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36 Scalabilities of FETI for variational inequalities and contact shape optimization

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Introduction

We review our work on development of an efficient algorithm for numerical solution of variational inequalities and their application to the solution of multi-body contact shape optimization problems solved by the gradient methods. The method presented exploits optimal features of the linear FETI domain decomposition method with the natural coarse grid and a special structure of quadratic programming problems arising in dual formulation of the state problem. Results of numerical experiments are reported that document both numerical and parallel scalability of the algorithm for the solution of a model variational inequality and illustrate its efficiency in the solution of a contact shape optimization problem with the semi-analytic sensitivity analysis.

Following [DFS98, DGS00a, DGS00b], we start our exposition by describing the discretized variational inequality as a convex quadratic programming (QP) problem with a block diagonal stiffness matrix and general equality and inequality constraints. Then we show that the difficulties arising from general inequality constraints and possible semi-definiteness can be essentially reduced by the application of the duality theory. The matrix of the dual quadratic form turns out to be positive definite with a spectrum that is more favorably distributed for application of the conjugate gradient based methods than its primal counterpart. The performance of the method can be further improved by means of the natural coarse space projectors[FMR94]. The algorithm and the corresponding theoretical results are then reviewed in Section 36.

In Section 36, we show that the algorithm complies well with the semi-analytic method [HN96, DVR01] for evaluation of the gradients of the cost function that are necessary for implementation of the feasible direction method. In particular, it turns out that the gradient may be evaluated with only one decomposition of the stiffness matrix, regardless of the number of the design variables.

The algorithm has been implemented by means of PETSc [BGMS97] package on SP2 for the solution of a model problem. The results of numerical experiments indicate both numerical and parallel scalability of the algorithm. For solution of 2D contact and contact shape optimization problems, the algorithm has been implemented into the system ODESSY [RKO91] developed at the Institute of Mechanical Engineering of the Aalborg University. Reported numerical experiments indicate again high performance of the algorithm in the solution of the contact shape optimization problems. Let us recall that interesting results concerning numerical scalabity of a different algorithm for variational inequalities can be found in Schöberl [Sch98].

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Discretized variational inequality and duality

Let $\mathbb{K}$ denote a closed convex subset of a Sobolev space $\mathbb{V}$ defined on a domain Ω in $\mathbb{R}^d,\ d = 2, 3$ with sufficiently smooth boundary Γ, and consider a problem to find $u \in \mathbb{K}$ so that

$$a(u, v-u) \geq b(v-u) \text{ for all } v \in \mathbb{K}, \tag{1}$$

where a and b are a symmetric positive semidefinite bilinear form and a linear functional, respectively. We restrict our attention to problems (1) arising from discretization of free boundary elliptic problems [Glo83] with a spatial domain Ω comprising subdomains $\Omega^1, \ldots, \Omega^s$. An important special case is a problem to find an equilibrium of a system of elastic bodies in contact, possibly with auxiliary domain decomposition [DGS00b].

The finite element discretization of $\Omega = \Omega^1 \cup \ldots \cup \Omega^s$ with a suitable numbering of nodes results in the QP problem to find

$$\min \frac{1}{2} u^T K u - f^T u \ \text{ subject to } \ N_1 u \leq c_1, \ \ N_2 u = c_2 \tag{2}$$

with a symmetric block-diagonal matrix $K = \mathrm{diag}(K_1, \ldots, K_s)$ of order n, $f \in \mathbb{R}^n$, an $m \times n$, $m \leq n$ full rank matrix N comprising blocks N_1 and N_2, and similarly $c \in \mathbb{R}^m$ comprising subvectors c_1 and c_2. The diagonal blocks K_p that correspond to the subdomains $\Omega^p, p = 1, \ldots, s$ are positive definite or semidefinite sparse matrices. Moreover, we assume that the nodes are numbered in such a way that $K_1, \ldots, K_s$ are banded matrices that can be effectively decomposed by the Cholesky factorization. If a contact problem of elasticity is considered, then the vector f describes the nodal forces arising from the volume forces or some other tractions, the matrix N_1 and the vector c_1 describe the linearized incremental non-interpenetration conditions, and the matrix N_2 with $c_2 = 0$ describe the "gluing" conditions on auxiliary interfaces. More details may be found in [DFS98].

