TFETI Scalable Solvers for Transient Contact Problems

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Summary. We review our results obtained by application of the TFETI domain decomposition method to implement the time step of the Newmark scheme for the solution of transient contact problems without friction. If the ratio of the decomposition and discretization parameters is kept uniformly bounded as well as the ratio of the time and space discretization, then the cost of the time step is proved to be proportional to the number of nodal variables. The algorithm uses our MPRGP algorithm for the solution of strictly convex bound constrained quadratic programming problems with optional preconditioning by the conjugate projector to the subspace defined by the trace of the rigid body motions on the artificial subdomain interfaces. The optimality relies on our results on quadratic programming, the theory of the preconditioning by a conjugate projector for nonlinear problems, and the classical bounds on the spectrum of the mass and stiffness matrices. The results are confirmed by numerical solution of 3D transient contact problems.

1 Introduction

The transient multibody contact problems are important in many applications arising in mechanical or civil engineering. However, it is not easy to provide a useful solution to realistic problems. The reasons include the lack of smoothness, which puts high demand on the construction of effective time discretization schemes, the strong nonlinearity arising from the non-interpenetration boundary conditions, and large dimension of the problems resulting from the space discretization. These complications stimulated extensive research activities both from the theoretical point of view (see, e.g., [4]), or the numerical point of view (see, e.g., [10], or [11]).

Numerical solution of transient contact problems usually comprises several steps. Starting from a week formulation of the conditions of equilibrium and boundary conditions, the problem is first discretized in space by the finite element method in a similar way as the related static problem. The resulting semidiscrete problem is then discretized by a suitable time discretization scheme. The time integration requires a special attention to guarantee stability of the algorithm and to avoid non-physical oscillations that result from application of the standard time discretization methods for unconstrained problems. Such schemes were proposed by many authors (see [6,

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7, 9, 10]). In our approach, we use a combination of the standard finite element space discretization with the contact stabilized Newmark scheme introduced by Krause and Walloth [9] that reduces the solution of the transient contact problem to a sequence of strictly convex quadratic programming (QP) problems with inequality constraints that describe the non-interpenetration conditions.

The final step amounts to the solution of QP problems of large dimension, possibly with millions of nodal variables and many inequality constraints. In this paper we propose to resolve the auxiliary problems by our variant of the FETI domain decomposition method called TFETI (total finite element tearing and interconnecting, Dostál et al. [1]). Our research has been motivated by our recent results in development of optimal algorithms for the frictionless static problems [1] that combine effective FETI preconditioning of both linear and nonlinear steps with our algorithms for the solution of bound constrained QP problems [3]. An important feature of our QP algorithms is the error estimate in terms of the bound on the condition number of the Hessian matrix of the cost function.

2 Transient Contact Problem and Its Discretization Using TFETI

The starting point of our exposition is the discretized transient multibody contact problem resulting from application of our TFETI domain decomposition. The reason is that a little is known about the solvability of the weak formulation of the transient contact problem (see, e.g., [4]), so we shall assume in what follows that its solution $\mathbf{u}$ exists. Moreover, we shall assume that $\mathbf{u}$ is sufficiently smooth so that $\ddot{\mathbf{u}}$ exists in some reasonable sense and can be approximated by finite differences. More specific choice of the solution space can be found, e.g., in [4] or in [6].

To discretize the multibody contact problem using TFETI, we tear each body from the part of the boundary with the Dirichlet boundary conditions, decompose each body into subdomains, assign each subdomain a unique number, and introduce new "gluing" conditions on the artificial subdomain interfaces and on the boundaries with imposed Dirichlet conditions. We denote the subdomains and their number by Ω^p and s, respectively. The gluing conditions require continuity of the displacements and of their normal derivatives across the subdomain interfaces. The procedure is the same as that for the static problem, [1].

