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Kestřánek, Zdeněk
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The Conjugate Projected Gradient Method -
Numerical Tests and Results

Zdeněk Kestřánek, Jiří Nedoma

Technical report No. 677

August 1996

Institute of Computer Science, Academy of Sciences of the Czech Republic
Pod vodárenskou věží 2, 182 07 Prague 8, Czech Republic
phone: 66053911 fax: (+422) 8585789
e-mail: zdenda@uivt.cas.cz

The Conjugate Projected Gradient Method - Numerical Tests and Results

Zdeněk Kestřánek, Jiří Nedoma ¹

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Abstract

In this paper the solution of the Friction Contact Problem and corresponding solvers are discussed. The model is based on Linear Elasticity, where small displacements are assumed. Then the condition of impenetration can be expressed by linear constraints. Mathematically, the problem leads to the saddle point problem. This formulation enables additional contact elements to be avoided, where a suitable stiffness parameter is needed. We discuss the continuous problem, the approximation and the discretized problem as well. The Conjugate Gradient Method without and with preconditioning is applied to solve the basic step of the discretized problem. We discuss several aspects concerning the *CG* method with projection of the gradient.

Keywords

Finite Element Method, Contact Problem, Quadratic Programming

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1 Introduction

The bridges are often constructed in difficult geological conditions, e.g. on undermining areas or on unstable slopes, simultaneously they have to satisfy a great static and dynamic loading. They consists of lower structure, upper structure and the bridge equipment. The foundations and bridge supports are included in lower structure, and the supporting structure in upper structure. We consider the simple type of a beam bridge with the lower structure to be massive. We study the case, when the pier is situated as far as the rigid footwall. In the model problem the neighbouring rocks are in a contact with the massive pier and then the effect of moving neighbouring rocks onto the deformation of the massive pier as well as of all construction of the bridge is numerically analyzed.

In this contribution the model of the bridge will be treated as the elastic contact problem. We test the conjugate gradient method without and with the preconditioning.

2 Classical formulation of the Contact Problem

Let us suppose, that we have S elastic bodies in a contact. Let these bodies occupy the bounded regions $\Omega^1, \Omega^2, \dots, \Omega^S \subset R^2$ with Lipschitz boundaries.

We look for the vector field of the displacements $\mathbf{u} = (u_1, u_2)$, the tensor field of small strains $e_{ij} = e_{ij}(\mathbf{u})$ and the stress tensor $\tau_{ij} = \tau_{ij}(\mathbf{u})$, $i, j = 1, 2$, on $\Omega^1 \cup \dots \cup \Omega^S$.

Let the boundary $\partial\Omega$ be divided into disjunct parts

$$\begin{aligned} \Gamma_u, \Gamma_\tau, \Gamma_c, \Gamma_0, R, \quad \partial\Omega &= \Gamma_u \cup \Gamma_\tau \cup \Gamma_c \cup \Gamma_0 \cup R, \\ \Gamma_u &= \bigcup_{i=1}^S \Gamma_u^i, \quad \Gamma_\tau = \bigcup_{i=1}^S \Gamma_\tau^i, \quad \Gamma_0 = \bigcup_{i=1}^S \Gamma_0^i, \quad \Gamma_c = \bigcup_{k,l} \Gamma_c^{kl}, \\ \Gamma_c^{kl} &= \bar{\Gamma}_c^k \cap \bar{\Gamma}_c^l, \quad k, l \in \{1, \dots, S\}, \quad k < l, \end{aligned}$$

and the surface measure of R be zero.

Let on $\Gamma_c = \bigcup_{k,l} \Gamma_c^{kl}$ normal and tangential components of the displacement vector \mathbf{u} and the stress tensor τ be defined by

$$u_n = u_i n_i, \quad u_t = u_i t_i, \quad \tau_n = \tau_i n_i, \quad \tau_t = \tau_i t_i, \quad (2.1)$$

where n_i are the components of outward normal to $\partial\Omega^k$, $\tau_i = \tau_{ij} n_j$, and $\mathbf{t} = (-n_2, n_1)$ represents the tangential vector to $\partial\Omega^k$.

Then we have to solve the following

problem (\mathcal{P}_c): Find \mathbf{u} that satisfies the equilibrium equations

$$\frac{\partial \tau_{ij}}{\partial x_j}(\mathbf{u}) + F_i = 0 \quad i, j = 1, 2, \quad (2.2)$$

and the boundary conditions

$$u_i = u_{0i} \quad \text{on } \Gamma_u, \quad (2.3)$$

$$\tau_{ij} n_j = P_i \quad \text{on } \Gamma_\tau, \quad (2.4)$$

$$u_n^k - u_n^l \leq 0, \quad \tau_n^k = -\tau_n^l \leq 0, \quad (u_n^k - u_n^l) \tau_n^k = 0, \quad \text{on } \Gamma_c^{kl} \quad (2.5)$$

$$\begin{aligned}
& |\tau_t^{kl}| \leq g^{kl} && \text{on } \Gamma_c^{kl} \\
|\tau_t^{kl}| < g^{kl} \Rightarrow u_t^k - u_t^l = 0, && \\
|\tau_t^{kl}| = g^{kl} \Rightarrow \exists \lambda \geq 0 \text{ such that } u_t^k - u_t^l = -\lambda \tau_t^{kl}, &&
\end{aligned} \tag{2.6}$$

$$u_n = 0, \quad \tau_t = 0 \quad \text{on } \Gamma_0, \tag{2.7}$$

where F_i are the components of body forces vector,
 u_{0i} the prescribed displacement vector,
 P_i the surface loads
and g^{kl} are the prescribed friction forces.

(2.5) are the Signorini conditions on an unilateral contact, (2.6) represents Coulomb's friction law and (2.7) describes the conditions on a bilateral contact. We suppose that the relation between stress and displacement is governed by the generalized Hooke's law

$$\tau_{ij}(\mathbf{u}) = c_{ijkm} e_{km}(\mathbf{u}) \quad i, j = 1, 2, \tag{2.8}$$

where we use the Einstein's summation convention,
and the small strain tensor e_{ij} is defined by

$$e_{ij}(\mathbf{u}) = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad i, j = 1, 2 \tag{2.9}$$

DEFINITION 2.1. The function \mathbf{u} is a classical solution of the Contact Problem if it satisfies (2.3-2.7) with (2.8) and (2.9).

The coefficients c_{ijkm} in (2.8), $c_{ijkm} \in L^\infty(\Omega)$, satisfy symmetry conditions

$$c_{ijkm} = c_{jikm} = c_{kmij}. \tag{2.10}$$

Moreover, there exists a constant $c_0 > 0$ such, that

$$c_{ijkm}(x) e_{ij} e_{km} \geq c_0 e_{ij} e_{ij} \tag{2.11}$$

is valid for all sym. matrices e_{ij} and almost everywhere in Ω .

In the case of isotropic bodies and plane strain

$$c_{1112} = \lambda, \quad c_{1212} = \mu,$$

the same holds for symmetric components (cf.(2.10)), and

$$c_{1111} = c_{2222} = \lambda + 2\mu, \quad c_{ijkm} = 0 \quad \text{otherwise.}$$

3 Variational formulation

For the definition of the classical solution, it is necessary to assume its sufficient smoothness. However, in the case when this assumption is not valid, it is possible to define the solution by using the minimum potential energy principle.

First of all, we introduce the space of all functions with finite energy by

$$\mathcal{H}^1(\Omega) \equiv \{\mathbf{v} | \mathbf{v} = (\mathbf{v}^1, \mathbf{v}^2, \dots, \mathbf{v}^S) \in [H^1(\Omega^1)]^2 \times \dots \times [H^1(\Omega^S)]^2\}. \quad (3.1)$$

The norm is defined as

$$\|\mathbf{v}\|^2 = \|\mathbf{v}\|_{\mathcal{H}^1(\Omega)}^2 = \sum_{l=1}^S \|\mathbf{v}^l\|_{[H^1(\Omega^l)]^2}^2 = \sum_{l=1}^S \sum_{i=1}^2 \|v_i^l\|_1^2. \quad (3.2)$$

Similarly we define the space $\mathcal{H}^2(\Omega)$

$$\mathcal{H}^2(\Omega) \equiv \{\mathbf{v} | \mathbf{v} = (\mathbf{v}^1, \mathbf{v}^2, \dots, \mathbf{v}^S) \in [H^2(\Omega^1)]^2 \times \dots \times [H^2(\Omega^S)]^2\}. \quad (3.3)$$

We will also use the space

$$[W^{1,\infty}(\Gamma)]^2 \equiv \{\mathbf{v} | \frac{\partial v_i}{\partial t} \in L^\infty(\Gamma)\}, \quad (3.4)$$

where $\mathbf{v} = \mathbf{v}(\mathbf{x})$, $\mathbf{x} = \mathbf{x}(t)$ is the parametrization of the abscissa Γ , $i = 1, 2$.

Furthermore, we define the seminorm

$$|\mathbf{v}|^2 = \int_{\Omega} e_{ij}(\mathbf{v}) e_{ij}(\mathbf{v}) d\mathbf{x}. \quad (3.5)$$

We introduce the sets of virtual displacements by

$$V \equiv \{\mathbf{v} \in \mathcal{H}^1(\Omega) | \mathbf{v} = \mathbf{u}_0 \quad \text{on } \Gamma_u, \quad v_n = 0 \quad \text{on } \Gamma_0\}, \quad (3.6)$$

where $\mathbf{u}_0 \in \mathcal{H}^1(\Omega)$, and the set of all admissible displacements by

$$K \equiv \{\mathbf{v} \in V | v_n^k - v_n^l \leq 0 \quad \text{on } \Gamma_c^{kl}\} \quad (3.7)$$

REMARK 3.1. For simplicity we will assume $\mathbf{u}_0 \equiv 0$ on Γ_u .

Let the potential energy functional be of the following form

$$\mathcal{L}(\mathbf{v}) = \mathcal{L}_0(\mathbf{v}) + j_0(\mathbf{v}) \quad , \quad (3.8)$$

where

$$\mathcal{L}_0(\mathbf{v}) = \frac{1}{2} A(\mathbf{v}, \mathbf{v}) - L(\mathbf{v}) \quad , \quad (3.9)$$

$$A(\mathbf{u}, \mathbf{v}) = \int_{\Omega} c_{ijkl} e_{ij}(\mathbf{u}) e_{kl}(\mathbf{v}) d\mathbf{x} \quad (3.10)$$

$$L(\mathbf{v}) = \int_{\Omega} F_i v_i d\mathbf{x} + \int_{\Gamma_\tau} P_i v_i ds \quad , \quad (3.11)$$

$$j_0(\mathbf{v}) = \int_{\Gamma_c^{kl}} g^{kl} |v_t^k - v_t^l| ds \quad \text{and} \quad (3.12)$$

$$\mathbf{F} \in [L^2(\Omega)]^2, \mathbf{P} \in [L^2(\Gamma_\tau)]^2, g^{kl} \in [L^\infty(\Gamma_c^{kl})]^2.$$

Regarding (2.10), (2.11) and Schwartz inequality, we have

$$c_0|\mathbf{v}|^2 \leq A(\mathbf{v}, \mathbf{v}) \quad , \quad (3.13)$$

$$A(\mathbf{u}, \mathbf{v}) \leq C_1|\mathbf{u}||\mathbf{v}| \quad , \quad (3.14)$$

$$|\mathbf{v}|^2 \leq C_2\|\mathbf{v}\|^2 \quad , \quad (3.15)$$

We will now define the variational solution.

