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41. Toward scalable FETI algorithm for variational inequalities with applications to composites

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1. Introduction. In this paper we review our results related to development of scalable algorithms for solution of variational inequalities. After describing a model problem, we apply the FETI methodology to reduce it to the quadratic programming problem with equality and non-negativity constraints. Then we present the basic algorithm with a "natural coarse grid" proposed by Dostál, Friedlander, Santos and Gomes [9, 10, 12] and report recent theoretical results that may be used either to prove scalability of parts of the basic algorithm or to modify the basic algorithm so that it is scalable. Finally we give results of parallel solution of the model problem discretized by up to more than eight million of nodal variables and show application of the algorithm to analysis of fibrous composite material that was studied by Wriggers [20]. The results related to development of scalable algorithms for elliptic variational inequalities include experimental evidence of numerical scalability of the algorithm based on monotone multigrid [17] by Kornhuber. Another interesting algorithm was proposed by Schöberl [18]. Also the authors of the original FETI method proposed its adaptation to the solution of variational inequalities and gave experimental evidence of numerical scalability of their algorithm with a coarse grid initial approximation [14]. Let us recall that the FETI (Finite Element Tearing and Interconnecting) method proposed by Farhat and Roux [16] for solving of linear elliptic boundary value problems is based on the decomposition of the spatial domain into non-overlapping subdomains that are "glued" by Lagrange multipliers. Using the so called "natural coarse grid", Farhat, Mandel and Roux [15] modified the basic FETI algorithm so that they were able to prove its numerical scalability. These results are key ingredients in our research.

2. Model problem. Let $\Omega = \Omega^1 \cup \Omega^2$, $\Omega^1 = (0,1) \times (0,1)$ and $\Omega^2 = (1,2) \times (0,1)$ denote open domains with boundaries Γ^1, Γ^2 decomposed into $\Gamma_u^1 = \{(x_1,x_2) \in \Gamma^1 : x_1 = 0\}$, $\Gamma_c^i = \{(x_1,x_2) \in \Gamma^i : x_1 = 1\}$, and Γ_f^i formed by the remaining sides of $\Omega^i, i = 1,2$. Let $H^1(\Omega^i)$ denote the Sobolev space of first order on the space $L^2(\Omega^i)$ of the functions on Ω^i whose squares are integrable in the sense of Lebesgue. Let

$$V^1 = \left\{v \in H^1(\Omega^1) : v^1 = 0 \quad \text{on} \quad \Gamma_u^1\right\}$$

denote the closed subspace of $H^1(\Omega^1)$, $V^2 = H^1(\Omega^2)$, and let

$$V = V^1 \times V^2 \qquad \text{and} \qquad \mathcal{K} = \left\{(v^1,v^2) \in V : v^2 - v^1 \geq 0 \quad \text{on} \quad \Gamma_c\right\}$$

denote a closed subspace and a closed convex subset of $\mathcal{H} = H^1(\Omega^1) \times H^1(\Omega^2)$, respectively. The relations on the boundaries are in terms of traces. On $\mathcal{H}$ we shall define a symmetric bilinear form

$$a(u,v) = \sum_{i=1}^{2} \int_{\Omega_i} \left(\frac{\partial u^i}{\partial x}\frac{\partial v^i}{\partial x} + \frac{\partial u^i}{\partial y}\frac{\partial v^i}{\partial y} \right) d\Omega$$

and a linear form

$$\ell(v) = \sum_{i=1}^{2} \int_{\Omega_i} f^i v^i d\Omega,$$

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where $f^i \in L^2(\Omega^i), i = 1, 2$ are the restrictions of

$$f(x,y) = \left\{ \begin{array}{c} -3 \quad \text{for} \quad (x,y) \in (0,1) \times [0.75, 1) \\ 0 \quad \text{for} \quad (x,y) \in (0,1) \times [0, 0.75) \quad \text{and} \quad (x,y) \in (1,2) \times [0.25, 1) \\ -1 \quad \text{for} \quad (x,y) \in (1,2) \times [0, 0.25) \end{array} \right\}.$$

Thus we can define a problem

$$\text{Minimize} \;\; q(u) = \frac{1}{2} a(u,u) - \ell(u) \;\; \text{subject to} \;\; u \in \mathcal{K}. \tag{2.1}$$

More details about this model problem including a discussion of the existence and uniqueness may be found in [9].