Using finite element discretization in space we get the following semidiscrete problem at time τ

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} \;=\; \mathbf{f} - \mathbf{B}_I^T \boldsymbol{\lambda}_I^T - \mathbf{B}_E^T \boldsymbol{\lambda}_E, \tag{1}$$

$$\mathbf{B}_I\mathbf{u} \le \mathbf{c}_I, \quad \mathbf{B}_E\mathbf{u} = \mathbf{c}_E, \quad \boldsymbol{\lambda}_I \ge \mathbf{o}, \quad \boldsymbol{\lambda}^T(\mathbf{B}\mathbf{u} - \mathbf{c}) = 0, \tag{2}$$

with the discrete Newton equation of motion (1) and the equality and inequality constraints (2) resulting from the gluing, Dirichlet, and non-interpenetration conditions enforced by Lagrange multipliers.

The TFETI based finite element semi-discretization in space of the subdomains $\Omega^p,\ p = 1,\dots,s$, results in the block diagonal stiffness matrix $\mathbf{K} = \mathrm{diag}\,(\mathbf{K}_1,\dots,\mathbf{K}_s)$

of the order n with the sparse positive semidefinite diagonal blocks $\mathbf{K}_p$ that correspond to the subdomains Ω^p. The same structure has a positive definite mass matrix $\mathbf{M} = \operatorname{diag}(\mathbf{M}_1, \ldots, \mathbf{M}_s)$. The decomposition induces also the block structure of the vector of nodal forces $\mathbf{f} = \mathbf{f}_\tau \in \mathbb{R}^n$ at time τ and the vector of nodal displacements $\mathbf{u} = \mathbf{u}_\tau \in \mathbb{R}^n$ at time τ.

The matrix $\mathbf{B}_I \in \mathbb{R}^{m_I \times n}$ and the vector $\mathbf{c}_I \in \mathbb{R}^{m_I}$ describe the linearized non-interpenetration conditions and the matrix $\mathbf{B}_E \in \mathbb{R}^{m_E \times n}$ and the vector $\mathbf{c}_E \in \mathbb{R}^{m_E}$ enforce the prescribed zero displacements on the part of the boundary with imposed Dirichlet condition and the continuity of the displacements across the auxiliary interfaces.

Finally, $\boldsymbol{\lambda}_I \in \mathbb{R}^{m_I}$ and $\boldsymbol{\lambda}_E \in \mathbb{R}^{m_E}$ denote the components of the vector of Lagrange multipliers $\boldsymbol{\lambda} = \boldsymbol{\lambda}_\tau \in \mathbb{R}^m$, $m = m_I + m_E$ at time τ. We use the notation

$$\boldsymbol{\lambda} = \begin{bmatrix} \boldsymbol{\lambda}_I \\ \boldsymbol{\lambda}_E \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} \mathbf{B}_I \\ \mathbf{B}_E \end{bmatrix}, \quad \text{and} \quad \mathbf{c} = \begin{bmatrix} \mathbf{c}_I \\ \mathbf{c}_E \end{bmatrix}. \tag{3}$$

For the time discretization, we use the contact-stabilized Newmark scheme introduced by Krause and Walloth [9] with the regular partition of the time interval $[0, T]$, $0 = \tau_0 < \tau_1 \ldots < \tau_{n_T} = T, \quad \tau_k = k\Delta, \quad \Delta = T/n_T, \quad k = 0, \ldots, n_T$. The scheme assumes that the acceleration vector is split at time τ_k into two components

$$\ddot{\mathbf{u}}_k = \ddot{\mathbf{u}}_k^{int} + \ddot{\mathbf{u}}_k^{con}, \quad \ddot{\mathbf{u}}_k^{int} = \mathbf{M}^{-1}(\mathbf{f}_k - \mathbf{K}\mathbf{u}_k), \text{ and } \ddot{\mathbf{u}}_k^{con} = -\mathbf{M}^{-1}\mathbf{B}^T\boldsymbol{\lambda}_k. \tag{4}$$

We obtain the solution algorithm in the form

Algorithm 2.1 Contact-stabilized Newmark algorithm.