DEFINITION 3.1. A function $\mathbf{u} \in K$ is the variational solution of the Contact Problem if it is the minimum of the potential energy functional on the set of all admissible displacements K i.e.

$$\mathcal{L}(\mathbf{u}) \leq \mathcal{L}(\mathbf{v}) \quad \forall \mathbf{v} \in K \quad . \quad (3.16)$$

We denote this minimization problem by (\mathcal{P}) .

It can be easily verified (e.g. [6],[11]), that under the assumption of sufficient smoothness of the classical solution, both classical and variational solution are equivalent.

THEOREM 3.1. There exists a unique solution of the problem (\mathcal{P}) . For the proof see e.g. [6],[10],[14],[15].

Since the term $j_0(\mathbf{v})$ is non-differentiable, we transform the minimization problem (\mathcal{P}) to the saddle point problem (\mathcal{P}') :

Find a pair $(\mathbf{u}, \lambda) \in K \times \Lambda$ such that

$$\mathcal{H}(\mathbf{u}, \mu) \leq \mathcal{H}(\mathbf{u}, \lambda) \leq \mathcal{H}(\mathbf{v}, \lambda) \quad \forall \mathbf{v} \in K, \quad \forall \mu \in \Lambda. \quad (3.17)$$

where

$$\mathcal{H}(\mathbf{v}, \mu) = \mathcal{L}_0(\mathbf{v}) + j_1(\mathbf{v}, \mu), \quad (3.18)$$

$$j_1(\mathbf{v}, \mu) = \int_{\Gamma_c^{kl}} g^{kl} \mu (v_i^k - v_i^l) ds \quad \text{and} \quad (3.19)$$

$$\Lambda = \{\mu | \mu \in L^2(\Gamma_c^{kl}), |\mu| \leq 1 \text{ a.e. on } \Gamma_c^{kl}\}. \quad (3.20)$$

4 Approximation

Consider the regular, consistent triangulation T_h of the regions Ω^s , $1 \leq s \leq S$, with nodes a_i . Let Ω^s have a polygonal boundary and h designate the longest side of the triangles. As the boundary is polygonal, it holds $\Gamma_c^{kl} = \bigcup_{j=1}^J \Gamma_{c_j}^{kl}$, $\Gamma_0 = \bigcup_{j=1}^{J'} \Gamma_{0j}$, where $\Gamma_{c_j}^{kl}$, Γ_{0j} are the abscissae, whose endpoints are the vertices of the region Ω . $J = J(k, l)$ is the number of straight lines on the unilateral contact boundary between the bodies k and l , and J' is the number of straight lines on the bilateral contact boundary. For every node a_i of the triangulation on Γ_c^{kl} , and on Γ_0 , define the set of indices

$\mathcal{N}_i^{kl} = \{j \in \{1, \dots, J\} | a_i \in \Gamma_{c_j}^{kl}\}$ and $\mathcal{N}_i = \{j \in \{1, \dots, J'\} | a_i \in \Gamma_{0j}\}$, respectively. (In plane problems \mathcal{N}_i has 1 or 2 members. In the latter case the node a_i is the vertex of the region laying inside Γ_c^{kl} or Γ_0). On the abscissae $\Gamma_{c_j}^{kl}$, let \mathbf{n}_j denote the outward normal to the boundary $\partial\Omega^k$. Let us define the finite dimensional approximations of V and K .

$$\begin{aligned} V_h &= \{ \mathbf{v}_h \in [C(\overline{\Omega}^1)]^2 \times \dots \times [C(\overline{\Omega}^S)]^2 | \mathbf{v}|_T \in [P_1(T)]^2 \ \forall T \in T_h; \\ &\quad \mathbf{v}_h(a_i)\mathbf{n}_j = 0, \ j \in \mathcal{N}_i, \ a_i \in \Gamma_0; \\ &\quad \mathbf{v}_h(a_i) = \mathbf{u}_0(a_i), \ a_i \in \Gamma_u \}, \end{aligned} \quad (4.1)$$

$$\begin{aligned} K_h &= \{ \mathbf{v}_h \in V_h | (\mathbf{v}_h^k - \mathbf{v}_h^l)(a_i)\mathbf{n}_j \leq 0, \\ &\quad j \in \mathcal{N}_i^{kl}, \ a_i \in \Gamma_c^{kl}, \ 1 \leq k \leq l \leq S \}. \end{aligned} \quad (4.2)$$

REMARK 4.1. It holds $K_h \subset K$.

We arrive at the definition of the approximate problem.

DEFINITION 4.1. A function $\mathbf{u}_h \in K_h$ is the solution of the approximate problem (\mathcal{P}_h) , if it is the minimum of the potential energy functional on the set of all admissible displacements, i.e.

$$\mathcal{L}(\mathbf{u}_h) \leq \mathcal{L}(\mathbf{v}_h) \quad \forall \mathbf{v}_h \in K_h. \quad (4.3)$$

THEOREM 4.1. There exists a unique finite element approximation of the problem (\mathcal{P}_h) .

For the proof see e.g. [6],[11],[14],[15].

To prove the convergence of the approximations to the exact solution we need the density lemma [7].

LEMMA 4.1. Let us assume that there is only a finite number of “end points” $\overline{\Gamma}_c^{kl} \cap \overline{\Gamma}_\tau, \overline{\Gamma}_u \cap \overline{\Gamma}_\tau, \overline{\Gamma}_u \cap \overline{\Gamma}_c^{kl}$. Then the set $K \cap [C^\infty(\overline{\Omega})]^2$ is dense in K .

We have the following result:

THEOREM 4.2. Let $K \subset V, K_h \subset V_h$ be sets defined above. Let the assumptions of Lemma 4.1. be fulfilled. Then for $\forall \mathbf{u} \in K$ there exists $\mathbf{u}_h \in K_h$ such that

$$\|\mathbf{u} - \mathbf{u}_h\|_1 \rightarrow 0 \quad \text{for } h \rightarrow 0.$$

Proof.

Let $\mathbf{u} \in K$. Due to Lemma 4.1. there exists a sequence $\{\mathbf{u}_k\} \subset K \cap [C^\infty(\overline{\Omega})]^2$ such that

$$\|\mathbf{u} - \mathbf{u}_k\|_1 \rightarrow 0 \quad \text{for } k \rightarrow \infty.$$

To the element $\mathbf{u}_k \in K \cap [C^\infty(\overline{\Omega})]^2$ there exists the element $\mathbf{r}_h \mathbf{u}_k$ - the linear Lagrange interpolation on the triangulation T_h . Thus

$$\|\mathbf{u}_k - \mathbf{r}_h \mathbf{u}_k\|_1 \leq ch |\mathbf{u}_k|_2$$

where $|\cdot|_2$ is the seminorm in $[H^2(\Omega)]^2$. Let $\mathbf{u}_h := \mathbf{r}_h \mathbf{u}_k$.

Then

$$\|\mathbf{u} - \mathbf{u}_h\|_1 \leq \|\mathbf{u} - \mathbf{u}_k\|_1 + \|\mathbf{u}_k - \mathbf{r}_h \mathbf{u}_k\|_1 \rightarrow 0 \text{ for } k \rightarrow \infty, h \rightarrow 0.$$

which completes the proof. \square

As it was mentioned in previous section, the functional \mathcal{L} is non-differentiable. Therefore, we define the approximate problem for (\mathcal{P}') .

Let

$$\Lambda_h = \{\mu \in \Lambda \mid \mu \in P_0(\cup_i \Gamma_{ci}^{kl})\}, \quad (4.4)$$

where Γ_{ci}^{kl} are the sides of triangles on the contact boundary Γ_c^{kl} .

The approximation of the problem (\mathcal{P}') has the form $(\mathcal{P}')_h$:

Find a pair $(\mathbf{u}_h, \lambda_h) \in K_h \times \Lambda_h$ such that

$$\mathcal{H}(\mathbf{u}_h, \mu) \leq \mathcal{H}(\mathbf{u}_h, \lambda_h) \leq \mathcal{H}(\mathbf{v}, \lambda_h) \quad \forall \mathbf{v} \in K_h, \quad \forall \mu \in \Lambda_h. \quad (4.5)$$

5 Numerical Realization

In the discrete form, the problem (3.17),(4.5) leads to the problem (\mathcal{P}_d) :

Find $(x, \lambda) \in K_d \times L$, such that

$$f(x, \mu) \leq f(x, \lambda) \leq f(y, \lambda) \quad \forall (y, \mu) \in K \times L, \quad (5.1)$$

where

$$f(y, \mu) = \frac{1}{2} y^T C y - y^T d + y^T G^T \mu \quad (5.2)$$

$$K_d = \{y \in R^N \mid A y \leq 0\} \text{ and } L = \{\mu \in R^P \mid |\mu_i| \leq 1\}. \quad (5.3)$$

REMARK 5.1. The global stiffness matrix C is of the type $N \times N$, block diagonal. Every block of it is sparse, symmetric, positive semidefinite matrix and corresponds to just one body of the model. In the coercive case (e.g.[11],[15]) C is positive definite, in the semi-coercive case [16] is positive semidefinite. (In our investigated case C is positive definite.) The stiffness matrix was stored in two formats: SKY-LINE (profile) format (e.g. [11]), and SPARSE (e.g. [1], [11]). The constraint matrix A is of the type $M \times N$, $M \ll N$; we assume its rows to be linearly independent. The friction matrix G is of type $P \times N$.

We will use the Uzawa algorithm for (\mathcal{P}_d) ([6], [11],[18],[15]):

- λ^0 ... initial guess
- if λ^k known, we solve the minimization problem
- $f(x, \lambda^k) \rightarrow \min$,
- obtaining x^k .

Then we correct
 $\lambda^{k+1} = \Pi_L(\lambda^k + \rho x^k G^T)$, $\rho > 0$,
 where Π_L is the projection R^P on L is defined by:

$$(\Pi_L(y))_i = \begin{cases} y_i & \text{if } |y_i| \leq 1, \\ \text{sgn } y_i & \text{if } |y_i| > 1. \end{cases} .$$

Clearly, the most expensive step is the minimization problem. Therefore, in next paragraphs we concentrate on it.

REMARK 5.2. By the contact equations we mean the equations with indices corresponding to some node on Γ_c .

