Quadratic Programming and Scalable Algorithms for Variational Inequalities

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Summary. We first review our recent results concerning optimal algorithms for the solution of bound and/or equality constrained quadratic programming problems. The unique feature of these algorithms is the rate of convergence in terms of bounds on the spectrum of the Hessian of the cost function. Then we combine these estimates with some results on the FETI method (FETI-DP, FETI and Total FETI) to get the convergence bounds that guarantee the scalability of the algorithms. i.e. asymptotically linear complexity and the time of solution inverse proportional to the number of processors. The results are confirmed by numerical experiments.

1 Introduction

One of the most impressive results in numerical analysis of the twentieth century was discovery that the systems of linear equations arising from the discretization of an elliptic partial differential equation may be solved by the multigrid or domain decomposition methods with asymptotically linear complexity. In this paper, we show how to extend these results to get scalable algorithms for variational inequalities. Our basic tool is the FETI method, which was proposed by Farhat and Roux [28] for parallel solution of problems described by elliptic partial differential equations. Its key ingredient is the 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. Observing that the equality constraints may be used to define so called "natural coarse grid", Farhat, Mandel and Roux [27] modified the basic FETI algorithm so that they were able to prove its numerical scalability. A similar results were achieved by the Dual-Primal FETI method (FETI–DP) introduced by Farhat et al. [26]; see also [32].

If the FETI procedure is applied to the contact problems, the resulting quadratic programming problem has not only the equality constraints, but also the non-negativity constraints. Even though the latter is a considerable complication as compared with the linear problem, the resulting problem is still easier to solve than the contact problem in displacements as it is smaller, better conditioned having constraints with simpler structure. Promising experimental results by Dureisseix and Farhat [24] support this claim and even indicate numerical scalability of their metod. Similar results were achieved also with the FETI–DP method by Avery, Rebel, Lesoinne and Farhat [1]. A different approach based on the augmented Lagrangian method was used by Dostál, Friedlander, Gomes and Santos [12, 13].

In this paper we review our recent improvements that resulted in development of theoretically supported scalable algorithms for variational inequalities that combine various FETI based domain decomposition methods with our optimal quadratic programming algorithms [6, 23, 7]. We present optimal algorithms based on scalable variant of FETI [27] or on its easier implementable variant called TFETI [19], on FETI–DP [26] and on optimal dual penalty [17]. Let us point out that the effort to develop scalable solvers for variational inequalities was not restricted to FETI. For example, developing ideas of Mandel [35], Kornhuber, Krause and Wohlmuth [33, 34, 40] gave an experimental evidence of numerical scalability of the algorithm based on monotone multigrid. Nice results concerning development of scalable algorithms were proved by Schöberl [37].

We start our exposition by presenting our MPRGP (Modified Proportioning with Reduced Gradient Projection) and SMALBE (Semimonotonic Augmented Lagrangians for Bound and Equality constrained problems) algorithms with in a sense optimal rates of convergence. Then we present a simple model problem and the FETI methodology [12] that turns the variational inequality into the quadratic programming problem with bound and possibly equality constraints. Combining these ingredients, we shall get new algorithms for numerical solution of boundary elliptic variational inequalities. A unique feature of these algorithms is theoretically guaranteed numerical scalability. We report results of numerical experiments that are in agreement with the theory and indicate high parallel and numerical scalability of the algorithm presented.

2 Bound Constrained Problems

Let us consider the problem

$$\text{minimize} \quad q(\mathbf{x}) \quad \text{subject to} \quad \mathbf{x} \in \Omega_B \tag{1}$$

with $q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathsf{A}\mathbf{x} - \mathbf{b}^T\mathbf{x}$, A a symmetric positive definite matrix, $\mathbf{b} \in I\!R^n$, $\Omega_B = \{\mathbf{x} : \mathbf{x} \geq \boldsymbol{\ell}\}$ and $\boldsymbol{\ell} \in I\!R^n$. The unique solution $\overline{\mathbf{x}}$ of (1) is fully determined by the Karush-Kuhn-Tucker optimality conditions [3] so that for $i = 1, \ldots, n$,

$$\overline{x}_i = \ell_i \text{ implies } \overline{g}_i \geq 0 \text{ and } \overline{x}_i > \ell_i \text{ implies } \overline{g}_i = 0, \tag{2}$$

where $\mathbf{g} = \mathbf{g}(\mathbf{x})$ denotes the gradient of q defined by

$$\mathbf{g} = \mathbf{g}(\mathbf{x}) = \mathsf{A}\mathbf{x} - \mathbf{b}. \tag{3}$$

The conditions (2) can be described alternatively by the *free gradient* $\boldsymbol{\varphi}$ and the *chopped gradient* $\boldsymbol{\beta}$ that are defined by

$$\varphi_i(\mathbf{x}) = g_i(\mathbf{x}) \text{ for } x_i > \ell_i, \varphi_i(\mathbf{x}) = 0 \text{ for } x_i = \ell_i,$$

$$\beta_i(\mathbf{x}) = 0 \text{ for } x_i > \ell_i, \beta_i(\mathbf{x}) = g_i^-(\mathbf{x}) \text{ for } x_i = \ell_i,$$

where we have used the notation $g_i^- = \min\{g_i, 0\}$. Thus the conditions (2) are satisfied iff the *projected gradient* $\mathbf{g}^P(\mathbf{x}) = \boldsymbol{\varphi}(\mathbf{x}) + \boldsymbol{\beta}(\mathbf{x})$ is equal to the zero. The algorithm for the solution of (1) that we describe here exploits a given constant $\Gamma > 0$, a test to decide about leaving the face and three types of steps to generate a sequence of the iterates $\{\mathbf{x}^k\}$ that approximate the solution of (1). The *expansion step* may expand the current active set and is defined by