Even though (2) is a standard convex QP problem, its numerical solution may be expensive. The reasons are that K is typically ill-conditioned or singular, and that the feasible set is so complex that projections onto it can hardly be effectively computed, so that it would be very difficult to achieve fast identification of the contact interface and fast solution of auxiliary linear problems. These complications may be essentially reduced by applying the duality theory of convex programming (e.g. [Dos95, DFS98]).

Following [DGS00a, DGS00b], let us first assume that the matrix K has a nontrivial null space that may be used to define the natural coarse grid [FMR94]. The Lagrangian associated with problem (2) is

$$L(u, \lambda) = \frac{1}{2} u^T K u - f^T u + \lambda^T (Nu - c), \tag{3}$$

where the vector of multipliers comprises subvectors λ_1, λ_2 that comply with the block structure of N, so that we can rewrite the problem (2) as the saddle point problem

$$\text{Find} \quad (\hat{u}, \hat{\lambda}) \quad \text{such that} \quad L(\hat{u}, \hat{\lambda}) = \sup_{\lambda_1 \geq 0} \inf_u L(u, \lambda). \tag{4}$$

If we eliminate u from (4), we shall get the minimization problem

$$\min \Theta(\lambda) \quad \text{s.t.} \quad \lambda_1 \geq 0 \quad \text{and} \quad R^T(f - N^T \lambda) = 0, \tag{5}$$

where R denotes a matrix whose columns span the null space of K, $K^\dagger$ denotes any matrix that satisfies $KK^\dagger K = K$, and

$$\Theta(\lambda) = \frac{1}{2}\lambda^T NK^\dagger N^T\lambda - \lambda^T(NK^\dagger f - c). \tag{6}$$

Once the solution $\hat{\lambda}$ of (5) is obtained, the vector u that solves (4) can be evaluated by means of explicit formulas that may be found in [Dos95, DFS98]. The Hessian of Θ is closely related to that of the basic FETI method by Farhat and Roux, so that its spectrum is relatively favorably distributed for application of the conjugate gradient method.

Even though problem (5) is much more suitable for computations than (2) and has been used for efficient solution of contact problems [DFS98], further improvement may be achieved by the natural coarse grid projectors of Farhat, Mandel and Roux [FMR94]. In this way, it is even possible to achieve that the effective spectral condition number of the Hessian of the Lagrangian involved in computations is bounded independently of both the penalty parameter and the number of subdomains [DGS00b]. It does not follow that the resulting algorithm is scalable as it is still necessary to find the active constraints of the solution.

If the stiffness matrix K is regular, than the same procedure leads to the dual problem

$$\min\ \Theta(\lambda) \quad \text{s.t.} \quad \lambda \geq 0. \tag{7}$$

Algorithm

The problem (7) comprises only bound constraints, so that efficient algorithms using projections and adaptive precision control [Dos97] may be used. To apply this algorithm also for the problem (5), we shall use a variant of the augmented Lagrangian type algorithm proposed by Conn, Gould and Toint [CGT91] for identification of stationary points for more general problems. However, the algorithm that we describe here is modified in order to exploit the specific structure of our problem. Main improvement is in a sense adaptive precision control in Step 1.

To simplify our notation, let us denote $F = NK^\dagger N^T$, $G = R^T N^T$, and $d = R^T f$, and let us introduce the augmented Lagrangian with the penalization parameter ρ and the multiplier μ for the equality constraints for problem (5) by

$$L(\lambda, \mu, \rho) = \frac{1}{2}\lambda^T F\lambda - \lambda^T f + \mu^T(G\lambda - d) + \frac{1}{2}\rho||G\lambda - d||^2.$$

If we denote by $g = g(\lambda, \mu, \rho)$ the gradient of L with respect to λ, then the *projected gradient* $g^P = g^P(\lambda, \mu, \rho)$ of L at λ is given component-wise by

$$g_i^P = g_i \text{ for } \lambda_i > 0 \text{ or } i \notin I \text{ and } g_i^P = g_i^- \text{ for } \lambda_i = 0 \text{ and } i \in I$$

with $g_i^- = \min(g_i, 0)$, where I is the set of indices of constrained entries of λ.

All the parameters that must be defined prior to the application of the algorithm are listed in Step 0.

Algorithm 3.1. (Simple bound and equality constraints)

Step 0. Initialization of parameters

Set $0 < \alpha < 1,\ 1 < \beta,\ \rho_0 > 0,\ \eta_0 > 0,\ M > 0,\ \mu^0,\ \lambda^0$.

