38

SYMMETRIZED SEMI-SMOOTH NEWTON METHOD FOR SOLVING 3D CONTACT PROBLEMS

38.1 INTRODUCTION

The dual algebraic formulation of discretized contact problems with Tresca friction in three space dimensions (3D) belongs to the class of problems called QCQP (Quadratically Constrained Quadratic Program, [1]) with a specific structure: the minimized function is strictly convex and quadratic subject to simple inequality bounds and separable quadratic constraints (spherical for isotropic and elliptical for orthotropic Tresca friction [3]).

For solving such problems we use an active set implementation of the semi-smooth Newton (SSN) method. However, the respective slanting function is given by non-symmetric matrices and this property can not be eliminated by simple linear algebra tools (unlike 2D case [5]). Fortunately, the slanting function at the minimizer does not contain some terms so that a symmetrization is possible. Neglecting these terms a-priori we get a symmetric approximation of the slanting function [6]. Then 3D contact problems can be treated analogously as 2D ones [5].

We propose a monotonous globalization strategy guaranteeing the R-linear convergence rate of the algorithm. To our knowledge, there is no such analysis for 3D frictional contact problems.

38.2 ALGEBRAIC CONTACT PROBLEMS WITH TRESCA FRICTION

The *primal-dual* algebraic formulation of discrete contact problems with Tresca friction reads as follows: find $(u^*, \lambda_\nu^*, \lambda_\tau^*) \in \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^{2m}$ satisfying

$$Ku + N^\top \lambda_\nu + T^\top \lambda_\tau - f = 0, \tag{38.1}$$

$$Nu - d \leq 0,\ \lambda_\nu \geq 0,\ \lambda_\nu^\top (Nu - d) = 0, \tag{38.2}$$

$$\left.\begin{array}{l} \|\bar{\lambda}_{\tau,i}\| \leq g_i \\ \|\bar{\lambda}_{\tau,i}\| < g_i \Rightarrow \bar{u}_{\tau,i} = 0 \\ \|\bar{\lambda}_{\tau,i}\| = g_i \Rightarrow \exists c_i \geq 0 :\ \bar{u}_{\tau,i} = c_i \bar{\lambda}_{\tau,i} \end{array}\right\} \quad i \in \mathcal{M}, \tag{38.3}$$

where $K \in \mathbb{R}^{n\times n}$ is symmetric, positive definite, $N \in \mathbb{R}^{m\times n}$, $T \in \mathbb{R}^{2m\times n}$, $f \in \mathbb{R}^n$, $d \in \mathbb{R}^m_+$, and g_i are entries of $g \in \mathbb{R}^m_+$. The symbols $\bar{u}_{\tau,i}$, $\bar{\lambda}_{\tau,i} \in \mathbb{R}^2$ in (38.3) denote $\bar{u}_{\tau,i} = ((Tu)_{2i-1}, (Tu)_{2i})^\top$, $\bar{\lambda}_{\tau,i} = (\lambda_{\tau,2i-1}, \lambda_{\tau,2i})^\top$, $\quad i \in \mathcal{M}$.

Let $q : \mathbb{R}^{3m} \to \mathbb{R}$ be the quadratic function defined by

$$q(\lambda) = \frac{1}{2}\lambda^\top A\lambda - \lambda^\top b,$$

where $\lambda = (\lambda_\nu^\top, \lambda_\tau^\top)^\top$, $A = BK^{-1}B^\top$ is symmetric, positive definite with the full row-rank matrix $B = \left(N^\top, T^\top\right)^\top$, $b = BK^{-1}f - c$, and $c = \left(d^\top, 0^\top\right)^\top$. $r(\lambda) = A\lambda - b$ is the gradient. Further, denote $\Lambda_\nu = \mathbb{R}^m_+$, $\Lambda_\tau = \Lambda_{\tau,1} \times \cdots \times \Lambda_{\tau,m}$, and $\Lambda_{\tau,i} = \{\bar{\lambda}_{\tau,i} \in \mathbb{R}^2 : \|\bar{\lambda}_{\tau,i}\| \leq g_i\}$, $i \in \mathcal{M}$, $\Lambda = \Lambda_\nu \times \Lambda_\tau$. Since (38.1)-(38.3) represent the Karush-Kuhn-Tucker conditions, after simple manipulations, we arrive at the *dual* formulation of the algebraic contact problem with Tresca friction: find $\lambda^* \in \Lambda$ such that