Let $M = \{z \in R^{M+P} | z_i \geq 0, i = 1, \dots, M; |z_i| \leq 1, i = M + 1, \dots, M + P\}$. In coercive case the problem (\mathcal{P}_d) can be further transformed to the form (\mathcal{P}_{d_2}) :

$$\frac{1}{2} z^T H z - z^T h \rightarrow \min \tag{5.4}$$

where

$$H = BC^{-1}B^T, \quad h = BC^{-1}d, \quad B = \begin{pmatrix} A \\ G \end{pmatrix}$$

This dual formulation enables us to use only the minimization algorithm (Conjugate gradients with projection) for the friction problem. However, to efficiently implement such algorithm, it is necessary to create Choleski decomposition of the stiffness matrix C .

In the next paragraphs, we discuss the conjugate gradient method with projection of the gradient without and with the preconditioning. This can be used for solving the most expensive step in the Uzawa algorithm - the minimization problem and in the dual method as well.

6 The conjugate gradient method with constraints

The principal idea of the algorithm [20] lies in the successive minimization of $f(x)$ on the facets created by constraints, for which the equality is satisfied. We solve minimization problem on each of such facets by using the conjugate gradient method (CGM). As CGM has finite number of steps and the number of facets is also finite (sometimes very great, however), it is obvious that the algorithm converges after a finite number of steps.

Denote by A_I the matrix whose rows have the indices $i \in I \subseteq \{1, \dots, M\}$.

LEMMA 6.1. Let the vectors $a_i, i \in I \subseteq \{1, \dots, M\}$ be linearly independent. Then the matrix $A_I A_I^T$ is regular.
 For the proof see [20].

Define the projection

$$\begin{aligned} P_I &= A_I^T \cdot (A_I A_I^T)^{-1} \cdot A_I & \text{if } I \neq \{\emptyset\} \\ P_I &= 0 & \text{if } I = \{\emptyset\} \end{aligned}$$

$$\begin{aligned} \text{Let } J &= \{i \in \{1, \dots, M\}, (x^k)^T a_i = 0\} \\ \text{and } u^k &= -(A_J A_J^T)^{-1} \cdot A_J f'(x^k) \quad k = 0, 1, \dots \end{aligned}$$

$$\begin{aligned} \text{It holds } P_J &= P_J^T, A_J(I - P_J) = 0, \\ f'(x^k) &= Cx^k - d, \text{ and} \\ (I - P_J)f'(x^k) &= f'(x^k) + A_J^T u^k. \end{aligned}$$

Now let x^0 be such that it satisfies $A_J x^0 = 0$. We introduce a new variable y by

$$x = x^0 + (I - P_J)y \quad (6.1)$$

and consider the function

$$F(y) = f(x^0 + (I - P_J)y). \quad (6.2)$$

Differentiating $F(y)$ using the chain rule and employing the symmetry of P_J we get

$$F'(y) = (I - P_J)f'(x) \quad (6.3)$$

LEMMA 6.2. Let y^k be the minimizer of $F(y)$. Then $x^k = x^0 + (I - P_J)y^k$ is the minimizer of $f(x)$ with constraints $A_J x = 0$.

Proof.

The gradient $F'(y)$ at the point y^k is equal zero.

$$\text{Then } (I - P_J)f'(x^k) = f'(x^k) - A_J(A_J A_J^T)^{-1} A_J f'(x^k) = 0$$

i.e.

$$f'(x^k) + A_J^T u^k = 0 \quad (6.4)$$

Since $A_J x^k = A_J x^0 + A_J(I - P_J)y^k = 0$, the vector x^k satisfies $A_J x^k = 0$ and therefore, it is a feasible point. Condition (6.4) is the necessary and sufficient condition for x^k to be the minimizer of $f(x)$ with constraints $A_J x = 0$. \square

Lemma 6.2 shows that the constrained problem can be transformed to the unconstrained one.

THEOREM 6.1. The problem of minimization of the quadratic functional $f(x)$ with constraints $A_J x = 0$ has a minimizer x^m , which can be found after a finite number of steps by the following algorithm:

Let x^0 be an initial approximation satisfying $A_J x = 0$

$$p^1 = -(I - P_J)f'(x^0),$$

For $k = 0, 1, 2, \dots$

$$x^{k+1} = x^k + \alpha^{k+1} p^{k+1},$$

$$p^{k+1} = -(I - P_J)f'(x^k) + \frac{\|(I - P_J)f'(x^k)\|^2}{\|(I - P_J)f'(x^{k-1})\|^2}p^k.$$

$$\alpha^{k+1} = -\frac{(f'(x^k), p^{k+1})}{(p^{k+1}, Cp^{k+1})}.$$

Proof.

We apply the CG algorithm onto the functional $F(y)$, i.e.:

let $y^0 = 0$ and let $p^1 = -F'(y^0)$. Then

$$y^{k+1} = y^k + \alpha^{k+1}p^{k+1},$$

$$p^{k+1} = -F'(y^k) + \frac{\|F'(y^k)\|^2}{\|F'(y^{k-1})\|^2}p^k,$$

$$\alpha^{k+1} = -\frac{(F'(y^k), p^{k+1})}{(p^{k+1}, (I - P_J)C(I - P_J)p^{k+1})}.$$

Now we transform the variable y to the original variable x . It is evident [20], that

$$(I - P_J)p^k = p^k. \quad (6.5)$$

$$x^{k+1} = x^0 + (I - P_J)y^{k+1}, \quad x^k = x^0 + (I - P_J)y^k,$$

then

$$x^{k+1} - x^k = (I - P_J)(y^{k+1} - y^k) = (I - P_J)\alpha^{k+1}p^k.$$

Hence

$$x^{k+1} = x^k + \alpha^{k+1}p^k.$$

Using $F'(y^k) = (I - P_J)f'(x^k)$, we find

$$p^{k+1} = -(I - P_J)f'(x^k) + \frac{\|(I - P_J)f'(x^k)\|^2}{\|(I - P_J)f'(x^{k-1})\|^2}p^k,$$

and (6.5), we find

$$\alpha^{k+1} = -\frac{((I - P_J)f'(x^k), p^{k+1})}{((I - P_J)p^{k+1}, C(I - P_J)p^{k+1})} = -\frac{(f'(x^k), p^{k+1})}{(p^{k+1}, Cp^{k+1})}. \quad \square$$

To analyze the rate of convergence of the method discussed then due to Lemma 6.2., we can investigate the functional $F(y)$.

Let us denote by

$$e^k = y^k - y^m$$

the error vector, where y^k is k -th approximation and y^m is the minimizer of $F(y)$. Let us denote by

$$\overline{C} = (I - P_J)C(I - P_J).$$

Let us set for any p^k

$$e^{k+1}(\alpha) = y^{k+1}(\alpha) - y = (y^k + \alpha p^k) - y.$$

The value α^k represents the value satisfying

$$\frac{d}{d\alpha}|e^{k+1}(\alpha)|_{\overline{C}}^2 \Big|_{\alpha=\alpha^k} = 0.$$

i.e. α^k is an optimal parameter minimizing the functional $F(y^k + \alpha p^k)$ among all possible $\alpha \in R$.

Let

$$r^k = F'(y^k) \quad k = 0, 1, \dots$$

Let us introduce the Krylov space of the order k by

$$K_k(r^0) = \text{span}\{p^0, p^1, \dots, p^{k-1}\}. \quad (6.6)$$

Due to choice $p^0 = r^0$ the Krylov space $K_k(r^0)$ can be alternatively defined by

$$K_k(r^0) = \text{span}\{r^0, r^1, \dots, r^{k-1}\}. \quad (6.7)$$

The following two lemmas can be proved (see e.g. [17]).

LEMMA 6.3. For $k \geq 0$ it holds

$$K_{k+1}(r^0) = \text{span}\{p^0, p^1, \dots, p^k\} = \text{span}\{r^0, \overline{C}r^0, \dots, \overline{C}^k r^0\}. \quad (6.8)$$

LEMMA 6.4. It holds

$$(r^j, r^m) = 0, (p^j, \overline{C}p^m) = 0 \text{ for } j \neq m. \quad (6.9)$$

With these results we can prove a fundamental convergence theorem.

THEOREM 6.2. For the CG-method the following estimate holds

$$|e^{k+1}|_{\overline{C}} \leq 2 \left(\frac{\kappa^{\frac{1}{2}}(\overline{C}) - 1}{\kappa^{\frac{1}{2}}(\overline{C}) + 1} \right)^k |e^0|_{\overline{C}}, \quad k = 0, 1, \dots \quad (6.10)$$

where

$$\kappa = \frac{\max\{|\lambda_i(\overline{C})| \mid i = 1, \dots, n\}}{\min\{|\lambda_i(\overline{C})| \mid i = 1, \dots, n\}}.$$

and where $|\cdot|_{\overline{C}}$ is the vector norm induced by the scalar product $(u, v)_{\overline{C}} = (\overline{C}u, v)$, $u, v \in R^n$.

Proof.

Since

$$y^{k+1} - y^0 = \sum_{s=0}^k \alpha^s p^s,$$

then taking $0 \leq j \leq k$, setting $y = C^{-1}d$ and using Lemma 6.4., we have

$$(\overline{C}p^j, y^{k+1} - y^0) = \alpha^j (\overline{C}p^j, p^j) = (p^j, r^j) = (\overline{C}p^j, y - y^j) = (\overline{C}p^j, y - y^0).$$

Thus $y^{k+1} - y^0$ is the orthogonal projection of $y - y^0$ onto the space spanned by p^0, \dots, p^k , with respect to the scalar product $(u, v)_{\overline{C}}$. Due to Lemma 6.3. $y^{k+1} - y^0$ is the projection of $y - y^0$ onto $K_{k+1}(r^0)$. Thus,

$$|y - y^{k+1}|_{\overline{C}} = |y - y^0 - (y^{k+1} - y^0)|_{\overline{C}} = \min_{w \in K_{k+1}(r^0)} |y - y^0 - w|_{\overline{C}}.$$

But $r^0 = \overline{C}(y^{k+1} - y)$, then any $w \in K_{k+1}(r^0)$ can be written in the form

$$w = \sum_{j=1}^{k+1} \gamma_j \overline{C}^j (y - y^0),$$

Let the set of all polynomials $p : R \rightarrow R$ of degree less than or equal to $k+1$ and such that $p(0) = 1$ be denoted by P_{k+1}^* . Then

$$|y - y^{k+1}|_{\overline{C}} = \min_{p \in P_{k+1}^*} |p(\overline{C})(y - y^0)|_{\overline{C}}.$$

Since $\overline{C} = \overline{C}^T > 0$, there exists orthonormal basis given by eigenvectors of \overline{C} , and that the eigenvalues λ_j of \overline{C} are strictly positive. If we expand $y - y^0$ with respect to these eigenvectors, then

$$|p(\overline{C})(y - y^0)|_{\overline{C}} \leq \max_{1 \leq j \leq n} |p(\lambda_j)| |y - y^0|_{\overline{C}}.$$