Step 0. $\{$*Initialization*$\}$

Set $\mathbf{u}_0$, $\dot{\mathbf{u}}_0$, $\widetilde{\mathbf{K}} = \frac{4}{\Delta^2}\mathbf{M} + \mathbf{K}$, $T > 0$, $n_T \in \mathbb{N}$, and $\Delta = T/n_T$.

for $k = 0, \ldots, n_T - 1$ **do**

Step 1. $\{$*Predictor displacement computation*$\}$

$$\min \left[\tfrac{1}{2} \left(\mathbf{u}_{k+1}^{pred}\right)^T \mathbf{M}\mathbf{u}_{k+1}^{pred} - \left(\mathbf{M}\mathbf{u}_k + \Delta\mathbf{M}\dot{\mathbf{u}}_k - \mathbf{B}^T\boldsymbol{\lambda}_k^{pred}\right)^T \mathbf{u}_{k+1}^{pred} \right]$$

subject to $\mathbf{B}_I\mathbf{u}_{k+1}^{pred} \le \mathbf{c}_I$, and $\mathbf{B}_E\mathbf{u}_{k+1}^{pred} = \mathbf{c}_E$

Step 2. $\{$*Contact-stabilized displacement computation*$\}$

$$\min \left[\tfrac{1}{2}\mathbf{u}_{k+1}^T \widetilde{\mathbf{K}}\mathbf{u}_{k+1} - \left(\tfrac{4}{\Delta^2}\mathbf{M}\mathbf{u}_{k+1}^{pred} - \mathbf{K}\mathbf{u}_k + \mathbf{f}_k + \mathbf{f}_{k+1} - \mathbf{B}^T\boldsymbol{\lambda}_k\right)^T \mathbf{u}_{k+1} \right]$$

subject to $\mathbf{B}_I\mathbf{u}_{k+1} \le \mathbf{c}_I$ and $\mathbf{B}_E\mathbf{u}_{k+1} = \mathbf{c}_E$

Step 3. $\{$*Velocity evaluation*$\}$

$$\dot{\mathbf{u}}_{k+1} = \dot{\mathbf{u}}_k + \tfrac{2}{\Delta}\left(\mathbf{u}_{k+1} - \mathbf{u}_{k+1}^{pred}\right)$$

end

The matrix $\widetilde{\mathbf{K}}$ introduced in *Step 0* is called an *effective stiffness matrix*. Let us note that we omit the factor '1/2' in the term $\mathbf{B}^T\boldsymbol{\lambda}_k^{pred}$ in the predictor step.

3 Optimal Solver with Bound on the Condition Number of the Hessian of the Dual Energy Function

The favorable distribution of the spectrum of the mass matrix $\mathbf{M}$ is sufficient to implement Step 1 by using the dual theory and the standard MPRGP algorithm described in [3] with asymptotically linear complexity. To develop an optimal algorithm for Step 2, we shall distinguish two cases. If the time steps are sufficiently short, then the effective stiffness matrix can be considered as a perturbation of the well conditioned mass matrix, so it is enough to use again our MPRGP algorithm to prove the numerical scalability and demonstrate it by numerical experiments. On the other hand, if we use longer time steps, the effective stiffness matrix has very small eigenvalues which obviously correspond to the eigenvectors that are near the kernel of $\mathbf{K}$. This observation was fully exploited for linear problems by Farhat et al. [5] who used the conjugate projectors to the natural coarse grid to achieve scalability with respect to the time step. Unfortunately, this idea can not be applied in full extent to the contact problems as we do not know a priori which boundary conditions are applied to the subdomains associated with the contact interface. However, we can still define the preconditioning by the trace of the rigid body motions on the artificial subdomain interfaces. To implement this observation, we use our preconditioning by conjugate projector for partially constrained strictly convex quadratic programming problems of the form