$$\lambda^* = \arg\min q(\lambda) \quad \text{subject to } \lambda \in \Lambda. \tag{38.4}$$

As q is strictly convex, quadratic and Λ is the closed and convex set, it is well known that there exists the unique solution $\lambda^* \in \Lambda$ to (38.4).

Now we reformulate (38.1)-(38.3) as a system of nonsmooth equations. We introduce the projections $P_{\Lambda_\nu} : \mathbb{R}^m \to \Lambda_\nu$, $P_{\Lambda_\tau} : \mathbb{R}^{2m} \to \Lambda_\tau$. $P_{\Lambda_\nu}(\lambda_\nu) = (\phi(\lambda_{\nu,1})^\top, \ldots, \phi(\lambda_{\nu,m})^\top)^\top$, where $\phi(\lambda_{\nu,i}) = \max\{0, \lambda_{\nu,i}\}, \quad i \in \mathcal{M}$ and $P_{\Lambda_\tau}(\lambda_\tau) = (\psi_{g_1}(\bar{\lambda}_{\tau,1})^\top, \ldots, \psi_{g_m}(\bar{\lambda}_{\tau,m})^\top)^\top$, where

$$\psi_{g_i}(\bar{\lambda}_{\tau,i}) = \begin{cases} \bar{\lambda}_{\tau,i} & \text{if } \|\bar{\lambda}_{\tau,i}\| \leq g_i, \\ \dfrac{g_i}{\|\bar{\lambda}_{\tau,i}\|}\,\bar{\lambda}_{\tau,i} & \text{if } \|\bar{\lambda}_{\tau,i}\| > g_i. \end{cases}$$

Let

$$G : \mathbb{R}^{n+3m} \to \mathbb{R}^{n+3m}, \quad y = \left(u^\top, \lambda_\nu^\top, \lambda_\tau^\top\right)^\top \in \mathbb{R}^{n+3m}$$

be the function defined by

$$G(y) = \begin{pmatrix} Ku + N^\top \lambda_\nu + T^\top \lambda_\tau - f \\ \lambda_\nu - P_{\Lambda_\nu}(\lambda_\nu + \rho(Nu - d)) \\ \lambda_\tau - P_{\Lambda_\tau}(\lambda_\tau + \rho Tu) \end{pmatrix}, \tag{38.5}$$

where $\rho > 0$ is an arbitrary but fixed parameter. It is easy to show that (38.1)-(38.3) and the equation

$$G(y) = 0 \tag{38.6}$$

have the same (unique) solution $y^* = ({u^*}^\top, {\lambda_\nu^*}^\top, {\lambda_\tau^*}^\top)^\top$. The SSN method can be used.

38.3 SEMI-SMOOTH NEWTON METHOD

It is convenient to use the concept of a slant differentiability ([2,4]) on the equation (38.6). Below, we will use an active/inactive set terminology and the indicator matrices. Concerning the unilateral contact law (38.2), we use $\mathcal{A}_\nu, \mathcal{I}_\nu \subseteq \mathcal{M}$ be the *active*, and *inactive* set at y, respectively: $\mathcal{A}_\nu = \{i \in \mathcal{M} : 0 \leq \lambda_{\nu,i} + \rho(Nu - d)_i\}$, $\mathcal{I}_\nu = \mathcal{M} \setminus \mathcal{A}_\nu$. For the Tresca friction law (38.2) we use $\mathcal{A}_\tau, \mathcal{I}_\tau \subseteq \mathcal{M}$, where $\mathcal{A}_\tau = \{i \in \mathcal{M} : \|\bar{\lambda}_{\tau,i} + \rho\bar{u}_{\tau,i}\| \leq g_i\}$, and $\mathcal{I}_\tau = \mathcal{M} \setminus \mathcal{A}_\tau$. Now, after the slant differentiation of the term (38.5), we arrive at

