Scalable Hybrid TFETI-DP Methods for Large Boundary Variational Inequalities

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1 Introduction

Variants of the FETI (finite element tearing and interconnecting) methods introduced by Farhat and Roux [8] belong to the most powerful methods for the massively parallel solution of large discretized elliptic partial differential equations. The basic idea is to decompose the domain into subdomains connected by Lagrange multipliers and then eliminate the primal variables to get a small coarse problem and local problems that can be solved in parallel. If applied to variational inequalities, the procedure simultaneously transforms the general inequality constraints into bound constraints. This simple observation and development of specialized quadratic programming algorithms [2] with optimal convergence rate have been at the heart of the generalization of the classical scalability results to variational inequalities [4]. The algorithms have been applied to solve contact problems discretized by billions of nodal variables [6].

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The bottleneck of the original FETI is caused by the coarse problem, which has the dimension which is proportional to the number of subdomains. The coarse problem is typically solved by a direct solver – its cost is negligible for a small number of subdomains. However, it starts to dominate when the number of subdomains is large, currently some tens of thousands of subdomains.

Here we introduce a model problem, the semi-coercive scalar variational inequality, describe its discretization and decomposition into subdomains and clusters, reduce the problem by duality to bound and equality constrained problems, give results on numerical scalability of the algorithms, and demonstrate their performance by numerical experiments. The analysis uses recently proved bounds on the spectrum of the Schur complements of the clusters interconnected by edge/face averages. The bounds for 2D and 3D scalar problems have been published in [5] and [3]; the development of the theory for elasticity is in progress. The results extend the scope of scalability of powerful massively parallel algorithms for the solution of variational inequalities [6] and show the unique efficiency of H-TFETI-DP coarse grid split between the primal and dual variables. We illustrate the analysis on a simple model problem but also include numerical experiments with 3D elastic contact problem with the clusters interconnected by average face rigid body motions.

Throughout the paper, we use the following notation. For any matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$ and subsets $\mathcal{I} \subseteq \{1,\dots,m\}$ and $\mathcal{J} \subseteq \{1,\dots,n\}$, we denote by $\mathbf{A}_{\mathcal{I}\mathcal{J}}$ a submatrix of $\mathbf{A}$ with the rows $i \in \mathcal{I}$ and columns $j \in \mathcal{J}$. If $m = n$ and $\mathbf{A} = \mathbf{A}^T$, then $\lambda_i(\mathbf{A})$, $\lambda_{\min}(\mathbf{A})$, $\lambda_{\max}(\mathbf{A})$ denote the eigenvalues of $\mathbf{A}$,

$$\lambda_{\max}(\mathbf{A}) = \lambda_1(\mathbf{A}) \geq \lambda_2(\mathbf{A}) \geq \cdots \lambda_n(\mathbf{A}) = \lambda_{\min}(\mathbf{A}).$$

The smallest nonzero eigenvalue of $\mathbf{A}$ is denoted by $\overline{\lambda}_{\min}(\mathbf{A})$. The Euclidean norm and zero vector a denoted by $\|\,.\,\|$ and $\mathbf{o}$, respectively.

2 Model problem

For simplicity, we shall reduce our analysis to a simple model problem, but our reasoning is also valid for more general cases. Let $\Omega = \Omega^1 \cup \Omega^2$, where $\Omega^1 = (0,1)\times(0,1)$ and $\Omega^2 = (1,2)\times(0,1)$ denote square domains with the boundaries Γ^1, Γ^2; their parts Γ_u^i, Γ_f^i, Γ_c^i are formed by the sides of Ω^i, $i = 1,2$, as in Fig. 1.

Let $H^1(\Omega^i)$, $i = 1,2$, denote the subspace of $L^2(\Omega^i)$ of elements with the first derivatives in $L^2(\Omega^i)$. Let

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

denote closed subspaces of $H^1(\Omega^i)$, let $\mathcal{H} = H^1(\Omega^1)\times H^1(\Omega^2)$, and let

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

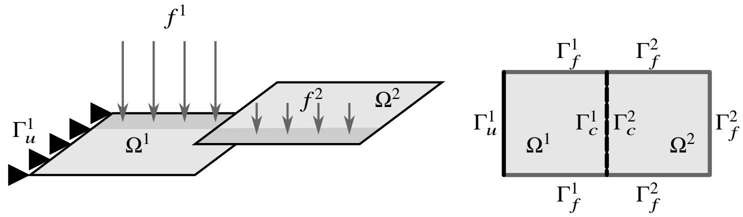

Fig. 1: Coercive model problem (left) and boundary conditions (right)

denote a closed subspace and a closed convex subset of $\mathcal{H}$, respectively. The relations on the boundaries are in terms of traces. On $\mathcal{H}$, we define a symmetric bilinear form

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

and a linear form

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

where $f^i \in L^2(\Omega^i)$, $i = 1, 2$, are nonzero and nonpositive. Thus we can define a problem to find

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

The solution of the model problem can be interpreted as the displacement of two membranes under the traction f. The left edge of the right membrane cannot penetrate below the right edge of the left membrane.

3 Domain decomposition and discretization

To enable efficient application of domain decomposition methods, we optionally decompose each Ω^i into $p = 1/H_s \times 1/H_s$, $i = 1, 2$, square subdomains. Misusing a little the notation, we assign to each subdomain of Ω^1 a unique number $i \in \{1, \dots, p\}$ and to each subdomain of Ω^2 a unique number $i \in \{p+1, \dots, s\}$, $s = 2p$, as in Fig. 2. We call H_s a *decomposition parameter*.

