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FETI BASED PARALLEL SOLUTION OF CONTACT SHAPE OPTIMIZATION PROBLEMS

V. Vondrák, T. Kozubek, Z. Dostál [1]

Summary: *The paper deals with parallel solution of contact shape optimization problems. We propose for the parallel solution of the state problem a domain decomposition technique based on the Finite Element Tearing and Interconnecting (FETI) method originally proposed in (Farhat and Roux, 1991; Farhat et al., 1994). Although this method was proposed for linear problems, it was adopted to solution of the contact problems (Dostál and Vondrák, 1997; Dostál et al., 2000). In this paper, we describe a new variant of this method that we call Total FETI (Dostál et al., 2005). We exploit the same method for the efficient parallel solution of sensitivity analysis which shows to be the most expensive part of the shape optimization process. The efficiency of proposed method will be demonstrated on numerical examples.*

1. Introduction

The contact shape optimization problem is one of the computationally most challenging problems. The reason is that not only the cost function is a nonlinear implicit function of the design variables, but that its evaluation requires also a solution of the highly nonlinear variational inequality, which describes the equilibrium of a system of elastic bodies in mutual contact. Since the cost function must be evaluated many times in the solution process, it is obvious that the solution of contact problem is a key ingredient of any effective algorithm for the solution of contact shape optimization problems.

The approach that we propose here is based on the Finite Element Tearing and Interconnecting (FETI) domain decomposition method, which was originally proposed by Farhat and Roux in (Farhat and Roux, 1991; Farhat et al., 1994) for parallel solving of the linear problems described by elliptic partial differential equations. Its key ingredient is decomposition of the spatial domain into non-overlapping subdomains that are ”glued” by Lagrange multipliers, so that, after eliminating the primal variables, the original problem is reduced to a small, relatively well conditioned, typically equality constrained quadratic programming problem that is solved iteratively. If the FETI procedure is applied to an elliptic variational inequality, the resulting quadratic programming problem has not only the equality constraints, but also the box constraints. Even though the latter is a considerable complication as compared with linear problems, it seems that the FETI procedure should be even more powerful for the solution

[1] doc. Mgr. Vít Vondrák, Ph.D., doc. Ing. Tomáš Kozubek, Ph.D., prof. RNDr. Zdeněk Dostál, DSc. Dept. of Applied Mathematics, VŠB-TU Ostrava, 17. listopadu 15, 70833 Ostrava-Poruba, tel. +420 596 993 489, e-mail vit.vondrak@vsb.cz

of variational inequalities than for the linear problems (Dostál, 2004, 2005; Dostál and Horák, 2004). The reason is that FETI not only reduces the original problem to a smaller and better conditioned one, but it also replaces for free all the inequalities by the bound constraints.

In this paper, we exploit the parallel implementation of our scalable algorithm for contact problem to the minimization of the compliance of the system of elastic bodies subject to the volume constraint and some additional constraints. We start our exposition by recalling some theoretical results and formulae for derivatives of the solution with respect to the design variables. In particular, it turns out that the derivatives of the solution may be evaluated by the solution of variational inequalities with the same operator as the state problem. We describe our Total FETI (TFETI) method for the solution of the resulting variational inequalities in two steps. First, using the duality theory, the problem to find the minimum of the energy functional subject to the kinematically admissible displacements is reduced to the contact interface. Then we exploit an efficient algorithm for the solution of the quadratic programming problems with simple bounds and possibly some equalities. An especially attractive feature of this approach is not only high precision of the gradient, but also the fact that relatively expensive factorization of the stiffness matrices of the subdomains is carried out only once for each update of the design variables. Moreover, the factorization update concerns only the subdomains affected by the update and we usually have good initial approximations for the solution. The efficiency of the proposed algorithms will be demonstrated on the numerical experiments.

2. Contact problems and Total FETI

Let us start our exposition introducing Total FETI method for the solution of contact problem of elastic bodies. Assuming that the bodies in potential contact are built from the subdomains $\Omega^{(s)}$, the equilibrium of the system may be described as a solution u of the problem

$$\min j(v) \quad \text{subject to} \quad \sum_{s=1}^{N_s} B_I^{(s)} v^{(s)} \le g_I \quad \text{and} \quad \sum_{s=1}^{N_s} B_E^{(s)} v^{(s)} = o, \tag{1}$$

where $j(v)$ is the energy functional defined by

$$j(v) = \sum_{s=1}^{N_s} \frac{1}{2} v^{(s)T} K^{(s)} v^{(s)} - v^{(s)T} f^{(s)},$$

$v^{(s)}$ and $f^{(s)}$ denote the admissible subdomain displacements and the subdomain vector of prescribed forces, $K^{(s)}$ is the subdomain stiffness matrix, $B^{(s)}$ is a block of the matrix $B = \left[B_I^T, B_E^T\right]^T$ that corresponds to $\Omega^{(s)}$, and g_I is a vector collecting the gaps between the bodies in the reference configuration. The matrix B_I and the vector g_I arise from the nodal or mortar description of non-penetration conditions, while B_E describes the "gluing" of the subdomains into the bodies and the Dirichlet boundary conditions.

