the stopping criterium

$$\|g^P(\lambda, \mu, 0)\| \leq 10^{-4} \|d\| \quad \text{and} \quad \|G\lambda\| \leq 10^{-4} \|f\|.$$

The results are summarized in Tables 1-4. These tables contain, besides the discretization and decomposition parameters, the number of iterations in the outer loop of the augmented Lagrangian algorithm, the number of the conjugate gradient iterations in the inner loops of the algorithm for the solution of bound constrained QP problems, the number of multiplications by the matrix  $F$  that dominates the cost in each inner iteration, and the times of serial implementation in seconds. If not specified explicitly, we use the values of parameters suggested at Algorithms 6.1 and 6.2,  $\mu^0 = 0$ ,  $\lambda_I^0 = -\bar{\lambda}_I$  and  $\lambda_E^0 = 0$ .

Table 1 shows the performance of the algorithm with decomposition into strips with  $H_x \in \{1/2, 1/8, 1/32\}$  for a fixed discretization parameter  $h = 1/128$  and some variants of our algorithm. The horizontal dimension  $H_x$  of the vertical strips is in the first column. The primal dimension of

Table 1.  
 Convergence with the decomposition into strips  
 for  $h = 1/128$  and  $H_y = 1$ .

$H_x$	Orth.	Proj.	Outer iter.	cg iter.	M-V prod.	Time sec.
1/2	no	no	11	115	249	146.1
	yes	no	9	115	240	140.6
	yes	yes	4	44	92	59.8
1/8	no	no	8	663	1342	805.9
	yes	no	8	181	370	223.6
	yes	yes	4	77	158	97.1
1/32	no	no	6	6425	12856	7321.7
	yes	no	6	361	728	409.4
	yes	yes	5	185	375	212.3

the problems ranges between 33411 and 41151, and their dual dimension between 387 and 8127. We can observe that the rate of convergence deteriorates with an increasing number of subdomains and resulting increasing aspect ratio, but that orthogonalization (orth.) and projectors to the natural coarse space (proj.) improve the performance considerably.

Table 2 shows the performance of the algorithm with projections to the natural coarse space on the regular decomposition for various values of the discretization parameter  $h$ . The regular decompositions are characterized by  $H = H_x = H_y = 32h$ . In particular, examining the column with the number of the conjugate gradient iterations per face, we can observe near optimal performance of the iterative solver in faces. The results with the preconditioner (6.1) are in Table 3.

These results are completed by Table 4, which illustrates the sensitivity of the algorithm with projections to the balancing parameter  $M$  and to the initial penalization parameter  $\rho_0$ . In particular, we can observe the elimination of the negative effect of the penalization predicted by the theory using orthogonalization and projectors.

The experiments with the model problem were run on a SUN Sparc

Table 2.  
Near optimality of algorithm with  
the natural coarse grid projectors for  $H = H_x = H_y$ .

$h$	$H$	Primal dim	Dual dim.	Outer iter.	cg iter.	cg per face	M-V prod.	Time sec.
1/64	1/2	8646	326	4	32	3.56	69	2.6
1/128	1/4	34716	1692	5	47	3.11	100	14.3
1/256	1/8	139128	7544	5	55	5.00	115	66.8
1/512	1/16	557040	31728	6	107	5.63	223	590.5

Table 3.  
Near optimality of algorithm with  
the preconditioning in faces for  $H = H_x = H_y$ .

$h$	$H$	Primal dim	Dual dim.	Outer iter.	cg iter	cg per face	M-V prod.	Time sec.
1/64	1/2	8646	326	4	23	2.56	50	1.9
1/128	1/4	34716	1692	4	35	2.92	75	10.9
1/256	1/8	139128	7544	5	47	3.61	99	58.3
1/512	1/16	557040	31728	6	81	5.40	169	476.2

Table 4.  
 Effect of  $\rho_0$  and  $M$   
 for  $H_x = H_y = 1/8$  and  $h = 1/128$ .