$$\min_{\boldsymbol{\lambda}} \frac{1}{2}\boldsymbol{\lambda}^T\widetilde{\mathbf{F}}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T\mathbf{d} \text{ subject to } \boldsymbol{\lambda}_{\mathscr{I}} \geq \mathbf{o} \tag{5}$$

which arises directly from the application of the dual theory on the problem in Step 2 of Algorithm 2.1. Such a method complies with our MPRGP-P algorithm for the solution of strictly convex bound constrained problems described in [3]. We keep the iterations in the subspace with the solution which is defined by the trace of the rigid body motions on the artificial interfaces between subdomains excluding the contact interface. Even though the necessity to keep the coarse grid away from the contact interface prevented us from proving the optimality with respect to the time step, we give the proof of optimality of our algorithm provided the ratio of the time step and the space discretization parameter is kept uniformly bounded and show that the optimality can be observed by numerical experiments (see [2] for details). Moreover, MPRGP-P algorithm has the rate of convergence in terms of the norm of the projected gradient and the bound on the condition number of the Hessian matrix of the cost functional. Therefore all we need to guarantee optimality is a uniform bound on the condition number of the Hessian.

In [2], we used the standard arguments to prove the following lemma which gives the required bound.

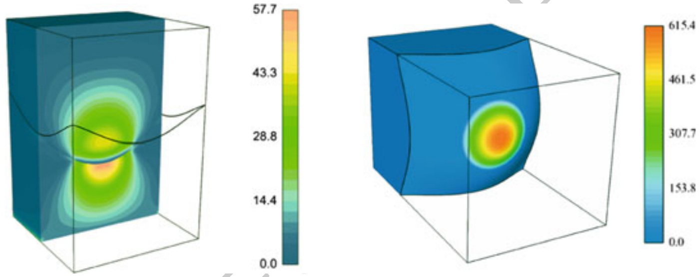
Lemma 1. *Let $B_1\|\boldsymbol{\lambda}\|^2 \leq \|\mathbf{B}^T\boldsymbol{\lambda}\|^2 \leq B_2\|\boldsymbol{\lambda}\|^2$ and let the elements have a regular shape and size. Then*

$$C_1\frac{h^2\Delta^2}{h^d\,(h^2+\Delta^2)}\|\boldsymbol{\lambda}\|^2 \leq \boldsymbol{\lambda}^T\widetilde{\mathbf{F}}\boldsymbol{\lambda} \leq C_2\frac{\Delta^2}{h^d}\|\boldsymbol{\lambda}\|^2, \tag{6}$$

with constants B_1, B_2, C_1, and C_2 independent of h, H, and Δ. Moreover, if $C > 0$ is any constant, then for any $0 < \Delta \leq Ch$ the condition number $\kappa(\widetilde{\mathbf{F}})$ satisfies $\kappa(\widetilde{\mathbf{F}}) \leq \frac{C_2}{C_1}(1 + C^2)$.

4 Numerical Experiments

The described algorithms were implemented in `MatSol` library [8] developed in Matlab environment and tested on the solution of 3D frictionless transient contact problems. For all computations we used the HP Blade system, model BLc7000 and as parallel programming environment we used Matlab Distributed Computing Engine. All the computations were carried out with the relative stopping tolerance $\varepsilon = 10^{-4}$.



a) Von Mises stress in τ_1 [MPa] b) Contact pressure in τ_1 [MPa]

Fig. 1. Results of 3D benchmark

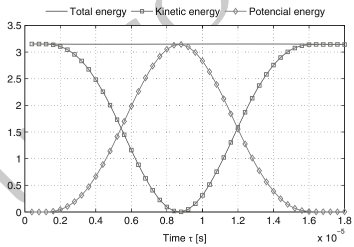


Fig. 2. Energy conservation (ton·mm^2·s^{-2})