To simplify the presentation of basic ideas, we can describe the equilibrium in terms of the global stiffness matrix K, the vector of global displacements u, and the vector of global loads f. In the TFETI method, we have

$$K = \mathrm{diag}(K^{(1)}, \ldots, K^{(N_s)}), \quad u = \begin{bmatrix} u^{(1)} \\ \vdots \\ u^{(N_s)} \end{bmatrix}, \quad \text{and} \quad \mathrm{f} = \begin{bmatrix} f^{(1)} \\ \vdots \\ f^{(N_s)} \end{bmatrix},$$

where $K^{(s)}$, $s = 1, \ldots, N_s$, is a positive semidefinite matrix. The energy function reads

$$j(v) = \frac{1}{2} v^T K v - f^T v$$

and the vector of global displacements u solves

$$\min j(v) \quad \text{subject to} \quad B_I v \le g_I \quad \text{and} \quad B_E v = o. \tag{2}$$

Alternatively, the global equilibrium may be described by the Karush–Kuhn–Tucker conditions (see, e.g., (Dostál, 2007))

$$Ku = f - B^T \lambda, \quad \lambda_I \ge o, \quad \lambda^T (Bu - g) = o, \tag{3}$$

where $g = \left[g_I^T, o^T \right]^T$ and $\lambda = \left[\lambda_I^T, \lambda_E^T \right]^T$ denotes the vector of Lagrange multipliers which may be interpreted as the reaction forces. The problem (3) differs from the linear problem by the non-negativity constraint on the components of reaction forces λ_I and by the complementarity condition.

We can use the left equation of (3) and the sparsity pattern of K to eliminate the displacements. We shall get the problem to find

$$\max \Theta(\lambda) \quad \text{s.t.} \quad \lambda_I \ge o \quad \text{and} \quad R^T (f - B^T \lambda) = o, \tag{4}$$

where

$$\Theta(\lambda) = -\frac{1}{2} \lambda^T B K^\dagger B^T \lambda + \lambda^T (B K^\dagger f - g) - \frac{1}{2} f K^\dagger f, \tag{5}$$

$K^\dagger$ denotes a generalized inverse that satisfies $K K^\dagger K = K$, and R denotes the full rank matrix whose columns span the kernel of K. The action of K^+ can be effectively evaluated by a variant of LU–SVD decomposition (Farhat and Géradin, 1998). Recalling the FETI notation

$$F = B K^\dagger B^T, \quad \widetilde{e} = R^T f, \quad G = R^T B^T, \quad \widetilde{d} = B K^\dagger f - g,$$

we can modify (4) to

$$\min \widetilde{\theta}(\lambda) \quad \text{s.t.} \quad \lambda_I \ge 0 \quad \text{and} \quad G\lambda = \widetilde{e}, \tag{6}$$

where

$$\widetilde{\theta}(\lambda) = \frac{1}{2} \lambda^T F \lambda - \lambda^T \widetilde{d}.$$

3. Contact shape optimization

Let us now assume that the shape of the bodies $\Omega_1, ..., \Omega_p$ is controlled by a vector of design variables α. The energy functional of the contact problem will have the form

$$j(v, \alpha) = \frac{1}{2} v^T K(\alpha) v - v^T f(\alpha), \tag{7}$$

where the stiffness matrix $K(\alpha)$ and possibly the vector of external nodal forces $f(\alpha)$ depend on α. The matrix B_I and the vector g_I that describe the linearized condition of non-interpenetration also depend on α, so that the solution $u(\alpha)$ of the contact problem with the region $\Omega_i = \Omega_i(\alpha)$ can be find as the solution of the minimization problem

$$\min j(v, \alpha) \quad \text{subject to} \quad v \in C(\alpha), \tag{8}$$

where

$$C(\alpha) = \{v : B_I(\alpha)v \leq g_I(\alpha)\}.$$

Now, we shall consider the contact shape optimization problem to find

$$\min\{\mathcal{J}(\alpha) : \alpha \in D_{adm}\}, \tag{9}$$

where $\mathcal{J}(\alpha)$ is the cost function that derives optimality criterion for design of body $\Omega_i(\alpha)$. The set of admissible design variables D_{adm} defines all feasible designs. For example, if the cost function is defined by $\mathcal{J}(\alpha) \equiv J(v, \alpha)$, then the minimal compliance problem is obtained. Set of admissible design parameters could be given for example by

$$D_{adm} = \{l \leq \alpha \leq r : \text{vol}(\Omega(\alpha)) = \text{vol}(\Omega(0))\} \tag{10}$$

It has been proved that the minimal compliance problem has at least one solution and that the function $J(u, \alpha)$ considered as a function of α has derivatives under natural assumption (Haslinger and Neittanmaki, 1996).