Step 1. Find λ^k so that $||g^P(\lambda^k, \mu^k, \rho_k)|| \leq M||G\lambda^k||$.

Step 2. If $||g^P(\lambda^k, \mu^k, \rho_k)||$ and $||G\lambda^k||$ are sufficiently small, then stop.

Step 3. $\mu^{k+1} = \mu^k + \rho_k G\lambda^k$

Step 4. $If||G\lambda^k|| \leq \eta_k$

Step 4a. then $\rho_{k+1} = \rho_k, \eta_{k+1} = \alpha\eta_k$

Step 4b. else $\rho_{k+1} = \beta\rho_k, \eta_{k+1} = \eta_k$

end if.

Step 5. Increase k and return to Step 1.

An implementation of Step 1 is carried out by the minimization of the augmented Lagrangian L subject to $\lambda \geq 0$ by an efficient algorithm that can be found in [Dos97]. The proposed algorithm has been proved [DFS01] to converge for any set of parameters that satisfy the prescribed relations. Moreover, an estimate of the rate of convergence of the approximations of the Lagrange multipliers has been proved that does not have any term that accounts for inexact solution of the bound constrained problems that are solved in Step 1, and it was proved that the penalty parameter is uniformly bounded. These results give theoretical support to Algorithm 3.1.

Discretized contact shape optimization problem

Let us now consider a contact shape optimization problem assuming for simplicity that the bodies occupy in a reference configuration subdomains $\Omega^1, \ldots, \Omega^s$ and that the shape of the first region Ω^1 depends on a vector of design variables α, so that the energy functional will have the form

$$j(u,\alpha) = \frac{1}{2}u^T K(\alpha)u - f^T(\alpha)u, \tag{8}$$

where the stiffness matrix $K(\alpha)$ and possibly the vector of nodal forces $f(\alpha)$ depend on α. The matrix N and the vector c now describe the linearized incremental conditions of non-interpenetration so that they also depend on α and the solution $u(\alpha)$ of the contact problem with the region $\Omega^1 = \Omega^1(\alpha)$ satisfies

$$u(\alpha) = \arg\min\{j(u,\alpha) : u \in C(\alpha)\}, \tag{9}$$

where

$$C(\alpha) = \{u : N(\alpha)u \leq c(\alpha)\}.$$

We shall consider the contact shape optimization problem to find

$$\min\{J(\alpha) : \alpha \in D_{adm}\}, \tag{10}$$

where $J(\alpha)$ is the cost functional that defines the cost function for design of body $\Omega^1(\alpha)$. The set of admissible design variables D_{adm} defines all feasible designs. For example, we can consider the cost functional $J(\alpha) \equiv -j(u,\alpha)$ that defines the minimal compliance problem. The set of admissible design parameters will be defined by

$$D_{adm} = \{-l \leq \alpha \leq r : \text{vol}(\Omega(\alpha)) \leq \text{vol}(\Omega(0))\}, \tag{11}$$

where l, r are given vectors with non-negative entries that define bounds on the design variables, and vol(.) is a mapping that assigns to each domain its volume. It has been proved that the minimal compliance problem has at least one solution and that the functional $j(u,\alpha)$ considered as a function of α is differentiable under reasonable assumptions [HN96].

If we want to exploit differentiability of problem (10), we must evaluate effectively partial derivatives of u with respect to the design variables $\alpha_1, \ldots, \alpha_k$. Our experience shows that the semi-analytic sensitivity analysis [HN96] is a method of choice. Let us denote by $I = \{1,...,m\}$ the set of indices of the Lagrange multipliers λ, $I_s = \{i \in I : N_{ij}(\alpha)u_j(\alpha) = d_i(\alpha) \wedge \lambda_i(\alpha) > 0\}$ the set of indices that correspond to couples of nodes in strong contact, and $I_w = \{i \in I : N_{ij}(\alpha)u_j(\alpha) = d_i(\alpha) \wedge \lambda_i(\alpha) = 0\}$ the set of indices that correspond to couples of nodes in weak contact. We have used the standard summing convention. Analysis of the Karush-Kuhn-Tucker conditions [HN96] enables to evaluate the directional derivative $u'(\alpha,\beta)$ in the direction β by solving the quadratic programming problem

