Total-FETI method for solving contact elasto-plastic problems

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1 Introduction

Contact problems with elasto-plastic bodies can be solved for example by primal-dual active set strategy, see e.g. [12]. In this paper, we propose a numerical method that combines the semi-smooth Newton method with the Total-FETI (TFETI) domain decomposition method and SMALSE method [1].

We consider a frictionless contact boundary condition between two bodies denoted as $\Omega^1, \Omega^2 \subset \mathbb{R}^3$, see Fig. 1. We assume that the bodies are fixed on the parts $\Gamma_U^1, \Gamma_U^2 \neq \emptyset$ of the boundaries. The load is represented by surface (prescribed on the boundaries parts Γ_N^1, Γ_N^2) and volume forces. The material of the bodies is described by the elasto-plastic constitutive model with the von Mises yield criterion and linear isotropic hardening [10]. For the sake of simplicity, we confine ourselves on one-step problem formulated in displacement. It leads to a minimization of the convex and smooth functional on a convex set. However the stress-strain relation is not smooth.

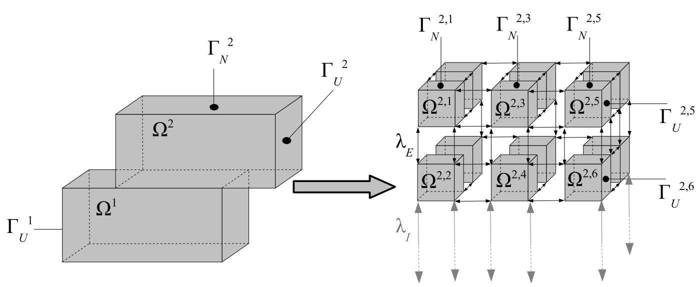

Fig. 1 Scheme of the geometry and domain decomposition

The problem is approximated by the finite element method. The finite element partition will be denoted as $\mathcal{T}_h = \mathcal{T}_h^1 \cup \mathcal{T}_h^2$ and consists of simplicial elements. In particular, displacement fields are approximated by continuous, piecewise linear functions and strain (stress) fields are approximated by piecewise constant functions. We will not investigate in detail the influence of domain and load approximation.

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Since we will apply the TFETI domain decomposition method [2], we tear the bodies from the part of the boundary with the Dirichlet boundary condition, decompose it into subdomains, assign each subdomain by a unique number, and introduce new “gluing” conditions on the artificial intersubdomain boundaries and on the boundaries with imposed Dirichlet condition. In particular, the domain $\Omega_h^i \equiv \Omega^i$ is decomposed into a system of s_i disjoint polyhedral subdomains $\Omega^{i,p} \subset \Omega^i$, $p = 1,2,\dots,s_i$, $i = 1,2$, see Fig. 1. The partition is conforming with the finite element partition $\mathscr{T}_h$.

The discretized problem can be classified as an optimization problem with simple equality and inequality contraints. In Section 2, we introduce and describe an algebraic formulation of the problem. We use the semi-smooth Newton method to approximate a non-quadratic functional by a quadratic one, see Section 3. The corresponding problem of quadratic programming is solved by the Total-FETI domain decomposition method in combination with SMALSE method, see Section 4. The elasto-plastic problem with contact was implemented into the MatSol library [8]. We illustrate the performance of our algorithm on a 3D benchmark problem in Section 5.