4. Sensitivity analysis

The goal of the sensitivity analysis is to find the influence of design change to the solution of the state problem and to the value of the cost function. It means that we are looking for the directional derivative of the solution of the state problem

$$u'(\alpha, \beta) = \lim_{t \to 0^+} \frac{u(\alpha + t\beta) - u(\alpha)}{t} \tag{11}$$

where β denotes the direction of this directional derivative which is substituted during computation by the vectors $\Delta\alpha = (0, \ldots, 0, \Delta\alpha_i, 0, \ldots, 0)^T$ for $i = 1, \ldots, k$, where k is the number of design variables that control the design of bodies.

The simplest method for computation of this derivative is to use the overall forward finite difference approximation $\Delta u / \Delta\alpha_i$ to the design sensitivity $\partial u / \partial\alpha_i$ that is given by

$$\frac{\partial u(\alpha)}{\partial \alpha_i} = \frac{\Delta_i u(\alpha)}{\Delta \alpha_i} = \frac{u(\alpha_1, \ldots, \alpha_i + \Delta\alpha_i, \ldots, \alpha_k) - u(\alpha_1, \ldots, \alpha_k)}{\Delta\alpha_i} \tag{12}$$

It follows that the overall finite difference method for evaluation of the gradient of u as a function of the design variables α requires $k + 1$ solutions of (8). An unpleasant complication is that the Hessian of this problem is different for each auxiliary problem so that we have to carry out $k + 1$ times the decomposition of the block K_i that corresponds to the body whose shape is to be computed.

This major drawback of the finite difference method can be resolved introducing the analytic or semi-analytic method of sensitivity analysis for contact problems. Some comparisons of the efficiency of these methods and overall finite difference method on practical problems solved by classical FETI method can be found in (Dostál et al., 1998, 2001, 2002). In the rest of this section, the semi-analytic approach for variational inequalities solved by Total FETI method will be described.

Let the set $I = \{i : b_{i*}(\alpha)u = c_i(\alpha)\}$ denote the set of indices of active constraints $B(\alpha)u \leq c(\alpha)$, let $b_{i*}(\alpha)$ denote the i^{th} row of matrix $B(\alpha)$, and let the vector u denote the solution of the state problem (8). Further, for analysis of all possible cases, we split the set I into the two sets

$$I_s = \{i : i \in I \wedge \lambda_i > 0\},$$
$$I_w = \{i : i \in I \wedge \lambda_i = 0\}, \tag{13}$$

where I_s is the set of indices of nodal variables in, so called, strong constraint, I_w is the set of indices in weak constraint, and λ is the solution of the dual formulation of the state problem (8). Using formal differentiation of the Karush-Kuhn-Tucker conditions of problem (8) and some simplification, we obtain the new problem

$$\min_{z \in \tilde{G}(\alpha,\beta)} \tilde{\mathcal{H}}(\alpha,\beta), \tag{14}$$

where

$$\begin{aligned} \tilde{\mathcal{H}}(\alpha,\beta) &= \frac{1}{2} z^\top K(\alpha) z - \tilde{f}^\top(\alpha,\beta) z, \\ \tilde{G}(\alpha,\beta) &= \{z : B_w(\alpha) z \le c_w(\alpha,\beta), B_s(\alpha) z = c_s(\alpha,\beta)\}, \end{aligned}$$

and

$$\begin{aligned} &\tilde{f}(\alpha,\beta) = f'(\alpha,\beta) - K'(\alpha,\beta)u - B'^\top(\alpha,\beta)\lambda, \\ &B_w(\alpha) = (b_{j*}(\alpha))_{j \in I_w}, \qquad c_w(\alpha,\beta) = \left(f'(\alpha,\beta) - b'_{j*}(\alpha,\beta)u\right)_{j \in I_w}, \\ &B_s(\alpha) = (b_{j*}(\alpha))_{j \in I_s}, \qquad c_s(\alpha,\beta) = \left(f'(\alpha,\beta) - b'_{j*}(\alpha,\beta)u\right)_{j \in I_s}. \end{aligned}$$

The symbols $K'(\alpha,\beta)$, $f'(\alpha,\beta)$ and $B'(\alpha,\beta)$ represent directional derivatives in direction β; see the definition of $u'(\alpha,\beta)$. At this place it is important to notice that these derivatives can be simply evaluated. It has been proved (Haslinger and Neittanmaki, 1996) that the solution of this problem is the directional derivative $u'(\alpha,\beta)$ of solution of problem (8).