For $p(\lambda)$ we take the polynomial \hat{P}_{k+1} with the property that

$$\max_{\lambda_1 \leq \lambda \leq \lambda_N} |\hat{P}_k(\lambda)| = \min_{P_{k+1} \in P_{k+1}^*} \max_{\lambda_1 \leq \lambda \leq \lambda_N} |P_{k+1}(\lambda)|.$$

The solution of this problem is the Chebyshev polynomial of degree $k+1$, i.e.:

$$p(y) = \frac{T_{k+1}\left(\frac{\lambda_{max} + \lambda_{min} - 2y}{\lambda_{max} - \lambda_{min}}\right)}{T_{k+1}\left(\frac{\lambda_{max} + \lambda_{min}}{\lambda_{max} - \lambda_{min}}\right)},$$

Since ([2], [17])

$$|T_{k+1}(w)| \leq 1, \quad |w| \leq 1,$$

we find that

$$\begin{aligned} \max_{y \in (\lambda_{min}, \lambda_{max})} |p(y)| &\leq \left[T_{k+1}\left(\frac{\lambda_{max} + \lambda_{min}}{\lambda_{max} - \lambda_{min}}\right) \right]^{-1} \\ &\leq \left[1 + \left(\frac{\lambda_{max}^{\frac{1}{2}} - \lambda_{min}^{\frac{1}{2}}}{\lambda_{max}^{\frac{1}{2}} + \lambda_{min}^{\frac{1}{2}}} \right)^{2k+2} \right]^{-1} \\ &\quad \cdot \left(\frac{\lambda_{max}^{\frac{1}{2}} - \lambda_{min}^{\frac{1}{2}}}{\lambda_{max}^{\frac{1}{2}} + \lambda_{min}^{\frac{1}{2}}} \right)^{k+1}, \end{aligned}$$

from which (6.10) follows. \square

7 Algorithm

We may now express the scheme of the algorithm as follows

```

SUBROUTINE CGC( $J', x, f'$ )
 $x^0$  ... the initial guess, which satisfies the constraints
IT = 0
 $f'(x^0) = Cx^0 - d$ 
DO WHILE ( IT < MAXIT )
  Set J
  CALL PROJECT( $J, f'(x^0), u^0, (I - P_J)f'(x^0)$ )

  IF ( $\|(I - P_J)f'(x^0)\| \approx 0$ ) THEN
    IF ( $u_i^0 \geq 0 \forall i \in J$ ) THEN
       $x^* = x^0$  { solution }
      GOTO 2
    ELSE
       $j := \{ i \in J \mid u_i^0 < 0 \}$ 
       $J' = J - \{j\}$ 
    ENDIF
  ELSE
     $J' = J$ 
  ENDIF

  CALL CG( $J', x^0, f'(x^0)$ )
IT = IT + 1
ENDDO
{ maximum number of iterations reached }

2 END

```

SUBROUTINE CG(J', x, f')
 { Conjugate gradients - unlike the standard CGM, the projection $(I - P_{J'})f'(x^k)$ instead of the gradient $f'(x^k)$ is used. The non-active constraints are also checked in every iteration, the new step length $\alpha^{k+1} := \min(\alpha^{k+1}, \bar{\alpha}^{k+1})$, where $\bar{\alpha}^{k+1} = \min_{\mathcal{M}} \frac{-(a_i, x^k)}{(a_i, p^{k+1})}$ and $\mathcal{M} := \{i \mid i \notin J' \wedge (a_i, p^{k+1}) > 0\}$. }
 is corrected.

Input: J', x

Output: x, f'

$k = 0$

$x^0 = x$

$f'(x^0) = f'$ { from previous iteration }

DO WHILE ($k < \text{MAXIT2}$)

CALL PROJECT($J', f'(x^k), u, (I - P_{J'})f'(x^k)$)

$g = -(I - P_{J'})f'(x^k)$

$r^{k+1} = \|g\|^2$

IF ($r^{k+1} < \epsilon$) THEN

$x = x^k$

$f' = f'(x^k)$

RETURN

ENDIF

IF ($k = 0$) THEN $p^1 = g$

ELSE $\beta^{k+1} = r^{k+1}/r^k$

$p^{k+1} = g + \beta^{k+1}p^k$

ENDIF

$\alpha 1 = r^{k+1}$

$\alpha 2 = (p^{k+1}, Cp^{k+1})$ { scal. product in R^N }

IF ($\alpha 1 < \min(1.0, |\alpha 2|) * \text{MAXVAL}$) THEN

$\alpha^{k+1} = \alpha 1/\alpha 2$

ELSE

$\alpha^{k+1} = \text{MAXVAL}$

ENDIF

$\mathcal{M} := \{i | i \notin J' \wedge (a_i, p^{k+1}) > 0\}$

IF $\mathcal{M} \neq \{\emptyset\}$ THEN

$\bar{\alpha}^{k+1} = \min_{\mathcal{M}} \frac{b_i - (a_i, x^k)}{(a_i, p^{k+1})}$ { $b_i = 0$ in our case }

ELSE $\bar{\alpha}^{k+1} = \text{MAXVAL}$

ENDIF

IF ($\bar{\alpha}^{k+1} < \alpha^{k+1}$) THEN

$x = x^k + \bar{\alpha}^{k+1}p^{k+1}$

$f' = f'(x^k) + \bar{\alpha}^{k+1}Cp^{k+1}$

RETURN

ELSEIF ($\alpha^{k+1} = \text{MAXVAL}$) THEN

STOP

ELSE

$x^{k+1} = x^k + \alpha^{k+1}p^{k+1}$

$f'(x^{k+1}) = f'(x^k) + \alpha^{k+1}Cp^{k+1}$

ENDIF

$dd = \|x^{k+1} - x^k\| / (\max(1, \|x^k\|))$

IF ($dd < \epsilon$) THEN

$x = x^{k+1}$
 $f' = f'(x^{k+1})$
RETURN
ENDIF

$k = k + 1$

ENDDO

$x = x^k$ { point obtained after max. num. of iterations }
 $f' = f'(x^k)$

RETURN

SUBROUTINE PROJECT($J, f'(x), u, (I - P_J)f'(x)$)
 { The calculation of $u = -(A_J A_J^T)^{-1} \cdot A_J f'(x)$ and $(I - P_J)f'(x) = f'(x) + A_J^T u$ by the CG Method }

Input: $J, f'(x)$

Output: $u, (I - P_J)f'(x)$

RETURN

REM. 7.1. We set $x^0 = (0, \dots, 0)$ for the initial guess.

REM. 7.2. Denote the value of $\|(I - P_J)f'(x^0)\|$ in IT -th iteration ($0 \leq IT < MAXIT$) by pg^{IT} . Then $pg^{IT} \approx 0$ numerically represents the comparison $[pg^{IT+1} / \max(1.0, pg^{IT})] < \epsilon$. Similarly, we use the test $u_i^0 / u > (-\epsilon)$, where $u = \max(1.0, u_i^0)$ and $u_i^0 = \max_{m \in J}(0.0, u_m^0)$, for the multipliers u_i^0 . In semicoercive cases it is also necessary to test the magnitudes of x^k and p^k .

REM. 7.3. It is convenient to use the following strategy which is similar to [8]. We choose less strict tolerance for subproblems (subr. *CG*) in the first several iterations within the *CGC* subroutine. The tolerance is set to more strict value after a limited number of these iterations. We can get remarkable acceleration of the process.

REM. 7.4. If C is positive definite (cf. Rem. 5.1.), it can occur

$$(f'(x^k), p^{k+1}) \neq 0 \text{ and } (p^{k+1}, Cp^{k+1}) = 0.$$

In this case $f(x^k + \alpha p^{k+1})$ is decreasing when α is increasing. If $\bar{\alpha}^{k+1} = MAXVAL$, then f on K_d is not bounded from below.

On the basis of the fact that $\bar{\alpha}^1 > 0$ (see Subroutine *CG*), we can prove that the *CG* algorithm makes a non-zero step (i.e. does not cycle) in the same way as in [20].

If the implication

$$j \in J \Rightarrow (j \in J' \vee (a_j, p^1) \leq 0).$$

is valid then it follows from the formula for $\bar{\alpha}^1$ in the subroutine *CG* that $\bar{\alpha}^1 > 0$. Therefore, it is sufficient to focus the case $\|(I - P_J)f'(x^0)\| \approx 0$ and the removed index $j \in J - J'$.

LEMMA 7.1. Let $\|(I - P_J)f'(x^0)\| = 0$. Let $A_{J'}$ be created from A_J by removing the row with index $j|u_j^0 < 0$.

Then $(a_j, p^1) < 0$, $j \in J - J'$.

For the proof see [20].

If the condition for removing more indices is fulfilled then, similarly as in [4], we choose the one with the greatest absolute value.

However, the condition $(a_j, p^1) < 0$ $j \in J - J'$ may be fulfilled even in the case when more indices $\{j|u_j^0 < 0\}$ are removed (e.g. for all with $j|u_j^0 < (-\epsilon)$ cf. Rem. 7.2.). The following lemma shows this. In some cases we can accelerate the algorithm very much through these means.

LEMMA 7.2. Let $\|(I - P_J)f'(x^0)\| = 0$. Let $A_{J'}$ be created from A_J by removing the rows with indices $j|u_j^0 < 0$. Furthermore, let the rows of A_J satisfy $(a_i, a_j) = 0$, $i \neq j$, $i, j \in J$.

Then $(a_j, p_1) < 0$, $j \in J - J'$.

Proof.

$$\begin{aligned} 0 &= (I - P_J)f'(x^0) = f'(x^0) + A_J^T u^0 = f'(x^0) + A_{J'}^T u^0 + A_{J-J'}^T u''^0 \\ -p^1 &= (I - P_{J'})f'(x^0) = f'(x^0) + A_{J'}^T v^0 \quad , \end{aligned}$$

where $v^0 = -(A_{J'} A_{J'}^T)^{-1} A_{J'} f'(x^0)$. Subtracting and multiplying by the vector a_j , $j \in J - J'$, we obtain $(a_j, p^1) = c \cdot u_{j''}^0$ where $c = (a_j, a_j) > 0$ and from the assumption $u''^0 < 0$.

Thus, $(a_j, p^1) < 0$. \square

COROLLARY. Let the assumptions of the previous lemma be fulfilled.

Then $\bar{\alpha}^1 > 0$, and as a result the algorithm *CGC* is not cycling. \square

The condition for the rows of A_J is fulfilled in “two bodies contact”. It may be slightly violated in a general case and also when the preconditioning is used. Nevertheless for such cases we often have an acceleration as well.