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \overline{\alpha}\widetilde{\boldsymbol{\varphi}}(\mathbf{x}^k) \tag{4}$$

with the fixed steplength $\overline{\alpha} \in (0, \|\mathsf{A}\|^{-1}]$ and the *reduced free gradient* $\widetilde{\boldsymbol{\varphi}}(\mathbf{x})$ with the entries $\widetilde{\varphi}_i = \widetilde{\varphi}_i(\mathbf{x}) = \min\{(x_i - \ell_i)/\overline{\alpha}, \varphi_i\}$. If the inequality

$$||\boldsymbol{\beta}(\mathbf{x}^k)||^2 \leq \Gamma^2 \widetilde{\boldsymbol{\varphi}}(\mathbf{x}^k)^\top \boldsymbol{\varphi}(\mathbf{x}^k) \tag{5}$$

holds then we call the iterate $\mathbf{x}^k$ *strictly proportional.* The test (5) is used to decide which component of the projected gradient $\mathbf{g}^P(\mathbf{x}^k)$ will be reduced in the next step. The *proportioning step* may remove indices from the active set and is defined by

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_{cg}\boldsymbol{\beta}(\mathbf{x}^k) \tag{6}$$

with the steplength α_{cg} that minimizes $q\left(\mathbf{x}^k - \alpha\boldsymbol{\beta}(\mathbf{x}^k)\right)$. It is easy to check [3] that α_{cg} that minimizes $q(\mathbf{x} - \alpha\mathbf{d})$ for a given $\mathbf{d}$ and $\mathbf{x}$ may be evaluated by the formula

$$\alpha_{cg} = \alpha_{cg}(\mathbf{d}) = \frac{\mathbf{d}^\top \mathbf{g}(\mathbf{x})}{\mathbf{d}^\top \mathsf{A}\mathbf{d}}. \tag{7}$$

The *conjugate gradient step* is defined by

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_{cg}\mathbf{p}^k \tag{8}$$

where $\mathbf{p}^k$ is the conjugate gradient direction [3] which is constructed recurrently. The recurrence starts (or restarts) from $\mathbf{p}^s = \boldsymbol{\varphi}(\mathbf{x}^s)$ whenever $\mathbf{x}^s$ is generated by the expansion or proportioning step. If $\mathbf{p}^k$ is known, then $\mathbf{p}^{k+1}$ is given [3] by

$$\mathbf{p}^{k+1} = \boldsymbol{\varphi}(\mathbf{x}^{k+1}) - \gamma\mathbf{p}^k, \quad \gamma = \frac{\boldsymbol{\varphi}(\mathbf{x}^{k+1})^\top \mathsf{A}\mathbf{p}^k}{(\mathbf{p}^k)^\top \mathsf{A}\mathbf{p}^k}. \tag{9}$$

Algorithm 1. Modified proportioning with reduced gradient projections (MPRGP).
Let $\mathbf{x}^0 \in \Omega$, $\overline{\alpha} \in (0, \|\mathsf{A}\|^{-1}]$, and $\Gamma > 0$ be given. For $k \geq 0$ and $\mathbf{x}^k$ known, choose $\mathbf{x}^{k+1}$ by the following rules:
Step 1. If $\mathbf{g}^P(\mathbf{x}^k) = \mathbf{o}$, set $\mathbf{x}^{k+1} = \mathbf{x}^k$.
Step 2. If $\mathbf{x}^k$ is strictly proportional and $\mathbf{g}^P(\mathbf{x}^k) \neq \mathbf{o}$, try to generate $\mathbf{x}^{k+1}$ by the conjugate gradient step. If $\mathbf{x}^{k+1} \in \Omega$, then accept it, else use the expansion step.
Step 3. If $\mathbf{x}^k$ is not strictly proportional, define $\mathbf{x}^{k+1}$ by proportioning.

Algorithm 1 has been proved to enjoy the R-linear rate of convergence in terms of the spectral condition number [23].

To formulate the optimality results, let $\mathcal{T}$ denote any set of indices and assume that for any $t \in \mathcal{T}$ there is defined the problem

$$\text{minimize} \quad q_t(\mathbf{x}) \quad \text{s.t.} \quad \mathbf{x} \in \Omega_B^t \tag{10}$$

with $\Omega_B^t = \{\mathbf{x} \in I\!R^{n_t} : \mathbf{x} \geq \boldsymbol{\ell}\}$, $q_t(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathsf{A}_t \mathbf{x} - \mathbf{b}_t^\top \mathbf{x}$, $\mathsf{A}_t \in I\!R^{n_t \times n_t}$ symmetric positive definite, and $\mathbf{b}_t, \mathbf{x}, \boldsymbol{\ell}_t \in I\!R^{n_t}$. Our optimality result then reads as follows.

Theorem 1. *Let the Hessian matrices* $\mathsf{A}_t = \boldsymbol{\nabla}^2 q_t$ *of (10) satisfy*

$$0 < a_{\min} \leq \lambda_{\min}(\mathsf{A}_t) \leq \lambda_{\max}(\mathsf{A}_t) \leq a_{\max},$$

let $\{\mathbf{x}_t^k\}$ *be generated by Algorithm 1 for (10) with a given* $\mathbf{x}_t^0 \in \Omega_B^t$, $\overline{\alpha} \in (0, a_{\max}^{-1}]$, *and let* $\Gamma > 0$. *Let there be a constant* a_b *such that* $\|\mathbf{x}_t^0\| \leq a_b \|\mathbf{b}_t\|$ *for any* $t \in \mathcal{T}$.
(i) If $\epsilon > 0$ *is given, then the approximate solution* $\overline{\mathbf{x}}_t$ *of (10) which satisfies*

$$\|\mathbf{x}_t^k - \overline{\mathbf{x}}_t\| \leq \epsilon \|\mathbf{b}_t\|$$

may be obtained at $O(1)$ *matrix-vector multiplications by* A_t.
(ii) If $\epsilon > 0$ *is given, then the approximate solution* $\mathbf{x}_t^k$ *of (10) which satisfies*

$$\|\mathbf{g}_t^P(\mathbf{x}_t^k)\| \leq \epsilon \|\mathbf{b}_t\|$$

may be obtained at $O(1)$ *matrix-vector multiplications by* A_t.