2 Algebraic formulation of the contact problem for elasto-plastic bodies

Algebraic formulation of the problem will be related to the domain decomposition. It means that a displacement vector $\mathbf{v} \in \mathbb{R}^n$ has the following structure:

$$\mathbf{v} = \left(\mathbf{v}_{1,1}^T, \mathbf{v}_{1,2}^T, \dots, \mathbf{v}_{1,s_1}^T, \mathbf{v}_{2,1}^T, \dots, \mathbf{v}_{2,s_2}^T\right)^T,$$

where $\mathbf{v}_{i,p}$ denotes the displacement vector on $\Omega^{i,p}$, $i = 1,2$. We define the space

$$\mathscr{V} := \left\{\mathbf{v} \in \mathbb{R}^n \mid \mathbf{B}_E\mathbf{v} = \mathbf{o}\right\}, \tag{1}$$

and the set of admissible displacement

$$\mathscr{K} := \left\{\mathbf{v} \in \mathbb{R}^n \mid \mathbf{B}_E\mathbf{v} = \mathbf{o},\ \mathbf{B}_I\mathbf{v} \le \mathbf{c}_I\right\}. \tag{2}$$

Here the equality constraint matrix $\mathbf{B}_E \in \mathbb{R}^{m_E \times n}$ represents the gluing conditions among neighbouring subdomains and the Dirichlet boundary conditions. The inequality constraint matrix $\mathbf{B}_I \in \mathbb{R}^{m_I \times n}$ represents the non-penetration condition on the contact zones. Notice that $\mathscr{K}$ is convex and closed.

Let $\mathbf{K}_e \in \mathbb{R}^{n \times n}$ be a block diagonal matrix consisting of the elastic stiffness matrices $\mathbf{K}_e^{i,p}$ defined on each subdomain $\Omega^{i,p}$, $i = 1,2$, $p = 1,\dots,s_i$. Due to the presence of the Dirichlet boundary conditions on both subdomains and the Korn inequality, we can define the energy norm on $\mathscr{V}$:

$$\|\mathbf{v}\|_e := \sqrt{\mathbf{v}^T\mathbf{K}_e\mathbf{v}} = \sqrt{\sum_{i=1}^{2}\sum_{p=1}^{s_i}\mathbf{v}_{i,p}^T\mathbf{K}_e^{i,p}\mathbf{v}_{i,p}}, \quad \mathbf{v} = \left(\mathbf{v}_{1,1}^T,\ldots,\mathbf{v}_{1,s_1}^T,\mathbf{v}_{2,1}^T,\ldots,\mathbf{v}_{2,s_2}^T\right)^T \in \mathscr{V}.$$

Notice that the using of this norm is suitable from mechanical and mathematical points of view since some of the below estimates (mainly (6)) are independent of the domain decomposition and the discretization parameter h of the mesh.

The algebraic formulation of the contact elasto-plastic problem can be written as the following optimization problem [1]:

$$\text{Find } \mathbf{u} \in \mathscr{K} \;:\; J(\mathbf{u}) \le J(\mathbf{v}) \quad \forall \mathbf{v} \in \mathscr{K}, \tag{3}$$

where

$$J(\mathbf{v}) := \Psi(\mathbf{v}) - \mathbf{f}^T\mathbf{v}, \quad \mathbf{v} \in \mathbb{R}^n. \tag{4}$$

Here the vector $\mathbf{f} = \left(\mathbf{f}_{1,1}^T,\ldots,\mathbf{f}_{1,s_1}^T,\mathbf{f}_{2,1}^T,\ldots,\mathbf{f}_{2,s_2}^T\right)^T \in \mathbb{R}^n$ represents the load consisting of the volume and surface forces, and the initial stress state. The functional Ψ represents the inner energy and has the structure

$$\Psi(\mathbf{v}) = \left(\Psi_{1,1}(\mathbf{v}_{1,1})^T,\ldots,\Psi_{1,s_1}(\mathbf{v}_{1,s_1})^T,\Psi_{2,1}(\mathbf{v}_{2,1})^T,\ldots,\Psi_{2,s_2}(\mathbf{v}_{2,s_2})^T\right)^T.$$