M	Initial $\rho_0$	Final $\rho$	Outer iter.	cg iter.	M-V prod.	Time sec.
$10^3$	$10^3$	$10^5$	5	46	97	9.9
	$10^4$	$10^5$	4	41	86	8.9
	$10^5$	$10^6$	4	51	108	11.0
	$10^6$	$10^8$	4	58	121	12.2
$10^4$	$10^4$	$10^5$	4	41	86	8.9
	$10^5$	$10^6$	4	51	108	11.0
	$10^6$	$10^7$	4	58	121	12.2
$10^5$	$10^5$	$10^6$	3	45	93	9.5
	$10^6$	$10^7$	4	56	117	11.9

Ultra1 computer, under SunOS 5.5.1, using the f77 (version 4.0) FORTRAN compiler and double precision. The auxiliary problems were solved by QUACON, a routine developed in the Institute of Mathematics, Statistics and Scientific Computation at Unicamp [4].

**Problem 2.** To test performance of our algorithm on a more realistic problem, we have also considered a 3D contact problem (Figure 6) proposed by Hittinger in [33] and solved in [13]. The 2D version of this problem was solved in [33] and [9, 10, 11]. The problem comprises three elastic blocks with boundary conditions defined by prescribed zero normal displacements on the vertical boundaries and on the bottom of the model with exception of the boundaries of the excavation in the bottom block. The blocks are considered isotropic with Young modulus  $E=10000\text{MPa}$  and Poisson ratio 0.25. The only external forces considered are gravitational volumetric forces with density  $2.5\text{g/cm}^3$ . The problem was discretized by the finite element method so that the resulting discrete problem comprised 6419 nodal variables and 382 dual variables. The bandwidth of the stiffness matrix of each

block is 165. The problem was solved to the precision

$$\|g^P(\lambda, \mu, 0)\| \leq 10^{-4}\|\tilde{d}\| \quad \text{and} \quad \|G\lambda\| \leq 10^{-4}\|f\|$$

defined to comply with our earlier experiments with the basic algorithm without the natural coarse space preconditioning [13]. The solution  $\lambda$  of the problem that is proportional to the contact nodal forces is in Figure 7. The problem is semicoercive due to the two “floating” upper blocks. We have not used any secondary decomposition so that our coarse grid was formed just by the two dimensional null space of the stiffness matrix that is generated by independent vertical movements of the upper two blocks.

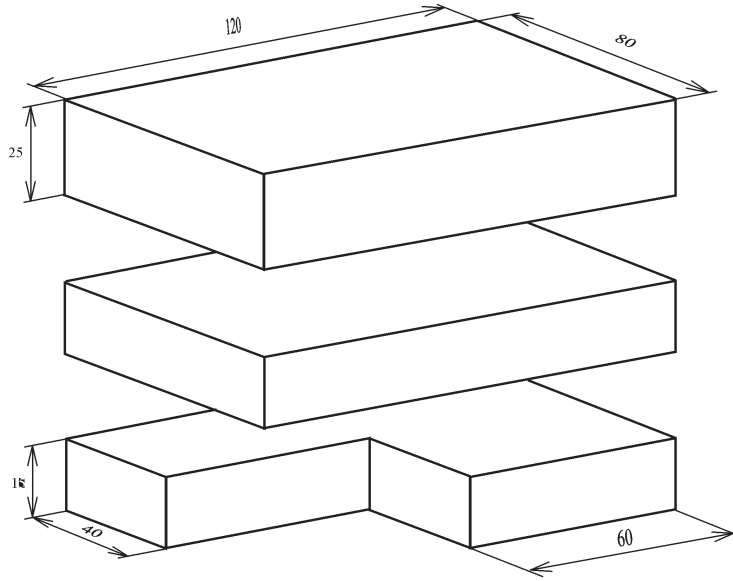


Figure 6: Block structure

The performance of our algorithm with various values of the balancing parameter  $M$  and the initial penalty parameter  $\rho_0$  is reported in Table 5.