Proof. See [23].

Numerical experiments and implementation details may be found in [23].

3 Bound and Equality Constrained Problems

We shall now be concerned with the problem of finding the minimizer of the strictly convex quadratic function $q(\mathbf{x})$ subject to the bound and linear equality constraints, that is

$$\text{minimize} \quad q(\mathbf{x}) \quad \text{subject to} \quad \mathbf{x} \in \Omega_{BE} \tag{11}$$

with $\Omega_{BE} = \{\mathbf{x} \in I\!R^n : \mathbf{x} \geq \boldsymbol{\ell} \text{ and } \mathsf{C}\mathbf{x} = \mathbf{o}\}$ and $\mathsf{C} \in I\!R^{m \times n}$. We do not require that C is a full row rank matrix, but we shall assume that Ω_{BE} is not empty. Let us point out that confining ourselves to the homogeneous equality constraints does not mean any loss of generality, as we can use a simple transform to reduce any non-homogeneous equality constraints to our case. The algorithm that we describe here combines in a natural way the augmented Lagrangians and MPRGP described above. It is related to the earlier work of Friedlander and Santos with the present author [11]. Let us recall that the basic scheme that we use was proposed by Conn, Gould and Toint [4] who adapted the augmented Lagrangian method to the solution of the problems with a general cost function subject to general equality constraints and simple bounds.

Algorithm 2. (Semi-monotonic augmented Lagrangians for bound and equality constraints (SMALBE)

Given $\eta > 0,\ \beta > 1,\ M > 0,\ \rho_0 > 0,$ and $\boldsymbol{\mu}^0 \in I\!R^m$, set $k = 0$.

Step 1. {Inner iteration with adaptive precision control.}
Find $\mathbf{x}^k$ such that

$$\|\mathbf{g}^P(\mathbf{x}^k, \boldsymbol{\mu}^k, \rho_k)\| \leq \min\{M\|\mathsf{C}\mathbf{x}^k\|, \eta\}. \tag{12}$$

Step 2. {Update $\boldsymbol{\mu}$.}

$$\boldsymbol{\mu}^{k+1} = \boldsymbol{\mu}^k + \rho_k \mathsf{C}\mathbf{x}^k. \tag{13}$$

Step 3. {Update ρ provided the increase of the Lagrangian is not sufficient.}
If $k > 0$ and

$$L(\mathbf{x}^k, \boldsymbol{\mu}^k, \rho^k) < L(\mathbf{x}^{k-1}, \boldsymbol{\mu}^{k-1}, \rho_{k-1}) + \frac{\rho_k}{2}\|\mathsf{C}\mathbf{x}^k\|^2 \tag{14}$$

then

$$\rho_{k+1} = \beta\rho_k, \tag{15}$$

else

$$\rho_{k+1} = \rho_k. \tag{16}$$

Step 4. Set $k = k + 1$ and return to *Step 1.*

In (14), we use the augmented Lagrangian defined by

$$L(\mathbf{x}, \boldsymbol{\mu}, \rho) = q(\mathbf{x}) + \boldsymbol{\mu}^\top \mathsf{C}\mathbf{x} + \frac{\rho_k}{2}\|\mathsf{C}\mathbf{x}\|^2. \tag{17}$$

Algorithm 2 has been shown to be well defined [11], that is, any convergent algorithm for the solution of the auxiliary problem required in Step 1 which guarantees convergence of the projected gradient to zero will generate either $\mathbf{x}^k$ that satisfies (12) in a finite number of steps or a sequence of approximations that converges to the solution of (11). To present explicitly the optimality of Algorithm 2 with Step 1 implemented by Algorithm 1, let $\mathcal{T}$ denote any set of indices and let for any $t \in \mathcal{T}$ be defined the problem

$$\text{minimize} \quad q_t(\mathbf{x}) \quad \text{s.t.} \quad \mathbf{x} \in \Omega_{BE}^t \tag{18}$$

with $\Omega_{BE}^t = \{\mathbf{x} \in I\!R^{n_t} : \mathsf{C}_t\mathbf{x} = \mathbf{o} \ \text{ and } \ \mathbf{x} \geq \boldsymbol{\ell}_t\}$, $q_t(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathsf{A}_t \mathbf{x} - \mathbf{b}_t^\top \mathbf{x}$, $\mathsf{A}_t \in I\!R^{n_t \times n_t}$ symmetric positive definite, $\mathsf{C}_t \in I\!R^{m_t \times n_t}$, and $\mathbf{b}_t, \boldsymbol{\ell}_t \in I\!R^{n_t}$. Our optimality result reads as follows.