Further Ψ is a potential to the non-linear elasto-plastic operator $F : \mathbb{R}^n \to \mathbb{R}^n$, i.e. $D\Psi(\mathbf{v}) = F(\mathbf{v})$, $\forall \mathbf{v} \in \mathbb{R}^n$. The function F is generally nonsmooth but Lipschitz continuous. It enables us to define a generalized derivative $K : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ of F in the sense of Clark, i.e. $K(\mathbf{v}) \in \partial F(\mathbf{v})$, $\mathbf{v} \in \mathbb{R}^n$. Notice that $K(\mathbf{v})$ is symmetric, block diagonal and sparse matrix. Moreover the following properties of F and K hold [11]:

1. $$F(\mathbf{v}+\mathbf{w}) - F(\mathbf{v}) = \int_0^1 K(\mathbf{v}+\theta\mathbf{w})\mathbf{w}\,\mathrm{d}\theta \quad \forall \mathbf{v},\mathbf{w} \in \mathbb{R}^n. \tag{5}$$
2. $K(\mathbf{v})$ is uniformly positive definite and bounded with respect to $\mathbf{v} \in \mathscr{V}$:
$$\exists \nu \in (0,1): \quad \nu\|\mathbf{w}\|_e^2 \le \mathbf{w}^T K(\mathbf{v})\mathbf{w} \le \|\mathbf{w}\|_e^2 \quad \forall \mathbf{v},\mathbf{w} \in \mathscr{V}. \tag{6}$$
3. F is strongly semismooth [9] on $\mathscr{V}$, which yields that for any $\mathbf{v} \in \mathscr{V}$ and any of sufficiently small $\mathbf{w} \in \mathscr{V}$:
$$F(\mathbf{v}+\mathbf{w}) - F(\mathbf{v}) - K(\mathbf{v}+\mathbf{w})\mathbf{w} = O(\|\mathbf{w}\|_e^2). \tag{7}$$

Notice that (5) and (6) yield that Ψ is coercive and strictly convex on $\mathscr{V}$. Hence the problem (4) has a unique solution and can be equivalently written as the following variational inequality:

$$\text{Find } \mathbf{u} \in \mathscr{K} \;:\; F(\mathbf{u})^T(\mathbf{v}-\mathbf{u}) \ge \mathbf{f}^T(\mathbf{v}-\mathbf{u}) \quad \forall \mathbf{v} \in \mathscr{K}. \tag{8}$$

The estimate (7) will be important for showing that the semi-smooth Newton method defined in the next section has a local quadratic convergence.

3 Semi-smooth Newton method for optimization problem

The investigated problem (3) contains two nonlinearities – the non-quadratic functional J (due to Ψ) and the non-penetration conditions including in the convex set $\mathscr{K}$. By the semismooth Newton method, we will approximate Ψ by a quadratic functional similarly as in the Taylor expansion:

$$\Psi(\mathbf{u}) \approx \Psi(\mathbf{u}^k) + F(\mathbf{u}^k)^T(\mathbf{u}-\mathbf{u}^k) + \frac{1}{2}(\mathbf{u}-\mathbf{u}^k)^T K(\mathbf{u}^k)(\mathbf{u}-\mathbf{u}^k),$$

for a given approximation $\mathbf{u}^k \in \mathscr{K}$ of the solution $\mathbf{u}$ to the problem (3). Let us denote $\mathbf{f}_k = \mathbf{f} - F(\mathbf{u}^k)$, $\mathbf{K}_k = K(\mathbf{u}^k)$ and define:

$$\mathscr{K}_k := \mathscr{K} - \mathbf{u}^k = \left\{\mathbf{v} \in \mathbb{R}^n \; ; \; \mathbf{B}_E\mathbf{v} = \mathbf{o},\, \mathbf{B}_I\mathbf{v} \le \mathbf{c}_{I,k},\, \mathbf{c}_{I,k} := \mathbf{c}_I - \mathbf{B}_I\mathbf{u}^k\right\},$$

$$J_k(\mathbf{v}) := \frac{1}{2}\mathbf{v}^T\mathbf{K}_k\mathbf{v} - \mathbf{f}_k^T\mathbf{v}, \quad \mathbf{v} \in \mathscr{K}_k. \tag{9}$$