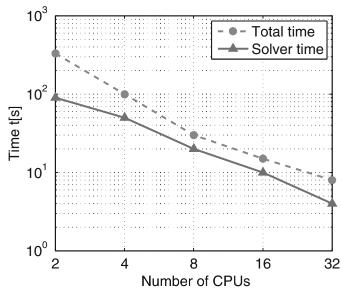


Fig. 3. Parallel scalability

3D impact problem

Our first academic benchmark is a 3D impact between the curved 3D elastic boxes of size 10 (mm) depicted in Fig. 1. Material constants are defined by the Young modulus $E = 2.1 \cdot 10^5$ (MPa), the Poisson ratio $\nu = 0.3$, and the density $\rho = 7.85 \cdot 10^{-9}$ (ton/mm^3). The initial gap between the curved boxes is set to 0.001 (mm). We prescribe the initial velocity $-1{,}000$ (mm/s) on the upper body in the x_3 direction. The upper body is floating in space and the lower body is fixed along the bottom side. The linearized non-interpenetration condition was imposed on the contact interface. For the time discretization, we use Algorithm 2.1 with the constant time step $\Delta = 4 \cdot 10^{-7}$ and solve the impact of bodies in the time interval $\tau = [0, 45\Delta]$.

The von Mises stress distribution and the normal contact pressure along the contact interface in time $\tau_1 = 22\Delta$ are depicted in Figs. 1a, b, respectively. The energy development is shown in Fig. 2. We can see the constant total energy curve as expected.

In Table 1, we report the numerical scalability of our algorithm for the constant time step $\Delta_1 = 1 \cdot 10^{-3}$ and $\Delta_2 = 1 \cdot 10^{-5}$ and with or without conjugate projectors. We kept $H/h = 10$. Moreover, in last two lines of the table, we report the same characteristics but with the time step dependent on the discretization step h, i.e., $\Delta_{1,h} = 3h\Delta_1$.

We can observe that the number of matrix-vector multiplications, the most expensive component of our algorithm, stays constant for the smaller time step Δ_2 as expected and increases only mildly in agreement with the theory for the case of the larger time step Δ_1 if we use conjugate projectors. If we simultaneously choose the time step Δ proportional to h, i.e., $\Delta = \Delta_h$, then the number of matrix-vector multiplications stays the same as predicted by the theory.

Parallel scalability of our algorithm is depicted in Fig. 3, where we keep the number of elements fixed and increase the number of CPUs (subdomains).

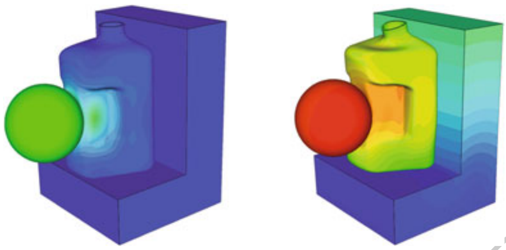
Number of subdomains		16	54	128	250
Primal variables		196 608	663 552	1 572 864	3 072 000
Dual variables		21 706	81 652	214 699	443 920
		Hessian multiplications			
MPRGP	Δ_1	67	86	113	191
MPRGP - P	Δ_1	60	67	85	112
MPRGP	Δ_2	39	40	40	42
MPRGP - P	Δ_2	40	40	40	42
MPRGP	$\Delta_{1,h}$	67	72	76	78
MPRGP - P	$\Delta_{1,h}$	60	63	67	69

Table 1. Numerical scalability of 3D impact problem - Δ constant or dependent on h