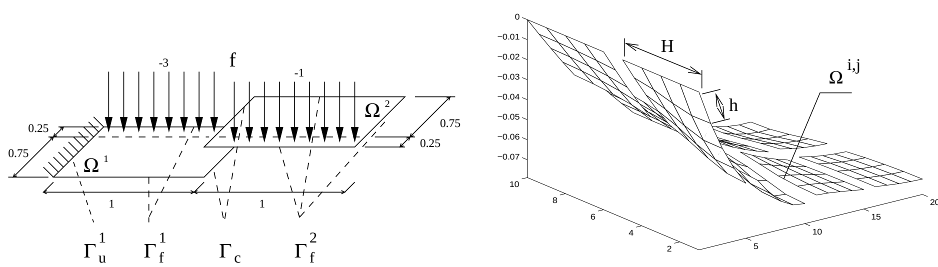

Figure 2.1: Model problem and its solution

3. Domain decomposition and discretized problem with a natural coarse grid. To enable efficient application of the domain decomposition methods, we can optionally decompose each Ω^i into square subdomains $\Omega^{i1}, \ldots, \Omega^{ip}, p = s^2 > 1$. The continuity in Ω^1 and Ω^2 of the global solution assembled from the local solutions u^{ij} will be enforced by the "gluing" conditions $u^{ij}(x) = u^{ik}(x)$ that should be satisfied for any x in the interface $\Gamma^{ij,ik}$ of Ω^{ij} and Ω^{ik}. After modifying appropriately the definition of problem (2.1), introducing regular grids in the subdomains Ω^{ij} that match across the interfaces $\Gamma^{ij,kl}$, indexing contiguously the nodes and entries of corresponding vectors in the subdomains, and using the finite element discretization, we get the discretized version of problem (2.1) with the auxiliary domain decomposition that reads

$$\min \frac{1}{2} x^T A x - f^T x \quad \text{s.t.} \quad B_I x \le 0 \quad \text{and} \quad B_E x = 0. \tag{3.1}$$

In (3.1), A denotes a positive semidefinite stiffness matrix, the full rank matrices B_I and B_E describe the discretized inequality and gluing conditions, respectively, and f represents the discrete analog of the linear term $\ell(u)$. Details may be found in [9]. Introducing the notation

$$\lambda = \begin{bmatrix} \lambda_I \\ \lambda_E \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} B_I \\ B_E \end{bmatrix},$$

we can observe that B is a full rank matrix and write the Lagrangian associated with problem (3.1) briefly as

$$L(x, \lambda) = \frac{1}{2} x^T A x - f^T x + \lambda^T B x.$$

It is well known that (3.1) is equivalent to the saddle point problem

$$\text{Find} \quad (\overline{x}, \overline{\lambda}) \quad \text{s.t.} \quad L(\overline{x}, \overline{\lambda}) = \sup_{\lambda_I \geq 0} \inf_x L(x, \lambda). \tag{3.2}$$

After eliminating the primal variables x from (3.2), we shall get the minimization problem

$$\min \Theta(\lambda) \quad \text{s.t.} \quad \lambda_I \geq 0 \quad \text{and} \quad R^T(f - B^T\lambda) = 0, \tag{3.3}$$

where

$$\Theta(\lambda) = \frac{1}{2}\lambda^T B A^\dagger B^T \lambda - \lambda^T B A^\dagger f, \tag{3.4}$$