Then the Newton step is following:

$$\mathbf{u}^{k+1} = \mathbf{u}^k + \delta\mathbf{u}^k, \quad \mathbf{u}^{k+1} \in \mathscr{K},$$

where $\delta\mathbf{u}^k \in \mathscr{K}_k$ is a unique minimum of J_k on $\mathscr{K}_k$:

$$J_k(\delta\mathbf{u}^k) \le J_k(\mathbf{v}) \qquad \forall \mathbf{v} \in \mathscr{K}_k, \tag{10}$$

or equivalently $\delta\mathbf{u}^k \in \mathscr{K}_k$ solves the following inequality:

$$\left(\mathbf{K}_k\delta\mathbf{u}^k\right)^T(\mathbf{v}-\delta\mathbf{u}^k) \ge \mathbf{f}_k^T(\mathbf{v}-\delta\mathbf{u}^k) \quad \forall \mathbf{v} \in \mathscr{K}_k. \tag{11}$$

Notice that if we substitute $\mathbf{v} = \mathbf{u}^{k+1} \in \mathscr{K}$ into (8) and $\mathbf{v} = \mathbf{u} - \mathbf{u}^k \in \mathscr{K}_k$ into (11), then by adding we obtain the inequality

$$\left(K(\mathbf{u}^k)\delta\mathbf{u}^k\right)^T(\mathbf{u}-\mathbf{u}^{k+1}) \ge \left(F(\mathbf{u}) - F(\mathbf{u}^k)\right)^T(\mathbf{u}-\mathbf{u}^{k+1}),$$

which can be arranged into the form

$$(\mathbf{u}^{k+1}-\mathbf{u})^T K(\mathbf{u}^k)(\mathbf{u}^{k+1}-\mathbf{u}) \le \left(F(\mathbf{u}^k) - F(\mathbf{u}) - K(\mathbf{u}^k)(\mathbf{u}^k-\mathbf{u})\right)^T(\mathbf{u}-\mathbf{u}^{k+1}).$$

Hence one can simply derive local quadratic convergence of the semi-smooth Newton method by (6) and (7) provided that $\mathbf{u}^k$ is sufficiently close to $\mathbf{u}$.

4 TFETI method for the inner problem

Notice that the structures and properties of the matrices $\mathbf{K}_k \in \mathbb{R}^{n\times n}$, $k = 0,1,2,\ldots$, are very similar to the corresponding elastic matrix $\mathbf{K}_e$ as follows from Section 2. Therefore we can solve the inner problem (10) in the same way as a contact problem with elastic bodies, see e.g. [4, 5].

Here we use the TFETI domain decomposition method for solving (10). For more detail see e.g. [3] and [1]. The method is based on enforcing all the constraints by the Lagrange multipliers. In particular, we use two types of Lagrange multipliers, namely $\lambda_I \in \mathbb{R}^{m_I}$, $\lambda_I \geq \mathbf{o}$ related to the non-penetration condition, $\lambda_E \in \mathbb{R}^{m_E}$ related to the "gluing" and Dirichlet conditions. To simplify the notation, we denote

$$\lambda = \begin{bmatrix} \lambda_E \\ \lambda_I \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} \mathbf{B}_E \\ \mathbf{B}_I \end{bmatrix}, \quad \mathbf{c}_k = \begin{bmatrix} \mathbf{o} \\ \mathbf{c}_{I,k} \end{bmatrix},$$

and

$$\Lambda = \{\lambda = (\lambda_E^T, \lambda_I^T)^T \in \mathbb{R}^{m_E+m_I} :\ \lambda_I \geq \mathbf{o}\}.$$