$$\min_{\substack{N_w(\alpha)z \leq d_w(\alpha,\beta)\\ N_s(\alpha)z = d_s(\alpha,\beta)}} \frac{1}{2} z^T K(\alpha) z - z^T(f'(\alpha,\beta) - K'(\alpha,\beta)u(\alpha) + N'^T(\alpha,\beta)\lambda(\alpha)), \tag{12}$$

where $K'(\alpha,\beta)$, $f'(\alpha,\beta)$ and $N'(\alpha,\beta)$ denote computable directional derivatives of the stiffness matrix, traction vector and the constraint matrix, respectively. Matrices $N_w(\alpha)$ and $N_s(\alpha)$ are formed by the rows of the matrix $N(\alpha)$ with the indices that belong to I_w and I_s, respectively. Similarly, the vectors $d_w(\alpha,\beta)$ and $d_s(\alpha,\beta)$ are formed by the entries of $d'(\alpha,\beta) - N'(\alpha,\beta)u(\alpha)$ with indices in I_w and I_s, respectively. Solving (12) for $\beta = e_i,\ i = 1,...,m$, where e_i are the standard unit vectors, we evaluate the gradient of the state problem. Denoting $\bar{f}(\alpha,\beta) = f'(\alpha,\beta) - K'(\alpha,\beta)u(\alpha) + N'^T(\alpha,\beta)\lambda(\alpha)$, we can see that the problem (12) has the same structure as the problem (2), so that we can rewrite (12) into the dual form.

It turns out that the semi-analytic sensitivity analysis based on the dual formulation requires only one assembly and decomposition of the stiffness matrix. More information may be found in [HN96, VDR99, DVR01].

Numerical experiments

We have tested our algorithm on the solution of a simple model problem

$$\begin{array}{ll} \text{Minimize} & q(u_1,u_2) = \displaystyle\sum_{i=1}^{2} \left(\int_{\Omega^i} |\nabla u_i|^2 d\Omega - \int_{\Omega^i} f u_i d\Omega \right) \\ \text{subject to} & u_1(0,y) \equiv 0 \text{ and } u_1(1,y) \leq u_2(1,y) \text{ for } y \in [0,1], \end{array}$$

where $\Omega^1 = (0,1)\times(0,1)$, $\Omega^2 = (1,2)\times(0,1)$, $f(x,y) = -3$ for $(x,y) \in (0,1)\times[0.75,1)$, $f(x,y) = 0$ for $(x,y) \in (0,1)\times(0,0.75)$, $f(x,y) = -1$ for $(x,y) \in (1,2)\times(0,0.25)$ and

$f(x, y) = 0$ for $(x, y) \in (1, 2) \times (0.25, 1)$. This problem is semicoercive due to the lack of Dirichlet data on the boundary of Ω^2.

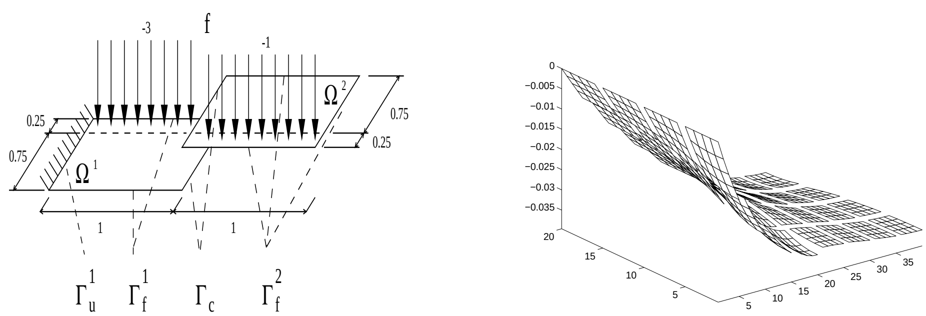
The solution of our model problem may be interpreted as the displacement of two membranes under the traction f. The left membrane is fixed on the left and the left edge of the right membrane is not allowed to penetrate below the edge of the left membrane as indicated in Figure 1a. The solution is unique because the right membrane is pressed down. More details about this model problem including some other results may be found in [DGS00a].

The model problem was discretized by regular grids defined by the stepsize $h = 1/n$ with $n + 1$ nodes in each direction per subdomain Ω^i, $i = 1, 2$. Each subdomain Ω^i was decomposed into $N \times N$ identical rectangles with dimensions $H = 1/N$. The solution of the model problem discretized by $H = 1/4$ and $h = 1/16$ can be seen in Figure 1b.