We have also used the algorithm with projectors to the natural coarse grid to solve the problem to the higher feasibility precision

$$\|g^P(\lambda, \mu, 0)\| \leq 10^{-4}\|\tilde{d}\| \quad \text{and} \quad \|G\lambda\| \leq 10^{-6}\|f\|$$



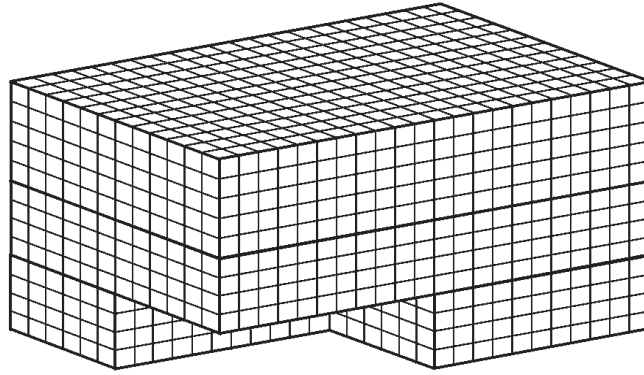


Figure 7: Discretized block structure

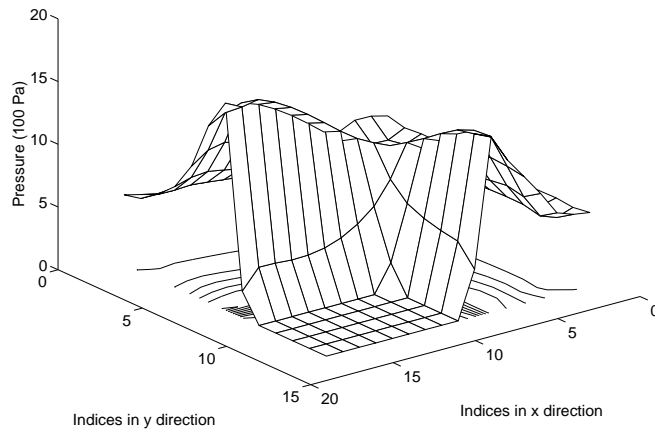


Figure 8: Contact stress between the upper two blocks

Table 5.  
 Convergence for block problem  
 without secondary decomposition.

$M$	$\rho_0$	Orth.	Proj.	Final $\rho$	Outer iter.	cg iter.	M-V prod.
$10^2$	$10^2$	no	no	$10^3$	3	381	669
		yes	no	$10^3$	3	459	787
		yes	yes	$10^2$	4	276	438
$10^2$	$10^3$	no	no	$10^3$	3	493	845
		yes	no	$10^3$	3	430	740
		yes	yes	$10^3$	4	211	298
$10^3$	$10^3$	no	no	$10^3$	3	473	843
		yes	no	$10^3$	3	503	871
		yes	yes	$10^3$	4	211	298

to see the sensitivity of performance on the feasibility tolerance. The results are in Table 6. The last two columns show the final feasibility and minimization errors labeled by  $\epsilon_f$  and  $\epsilon_p$ , respectively. The stopping criterion requires  $\epsilon_f \leq 2.88 * 10^{-4}$  and  $\epsilon_p \leq 1.65 * 10^{-4}$ . We were not able to solve the problem to higher feasibility precision with the basic algorithm in comparable time.

The considerably better performance of the algorithm with coarse grid projections is rather surprising if we take into account that the dimension of the coarse grid is only two. Again, as predicted by the theory, we observe no negative effect of high penalization parameter on the performance of the algorithm. We believe that the results indicate that the algorithms presented are efficient.

The solution of the contact problem was carried out on a PC-586/200 type computer, DOS operating system, Microsoft **Fortran 77** and double precision. The stiffness matrices of blocks of Problem 2 were generated by experimental code of Blaheta and Kohut [5] and the auxiliary problems were solved by **QUACAN**, a routine developed in the Institute of Mathematics, Statistics and Scientific Computation at Unicamp [26].

Table 6.  
Effect of  $\rho_0$  and  $M$  on algorithm with the natural coarse grid  
Block problem with higher feasibility precision

M	Initial $\rho_0$	Final $\rho$	Outer iter.	cg iter.	M-V prod.	$\epsilon_f$	$\epsilon_p$
$10^1$	$10^1$	$10^1$	4	230	378	3.45E-7	9.01E-5
	$10^2$	$10^2$	4	276	438	4.93E-7	1.39E-4
	$10^3$	$10^3$	4	284	437	9.36E-6	1.60E-4
$10^2$	$10^2$	$10^2$	4	276	438	4.93E-6	1.39E-4
	$10^3$	$10^3$	4	211	298	8.92E-8	1.50E-4
$10^3$	$10^3$	$10^3$	4	211	298	8.92E-8	1.50E-4

## 7 Comments and conclusions

We have described a new domain decomposition algorithm for the solution of coercive and semicoercive frictionless contact problems of elasticity. The method reduces the problem to the contact interface so that it directly computes the tractions on the contact interface. The stress and strain distribution may then be obtained by the solution of standard linear problems for each body separately.