Theorem 2. *Let* $\{\mathbf{x}_t^k\}, \{\boldsymbol{\mu}_t^k\}$ *and* $\{\rho_{t,k}\}$ *be generated by Algorithm 2 for (18) with* $\|\mathbf{b}_t\| \geq \eta_t > 0$, $\beta > 1$, $M > 0$, $\rho_{t,0} = \rho_0 > 0$, $\boldsymbol{\mu}_t^0 = \mathbf{o}$. *Let Step 1 of Algorithm 2 be implemented by Algorithm 1 (MPRGP) which generates the iterates* $\mathbf{x}_t^{k,0}, \mathbf{x}_t^{k,1}, \ldots, \mathbf{x}_t^{k,l} = \mathbf{x}_t^k$ *for the solution of (18) starting from* $\mathbf{x}_t^{k,0} = \mathbf{x}_t^{k-1}$ *with* $\mathbf{x}_t^{-1} = \mathbf{o}$, *where* $l = l_{k_t}$ *is the first index satisfying*

$$\|\mathbf{g}^P(\mathbf{x}_t^{k,l}, \boldsymbol{\mu}_t^k, \rho_k)\| \leq M\|\mathsf{C}_t\mathbf{x}_t^{k,l}\| \tag{19}$$

or

$$\|\mathbf{g}^P(\mathbf{x}_t^{k,l}, \boldsymbol{\mu}_t^k, \rho_k)\| \leq \epsilon\|\mathbf{b}_t\| \min\{1, M^{-1}\}. \tag{20}$$

Let $0 < a_{\min} < a_{\max}$ *and* $0 < c_{\max}$ *be given and let the class of problems (18) satisfy*

$$a_{\min} \leq \lambda_{\min}(\mathsf{A}_t) \leq \lambda_{\max}(\mathsf{A}_t) \leq a_{\max} \quad \text{and} \quad \|\mathsf{C}_t\| \leq c_{\max}. \tag{21}$$

Then Algorithm 2 generates an approximate solution $\mathbf{x}_t^{k_t}$ *of any problem (18) which satisfies*

$$\|\mathbf{g}^P(\mathbf{x}_t^{k_t}, \boldsymbol{\mu}_t^{k_t}, \rho_{t,k_t})\| \leq \epsilon\|\mathbf{b}_t\| \quad \text{and} \quad \|\mathsf{C}_t\mathbf{x}_t^{k_t}\| \leq \epsilon\|\mathbf{b}_t\| \tag{22}$$

at $O(1)$ *matrix-vector multiplications by the Hessian of the augmented Lagrangian* L_t.

Proof. See [7, 8].

4 Model Problem

To simplify our exposition, we restrict our attention to a simple scalar variational inequality. The computational domain is $\Omega = \Omega^1 \cup \Omega^2$, where $\Omega^1 = (0,1) \times (0,1)$ and $\Omega^2 = (1,2) \times (0,1)$, with boundaries Γ^1 and Γ^2, respectively. We denote by Γ_u^i, Γ_f^i, and Γ_c^i the fixed, free, and potential contact parts of Γ^i, $i = 1, 2$. We assume that Γ_u^1 has non-zero measure, i.e., $\Gamma_u^1 \neq \emptyset$. For a coercive model problem, $\Gamma_u^2 \neq \emptyset$, while for a semicoercive model problem, $\Gamma_u^2 = \emptyset$; see Figure 1. Let $H^1(\Omega^i), i = 1, 2$ denote the Sobolev space of the first order in the space $L^2(\Omega^i)$ of functions on Ω^i whose squares are integrable in the Lebesgue sense. Let

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

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

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

denote the closed subspace and the 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

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

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

$$f(x, y) = \begin{cases} -1| - 3 \quad \text{for} \quad (x, y) \in (0, 1) \times [0.75, 1), \\ \;\; 0| \;\; 0 \;\; \text{for } (x, y) \in (0, 1) \times [0, 0.75) \text{ and } (x, y) \in (1, 2) \times [0.25, 1), \\ -3| - 1 \quad \text{for} \quad (x, y) \in (1, 2) \times [0, 0.25), \end{cases}$$

for coercive | semicoercive model problem. Thus we can define a problem to find

$$\min \quad q(u) = \frac{1}{2} a(u, u) - \ell(u) \;\; \text{subject to} \;\; u \in \mathcal{K}. \tag{23}$$

The solution of the model problem may be interpreted as the displacement of

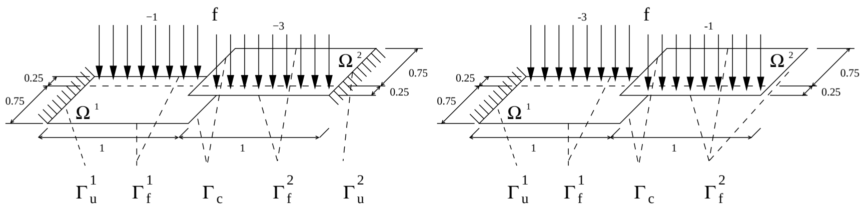

Fig. 1. The coercive (left) and semicoercive (right) model problem

two membranes under the traction f. The membranes are fixed as in Fig. 1 and the left edge of the right membrane is not allowed to penetrate below the right edge of the left membrane. In the first case, when the Dirichlet conditions are prescribed on the parts $\Gamma_u^i, i = 1, 2$ of the boundaries with a positive measure, the quadratic form a is coercive which guarantees the existence and uniqueness of the solution [31]. In the second case, only the left membrane is fixed on the outer edge and the right membrane has no prescribed displacement as in Fig. 1 (right), so that

$$\Gamma_u^1 = \{(0, y) \in I\!R^2 : y \in [0, 1]\}, \quad \Gamma_u^2 = \emptyset.$$

Even though a is in this case only semidefinite, the form q is still coercive due to the choice of f so that it has again the unique solution [31].