$$G^o(y) = \begin{pmatrix} K & N^\top & T^\top \\ -\rho D(\mathcal{A}_\nu)N & D(\mathcal{I}_\nu) & 0 \\ G^o_{31}(y) & 0 & G^o_{33}(y) \end{pmatrix},$$

where

$$\begin{aligned} G^o_{31}(y) &= -\rho D(\bar{\mathcal{A}}_\tau)T - \rho D(\bar{\mathcal{I}}_\tau)P^o_{\Lambda_\tau}(\lambda_\tau + \rho Tu)T, \\ G^o_{32}(y) &= 0, \\ G^o_{33}(y) &= D(\bar{\mathcal{I}}_\tau)(I - P^o_{\Lambda_\tau}(\lambda_\tau + \rho Tu)), \end{aligned}$$

and $P^o_{\Lambda_\tau}(\lambda_\tau + \rho Tu) = diag(\psi^o_{g_1}(\bar{y}_1), \ldots, \psi^o_{g_m}(\bar{y}_m)) \in \mathbb{R}^{2m\times 2m}$.

Each Newton iteration solves the linear system for y^{k+1}, i.e.

$$G^o(y^k)y^{k+1} = G^o(y^k)y^k - G(y^k). \tag{38.7}$$

38.3.1 Modified algorithm

The slanting function of the projection onto the circle reads as

$$\psi^o_\delta(y) = \begin{cases} I & \text{if } \|y\| \leq \delta, \\ \dfrac{\delta}{\|y\|}\Big(I - \dfrac{1}{\|y\|^2}\, yy^\top\Big) & \text{if } \|y\| > \delta, \end{cases}$$

where $I \in \mathbb{R}^{2\times 2}$. It is easy to show that $I - \frac{1}{\|y\|^2}\, yy^\top$ is the orthogonal projection onto $\langle y\rangle^\perp$ so that

$$\psi^o_\delta(y)\hat{y} = 0 \in \mathbb{R}^2 \quad \forall \hat{y} \in \langle y\rangle,\ \|y\| > \delta, \tag{38.8}$$

where $\langle\cdot\rangle$ denotes the linear span. Using this fact, the third block equation in (38.7) splits with respect to the active/inactive set:

$$-\rho T_{\bar{\mathcal{A}}_\tau} u^{k+1} = 0, \quad \bar{\lambda}^{k+1}_{\tau,i} - \psi^o_{g_i}(\bar{y}^k_i)\bar{y}^{k+1}_i = \psi_{g_i}(\bar{y}^k_i),\ i \in \mathcal{I}_\tau.$$

From (38.8) it follows that the terms $\psi_{g_i}^o(\bar{y}_i^k)\bar{y}_i^{k+1}$ tend to zero if the algorithm converges. Therefore we propose to omit them and to replace $G^o(y)$ by the following approximation:

$$\widetilde{G}^o(y) = \begin{pmatrix} K & N^\top & T^\top \\ -\rho D(\mathcal{A}_\nu)N & D(\mathcal{I}_\nu) & 0 \\ -\rho D(\bar{\mathcal{A}}_\tau)T & 0 & D(\bar{\mathcal{I}}_\tau) \end{pmatrix}. \tag{38.9}$$

Lemma 38.1 *Let G and $\widetilde{G}^o$ be given by (38.5), and (38.9), respectively. Suppose that y^* is the solution to $G(y) = 0$. If the sequence of the modified Newton iterations*

$$y^{k+1} = y^k - \widetilde{G}^o(y^k)^{-1}G(y^k) \tag{38.10}$$

converges, then its limit is y^*.