The approach combines a variant of the FETI method with projectors to the natural coarse grid and recently developed algorithms for the solution of special quadratic programming problems. A new feature of these algorithms is the adaptive control of precision of the solution of auxiliary problems with effective usage of the projections to the natural coarse grid.

The implementation of this approach deals separately with each body or subdomain, so that it is suitable for parallelization. Theoretical results are presented that guarantee convergence and high numerical scalability of the algorithm. In particular, the algorithm is shown to be in a sense optimal with respect to both penalization and discretization parameters. First numerical experiments are in agreement with the theory and give further evidence that the algorithms presented are efficient.

We believe that the performance of the algorithms may be further improved by adapting the standard regular preconditioners to the unconstrained minimization in faces. The first reported experimental results are encouraging but more research is necessary to get insight into the effect and

proper treatment of the preconditioners with the intervening projectors.

## References

- [1] O. Axelsson, A class of iterative methods for finite element equations. *Comp. Meth. in Appl. Mech. and Engng.*, 9 (1976), 127-137.
- [2] O. Axelsson, *Iterative Solution Methods*, Cambridge Univ. Press, Cambridge, 1995.
- [3] O. Axelsson, V. A. Barker, *Finite Element Solution of Boundary Value Problems*, Academic Press, London 1984.
- [4] R.H. Bielschowski, A. Friedlander, F.A.M. Gomes, J.M.Martínez, M. Raydan, An adaptive algorithm for bound constrained quadratic minimization, *Investigación Operativa*, 7 (1997), 67-102.
- [5] R. Blaheta, R. Kohut, Benchmarks and programs for testing iterative solvers for 3D problems of geomechanics, Report No. 9502, Institute of Geonics, Academy of Science of Czech Republic, Ostrava 1995.
- [6] F. Brezzi, M. Fortin, *Mixed and Hybrid Finite Element Methods*, Springer Verlag, New York, 1991.
- [7] 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 J. Num. Anal.* 28 (1991), 545-572.
- [8] Z. Dostál, Conjugate gradient method with preconditioning by projector, *Int. J. Comp. Math.* 23 (1988), 315-324.
- [9] Z. Dostál, Conjugate projector preconditioning for the solution of contact problems, *Int. J. Num. Met. Engng.* 34 (1992), 271-277.
- [10] Z. Dostál, Domain decomposition methods for modelling of deformable block structure, *Proceedings of Geomechanics'93*, Z. Rakowski ed., A. A. Balkema, Rotterdam (1994), 185-188.
- [11] Z. Dostál, Duality based domain decomposition with inexact subproblem solver for contact problems. *Contact Mechanics II*, eds. M.H. Aliabadi, C. Alessandri, Wessex Inst. of Technology, Southampton (1995), 461-468.