Then the Lagrangian associated with problem (10) reads as

$$L_k(\mathbf{v},\lambda) = \frac{1}{2}\mathbf{v}^T\mathbf{K}_k\mathbf{v} - \mathbf{f}_k^T\mathbf{v} + \lambda^T(\mathbf{B}\mathbf{v} - \mathbf{c}_k), \quad \mathbf{v} \in \mathbb{R}^n,\ \lambda \in \Lambda. \tag{12}$$

Using the convexity of the cost function and constraints, we can use the classical duality theory to reformulate problem (10) to get

$$J_k(\delta\mathbf{u}^k) = \min_{\mathbf{v}\in\mathscr{K}_k} J_k(\mathbf{v}) = \min_{\mathbf{v}\in\mathbb{R}^n}\sup_{\lambda\in\Lambda} L_k(\mathbf{v},\lambda) = \max_{\lambda\in\Lambda}\inf_{\mathbf{v}\in\mathbb{R}^n} L_k(\mathbf{v},\lambda) = \max_{\lambda\in\Lambda}\{-\Theta_k(\lambda)\}, \tag{13}$$

with

$$\Theta_k(\lambda) = \begin{cases} \frac{1}{2}\lambda^T\mathbf{B}\mathbf{K}_k^\dagger\mathbf{B}^T\lambda - \lambda^T(\mathbf{B}\mathbf{K}_k^\dagger\mathbf{f}_k - \mathbf{c}_k), & \mathbf{R}_k^T(\mathbf{f}_k - \mathbf{B}^T\lambda) = \mathbf{o}, \\ +\infty, & \text{otherwise}, \end{cases}$$

where $\mathbf{K}_k^\dagger$ is a pseudoinverse matrix to $\mathbf{K}_k$ and $\mathbf{R}_k \in \mathbb{R}^{n\times l}$ represents the null space of $\mathbf{K}_k$. More details to implementation of $\mathbf{B}\mathbf{K}_k^\dagger\mathbf{B}^T$ can be found in [6]. Thus the corresponding dual problem has the form:

$$\text{find } \lambda^k \in \Lambda : \quad \Theta_k(\lambda^k) \leq \Theta_k(\lambda) \quad \forall\lambda \in \Lambda. \tag{14}$$

We solve the dual problem by algorithm SMALSE-M [3]. The algorithm is based on active set strategy and it combines three steps: CG with preconditioning based on orthogonal projectors, expansion, and proportioning.

Once the solution λ^k of (14) is known, the solution of (10) can be evaluated in this way:

$$\delta\mathbf{u}^k = \mathbf{K}_k^\dagger(\mathbf{f} - \mathbf{B}^T\lambda^k) + \mathbf{R}_k\alpha_k, \quad \alpha_k = (\mathbf{R}_k^T\overline{\mathbf{B}}^T\overline{\mathbf{B}}\mathbf{R}_k)^{-1}\mathbf{R}_k^T\overline{\mathbf{B}}^T(\overline{\mathbf{c}}_k - \overline{\mathbf{B}}\mathbf{K}_k^\dagger(\mathbf{f}_k - \mathbf{B}^T\lambda^k)),$$

where the matrix $\overline{\mathbf{B}}$ and the vector $\bar{\mathbf{c}}_k$ are formed by the rows of $\mathbf{B}$ and $\mathbf{c}_k$ corresponding to all equality constraints and all active inequality constraints.

Notice that we use in fact the inexact Newton method with respect to computing of $\delta\mathbf{u}^k$.

5 Numerical experiments

In this section we illustrate the strong parallel scalability and the performance of numerical scalability of our approach on a numerical example. The geometry of the problem is depicted in Figure 1. The sizes of the bodies are $3000 \times 1000 \times 1000$. We use regular meshes generated in MatSol [8]. The Young modulus, the Poisson ratio, the initial yield stress for the von Mises criterion, and the hardening modulus are $E^i = 210000$, $\nu^i = 0.29$, $\sigma_y^i = 450$, and $H_m^i = 10000$, $i = 1,2$, respectively. The indicated traction force prescribed in the vertical direction is $g(x) = 150$, $x \in \Gamma_N^2$. The initial stress (or plastic strain) state is equal to zero.