Proof See [6]. □

Each iterative step (38.10) leads to the linear system that splits as follows:

$$\lambda_{\nu,\mathcal{I}_\nu}^{k+1} = 0,\ \bar{\lambda}_{\tau,i}^{k+1} = \psi_{g_i}(\bar{y}_i^k),\ i \in \mathcal{I}_\tau \tag{38.11}$$

and

$$\begin{pmatrix} K & N_{\mathcal{A}_\nu}^\top & T_{\bar{\mathcal{A}}_\tau}^\top \\ N_{\mathcal{A}_\nu} & 0 & 0 \\ T_{\bar{\mathcal{A}}_\tau} & 0 & 0 \end{pmatrix} \begin{pmatrix} u^{k+1} \\ \lambda_{\nu,\mathcal{A}_\nu}^{k+1} \\ \lambda_{\tau,\bar{\mathcal{A}}_\tau}^{k+1} \end{pmatrix} = \begin{pmatrix} f - T_{\bar{\mathcal{I}}_\tau}^\top \lambda_{\tau,\bar{\mathcal{I}}_\tau}^{k+1} \\ d_{\mathcal{A}_\nu} \\ 0 \end{pmatrix}.$$

To propose a computationally efficient inexact implementation, using simple manipulations to eliminate $\{u^k\}$ and therefore reformulating the active and inactive sets (without using u), we arrive at the dual implementation of the algorithm with the reduced gradient used as a stopping criterion.

Algorithm MSSN (Modified SSN method)

Given $\lambda^0 \in \mathbb{R}^{3m}$, $\rho > 0$, and $\varepsilon \geq 0$. Set $err^0 = \|\widetilde{r}_\rho(P_\Lambda(\lambda^0))\|$ and $k = 0$.

(*Step 1*) If $err^k \leq \varepsilon$, return $\lambda = P_\Lambda(\lambda^k)$, else go to *Step 2*.

(*Step 2*) Assembly the active/inactive sets at λ^k:

$$\mathcal{A}_\nu = \{i \in \mathcal{M} : \lambda_i^k - \rho r_i^k \geq 0\}, \quad \mathcal{I}_\nu = \mathcal{M} \setminus \mathcal{A}_\nu, \tag{38.12}$$

$$\mathcal{A}_\tau = \{i \in \mathcal{M} : \|\bar{\lambda}_{\tau,i}^k - \rho \bar{r}_i^k\| \leq g_i\}, \quad \mathcal{I}_\tau = \mathcal{M} \setminus \mathcal{A}_\tau. \tag{38.13}$$

(*Step 3*) Find λ^{k+1} so that

$$\lambda^{k+1} = \arg\min q(\lambda) \quad \text{subject to (38.11)}. \tag{38.14}$$

(*Step 4*) Set $err^{k+1} = \|\widetilde{r}_\rho(P_\Lambda(\lambda^{k+1}))\|$, $k = k + 1$ and go to *Step 1*.

The main difference between Algorithm MSSN and its 2D counterpart lies in the finite termination property. The 2D algorithm terminates in a finite number of steps (see [5]). Due to the projections onto the circles with infinitely many boundary points the Algorithm MSSN has to treat infinitely many linear systems.

38.4 INEXACT AND GLOBALLY CONVERGENT ALGORITHMS

Firstly, we propose an inexact implementation of the algorithm, i.e. the solution to (38.14) we get using the CG method. The adaptive precision control ((*Step 3.1*)) is used to accept inexact inner solutions. This variant of the algorithm we denote by ALGORITHM IMSSN.

The key idea to achieve the globally convergent variant of the algorithm is that the generated sequence $\{q(\lambda^k)\}$ will be monotonically decreasing. For that, we use the upper bound for ρ and ensure that all iterations belong to Λ, i.e. we choose $\lambda^0 \in \Lambda$ and terminate the CG loop before an iteration outside of Λ is generated (CGM_{feas}). To simplify our presentation we denote: $\mathcal{A} = \mathcal{A}_\nu \cup \{i+m : \ i \in \bar{\mathcal{A}}_\tau\}$ and $\mathcal{I} = \{1, 2, \ldots, 3m\} \setminus \mathcal{A}$.