Impact of three bodies

We have also tested our algorithms on the impact of three bodies. We considered the transient analysis of three elastic bodies in mutual contact (see Fig. 4). We prescribe the initial velocity 5,000 (mm/s) on the sphere in the x_1 direction. The L-shape body is fixed along the bottom side. Material constants are defined by the Young modulus $E = 2.1 \cdot 10^3$ (MPa), the Poisson ratio $\nu = 0.3$, and the density $\rho = 6 \cdot 10^{-9}$ (ton/mm^3). For the time discretization, we use the constant time step $\Delta = 1 \cdot 10^{-3}$ (s) and solve the impact of bodies in the time interval $\tau = [0, 150\Delta]$ (s). The total displacement in times $\tau_1 = 20\Delta$ and $\tau_2 = 80\Delta$ (s) of the problem discretized by $1.2 \cdot 10^5$

primal and $8.5 \cdot 10^3$ dual variables and decomposed into 32 subdomains using METIS is depicted in Fig. 4.



a) Total displacement in τ_1 b) Total displacement in τ_2

Fig. 4. Impact of bodies in time

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Bibliography

[1] Z. Dostál, T. Kozubek, V. Vondrák, T. Brzobohatý, and A. Markopoulos. Scalable TFETI algorithm for the solution of multibody contact problems of elasticity. *Internat. J. Numer. Methods Engrg.*, 82(11):1384–1405, 2010. ISSN 0029-5981.

[2] Z. Dostál, T. Kozubek, T. Brzobohatý, A. Markopoulos, and O. Vlach. Scalable TFETI with preconditioning by conjugate projector for transient frictionless contact problems of elasticity. submitted., 2011.

[3] Zdeněk Dostál. *Optimal quadratic programming algorithms*, volume 23 of *Springer Optimization and Its Applications*. Springer, New York, 2009. ISBN 978-0-387-84805-1. With applications to variational inequalities.

[4] Christof Eck, Jiří Jarušek, and Miroslav Krbec. *Unilateral contact problems*, volume 270 of *Pure and Applied Mathematics (Boca Raton)*. Chapman & Hall/CRC, Boca Raton, FL, 2005. ISBN 978-1-57444-629-6; 1-57444-629-0. doi: 10.1201/9781420027365. URL http://dx.doi.org/10.1201/9781420027365. Variational methods and existence theorems.

[5] C. Farhat, P.S. Chen, and J. Mandel. A scalable lagrange multiplier based domain decomposition method for time-dependent problems. *Internat. J. Numer. Methods Engrg.*, 38(22):3831–3853, 1995. ISSN 0029-5981.

[6] C. Hager and B. I. Wohlmuth. Analysis of a space-time discretization for dynamic elasticity problems based on mass-free surface elements. *SIAM J. Numer.*

Anal., 47(3):1863–1885, 2009. ISSN 0036-1429. doi: 10.1137/080715627. URL http://dx.doi.org/10.1137/080715627.

[7] Houari Boumediène Khenous, Patrick Laborde, and Yves Renard. Mass redistribution method for finite element contact problems in elastodynamics. *Eur. J. Mech. A Solids*, 27(5):918–932, 2008. ISSN 0997-7538. doi: 10.1016/j.euromechsol.2008.01.001. URL http://dx.doi.org/10.1016/j.euromechsol.2008.01.001.

[8] T. Kozubek, A. Markopoulos, T. Brzobohatý, R. Kučera, V. Vondrák, and Z. Dostál. Matsol - matlab efficient solvers for problems in engineering. "http://matsol.vsb.cz/", 2009.

[9] Rolf Krause and Mirjam Walloth. A time discretization scheme based on Rothe's method for dynamical contact problems with friction. *Comput. Methods Appl. Mech. Engrg.*, 199(1-4):1–19, 2009. ISSN 0045-7825. doi: 10.1016/j.cma.2009.08.022. URL http://dx.doi.org/10.1016/j.cma.2009.08.022.

[10] Tod A. Laursen. *Computational contact and impact mechanics*. Springer-Verlag, Berlin, 2002. ISBN 3-540-42906-9. Fundamentals of modeling interfacial phenomena in nonlinear finite element analysis.

[11] Peter Wriggers. *Computational contact mechanics*. John Wiley & Sons, Ltd., Chichester, West Sussex, England, 2002.