$A^\dagger$ denotes a generalized inverse that satisfies $AA^\dagger A = A$, and R denotes the full rank matrix whose columns span the kernel of A. Using the fact that $R^T B^T$ is a full rank matrix, it may be verified that the Hessian of Θ is positive definite. Even though problem (3.3) is much more suitable for computations than (3.1) and was used to efficient solving of the discretized variational inequalities [7], further improvement may be achieved by adapting some simple observations and the results of Farhat, Mandel and Roux [15]. Let us denote

$$F = BA^\dagger B^T, \qquad \widetilde{d} = BA^\dagger f,$$
$$\widetilde{G} = R^T B^T, \qquad \widetilde{e} = R^T f,$$

and let $\widetilde{\lambda}$ solve $\widetilde{G}\widetilde{\lambda} = \widetilde{e}$. Let $d = \widetilde{d} - F\widetilde{\lambda}$ and let G denote a regular matrix with orthonormal rows and the same kernel as $\widetilde{G}$, so that

$$Q = G^T G \qquad \text{and} \qquad P = I - Q$$

are the orthogonal projectors on the image space of G^T and on the kernel of G, respectively. Problem (3.3) may then be reduced to

$$\min \quad \frac{1}{2}\lambda^T PFP\lambda - \lambda^T Pd \quad \text{s.t} \quad G\lambda = 0 \quad \text{and} \quad \lambda_I \geq -\widetilde{\lambda_I}. \tag{3.5}$$

The Hessian $H_\rho = PFP + \rho Q$ of the augmented Lagrangian

$$L(\lambda, \mu, \rho) = \frac{1}{2}\lambda^T(PFP + \rho Q)\lambda - \lambda^T Pd + \mu^T G\lambda \tag{3.6}$$

is decomposed by the projectors P and Q whose image spaces are invariant subspaces of H_ρ. The key point is that the analysis by Farhat, Mandel and Roux [15] implies that the *spectral condition number* $\kappa(H_\rho)$ of H_ρ is *bounded independently* of h for a regular decomposition provided H/h is uniformly bounded, where h and H are the mesh and subdomain diameters, respectively.

4. Solution of bound and equality constrained quadratic programming problems and optimal penalty. Dostál, Friedlander and Santos [8] proposed a variant of the augmented Lagrangian type algorithm by Conn, Gould and Toint [3] that fully exploits the specific structure of problem (3.3). To describe it, let us recall that the gradient of the augmented Lagrangian 3.6 is given by

$$g(\lambda, \mu, \rho) = PFP\lambda - Pd + G^T(\mu + \rho G\lambda),$$

so that the *projected gradient* $g^P = g^P(\lambda, \mu, \rho)$ of L at λ is given componentwise by

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

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

Algorithm 4.1 (Quadratic programming with simple bound and equality constraints)

Step 0. Set $0 < \alpha < 1,\ 1 < \beta,\ \rho_0 > 0,\ \eta_0 > 0,\ M > 0,\ \mu^0$ and $k = 0$.

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

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 $||G\lambda^k|| \le \eta_k$

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 by one and return to Step 1.

The algorithm has been proved [8] to converge for any set of parameters that satisfy the prescribed relations. Moreover, it has been proved that the asymptotic rate of convergence is the same as for the algorithm with an exact solution of the auxiliary QP problems (i.e. $M = 0$) and that the penalty parameter is uniformly bounded. These results give theoretical support to Algorithm 4.1. The performance of the algorithm depends essentially on the rate of convergence of the method that minimizes L in the inner loop as the number of the outer iterations was rather small ranging from two to six. We use the active set strategy in combination with the proportioning conjugate gradient algorithm [4] and the gradient projection [18]. We managed to get the rate of convergence for the inner loop in terms of $\kappa(H_\rho)$ [6]. Combining this result with that on the boundedness of $\kappa(H_\rho)$, *we find that the rate of convergence in the inner loop does not depend on the discretization parameter* h . The best results were achieved with relatively high penalty parameters which may be explained by the fact that it is possible to give the rate of convergence for the conjugate gradient method for minimization of the quadratic form with the Hessian H_ρ that depends neither on ρ nor on the rank of G [5]. This suggests that we could try to enforce the equality constraints by the *penalty method*. Closer inspection reveals nice optimality property of the penalty method applied to 3.5, namely if H/h is bounded, then there is a constant C independent of h such that if $\|g^P(\lambda, 0, \rho)\| \le \epsilon\|Pd\|$, then

$$\|G\lambda\| \le \frac{C(1+\epsilon)}{\rho}\|Pd\|.$$

It follows that using the penalty in combination with the algorithm with the rate of convergence, it is possible to *get an approximate solution with the prescribed precision in a number of iterations independent of the discretization parameter* h. We shall give the details elsewhere. Another way to achieve scalability, at least for coercive problems, is to apply FETI-DP method [2].