ALGORITHM GIMSSN (Globally convergent IMSSN method)
Given $\lambda^0 \in \Lambda$, $\rho \in (0, 2\sigma_{\max}^{-1})$, $\varepsilon \geq 0$, and $r_{tol}, c_{fact} \in (0,1)$.
Set $err^0 = \|\widetilde{r}_\rho(\lambda^0)\|$, $tol^0 = r_{tol}/c_{fact}$, and $k = 0$.
(*Step 1*) If $err^k \leq \varepsilon$, return $\lambda = \lambda^k$, else go to step *Step 2*.
(*Step 2*) Assembly the active/inactive sets at λ^k by (38.12)-(38.13).
(*Step 3.1*) $tol^{k+1} = \min\{r_{tol} \times err^k/err^0, c_{fact} \times tol^k\}$.
(*Step 3.2*) $\lambda^{k+1,0} = P_\Lambda(\lambda^k - \rho r(\lambda^k))$.
(*Step 3.3*) $\lambda^{k+1} = \mathrm{CGM}_{feas}(A, b, \mathcal{A}, \lambda^{k+1,0}, tol^{k+1})$.
(*Step 4*) Set $err^{k+1} = \|\widetilde{r}_\rho(\lambda^{k+1})\|$, $k = k+1$, and go to *Step 1*.

The difference to the 2D case consists of treatment the spherical constraints that is hidden inside the evaluation of the projection P_Λ and in the feasibility test in CGM_{feas}.

Theorem 38.1 *Let $\lambda^0 \in \Lambda$, $\varepsilon = 0$, $\rho \in (0, 2\sigma_{\max}^{-1})$, and $r_{tol}, c_{fact} \in (0,1)$. Let $\sigma_{\min}$, $\sigma_{\max}$ be the smallest and largest eigenvalues of A, respectively, and let λ^* be the solution to (38.4). Let $\{\lambda^k\}$ denote the sequence generated by* ALGORITHM GIMSSN. *The following statement holds:*
(i) the sequence $\{q(\lambda^k)\}$ decreases so that

$$q(\lambda^{k+1}) - q(\lambda^*) \leq \eta(\rho)\,(q(\lambda^k) - q(\lambda^*)),$$

where

$$\eta(\rho) = \begin{cases} 1 - \rho\sigma_{\min} & \text{for } \rho \in (0, \sigma_{\max}^{-1}], \\ 1 - (2\sigma_{\max}^{-1} - \rho)\sigma_{\min} & \text{for } \rho \in [\sigma_{\max}^{-1}, 2\sigma_{\max}^{-1}); \end{cases}$$

(ii) if $\{\lambda^k\}$ is finite, then its last element is λ^*;
(iii) if $\{\lambda^k\}$ is infinite, then it converges to λ^* R-linearly so that

$$\|\lambda^k - \lambda^*\| \leq C\,\eta(\rho)^{k/2},$$

where $C = \sqrt{2(q(\lambda^0) - q(\lambda^*))/\sigma_{\min}}$.

Proof See [5], Theorem 3.

38.5 NUMERICAL EXPERIMENTS

We will assess performances of different algorithms for contact of two bricks given by the domains $\Omega_1 = (0,2) \times (0,1) \times (1,2)$ and $\Omega_2 = (0,2) \times (0,1) \times (0,1)$ (in [m]). The briks are made of isotropic, homogeneous materials characterized by the Young modulus 50000 [MPa] and the Poisson ratio 0.277 for Ω_1 and 0.35 for Ω_2. The decompositions of $\partial\Omega_1$ and $\partial\Omega_2$ are as follows:

$$\gamma_1^u = \{2\} \times (0,1) \times (1,2),\ \gamma_1^c = (0,2) \times (0,1) \times \{1\},\ \gamma_1^p = \partial\Omega_1 \backslash \overline{\gamma_1^u \cup \gamma_1^c},$$
$$\gamma_2^u = \{0\} \times (0,1) \times (0,1),\ \gamma_2^c = (0,2) \times (0,1) \times \{1\},\ \gamma_2^p = \partial\Omega_2 \backslash \overline{\gamma_2^u \cup \gamma_2^c}.$$