It is easy to see that the last problem is again a quadratic programming problem with linear constraints in the form of equalities and inequalities. This problem may be efficiently solved using Total FETI method which was described in Section 2.

The semi-analytic method for sensitivity analysis requires solution of k quadratic programming problems (14) with the same matrix $K^\dagger(\alpha)$. Using this method we exploit not only the advantages of Total FETI formulation of the problem, but we can use the decomposition and kernel of matrix $K(\alpha)$ from the solution of the state problem to the sequence of problems in the semi-analytic sensitivity analysis. Thus the semi-analytic approach requires only one decomposition of the stiffness matrix which compares favorably with k+1 decompositions of the overall finite difference approach.

5. Numerical experiments

Proposed algorithms were tested on the 3D Hertz problem which is depicted in Figure 1. The shape of the bottom body was parameterized with 9 and 16 design variables. The compliance was used as the shape optimization objective function with the constraints on feasible design and volume invariance. In case of problem with 16 design variables, the optimized design was obtained after 120 design iterations and the parallel solution of the one design step was six times faster then the standard sequential code. Solution times of the sequential and parallel sensitivity analysis are in Table 1. Comparison of the initial and optimized stress distribution is in Figures 1 and 2. All tests were run on HP Blade server with 18x AMD Opteron Dual Core and Matlab Parallel Computing Engine.

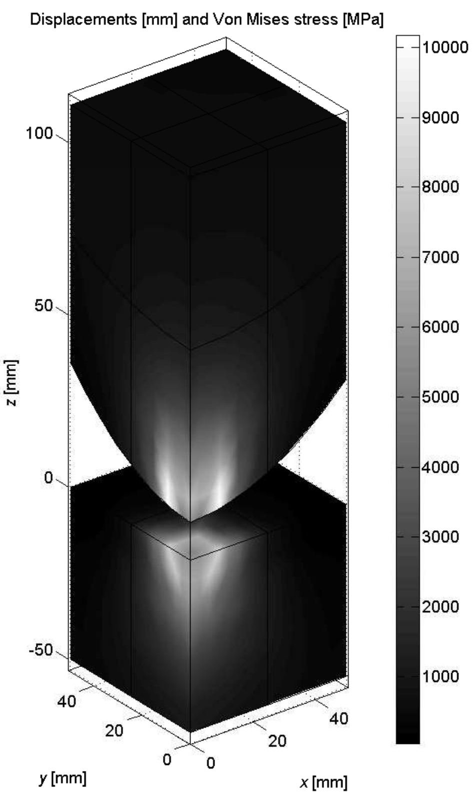

Figure 1: Initial design stress distribution

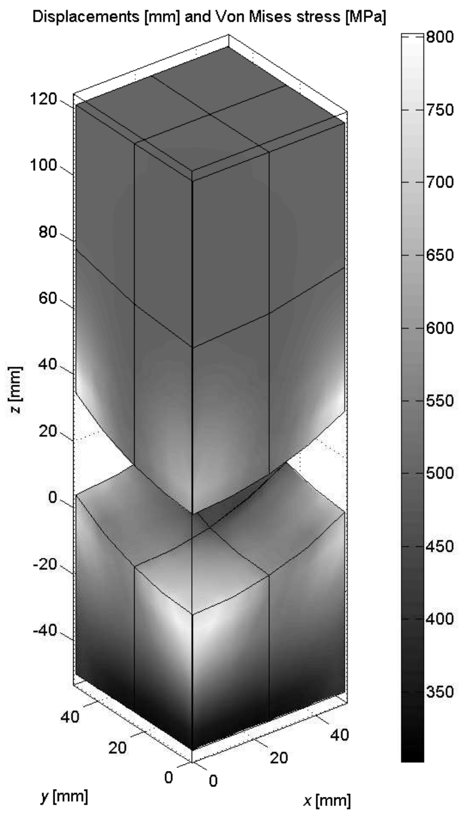

Figure 2: Optimized design stress distribution

Table 1: Performance of parallel sensitivity analysis

Problem	State problem	Sequential SA	Parallel SA	Speed-up
3D Hertz 9DV	15s	135s	30s	4.5x
3D Hertz 16DV	15s	240s	40s	6x

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