The model problem was solved for $h \in \{1/64, 1/128, 1/256, 1/512\}$, $H/h = 64$ with the stopping criterion

$$||g^P(\lambda, \mu, 0)|| \leq 10^{-4}||Nf|| \text{ and } ||G\lambda|| \leq 10^{-4}||d||.$$

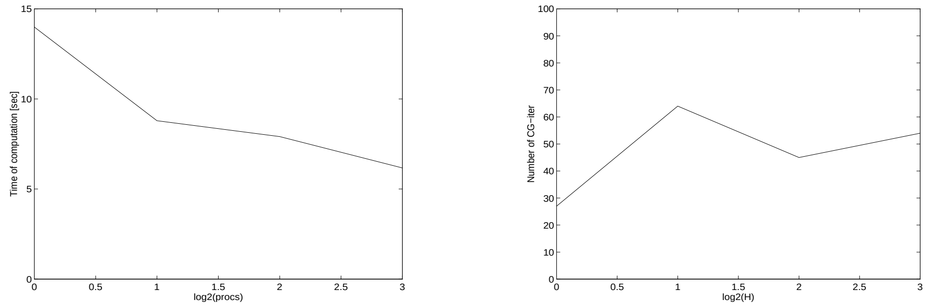
Both numerical and parallel scalabilities are demonstrated in Figure 2. Figure 2a demonstrates the dependence of elapsed time on the number of processors. Let us point out that the times were effected by the order and variety of used processors. Figure 2b then demonstrates high degree of numerical scalability of our algorithm for variational inequalities. In particular, the number of the conjugate gradient iterations ranged from 27 to 65 with only 54 iterations for the largest problem. The primal dimension ranged from 8450 to 540800. To solve the problem to the prescribed precision, it was necessary to identify about 350 active constraints on the contact interface comprising 520 couples of nodes that might have come into contact. The dual dimension was 14975.



(a) (b)

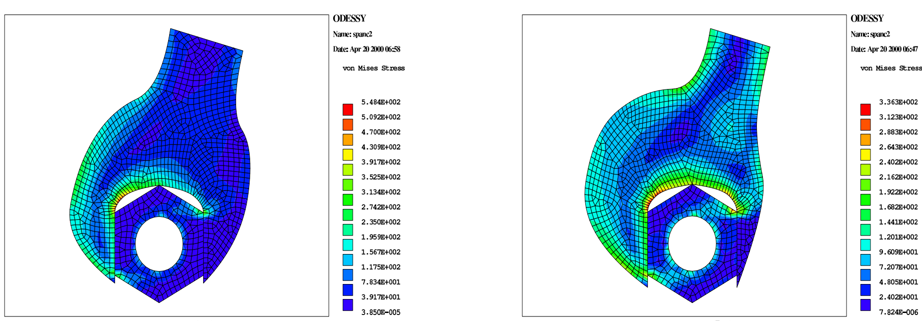
Figure 1: Model problem and its solution $h = 1/16, H = 1/4$

We have also tested our algorithm on the solution of a problem to find a shape of the spanner in Figure 3a that minimizes the maximum of von Mizes stress. To this end, we have implemented our algorithm into the system ODESSY developed at the Institute of Mechanical Engineering of the Aalborg University [RKO91]. The problem has been discretized by the finite element method using 2606 degrees of freedom with 46 couples of nodes that may get in contact. The admissible shape of the spanner was restricted by the box constraints on the design variables and by the upper bound on the volume. The initial and optimized designs are displayed in Figures 3a and 3b together with the values of the cost function. To get the results, we carried out 79 design steps.



(a) $h = 1/128, H = 1/4$ (b) $H/h = 64$

Figure 2: Parallel and numerical scalabilities



(a) (b)

Figure 3: Initial and optimized shape of the spanner

For comparison, we attempted to solve the problem also by the commercial software ANSYS. It turned out that the implementation of our algorithm in ODESSY was considerably more efficient. The analysis step in ODESSY required only 13 seconds, while it required 12 minutes to get a comparable result by ANSYS on the same computer. We were not able to carry out the optimization in ANSYS.