5 FETI and Total FETI Domain Decomposition

To enable efficient application of the domain decomposition methods, we can optionally decompose each Ω^i into square subdomains $\Omega^{i1}, \dots, \Omega^{ip}, p = s^2 > 1, i = 1, 2$. The outer subdomains Ω^{ij} can either inherit the Dirichlet boundary conditions from Γ_u^i as in the original FETI [28], or they can be treated as floating with the Dirichlet conditions enforced by the Lagrange multipliers. The latter approach was coined Total FETI (TFETI) [19]. 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 (23), 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 (23) with the auxiliary domain decomposition that reads

$$\min \frac{1}{2}\mathbf{u}^\top \mathsf{K}\mathbf{u} - \mathbf{f}^\top \mathbf{u} \quad \text{s.t.} \quad \mathsf{B}^I\mathbf{u} \le \mathbf{o} \quad \text{and} \quad \mathsf{B}^E\mathbf{u} = \mathbf{o}. \tag{24}$$

In (24), $\mathsf{K} = \operatorname{diag}[\mathsf{K}_1, \dots, \mathsf{K}_{2p}]$ denotes a positive semidefinite stiffness matrix, the full rank matrices B^I and B^E describe the discretized inequality and gluing conditions, respectively, and $\mathbf{f}$ represents the discrete analog of the linear term $\ell(u)$. Denoting

$$\boldsymbol{\lambda} = \begin{bmatrix} \boldsymbol{\lambda}^I \\ \boldsymbol{\lambda}^E \end{bmatrix} \quad \text{and} \quad \mathsf{B} = \begin{bmatrix} \mathsf{B}^I \\ \mathsf{B}^E \end{bmatrix},$$

we can write the Lagrangian associated with problem (30) briefly as

$$L(\mathbf{u}, \boldsymbol{\lambda}) = \frac{1}{2}\mathbf{u}^\top \mathsf{K}\mathbf{u} - \mathbf{f}^\top \mathbf{u} + \boldsymbol{\lambda}^\top \mathsf{B}\mathbf{u}.$$

It is well known that (24) is equivalent to the saddle point problem

$$\text{Find} \quad (\overline{\mathbf{u}}, \overline{\boldsymbol{\lambda}}) \quad \text{s.t.} \quad L(\overline{\mathbf{u}}, \overline{\boldsymbol{\lambda}}) = \sup_{\boldsymbol{\lambda}^I \ge \mathbf{o}} \inf_{\mathbf{u}} L(\mathbf{u}, \boldsymbol{\lambda}). \tag{25}$$

After eliminating the primal variables $\mathbf{u}$ from (25), we shall get the minimization problem

$$\min \Theta(\boldsymbol{\lambda}) \quad \text{s.t.} \quad \boldsymbol{\lambda}^I \geq \mathbf{o} \quad \text{and} \quad \mathsf{R}^\top(\mathbf{f} - \mathsf{B}^\top\boldsymbol{\lambda}) = \mathbf{o}, \tag{26}$$

where

$$\Theta(\boldsymbol{\lambda}) = \frac{1}{2}\boldsymbol{\lambda}^\top \mathsf{B}\mathsf{K}^\dagger\mathsf{B}^\top\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top\mathsf{B}\mathsf{K}^\dagger\mathbf{f}, \tag{27}$$

$\mathsf{K}^\dagger$ denotes a generalized inverse that satisfies $\mathsf{K}\mathsf{K}^\dagger\mathsf{K} = \mathsf{K}$, and R denotes the full rank matrix whose columns span the kernel of K. We shall choose R so that its entries belong to $\{0, 1\}$ and each column corresponds to some floating auxiliary subdomain Ω^{ij} with the nonzero entries in the positions corresponding to the indices of nodes belonging to Ω^{ij}. The action of $\mathsf{K}^\dagger = \operatorname{diag}[\mathsf{K}_1^\dagger, \dots, \mathsf{K}_{2p}^\dagger]$ can be evaluated in parallel at the cost comparable with the action of the inverse of the regular matrix with the same sparsity pattern [25]. When TFETI method is used, the implementation is easy as the kernels of K_i are known a priori. Even though problem (26) is much more suitable for computations than (24), further improvement may be achieved by adapting some simple observations and the results of Farhat, Mandel and Roux [27]. Let us denote

$$\mathsf{F} = \mathsf{B}\mathsf{K}^\dagger\mathsf{B}^\top, \quad \widetilde{\mathsf{G}} = \mathsf{R}^\top\mathsf{B}^\top, \quad \widetilde{\mathbf{e}} = \mathsf{R}^\top\mathbf{f}, \quad \widetilde{\mathbf{d}} = \mathsf{B}\mathsf{K}^\dagger\mathbf{f},$$

and let $\widetilde{\boldsymbol{\lambda}}$ solve $\widetilde{\mathsf{G}}\widetilde{\boldsymbol{\lambda}} = \widetilde{\mathbf{e}}$, so that we can transform the problem (26) to minimization on the subset of the vector space by looking for the solution in the form $\boldsymbol{\lambda} = \boldsymbol{\mu} + \widetilde{\boldsymbol{\lambda}}$. Since

$$\frac{1}{2}\boldsymbol{\lambda}^\top\mathsf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top\widetilde{\mathbf{d}} = \frac{1}{2}\boldsymbol{\mu}^\top\mathsf{F}\boldsymbol{\mu} - \boldsymbol{\mu}^\top(\widetilde{\mathbf{d}} - \mathsf{F}\widetilde{\boldsymbol{\lambda}}) + \frac{1}{2}\widetilde{\boldsymbol{\lambda}}^\top\mathsf{F}\widetilde{\boldsymbol{\lambda}} - \widetilde{\boldsymbol{\lambda}}^\top\widetilde{\mathbf{d}},$$