The proposed algorithms were parallelized using Matlab Distributed Computing Server and Matlab Parallel Toolbox. For all computations we use 28 cores with 2GB memory per core of the HP Blade system, model BLc7000. The stopping criterion of the Newton method is $\frac{\|\mathbf{u}^{k+1}-\mathbf{u}^k\|_e}{\|\mathbf{u}^{k+1}\|_e+\|\mathbf{u}^k\|_e} < 10^{-4}$ (see e.g. [7] or [11]). The stopping criterion for the SMALSE-M algorithm is described in [3]. We use the tolerance 10^{-7} for SMALSE-M.

The strong parallel scalability is depicted in Table 1. Here we consider the mesh with 174 902 nodes and 162 000 hexahedrons. The bodies are decomposed into 162 subdomains by MatSol. The number of primal variables is 646 866 and the number of dual variables is 130 189.

Number of cores	3	7	14	28
Number of plastic elems.	151 300	151 300	151 300	151 300
Number of Newton iters.	6	6	6	6
Total number of SMALSE-M iters.	67	67	67	67
Total number of multi. by Hessian	3 726	3 726	3 726	3 726
Time for last Newton iter.	6 976	1 259	778	537
Total time [sec]	26 828	6 481	4 091	2 926

Table 1 Strong paralel scalability.

In Table 2 we report "the numerical scalability" for different mesh levels. The most important is row with total number of multiplication by Hessian, where we can see, that the number of iterations grows only moderately. The total times are not mutually comparable since we could not keep a constant number of subdomain per one core due to the limitation on maximal number of the core.

Distribution of the von Mises stress and the total displacement for the finest mesh are depicted in Figures 2 and 3.

Mesh level	1	2	3	4
Mesh nodes	7 502	53 802	174 902	406 802
Mesh elements	6 000	48 000	162 000	384 000
Number of subdomains	6	48	162	384
Number of cores	4	25	28	28
Primal variables	23 958	191 664	646 866	1 533 312
Dual variables	2 453	33 933	130 189	326 969
Number of plastic elems.	6 624	48 141	151 300	356 384
Number of Newton iters.	6	6	6	6
Total number of SMALSE-M iters.	153	88	67	67
Total number of multi. by Hessian	1 951	3 106	3 726	5 375
Time for last Newton iter.	41	141	537	1 758
Total time [sec]	287	683	2 926	9 318

Table 2 Performance of ”the numerical scalability”.

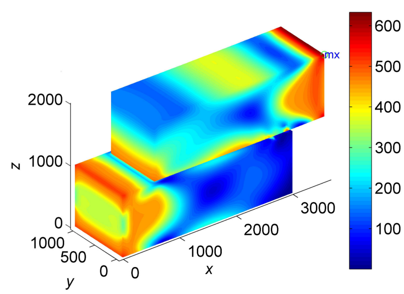

Fig. 2 von Mises stress distribution

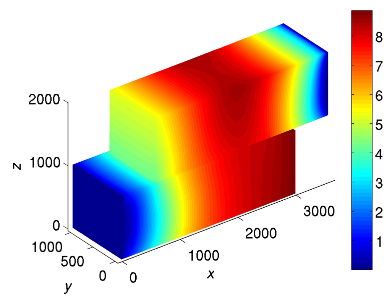

Fig. 3 total displacement

6 Conclusion

In this paper, we proposed a numerical method for solving contact elasto-plastic problems based on TFETI method and demonstrate its parallel and numerical scalability on a numerical example. The numerical realization and implementation of the problem were newly included into the MatSol library. In fact, the proposed method can be used or can be as a part of other contact inelastic problems than the considered frictionless contact problem of von Mises' elasto-plastic bodies with isotropic hardening.

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