5. Numerical experiments. In this section we report some results of numerical solution of the model problem of Section 2 and of a problem with the fibrous composite material in order to illustrate the performance of the algorithm, in particular its numerical and parallel scalability. To this end, we have implemented Algorithm 4.1 in C exploiting PETSc [1] to solve the basic dual problem (3.3) so that we could plug in the projectors to the natural coarse space (3.5) and the dual penalty method. Each domain $\Omega^i,\ i = 1, 2$ was first decomposed into identical rectangles Ω^{ij} with the sides H that were discretized by the regular grids defined by the stepsize h as in Figure 2.1. The stopping criterium $\left\|g^P(\lambda, \mu, 0)\right\| \le 10^{-4}\,\|d\|$ and $\|G\lambda\| \le 10^{-4}\left\|(\widetilde{G}G^T)^{-1}\widetilde{e}\right\|$ was used in all calculations.

Solution of the model problem for $h = 1/8$ and $H = 1/2$ is in Figure 2.1. The experiments were run on the Lomond 18-processor Sun HPC 6500 Ultra SPARC-II based SMP system with 400 MHz, 18 GB of shared memory, 90 GB disc space, nominal peak performance 14.4 GFlops, 16 kB level 1 and 8 MB level 2 cache of the EPCC Edinburgh, and on the SGI Origin 3800 128-processor R12000 shared memory (MIMD) system with 400 Mhz, 48.128 GB of RAM, 500 GB disc space, FDDI 1 Gb/sec of the Johannes Kepler University Linz. All the computations were carried out with parameters $M = 1, \rho_0 = 10, \Gamma = 1, \lambda^0 = \frac{1}{2}Bf$.

Table 5.1: Parallel scalability for 128 subdomains

processors	1	2	4	8	16	32	64	128
Time[sec]	1814.0	566.4	185.9	54.5	32.0	32.7	62.5	147.0

Table 5.2: Performance for varying decomposition and discretization

H	1	1/2	1/4	1/8
H/h \ procs	2	8	16	16
128	33282/129/41.95 28	133128/1287/89.50 59	532512/6687/74.9 36	2130048/29823/421.5 47
32	2178/33/0.20 17	8712/327/0.50 33	34848/1695/1.48 30	139392/7551/11.66 37
8	162/9/0.03 10	648/87/0.10 20	2592/447/0.39 23	10365/1983/2.06 27

Table 5.3: Highlights

h	H	prim. dim.	dual. dim.	num. of subdom.	procs	out. iter.	cg. iter.	time [sec]
1/1024	1/8	2130048	29823	128	32	2	47	167.8
1/2048	1/8	8454272	59519	128	64	2	65	1281.0

The selected results of the computations are summed up in Tables 5.1 - 5.4. Table 5.1 indicates that the algorithm presented enjoys high parallel scalability for problem with $h = 1/512, H = 1/8$, primal dimension 540800, and dual dimension 14975 that was solved on the computer SGI Origin. Table 5.2 indicates that Algorithm 4.1 may enjoy also high numerical scalability, even though the latter is so far supported by theory only for the inner loops of the algorithm. In particular, for varying decompositions and discretizations, the upper row of each field of the table gives the corresponding primal/dual dimensions and times in seconds on the Lomond, while the number in the lower row gives a number of the conjugate gradient iterations that were necessary for the solution of the problem to the given precision. We can see that the number of the conjugate gradient iterations for a given ratio H/h varies very moderately. The results for the largest problems using the SGI Origin are in Table 5.3. Optimality of dual penalty is illustrated in Table 5.4. We conclude that at least for our model problem, the experiments indicate that the cost of numerical solution of the variational inequalities may be comparable to the cost of solution of corresponding linear problem. To check the performance and robustness of our algorithm on a more challenging problem, we considered linear elastic response of a sample of fibrous composite material. For simplicity, we assumed that the fibers are inserted into the matrix