- [12] Z. Dostál, Duality based domain decomposition with proportioning for the solution of free boundary problems, *J. Comp. Appl. Math.* 63 (1995), 203-208.
- [13] Z. Dostál, A. Friedlander, S.A. Santos, Analysis of block structures by augmented Lagrangians with adaptive precision control, *Proc. of Geomechanics'96*, ed. Z. Rakowski, A. A. Balkema, Rotterdam (1997), 175-180.
- [14] Z. Dostál, Box constrained quadratic programming with proportioning and projections, *SIAM J.Opt.* 7 (1997), 871-887.
- [15] Z. Dostál, On preconditioning and penalized matrices, to appear in *Num. Lin. Alg. Appl.*
- [16] Z. Dostál, A. Friedlander, S.A. Santos, Augmented Lagrangians with adaptive precision control for quadratic programming with simple bounds and equality constraints, Technical Report RP 74/96, IMECC-UNICAMP, University of Campinas, October 1996.
- [17] Z. Dostál, A. Friedlander, S.A. Santos, Solution of coercive and semicoercive contact problems by FETI domain decomposition, *Contemporary Math.* 218 (1998), 82-93.
- [18] Z. Dostál, A. Friedlander, S.A. Santos, Augmented Lagrangians with adaptive precision control for quadratic programming with equality constraints, to appear in *Comp. Opt. Appl.*
- [19] Z. Dostál, F.A.M. Gomes, S.A. Santos, Duality-based domain decomposition with natural coarse-space for variational inequalities, Technical Report RP 63/98, IMECC-UNICAMP, University of Campinas, October 1998.
- [20] Z. Dostál, V. Vondrák, Duality based solution of contact problems with Coulomb friction, *Arch.Mech.* 49 (1997), 453-460.
- [21] G. Duvant, J. L. Lions, *Inequalities in Mechanics and Physics*, Springer Verlag, Berlin 1976.
- [22] C. Farhat, M. Gérardin, On the general solution by a direct method of a large scale singular system of linear equations: application to the analysis of floating structures, *Int. J. Num. Met. Eng.* 41 (1997), 675-696.

- [23] C. Farhat, F.-X. Roux, An unconventional domain decomposition method for an efficient parallel solution of large-scale finite element systems, *SIAM J. Sci. Stat. Comput.* 13 (1992), 379-396.
- [24] C. Farhat, P. Chen, F.-X. Roux, The dual Schur complement method with well posed local Neumann problems, *SIAM J. Sci. Stat. Comput.* 14 (1993), 752-759.
- [25] C. Farhat, J. Mandel, F.-X. Roux, Optimal convergence properties of the FETI domain decomposition method, *Comput. Methods Appl. Mech. Eng.* 115 (1994), 365-385.
- [26] A. Friedlander, J.M. Martínez, S.A. Santos, A new trust region algorithm for bound constrained minimization, *Applied Mathematics & Optimization* 30 (1994), 235-266.
- [27] A. Friedlander, J.M. Martínez, On the maximization of concave quadratic function with box constraints, *SIAM J. Opt.* 4 (1994), 177-192.
- [28] A. Friedlander, J.M. Martínez, M. Raydan, A new method for large scale box constrained quadratic minimization problems, *Optimization Methods and Software* 5 (1995) 57-74.
- [29] S. Fučík, A. Kufner, *Nonlinear Differential Equations*, Elsevier, Amsterdam 1980.
- [30] R. Glowinski, P. Le Tallec, *Augmented Lagrangians and Operator Splitting Methods*, SIAM, Philadelphia, 1989.
- [31] R. Glowinski, J. L. Lions, R. Trémoières, *Analyse Numérique des Inéquations Variationnelles*, Tom 1-2, Dunod, Paris, 1976.
- [32] G. H. Golub, C. F. Van Loan, *Matrix Computation*, The John Hopkins Univ. Press, Baltimore, 1985.
- [33] M. Hittinger, *Numerical Analysis of Topping Failures in Jointed Rocks*, Ph.D. Thesis, Univ. of California, Dept. of Civil Engng. (1978).
- [34] I. Hlaváček, J. Haslinger, J. Nečas, J. Lovíšek, *Solution of Variational Inequalities in Mechanics*, Springer Verlag, Berlin, 1988.
- [35] N. Kikuchi, J.T. Oden, *Contact Problems in Elasticity*, SIAM, Philadelphia, 1988.

- [36] M. Raous, L. Cangémi, M. Cocu, Friction and adhesion: variational formulation, numerical methods and application to fiber/matrix interface of composite materials. Book of Abstracts of 4th World Congress on Computational Mechanics, Buenos Aires 1998, I/396.
- [37] F.-X. Roux, Spectral analysis of interface operator, Proceedings of the 5th Int. Symp. on Domain Decomposition Methods for Partial Differential Equations, ed. D. E. Keyes et al., SIAM, Philadelphia (1992), 73-90.
- [38] F.-X. Roux et al., Efficient parallel coarse grid preconditioner to the FETI method, to appear in Contemporary Math. 218 (1998).
- [39] Simo J. S., Laursen J. A., An augmented Lagrangian treatment of contact problems involving friction, Comp.& Structures 42 (1992) 97-116.