8 The preconditioning

Consider again the problem (\mathcal{P}_d) , i.e.

$$f(x) = \frac{1}{2}x^T C x - x^T d \rightarrow \min \\ Ax \leq 0.$$

Now we assume C to be positive definite. Let W be a positive definite $N \times N$ matrix in the form $W = EE^T$. Let us introduce the transformation $y = E^T x$ and express (\mathcal{P}_d) in terms of a new variable y . Then

$$\bar{f}(y) = \frac{1}{2}y^T \bar{C} y - y^T \bar{d} \rightarrow \min \\ \bar{A} y \leq 0,$$

where

$$\bar{C} = E^{-1} C E^{-T}, \bar{d} = E^{-1} d, \bar{A} = A E^{-T}.$$

As $E^{-T} \bar{C} E^T = W^{-1} C$, the matrices \bar{C} and $W^{-1} C$ have the same eigenvalues. The convergence of CGM depends on the condition number $(\lambda_{max}/\lambda_{min})$ of the matrix C . The speed of the convergence is increasing when the condition number [1] is decreasing. The lowest condition number has a unity matrix. Therefore, we try to find W which is an easy invertible approximation of C or for which we can show that $W^{-1} C$ has lower condition number.

The preconditioning will be used when solving the problem on particular facets, i.e. in the subroutine *CG*. Let us write its steps for the transformed problem (\mathcal{P}_d) (without supplementary commands and tests).

SUBROUTINE PCG - 0 ($J', x\{= E^{-T} y\}, E^T, \bar{r}\{= f'\}$)

$$y^0 = y = E^T x \\ \bar{r}^0 = \bar{C} y^0 - \bar{d} \\ \bar{g}^0 = (I - \bar{P}_{J'}) \bar{r}^0 \\ \bar{p}^0 = -\bar{g}^0$$

for $k = 0, 1, \dots$

$$\alpha^k = (\bar{g}^k, \bar{g}^k) / (\bar{p}^k, \bar{C} \bar{p}^k)$$

$$\bar{\alpha}^k = \min_{\bar{M}} - \frac{(\bar{a}_i, y^k)}{(\bar{a}_i, \bar{p}^k)}$$

IF $(\bar{\alpha}^k < \alpha^k)$ *THEN*

$$y = y^k + \bar{\alpha}^k \bar{p}^k \\ \bar{f}' = \bar{r}^k + \bar{\alpha}^k \bar{C} \bar{p}^k \quad \{ \text{and return to CGC} \}$$

ELSE

$$y^{k+1} = y^k + \alpha^k \bar{p}^k \\ \bar{r}^{k+1} = \bar{r}^k + \alpha^k \bar{C} \bar{p}^k$$

ENDIF

$$\bar{g}^{k+1} = (I - \bar{P}_{J'}) \bar{r}^{k+1} \\ \beta^{k+1} = (\bar{g}^{k+1}, \bar{g}^{k+1}) / (\bar{g}^k, \bar{g}^k)$$

$$\bar{p}^{k+1} = -\bar{g}^{k+1} + \beta^{k+1}\bar{p}^k$$

At the same time $\bar{P}_{J'} = \bar{A}_{J'}^T (\bar{A}_{J'} \bar{A}_{J'}^T)^{-1} \bar{A}_{J'}$
and $\bar{\mathcal{M}}$ is connected with \mathcal{M} by the transformation $y = E^T x$.

Introducing a vector v^k by $v^k = E^{-T} \bar{p}^k$ and using

$$\begin{aligned} h^k &:= \bar{f}'(y^k) = E^{-1} f'(x^k), \\ (\bar{p}^k, \bar{C}\bar{p}^k) &= (v^k, C v^k) \quad \text{and} \\ (\bar{a}_i, \bar{p}^k) &= (a_i, v^k), \end{aligned}$$

we can write $PCG - 0$ in x variable.

```

SUBROUTINE PCG - 1 ( J', x, E^T, r {= f'} )
r^0 = f'   { from previous iteration }
h^0 = E^{-1} r^0
g^0 = (I - \bar{P}_{J'}) h^0
v^0 = -E^{-T} g^0

```

for $k = 0, 1, \dots$

$$\begin{aligned} \alpha^k &= (g^k, g^k) / (v^k, C v^k) \\ \bar{\alpha}^k &= \min_{\mathcal{M}} -\frac{(a_i, x^k)}{(a_i, v^k)} \end{aligned}$$

```

IF (\bar{\alpha}^k < \alpha^k) THEN
    x = x^k + \bar{\alpha}^k v^k
    f' = r^k + \bar{\alpha}^k C v^k   { and return to CGC }
ELSE
    x^{k+1} = x^k + \alpha^k v^k
    r^{k+1} = r^k + \alpha^k C v^k
    h^{k+1} = E^{-1} r^{k+1}
    g^{k+1} = (I - \bar{P}_{J'}) h^{k+1}
    \beta^{k+1} = (g^{k+1}, g^{k+1}) / (g^k, g^k)
    v^{k+1} = -E^{-T} g^{k+1} + \beta^{k+1} v^k
ENDIF

```

In the subroutine *PROJECT*, if it is called from *PCG - 1* (the calculation of \bar{g}), the multiplications $A_{J'} x$, $A_{J'}^T x$ are replaced by $\bar{A}_{J'} y$, $\bar{A}_{J'}^T y$, i.e. $A_{J'} E^{-T} y$, $E^{-1} A_{J'}^T y$. As E^{-T} is regular, $\bar{A}_{J'}$ also has linearly independent rows.

The matrix \bar{C} does not occur in the transformed problem.

9 A second approach to the preconditioning

In previous section, the projection matrix is very expensive to calculate. Therefore, it is desirable to modify the algorithm so that the projection matrix is created directly from the original constraint matrix. We write the preconditioned CG algorithm from previous section omitting the steps with the projection, i.e. we have the unconstrained version of this algorithm now.

SUBROUTINE PCG

$$r^0 = Cx^0 - d$$

$$g^0 = E^{-1}r^0$$

$$v^0 = -E^{-T}g^0$$

for $k = 0, 1, \dots$

$$\alpha^k = (g^k, g^k)/(v^k, Cv^k)$$

$$x^{k+1} = x^k + \alpha^k v^k$$

$$r^{k+1} = r^k + \alpha^k Cv^k$$

$$g^{k+1} = E^{-1}r^{k+1}$$

$$\beta^{k+1} = (g^{k+1}, g^{k+1})/(g^k, g^k)$$

$$v^{k+1} = -E^{-T}g^{k+1} + \beta^{k+1}v^k$$

If we consider a constrained problem, we may use Lemma 6.2 and modify directly *PCG*. We deal with the minimization of $\tilde{f}(x) = f(y) = f((I - P_{J'})x)$, therefore the quantities r^k , g^k and v^k , which concern the gradient are replaced by $(I - P_{J'})r^k$, $(I - P_{J'})g^k$ and $(I - P_{J'})v^k$, respectively.

We arrive at the following algorithm:

SUBROUTINE PCG - 2(J', x, E^T, f')

$$r^0 = f' \quad \{ \text{from previous iteration} \}$$

$$g^0 = (I - P_{J'})E^{-1}(I - P_{J'})r^0$$

$$v^0 = -(I - P_{J'})E^{-T}g^0$$

for $k = 0, 1, \dots$

$$\alpha^k = (g^k, g^k)/(v^k, Cv^k)$$

$$\bar{\alpha}^k = \min_{\mathcal{M}} -\frac{(a_i, x^k)}{(a_i, v^k)}$$

IF $(\bar{\alpha}^k < \alpha^k)$ *THEN*

$$x = x^k + \bar{\alpha}^k v^k$$

$$f' = r^k + \bar{\alpha}^k Cv^k \quad \{ \text{and return to CGC} \}$$

ELSE

$$x^{k+1} = x^k + \alpha^k v^k$$

$$r^{k+1} = r^k + \alpha^k Cv^k$$

$$g^{k+1} = (I - P_{J'})E^{-1}(I - P_{J'})r^{k+1}$$

$$\beta^{k+1} = (g^{k+1}, g^{k+1})/(g^k, g^k)$$

$$v^{k+1} = -(I - P_{J'})E^{-T}g^{k+1} + \beta^{k+1}v^k$$

ENDIF

Comparing with *PCG-1*, we have to calculate the projection three times during one iteration. This projection is, however, much simpler to calculate than the projection appearing in *PCG-1*. It is obvious, that the version *PCG-2* is much more efficient concerning time aspect. The numerical experiments confirm this, up to one exception, which is shown in Tab. 11.9 and Fig. 11.16.

10 The choice of the preconditioning matrix

The simplest choice is $W = D$, where D is the diagonal of the matrix C . In this case $E^T = D^{\frac{1}{2}}$ and it is sufficient to store only the vector.

Another possibility is the *SOR* decomposition [1],[2]. Let $C = D + L + L^T$. The preconditioning matrix is of the form

$$W = \frac{1}{2-\omega} \left(\frac{1}{\omega}D + L \right) \left(\frac{1}{\omega}D \right)^{-1} \left(\frac{1}{\omega}D + L \right)^T, \quad 0 < \omega < 2, \quad (10.1)$$

where the factor $\frac{1}{2-\omega}$ may be omitted. Thus

$$E^T = \left(\frac{1}{\omega}D \right)^{-\frac{1}{2}} \left(\frac{1}{\omega}D + L^T \right).$$

The condition number of $\bar{C} = W^{-1}C$, we denote it by $\kappa(\bar{C})$, may be under the certain assumptions smaller than $\kappa(C)$, as the following assertion shows [1].

THEOREM 10.1. Let C be positive definite and W be determined by (10.1). Let

$$\|D^{-\frac{1}{2}}LD^{-\frac{1}{2}}\|_{\infty} \leq \frac{1}{2}, \quad \|D^{-\frac{1}{2}}L^TD^{-\frac{1}{2}}\|_{\infty} \leq \frac{1}{2}.$$

Then

$$\min_{0 < \omega < 2} \kappa(\bar{C}) \leq \sqrt{\frac{1}{2}\kappa(C) + \frac{1}{2}}.$$

The optimal value of ω can be determined [1], if the numbers

$$\begin{aligned} \mu &= \max_{x \neq 0} (x^T Dx / x^T Hx), \\ \delta &= \max_{x \neq 0} \frac{x^T (LD^{-1}L^T - \frac{1}{4}D)x}{x^T Hx}, \end{aligned}$$

are estimated.

However, in our case (the presence of the constraints) the numerical experiments have shown that by choosing $\omega \neq 1$, the speed of the process does not change very much.

The incomplete factorization is more effective. Consider factorization $C = LL^T$, where L is a lower triangular matrix. The incomplete factorization, in the simplest form, lies on determining only such entries of L where the original matrix C has non-zeros. We will obtain certain “approximation” of C .