Table 5.4: Optimal enforcing of $\|G\lambda\| \,/\, \|d\|$

prim.dim./dual.dim.		1152/591	10368/1983	139392/7551	2130048/29823
$\|G\lambda\| \,/\, \|d\|$	$\rho = 10$	3.027e-03	3.108e-03	3.115e-03	3.117e-03
	$\rho = 1000$	3.144e-05	3.213e-05	3.222e-05	3.225e-05
	$\rho = 100000$	3.145e-07	3.212e-07	3.224e-07	

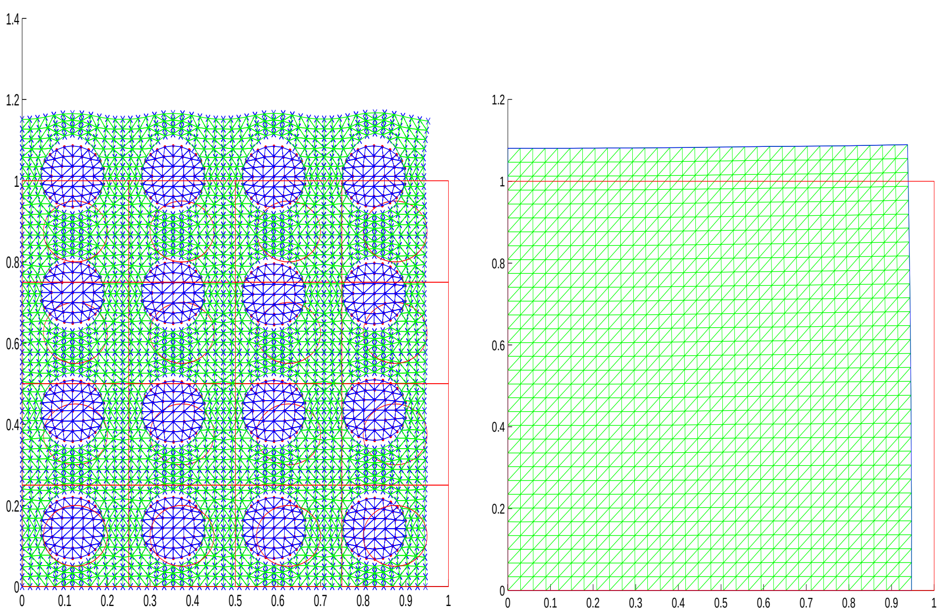

Figure 5.1: Fiber composite and homogeneous sample in strain

so that there is no adhesion. Such composites may be useful e.g. in design of materials with different response to strain and stress. The algorithm may be modified to model debonding of more realistic material as considered in Wriggers [20]. The problem is difficult due to the long, split, a priori unknown contact interface with many points in which the condition of strict complementarity is violated. We decomposed the space domain of the sample into squares, each square comprising two subdomains consisting of a circular fiber and corresponding part of the matrix, and discretized the problem as in Figure 5.1. The primal and dual dimensions of the problem were 6176 and 990, respectively. The number of outer iterations was only four, while the solution to the relative precision 1E-4 required 591 iterations with 157 faces examined. We conclude that the performance of the algorithm is acceptable even for problems where the results related to scalability mentioned above do not apply as in this case when the decomposition includes subdomains that are not simply connected.

6. Comments and conclusions. We have reviewed a domain decomposition algorithm for the solution of variational inequalities. The method combines a variant of the FETI method with projectors to the natural coarse grid and recently developed algorithms for the solution of special QP problems. We have also introduced the penalty approximation that is optimal in the sense that a fixed penalty parameter can enforce feasibility to the prescribed relative precision regardless of the discretization parameter. The theory gives relevant results concerning the scalability of main parts of the basic algorithm and yields full theoretical support of its variants presented in the paper. Numerical experiments with the model variational inequality discretized by up to more than eight million of nodal variables indicate that even the basic algorithm may enjoy full numerical and parallel scalability and confirm a kind of optimality for the dual penalty. Numerical solution of a problem with fibrous composite material confirm that the algorithm presented is effective for more challenging problems. In fact, it has already been exploited for solving 2D problems with Coulomb friction [11] and contact shape optimization [13, 19].

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