problem (26) is, after returning to the old notation, equivalent to

$$\min \quad \frac{1}{2}\boldsymbol{\lambda}^\top\mathsf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top\mathbf{d} \quad \text{s.t} \quad \mathsf{G}\boldsymbol{\lambda} = \mathbf{o} \quad \text{and} \quad \boldsymbol{\lambda}^I \geq -\widetilde{\boldsymbol{\lambda}}^I, \tag{28}$$

where $\mathbf{d} = \widetilde{\mathbf{d}} - \mathsf{F}\widetilde{\boldsymbol{\lambda}}$ and G denotes a matrix arising from the orthonormalization of the rows of $\widetilde{\mathsf{G}}$. Our final step is based on observation that the problem (28) is equivalent to

$$\min \quad \frac{1}{2}\boldsymbol{\lambda}^\top\mathsf{P}\mathsf{F}\mathsf{P}\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top\mathsf{P}\mathbf{d} \quad \text{s.t} \quad \mathsf{G}\boldsymbol{\lambda} = \mathbf{o} \quad \text{and} \quad \boldsymbol{\lambda}^I \geq -\widetilde{\boldsymbol{\lambda}}^I \tag{29}$$

where

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

denote the orthogonal projectors on the image space of $\mathsf{G}^\top$ and on the kernel of G.

Theorem 3. *If* F *and* P *denote the matrices of the problem (29) (generated either by FETI or TFETI), then the following spectral bounds hold:*

$$\lambda_{\max}(\mathsf{P}\mathsf{F}\mathsf{P}) \leq ||\mathsf{F}|| \ \leq \ C\frac{H}{h}; \quad \lambda_{\min}(\mathsf{P}\mathsf{F}\mathsf{P}|\mathrm{Im}\mathsf{P}) \ \geq \ \mathrm{C}.$$

Proof. See [27, 9].

6 FETI–DP Domain Decomposition and Discretization

We shall now assume that the subdomains are not completely separated, but joined in the joint corners that we shall call crosspoints. We call a crosspoint either a corner that belongs to four subdomains, or a corner that belongs to two subdomains and is located on $\partial\Omega^1 \setminus \Gamma_u^1$ or on $\partial\Omega^2 \setminus \Gamma_u^2$. An important feature for developing FETI–DP type algorithms is that a single degree of freedom is considered at each crosspoint, while two degrees of freedom are introduced at all the other matching nodes across subdomain edges as in FETI or TFETI. Using the finite element discretization, we get again the discretized version of problem (23) with the auxiliary domain decomposition

$$\min \frac{1}{2}\mathbf{u}^\top \mathsf{K}\mathbf{u} - \mathbf{f}^\top \mathbf{u} \quad \text{s.t.} \quad \mathsf{B}^I\mathbf{u} \le \mathbf{o} \quad \text{and} \quad \mathsf{B}^E\mathbf{u} = \mathbf{o}, \tag{30}$$

where the full rank matrices B^I and B^E describe the non-penetration (inequality) conditions and the gluing (equality) conditions, respectively, and $\mathbf{f}$ represents the discrete analog of the linear form $\ell(\cdot)$. In (30), using suitable numbering, $\mathsf{K} = \mathrm{diag}(\mathsf{K}^1, \mathsf{K}^2)$ is the block diagonal stiffness matrix with the nonzero blocks

$$\mathsf{K}^i = \begin{bmatrix} \mathsf{K}^i_{11} & & & \mathsf{K}^i_{1,p+1} \\ & \ddots & & \vdots \\ & & \mathsf{K}^i_{p,p} & \mathsf{K}^i_{p,p+1} \\ \mathsf{K}^i_{p+1,1} & \dots & \mathsf{K}^i_{p+1,p} & \mathsf{K}^i_{p+1,p+1} \end{bmatrix}.$$

The block K^1 corresponding to Ω^1 is nonsingular due to the Dirichlet boundary conditions on Γ_u^1. The block K^2 corresponding to Ω^2 is nonsingular for a coercive problem, and is singular, with the kernel made of a vector $\mathbf{e}$ with all the entries equal to 1, for a semicoercive problem. In the latter case, the kernel of K is spanned by the matrix $\mathsf{R} = \left[\mathbf{o}^\top, \mathbf{e}^\top\right]^\top$. Using the duality theory [3], we can again transform (30) to the dual problem. For a coercive problem, K is nonsingular and we obtain the problem of finding

$$\min \frac{1}{2}\boldsymbol{\lambda}^\top \mathsf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top \mathbf{d} \quad \text{s.t.} \quad \boldsymbol{\lambda}^I \ge \mathbf{o}, \tag{31}$$

with $\mathsf{F} = \mathsf{B}\ \mathsf{K}^{-1}\mathsf{B}^\top$ and $\mathbf{d} = \mathsf{B}\ \mathsf{K}^{-1}\mathbf{f}$. For an efficient implementation of F, it is important to exploit the structure of K; see [21] for more details. For a semicoercive problem, we obtain the problem of finding

$$\min \quad \frac{1}{2}\boldsymbol{\lambda}^\top \mathsf{F}\boldsymbol{\lambda} - \mathbf{d}^\top \boldsymbol{\lambda} \quad \text{s.t} \quad \mathsf{G}\boldsymbol{\lambda} = \mathbf{o} \quad \text{and} \quad \boldsymbol{\lambda}^I \ge -\widetilde{\boldsymbol{\lambda}}^I, \tag{32}$$

with $\mathbf{d} = \widetilde{\mathbf{d}} - \mathsf{F}\widetilde{\boldsymbol{\lambda}}$ and G and $\widetilde{\boldsymbol{\lambda}}$ defined similarly as in FETI. Our final step is again based on the observation that the Hessian of the augmented Lagrangian for problem (32) may be decomposed by the orthogonal projectors