Comments and conclusions

The FETI-based domain decomposition algorithms for the solution of coercive and semicoercive variational inequalities has been reviewed and tested. Presented results of solution of a model variational inequality indicate both numerical and parallel scalability of the algorithm. Development of the theory is in progress. Theoretical results published so far [DGS00b] guarantee the convergence and robustness of the method. The method has been applied to optimization of a spanner and the efficiency of the method has been confirmed also by comparison with the commercial software. The salient feature of the algorithm in contact shape optimization is the reduction in the costs in preparing domain decomposition based solutions for related QP problems that appear in the dual formulation of the sensitivity analysis. In particular, it turns out that for each design step, it is necessary to carry out the preparation step only once regardless the number of the design variables. Further improvement may be achieved by the application of the mixed finite element discretization [DHK00, WK01].

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References

[BGMS97]Satish Balay, William D. Gropp, Louis C. McInnes, and Barry F. Smith. *PETSc 2.0 User Manual*. Argonne National Laboratory, http://www.mcs.anl.gov/petsc/, 1997.

[CGT91]Andrew R. Conn, Nicholas I. M. Gould, and Philipe L. Toint. A globally convergent augmented lagrangian algorithm for optimization with general constraints and simple bounds. *SIAM J. Num. Anal.*, 28:545–572, 1991.

[DFS98]Zdeněk Dostál, Ana Friedlander, and Sandra A. Santos. Solution of coercive and semicoercive contact problems by FETI domain decomposition. *Contemporary Math.*, 218:82–93, 1998.

[DFS01]Zdeněk Dostál, Ana Friedlander, and Sandra A. Santos. Augmented lagrangians with adaptive precision control for quadratic programming with simple bounds and equality constraints. *SIAM J. Opt.*, 2001. submitted.

[DGS00a]Zdeněk Dostál, Francisco A. M. Gomes, and Sandra A. Santos. Duality based domain decomposition with natural coarse space for variational inequalities. *J. Comput. Appl. Math.*, 126:397–415, 2000.

[DGS00b]Zdeněk Dostál, Francisco A. M. Gomes, and Sandra A. Santos. Solution of contact problems by FETI domain decomposition. *Computer Meth. Appl. Mech. Engng.*, 190:1611–1627, 2000.

[DHK00]Zdeněk Dostál, Jaroslav Haslinger, and Radek Kučera. Implementation of fixed point method for duality based solution of contact problems with friction. *Int. J.Comput. Appl. Math.*, 2000. submitted.

[Dos95]Zdeněk Dostál. Duality based domain decomposition with proportioning for the solution of free boundary problems. *J. Comp. Appl. Math.*, 63:203–208, 1995.

[Dos97]Zdeněk Dostál. Box constrained quadratic programming with proportioning and projections. *SIAM J. Opt.*, 7:871–887, 1997.

[DVR01]Zdeněk Dostál, Vít Vondrák, and John Rasmussen. Efficient algorithms for contact shape optimization. In V. Schulz, editor, *Workshop Fast Solution of Discretized Optimization Problems*, pages 98–106, WIAS Berlin, 2001.

[FMR94]Charbel Farhat, Jan Mandel, and Francois-Xavier Roux. Optimal convergence properties of the FETI domain decomposition method. *Comput. Methods Appl. Mech. Engrg.*, 115:367–388, 1994.

[Glo83]Roland Glowinski. *Numerical Methods for Nonlinear Variational Problems*. Springer Verlag, New York, 1983.

[HN96]Jaroslav Haslinger and Pekka Neittaanmäki. *Finite element approximation for optimal shape, material and topology design*. John Wiley and Sons, London, 1996.

[RKO91]John Rasmussen, Oluf Krogh, and Niels Olhoff. *ODESSY System for Optimization*. IME Aalborg University, 1991.

[Sch98]Joachim Schöberl. Solving the signorini problem on the basis of domain decomposition techniques. *Computing*, 60:323–344, 1998.

[VDR99]Vít Vondrák, Zdeněk Dostál, and John Rasmussen. FETI domain decomposition algorithms for sensitivity analysis in contact shape optimization. In Choi-Hong Lai, Petter E. Bjørstad, Mark Cross, and Olof B. Widlund, editors, *11th International Conference on Domain Decomposition in Science and Engineering*, pages 561–567, Bergen, 1999. Domain Decomposition Press.

[WK01]Barbara Wohlmuth and Rolf Krause. Multigrid methods based on the unconstrained product space arising from mortar finite element discretizations. *SIAM J. Numer. Anal.*, 39:192–213, 2001.