The slip bound on γ_1^c is given by constant $g = 0.09$ (in [MPa]). The volume forces vanish for both bodies. The non-vanishing surface tractions act on the part of γ_1^p denoted by $L_8 = (0,2) \times (0,1) \times \{2\}$ and on the part of γ_2^p denoted by $L_6 = \{0\} \times (0,1) \times (1,2)$, they are given by the same constant functions $\boldsymbol{p}_1 = \boldsymbol{p}_2 = (0,0,-1)$ (in [MPa]). The problem is approximated by the linear finite elements over regular triangulations.

In tables below we report the number n_A of matrix-vector multiplications by A and the number *iter* of outer (Newton) iterations, i.e. the last value of k, for different DOFs n and m. The value n_A characterizes computational complexity.

Example 38.1. In Table 38.1 we compare efficiency of ALGORITHM IMSSN with the dual implementation of ALGORITHM SSN (a variant of the algorithm without the modification). We use few BiCGSTAB iterations [7] to get inexact solutions of inner linear systems. One can observe that computations based on symmetric inner linear systems are considerably more efficient.

Tab. 38.1 Symmetrized versus non-symmetrized variants of the SSN method.

	IMSSN	SSN
n/m	$iter/n_A$	$iter/n_A$
24576/256	10/161	9/1180
55566/441	9/143	9/1428
105456/676	10/185	11/2506
178746/961	10/190	10/2162
279936/1296	9/167	10/2298
413536/1681	10/216	10/2586

Source: own elaboration

CONCLUSION

We have analyzed the solution of contact problems with Tresca friction in 3D. The analysis is similar to the 2D case, see [5]. We have pointed out the main differences between these two cases. The 3D case is more complicated due to projections onto circles in $\mathbb{R}^2$ describing the friction law in 3D.

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SYMMETRIZED SEMI-SMOOTH NEWTON METHOD FOR SOLVING 3D CONTACT PROBLEMS

Abstract: *The semi-smooth Newton method for solving discretized contact problems with Tresca friction in three space dimensions is analyzed. The slanting function is approximated to get symmetric inner linear systems. The primal-dual algorithm is transformed into the dual one so that the conjugate gradient method can be used. The R-linear convergence rate is proved for an inexact globally convergent variant of the method. Numerical experiments conclude the paper. The contact problems are important in many practical applications, e.g., biological processes, design of machines, transportation systems, metal forming, or medicine (bone replacements).*

Keywords: *contact problem; Tresca friction; semi-smooth Newton method; conjugate gradient method; gradient projection; convergence rate.*

SYMETRIZOVANÁ NEHLADKÁ NEWTONOVA METODA PRO ŘEŠENÍ 3D KONTAKTNÍCH ÚLOH

Abstrakt: *V práci je analyzována nehladká Newtonova metoda pro řešení diskretizovaných kontaktních úloh s Trescovým třením ve třech prostorových dimenzích. Slanting funkce je aproximována za účelem získání symetrických vnitřních lineárních úloh. Pro použití metody sdružených gradientů je primárně-duální algoritmus převeden na duální. R-lineární rychlost konvergence je dokázána pro nepřesnou globálně konvergentní variantu metody. Závěrem jsou uvedeny numerické experimenty. Kontaktní úlohy mají řadu významných aplikací, např. biologické procesy, design strojů a přepravních systémů, tváření kovů nebo medicína (modelování kostních náhrad).*

Klíčová slova: *kontaktní úloha; Trescovo tření; nehladká Newtonova metoda; metoda sdružených gradientů; projekce gradientu; rychlost konvergence.*

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