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

on the image space of $\mathsf{G}^\top$ and on the kernel of G, respectively. Since $\mathsf{P}\boldsymbol{\lambda} = \boldsymbol{\lambda}$ for any feasible $\boldsymbol{\lambda}$, problem (32) is equivalent to

$$\min \quad \frac{1}{2}\boldsymbol{\lambda}^\top \mathsf{PFP}\boldsymbol{\lambda} - \boldsymbol{\lambda}^\top \mathsf{P}\mathbf{d} \quad \text{s.t} \quad \mathsf{G}\boldsymbol{\lambda} = \mathbf{o} \quad \text{and} \quad \boldsymbol{\lambda}^I \geq -\widetilde{\boldsymbol{\lambda}}^I. \tag{33}$$

The optimality follows from the following theorem.

Theorem 4. *If* F *denotes the matrix of the problem (32) generated by FETI–DP for the coercive problem, then the following spectral bounds hold:*

$$\lambda_{\max}(\mathsf{F}) = \|\mathsf{F}\| \ \leq \ C\left(\frac{H}{h}\right)^2; \quad \lambda_{\min}(\mathsf{F}) \ \geq \ C.$$

If F *and* P *denote the matrices of the problem (33) generated by FETI–DP for the semicoercive problem, then the following spectral bounds hold:*

$$\lambda_{\max}(\mathsf{PFP}|\mathrm{Im}\mathsf{P}) \leq \|\mathsf{F}\| \ \leq \ C\left(\frac{H}{h}\right)^2; \quad \lambda_{\min}(\mathsf{PFP}|\mathrm{Im}\mathsf{P}) \ \geq \ C.$$

Proof. See [21, 22].

7 Numerical Scalability

To show that Algorithm 2 with the inner loop implemented by Algorithm 1 is optimal for the solution of our model problems (or a class of problems) discretized by means of FETI, TFETI and FETI–DP, we shall use

$$\mathcal{T} = \{(H, h) \in I\!R^2 : H \leq 1,\ 2h \leq H \ \ \text{and} \ \ H/h \in I\!N\}$$

as the set of indices. Given a constant $C \geq 2$, we shall define a subset $\mathcal{T}_C$ of $\mathcal{T}$ by

$$\mathcal{T}_C = \{(H, h) \in I\!R^2 : H \leq 1,\ 2h \leq H,\ H/h \in I\!N \ \ \text{and} \ \ H/h \leq C\}.$$

For any $t \in \mathcal{T}$, and a given $\overline{\rho} > 0$, we shall define

$$\begin{aligned} &\mathsf{A}_t = \mathsf{PFP} + \overline{\rho}\mathsf{Q},\ \mathbf{b}_t = \mathsf{P}\mathbf{d} \\ &\mathsf{C}_t = \mathsf{G}, \qquad\qquad \boldsymbol{\ell}_t^I = -\widetilde{\boldsymbol{\lambda}}^I \ \ \text{and} \ \ \boldsymbol{\ell}_t^E = -\boldsymbol{\infty} \end{aligned}$$

with the vectors and matrices generated with the discretization and decomposition parameters H and h, respectively, so that the problem (29) is equivalent to the problem

$$\text{minimize} \ \ \Theta_t(\boldsymbol{\lambda}_t) \ \ \text{s.t.} \ \ \mathsf{C}_t\boldsymbol{\lambda}_t = 0 \ \ \text{and} \ \ \boldsymbol{\lambda}_t \geq \boldsymbol{\ell}_t \tag{34}$$

with $\Theta_t(\boldsymbol{\lambda}) = \frac{1}{2}\boldsymbol{\lambda}^\top \mathsf{A}_t\boldsymbol{\lambda} - \mathbf{b}_t^\top\boldsymbol{\lambda}$. Using these definitions and $\mathsf{G}\mathsf{G}^\top = \mathsf{I}$, we obtain

$$\|\mathsf{C}_t\| \leq 1 \quad \text{and} \quad \|\boldsymbol{\ell}_t^+\| = 0, \tag{35}$$

where for any vector $\mathbf{v}$ with the entries v_i, $\mathbf{v}^+$ denotes the vector with the entries $v_i^+ = \max\{v_i, 0\}$. Moreover, it follows by Theorem 4 that for any $C \geq 2$ there are constants $a_{\max}^C > a_{\min}^C > 0$ such that

$$a_{\min}^C \leq \alpha_{\min}(\mathsf{A}_t) \leq \alpha_{\max}(\mathsf{A}_t) \leq a_{\max}^C \tag{36}$$

for any $t \in \mathcal{T}_C$. Moreover, there are positive constants C_1 and C_2 such that $a_{\min}^C \geq C_1$ and $a_{\max}^C \leq C_2 C$. In particular, it follows that the assumptions of Theorem 5 (i.e. the inequalities (35) and (36)) of [8] are satisfied for any set of indices $\mathcal{T}_C,\ C \geq 2$, and we have the following result:

Theorem 5. *Let $C \geq 2$ denote a given constant, let $\{\boldsymbol{\lambda}_t^k\}, \{\boldsymbol{\mu}_t^k\}$ and $\{\rho_{t,k}\}$ be generated by Algorithm 2 (SMALBE) for (34) with $\|\mathbf{b}_t\| \geq \eta_t > 0$, $\beta > 1$, $M > 0$, $\rho_{t,0} = \rho_0 > 0$, and $\boldsymbol{\mu}_t^0 = \mathbf{o}$. Let $s \geq 0$ denote the smallest integer such that $\beta^s \rho_0 \geq M^2/a_{\min}$ and assume that Step 1 of Algorithm 2 is implemented by means of Algorithm 1 (MPRGP) with parameters $\Gamma > 0$ and $\overline{\alpha} \in (0, (a_{\max} + \beta^s \rho_0)^{-1}]$, so that it generates the iterates $\boldsymbol{\lambda}_t^{k,0}, \boldsymbol{\lambda}_t^{k,1}, \ldots, \boldsymbol{\lambda}_t^{k,l} = \boldsymbol{\lambda}_t^k$ for the solution of (34) starting from $\boldsymbol{\lambda}_t^{k,0} = \boldsymbol{\lambda}_t^{k-1}$ with $\boldsymbol{\lambda}_t^{-1} = \mathbf{o}$, where $l = l_{t,k}$ is the first index satisfying*

$$\|\mathbf{g}^P(\boldsymbol{\lambda}_t^{k,l}, \boldsymbol{\mu}_t^k, \rho_{t,k})\| \leq M \|\mathsf{C}_t \boldsymbol{\lambda}_t^{k,l}\| \tag{37}$$

or

$$\|\mathbf{g}^P(\boldsymbol{\lambda}_t^{k,l}, \boldsymbol{\mu}_t^k, \rho_{t,k})\| \leq \epsilon \|\mathbf{b}_t\| \min\{1, M^{-1}\}. \tag{38}$$

Then for any $t \in \mathcal{T}_C$ and problem (34), Algorithm 2 generates an approximate solution $\boldsymbol{\lambda}_t^{k_t}$ which satisfies

$$M^{-1} \|\mathbf{g}^P(\boldsymbol{\lambda}_t^{k_t}, \boldsymbol{\mu}_t^{k_t}, \rho_{t,k_t})\| \leq \|\mathsf{C}_t \boldsymbol{\lambda}_t^{k_t}\| \leq \epsilon \|\mathbf{b}_t\| \tag{39}$$

at $O(1)$ matrix-vector multiplications by the Hessian of the augmented Lagrangian L_t for (34) and $\rho_{t,k} \leq \beta^s \rho_0$.

Proof. See [9].

8 Numerical Experiments

We have implemented all three domain decomposition methods described above to the solution of both variants of the model problems of Fig. 1. The solution of both problems is in Fig. 2. For the solution of the quadratic programming problems generated by FETI1 and TFETI, we used the SMALBE algorithm of Section 3 with the inner loop generated by the MPRGP algorithm of Section 2. We have implemented the solver in C exploiting PETSc

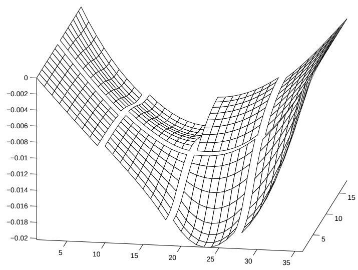

Fig. 3a: Coercive problem

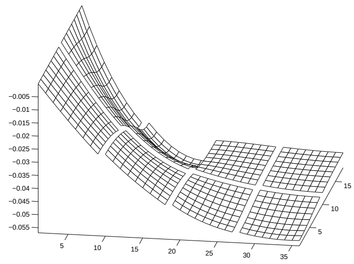

Fig. 3b: Semicoercive problem

Fig. 2. Solution of model problems

Table 1. Numerical scalability of FETI and TFETI for H/h=const and ρ=1e3

primal dim.	2312	9248	36992	133128	532512	2130048
FETI/TFETI dual dim.	167/201	863/931	3839/3975	1287/-	6687/-	29823/-
subdomains	8	32	128	8	32	128
FETI iterations	47	58	64	59	36	47
TFETI iterations	39	54	45	-	-	-

to solve the semicoercive model problem with varying decomposition and discretization parameters. The results of computations which were carried out to the relative precision 1e-4 are in Table 1.

Since the algorithms are closely related to the original FETI method, it is not surprising that they enjoy good parallel scalability as documented in Table 2. The experiments with semicoercive problem were run on the Lomond 52-processor Sun Ultra SPARC-III based system with 900 MHz, 52 GB of shared memory, nominal peak performance 93.6 GFlops, 64 kB level 1 and 8 MB level 2 cache in EPCC Edinburgh, to the relative precision 1e-4.

Table 2. Parallel scalability for semicoer.problem with prim.dim 540800, dual dim.14975, 2 outer iters, 43 cg iters, 128 subdomains using Lomond, ρ=1e3

processors	1	2	4	8	16	32
time [sec]	879	290	138	50	27	15

We have implemented also the basic FETI-DP algorithms for the solution of both coercive and semicoercive problems in MATLAB. We have used MPRGP of Section 2 for the solution of the coercive problems and the SMALBE algorithm of Section 3 with the inner loop generated by the MPRGP algorithm to the solution of the semicoercive problem to the relative precision 1e-6. The results are in Table 3.

Table 3. Numerical scalability of the basic FETI-DP for coer. and semicoer.problem, ρ=1e3

prim./dual/corner dim.	2312/153/10	9248/785/42	36992/3489/154
subdomains	8	32	128
cg iters for coer.problem	27	48	51
cg iters for semicoer.problem	41	57	63

9 Comments and Conclusions

We have reviewed our recent results related to application of the augmented Lagrangians with the FETI based domain decomposition method to the solution of variational inequalities using recently developed algorithms for the solution of special QP problems. In particular, we have shown that the solution of the discretized problem to a prescribed precision may be found in a number of iterations bounded independently of the discretization parameter. Numerical experiments with the model variational inequality are in agreement with the theory and indicate that the algorithms presented are efficient. The research in progress includes implementation of preconditioners, the mortar discretization and the generalization to the contact problems with friction.

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