Define $S_C = \{(i, j), c_{ij} \neq 0\}$. Proceeding from the Gaussian elimination, the steps of incomplete factorization can be written as follows:

$$\begin{aligned} & \text{for } r = 1, \dots, N - 1 \\ l_{ir} &= c_{ir}^{(r)} / c_{rr}^{(r)}, \\ c_{ij}^{(r+1)} &= \begin{cases} c_{ij}^{(r)} - l_{ir}c_{rj}^{(r)} & (r + 1 \leq j \leq N) \wedge [(i, j) \in S_C] \wedge (i \neq j), \\ 0 & (r + 1 \leq j \leq N) \wedge [(i, j) \notin S_C], \\ c_{ii}^{(r)} - l_{ir}c_{ri}^{(r)} & i = j. \end{cases} \end{aligned}$$

In another variant we add removed entries to the diagonal, i.e.

$$c_{ii}^{(r+1)} = c_{ii}^{(r)} - l_{ir}c_{ri}^{(r)} - \sum_{\substack{(i,k) \notin S_C \\ k=r+1}}^N l_{ir}c_{rk}^{(r)}.$$

Thus, in the matrix form

$$\begin{aligned} C &= EE^T + R = W + R, \\ R &= \sum_{r=1}^{N-1} R^{(r+1)}, \quad r^{(r+1)} = \begin{cases} 0 & (i, j) \in S_C, i \neq j, \\ c_{ij}^{(r)} - l_{ir}c_{rj}^{(r)} & (i, j) \notin S_C, \\ \sum_{k=r+1}^N l_{ir}c_{rk}^{(r)} & i = j. \end{cases} \end{aligned}$$

(The form of R follows from the description of the incomplete Gaussian elimination through lower triangular matrices L_r and from properties of these matrices.)

It is obvious that, in particular, the version with adding to the diagonal in the number of operations does not differ so much from a complete factorization. Its main advantage is in avoiding the fill-in which occurs in the complete factorization. This fact is not important in SKY-LINE format. Therefore, here we also test the complete factorization.

DEFINITION 10.1. C is \overline{M} -matrix, if

- (1) $c_{ii} > 0$ $i = 1, \dots, N - 1,$
- (2) $c_{ij} < 0$ $i \neq j,$
- (3) $\max \{j \mid (i \leq j \leq N) \wedge (c_{ij} \neq 0)\} > i$ for $1 \leq i < N$.

For this class of matrices the following theorem holds [1],[2].

THEOREM 10.2. The incomplete factorization is a stable process for the diagonal dominant \overline{M} -matrix in the following sense:

the number

$$q = \max_{i,j,r} |c_{ij}^{(r)}| / \max_{i,j} |c_{ij}|$$

is bounded from above (even $q = 1$).

Generally, it can be said that the number of iterations on particular facets is lower in the preconditioning (see Tabs. 11.3-11.9). In the first version of the preconditioning ($PCG - 1$), however, the calculations of the projection matrix are very expensive.

In the SKY-LINE format it is the best to carry out the complete factorization. While in the problems without constraints it would be redundant to perform the iterations after it, for this situation we do not have the solution yet, but we can achieve substantial acceleration of the CGM iterations. Only in this situation the convergence is faster (see Tab. 11.2) in the case of $PCG - 1$ than in the case without the preconditioning and also faster than for the version $PCG - 2$. Naturally, the disadvantage is the fill-in which arises due to the elimination.

11 Test example

We analyze the structure of a beam bridge on a nonstable slope as a model example (Fig.11.1). The model example was simplified in the sense, that the valley was arched by one prestressed concrete arch. Foundation of the bridge situated on the unstable slope is simulated by contact conditions with Coulombian friction. The movement of the unstable slope acting onto a bridge is simulated by the boundary conditions. Moreover, we suppose that the bridge is statically loaded by vehicles. As the movement of the slope is very slow, the model can be investigated as a quasistatic ([14]-[15]).

There are 5 subregions with different values of $E[Nm^{-2}]$ and μ varying from $E = 0.45d+11$ and $\mu = 0.17$ to $E = 0.73d+11$ and $\mu = 0.31$. The contact boundaries are located along the lines 10 – 15, 16 – 11 and 14 – 17. The movement of unstable slope is realized by the prescribed displacement $\mathbf{u}_0 = 0.1d-1 [m]$ between the vertices 11 and 20. The load $P = -0.1d+5 [Nm^{-2}]$ acts along the line 4 – 19, $g^{kl} = 0.1d+8 [Nm^{-2}]$.

Figs. 11.2-11.6 represent by turns deformations, stresses (τ_{11} , τ_{12} , τ_{22}) and principal stresses. The same quantities are depicted in Figs. 11.7-11.11 for the zoomed detail (see Fig. 11.1). We use scale factor 100 for the deformations. In Figs. 11.6 and 11.11 “ \longleftrightarrow ” represents tractions, “ $\rightarrow\leftarrow$ ” pressures.

Various types of preconditioners were tested on our model of the bridge (see Tabs. 11.2-11.9) - diagonal(P-DIAG), incomplete Choleski(P-ILL), incomplete Choleski with adding to the diagonal(P-ILLD), SOR decomposition(P-SOR). Also, the complete Choleski decomposition for the algorithm PCG-1 (P-LL(1)) and PCG-2 (P-LL(2)) was tested. The results are graphically shown on graphs (Figs. 11.12-11.16).

The statistics for this example is in Tab. 11.1.

Here NV - number of vertices, NEL - number of elements, NEQ - number of degrees of freedom, NCP - number of contact constraints, LIC and NWK - number

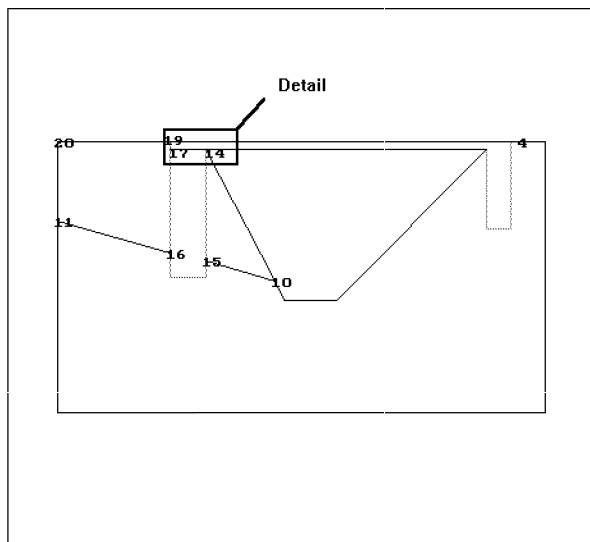


Figure 11.1:

Table 11.1:

<i>NV</i>	<i>NEL</i>	<i>NEQ</i>	<i>NCP</i>	<i>LIC</i>	<i>NWK</i>	<i>LJA</i>
380	551	716	10	4546	16378	40

Table 11.2:

<i>METHOD</i>	<i>TIME</i>
SPARSE	30"
P-DIAG	30"
P-SOR	19"
P-ILL	13"
P-ILLD	15"
SKY-LINE	29"
P-LL(1)	2"
P-LL(2)	3"

Table 11.3: Outer iterations - SPARSE

Iter.	Activ. Constr.	No. of Inner It.
1	10	547
2	3	558

Table 11.4: Outer iterations - P-DIAG

Iter.	Activ. Constr.	No. of Inner It.
1	10	431
2	3	128

of stored entries in the stiffness matrix for *SPARSE* and *SKY – LINE* formats.

Table 11.5: Outer iterations - P-SOR

Iter.	Activ. Constr.	No. of Inner It.
1	10	212
2	3	203

Table 11.6: Outer iterations - P-ILL

Iter.	Activ. Constr.	No. of Inner It.
1	10	141
2	3	128

Table 11.7: Outer iterations - P-ILLD

Iter.	Activ. Constr.	No. of Inner It.
1	10	141
2	3	128

Table 11.8: Outer iterations - SKY-LINE

Iter.	Activ. Constr.	No. of Inner It.
1	10	547
2	3	557

Table 11.9: Outer iterations - P-LL(1)

Iter.	Activ. Constr.	No. of Inner It.
1	10	2
2	3	2

Table 11.10: Outer iterations; 2. ver. of preconditioning - P-LL(2)

Iter.	Activ. Constr.	No. of Inner It.
1	10	18
2	3	8

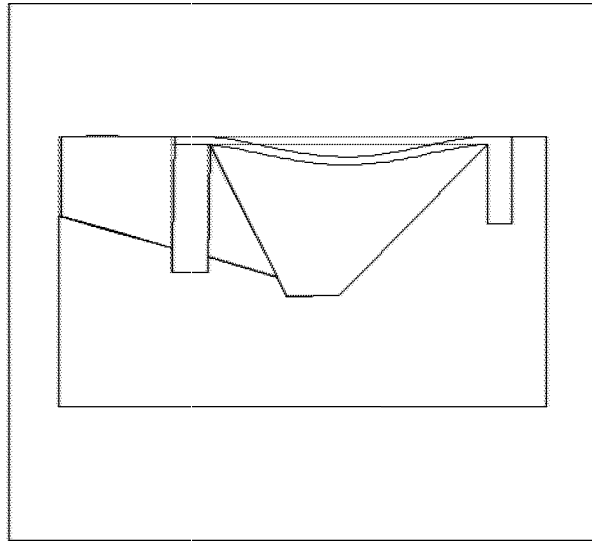


Figure 11.2:

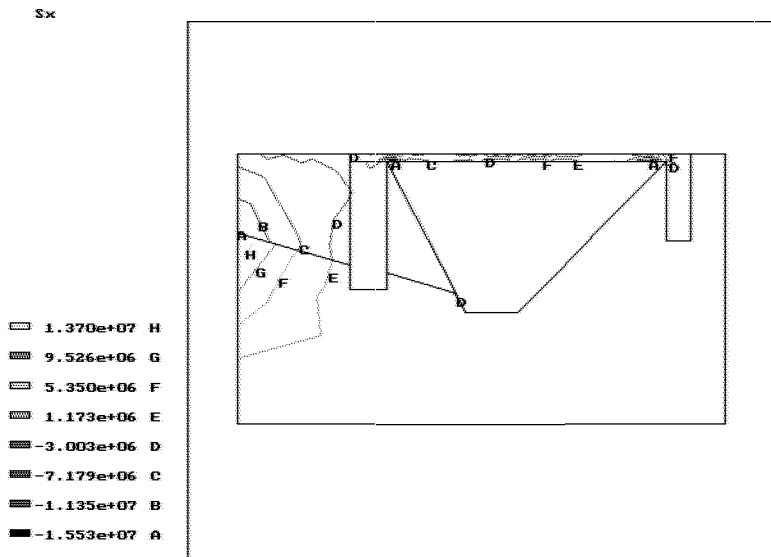


Figure 11.3:

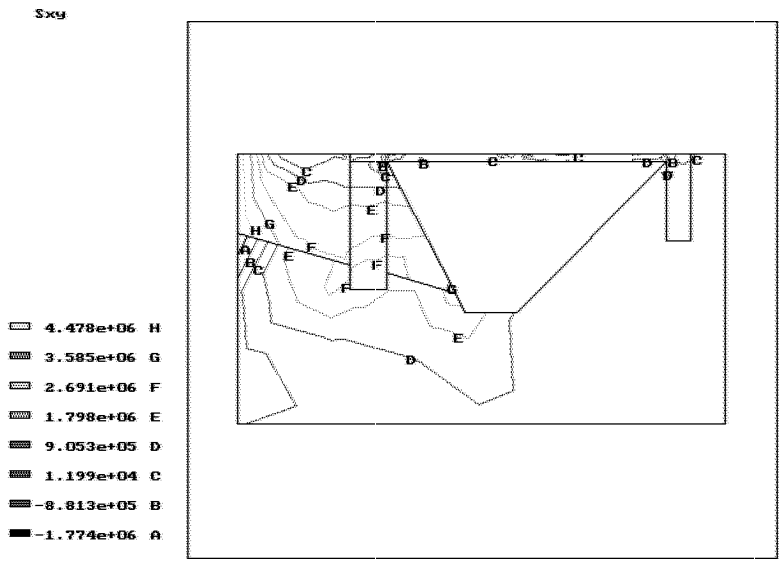


Figure 11.4:

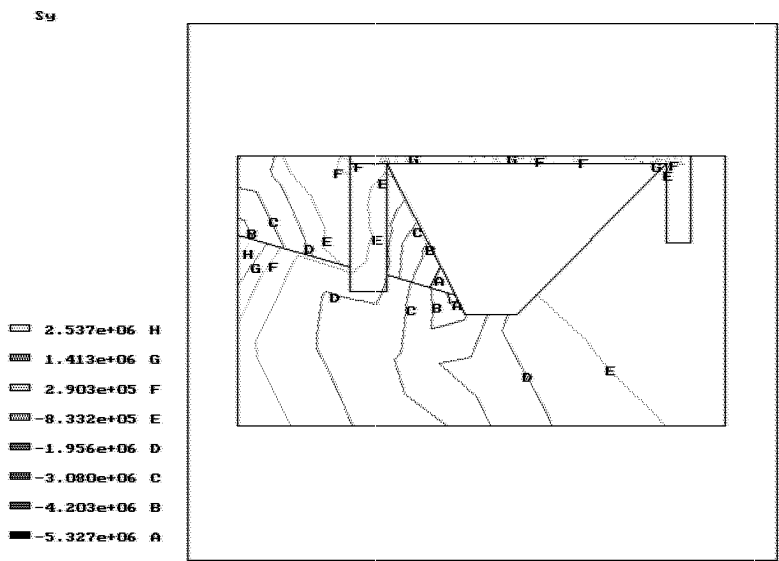


Figure 11.5:

Table 11.11:

<i>METHOD</i>	<i>ITER</i>	<i>TOT.TIME</i>
SPARSE	562	416"
P-DIAG	550	595"
P-SOR	541	1060"
P-ILL	527	600"
P-ILLD	535	592"
SKY-LINE	565	413"
P-LL(1)	531	219"
P-LL(2)	531	149"
DUAL		4"

The Table 11.2 compares the times for the versions without preconditioning and with the second version of preconditioning required by the *CGC* Method. The first version of the preconditioning (except *LL(1)*) is not shown as the times were greater than for the version without the preconditioning.

The Tables 11.3 - 11.9 show the statistics concerning outer iterations in Subr. *CGC* in Sec.7 .

The Table 11.11 shows the total times, including iterations of the Uzawa algorithm (cf. Sec.5), for all tested variants. The Uzawa method is the method with locally bounded step, which was confirmed in our experiments as compared with the dual method. On the other hand, the dual method can be used only under the additional assumption on the stiffness matrix.

For the greater value of the Uzawa algorithm iteration number (*ITER*), the number of inner iterations in *CGC* is almost comparable for the versions without and with the preconditioning. Therefore, we have no acceleration for the preconditioned versions (cf. Tab. 11.11).

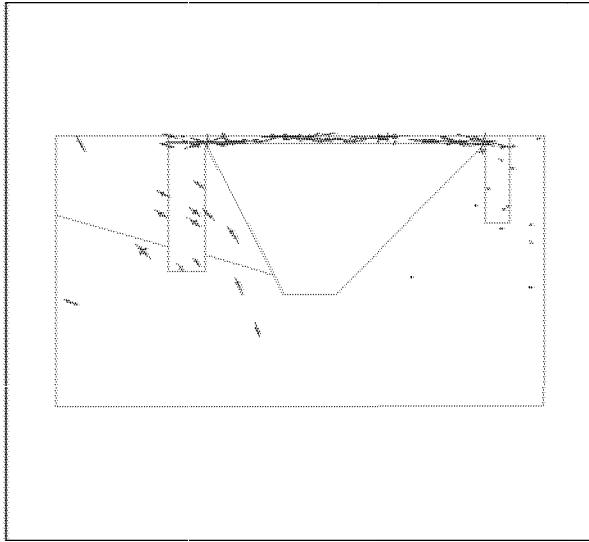


Figure 11.6:

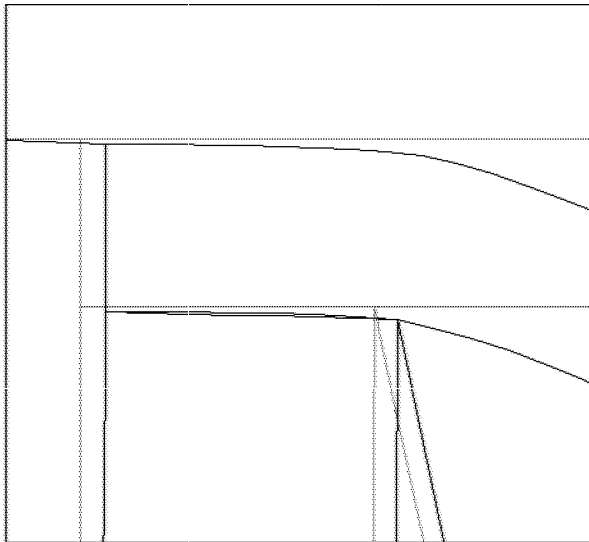


Figure 11.7:

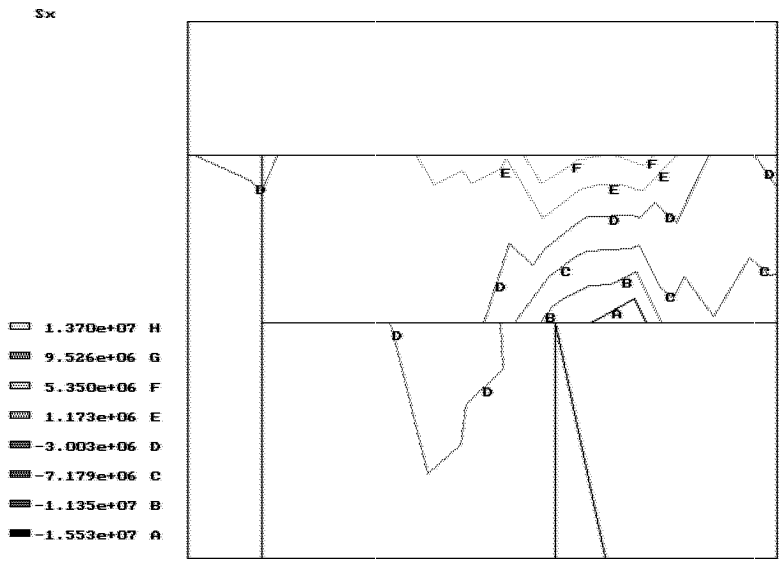


Figure 11.8:

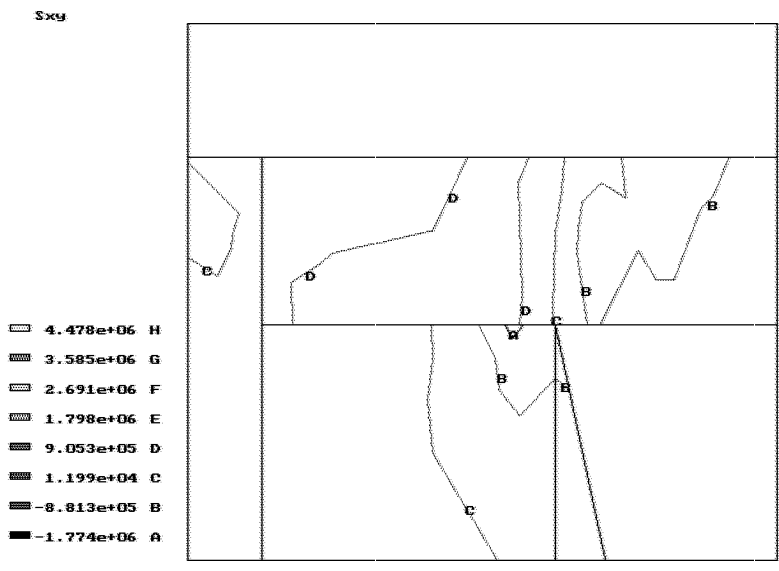


Figure 11.9:

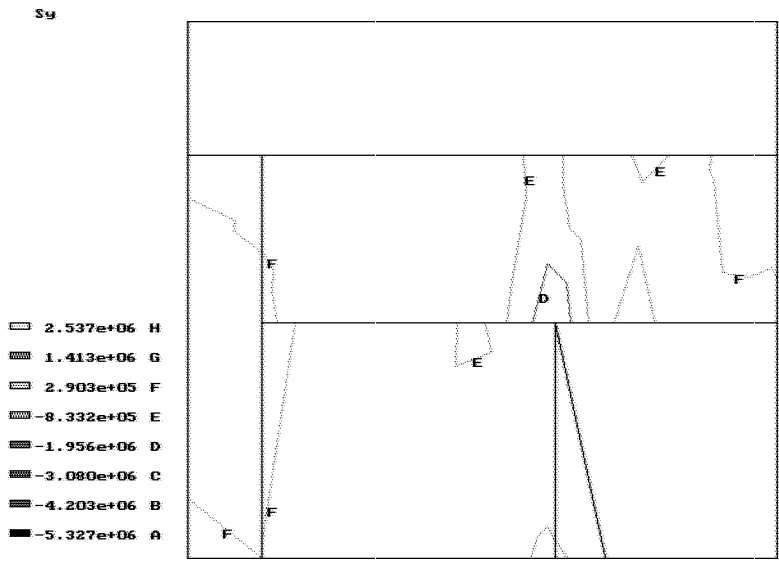


Figure 11.10:

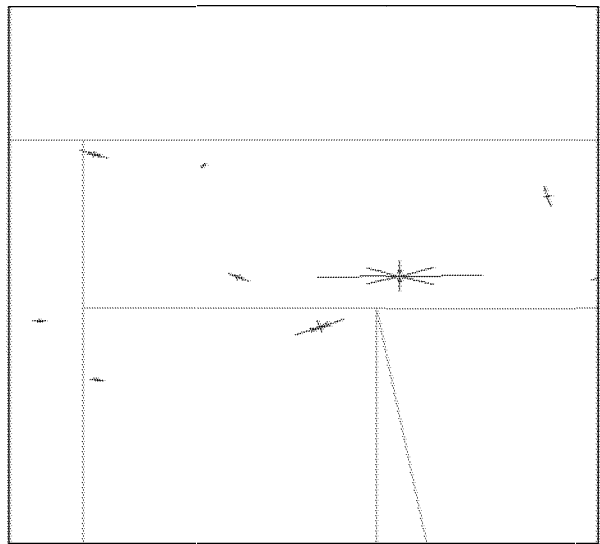


Figure 11.11:

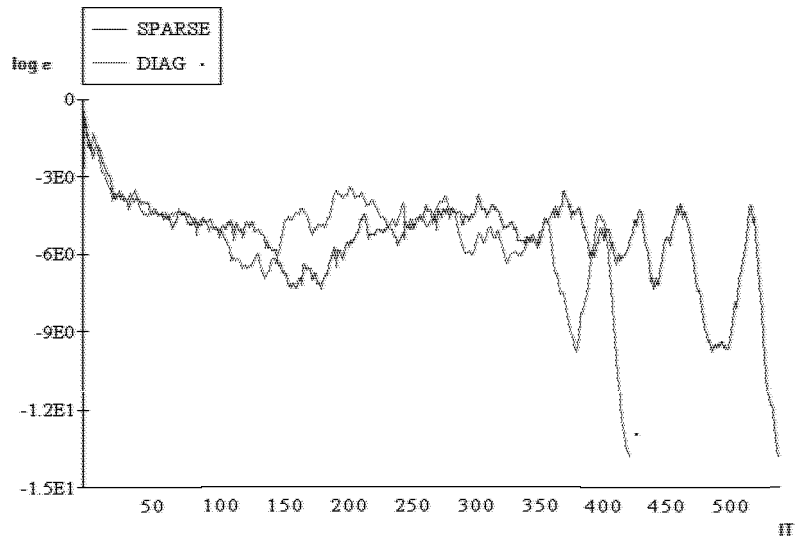


Figure 11.12:

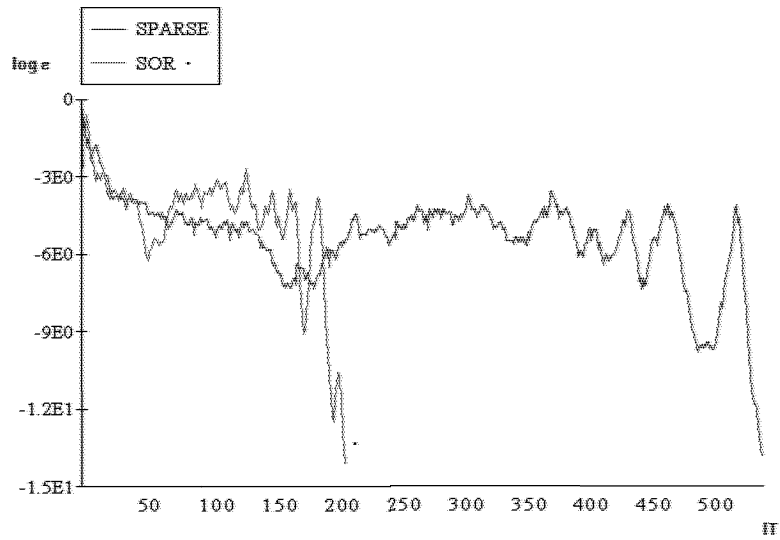


Figure 11.13:

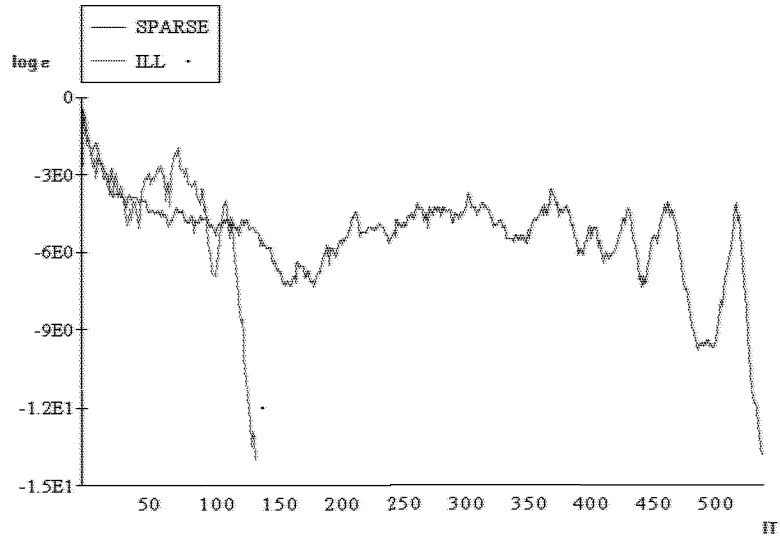


Figure 11.14:

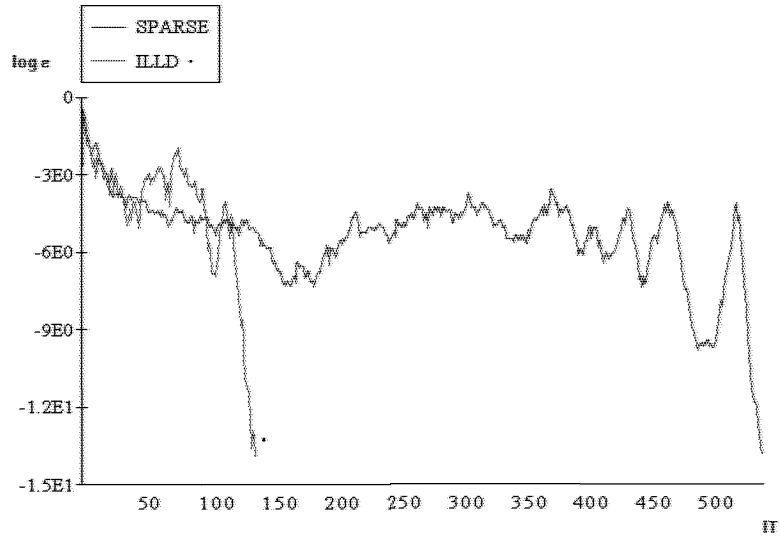


Figure 11.15:

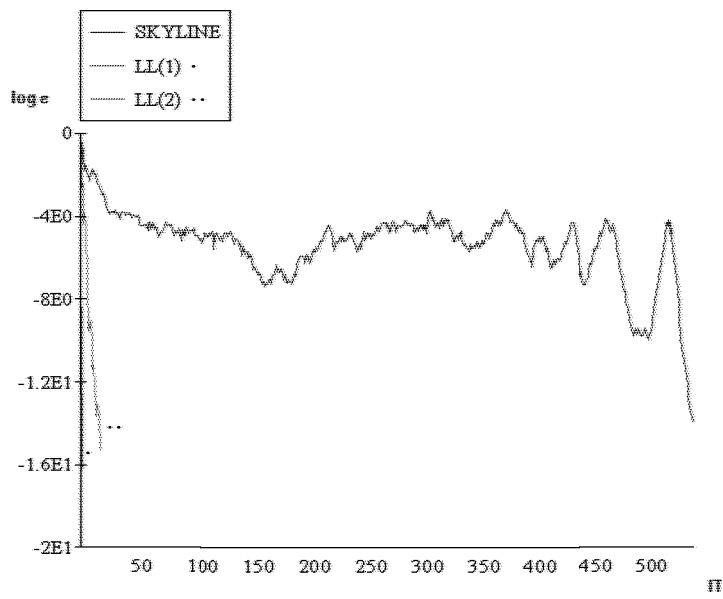


Figure 11.16:

Bibliography

- [1] Axelsson O., Barker V.A. : *Finite Element Solution of Boundary Value Problems. Theory and Computation.* Academic Press, New York, London 1984
- [2] Axelsson O. : *Iterative Solution Methods.* Cambridge Univ. Press, 1994
- [3] Bartoš M., Kestřánek Z. : *Numerical Solution of the Contact Problem. Application to a Simple Model of the Human Hip Joint.* Submitted to J.Comput.Appl.Math. 1994
- [4] Fletcher R. : *Practical Methods of Optimization, Vol.2: Constrained Optimization.* J. Wiley and Sons, New York 1981
- [5] Glowinski R., Lions J.L., Tremolières R. : *Numerical Analysis of Variational Inequalities.* North-Holland, Amsterdam 1981
- [6] Haslinger J., Hlaváček I., Lovíšek J., Nečas J. : *The Solution of Variational Inequalities in Mechanics.* Alfa, Bratislava 1983
- [7] Hlaváček I., Lovíšek J.: *A Finite Element Analysis for the Signorini Problem in Plane Elastostatics.* Aplikace Matematiky 22, 1977, pp 215-228
- [8] Horák J. : *Mathematical Modelling of the System "Moving Cutting Tool-Steady Rock". (In Czech)* TR HoÚ ČSAV, Ostrava 1990
- [9] Frank P.D., Healy M.J., Mastro R.A. : *Implementation for Large Quadratic Programs with Small Active Sets.* Journal of Optimization Theory and Applications, Vol.69, No.1, 1991, pp 109-127
- [10] Kestřánek Z. : *Comparison of Methods for Solving Contact Problem in Thermoelasticity.* In: Numerical Methods in Continuum Mechanics, Proc. of the Internat. Scient. Conf., Editional Centre VSZS Žilina, Stará Lesná-Slovakia 1994, pp 128-135
- [11] Kestřánek Z. : *Numerical Analysis of the Contact Problem - Comparison of Methods for Finding the Approximate Solution,* TR-648 ICS Prague 1995
- [12] Míka S., Šulcová I. : *The Saddle Point Algorithms. (In Czech)* In: Programs and Algorithms of Numerical Mathematics 5. Proc. Math. Inst. of Czech. Acad. Sci., 1990, pp 114-144

- [13] Nedoma J. : *On One Type of Signorini Problem without Friction in Linear Thermoelasticity*. Aplikace Matematiky 28, 1983, pp 393-407
- [14] Nedoma J. : *On the Signorini Problem with Friction in Linear Thermoelasticity. Quasicoupled 2D Case*. Aplikace Matematiky 32, 1987, pp 186-199
- [15] Nedoma J. : *Finite Element Analysis in Nuclear Safety*. TR-ICS Prague 1993
- [16] Nedoma J. : *Finite Element Analysis of Contact Problems in Thermoelasticity. The Semi-Coercive Case*. J.Comp.Appl.Mat. 50, 1994, pp 411-423
- [17] Nedoma J. : *Iterative CG-methods for Large Convex Quadratic Programming with Linear Constraints and Their Algorithms*. Report CP 940820 HIPERGEOS, Prague 1995
- [18] Nečas J., Hlaváček I. : *Mathematical Theory of Elastic and Elasto-plastic Bodies. An Introduction*. North Holland, Amsterdam 1981
- [19] Oden J.T., Kikuchi N. : *Contact Problems in Elasticity*. TICOM Report 79-8 July 1979. The University of Texas at Austin.
- [20] Pshenichny B.N., Danilin J.M. : *Numerical Methods in Extremal Problems*. Mir Publishers, Moscow 1978