To get a variational formulation of the decomposed problem, let

$$V_D^i = \left\{ v^i \in H^1(\Omega^i) : v^i = 0 \quad \text{on} \quad \Gamma_U \cap \Gamma^i \right\}, \quad i = 1, \dots s,$$

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

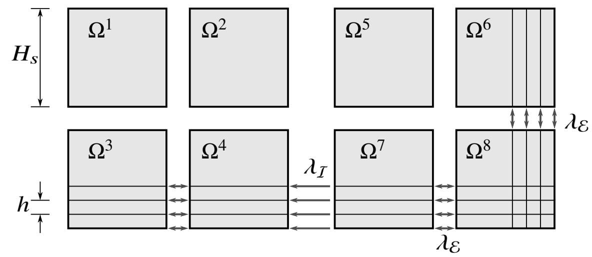

Fig. 2: Domain decomposition and discretization

$$
\begin{aligned}
V_D &= V_D^1 \times \cdots \times V_D^s,\\
\mathcal{K}_D^C &= \left\{ v \in V_D : v^j - v^i \geq 0 \ \text{ on } \ \Gamma_C^1 \cap \Gamma_C^2, \quad i \leq p < j \right\},\\
\mathcal{K}_D &= \left\{ v \in \mathcal{K}_D^C : v^i = v^j \ \text{ on } \ \Gamma^{ij} \right\}, \quad \Gamma^{ij} = \overline{\Gamma}^i \cap \overline{\Gamma}^j, \quad i,j \leq p \text{ or } \quad i,j > p.
\end{aligned}
$$

On V_D, we define the scalar product

$$(u,v)_D = \sum_{i=1}^{s} \int_{\Omega^i} u^i v^i \mathrm{d}\Omega,$$

and the forms

$$a_D(u,v) = \sum_{i=1}^{s} \int_{\Omega^i} \left(\frac{\partial u^i}{\partial x_1}\frac{\partial v^i}{\partial x_1} + \frac{\partial u^i}{\partial x_2}\frac{\partial v^i}{\partial x_2} \right) \mathrm{d}\Omega \quad \text{and} \quad \ell_D(v) = (f,v)_D.$$

Using the above notation, it is a standard exercise [6, Sect. 10.2] to prove that (1) is equivalent to the problem to find $u \in \mathcal{K}_D$ such that

$$q_D(u) \leq q_D(v), \quad q_D(v) = \frac{1}{2} a_D(v,v) - \ell_D(v), \quad v \in \mathcal{K}_D. \tag{2}$$

After introducing regular grids with the discretization parameter h in the subdomains Ω^i (see Fig. 2), and using Lagrangian finite elements for the discretization, we get the discretized version of problem (2) with auxiliary domain decomposition

$$\min \ \frac{1}{2}\mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{f}^T\mathbf{u} \quad \text{s.t.} \quad \mathbf{B}_I\mathbf{u} \leq \mathbf{o} \quad \text{and} \quad \mathbf{B}_E\mathbf{u} = \mathbf{o}. \tag{3}$$

In (3), $\mathbf{K} \in \mathbb{R}^{n\times n}$ denotes a block diagonal SPS (symmetric positive semidefinite) stiffness matrix, the full rank matrices $\mathbf{B}_I$ and $\mathbf{B}_E$ describe the non-penetration and interconnecting conditions, respectively, and $\mathbf{f}$ represents the discretized linear form $\ell_D(u)$. We can write the stiffness matrix and the vectors in the block form

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_1 & \mathbf{O} & \dots & \mathbf{O} \\ \mathbf{O} & \mathbf{K}_2 & \dots & \mathbf{O} \\ \dots & \dots & \dots & \dots \\ \mathbf{O} & \mathbf{O} & \dots & \mathbf{K}_s \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} \mathbf{u}_1 \\ \dots \\ \mathbf{u}_s \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} \mathbf{f}_1 \\ \dots \\ \mathbf{f}_s \end{bmatrix}, \quad s = 2p.$$

After a suitable scaling of the rows of $\mathbf{B} = [\mathbf{B}_E^T, \mathbf{B}_I^T]^T$, we can achieve $\mathbf{B}\mathbf{B}^T = \mathbf{I}$.

4 TFETI problem

To reduce the problem to the subdomain boundaries using duality theory, let us introduce the Lagrangian associated with problem (3) by

$$L(\mathbf{u}, \lambda_I, \lambda_E) = \frac{1}{2}\mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{f}^T\mathbf{u} + \lambda_I^T\mathbf{B}_I\mathbf{u} + \lambda_E^T\mathbf{B}_E\mathbf{u}, \tag{4}$$

where λ_I and λ_E are the Lagrange multipliers associated with the inequalities and equalities, respectively. Introducing the notation

$$\lambda = \begin{bmatrix} \lambda_I \\ \lambda_E \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} \mathbf{B}_I \\ \mathbf{B}_E \end{bmatrix},$$

we can observe that $\mathbf{B} \in \mathbb{R}^{m\times n}$ is a full rank matrix and write the Lagrangian as

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

The solution satisfies the KKT conditions, including

$$\mathbf{K}\mathbf{u} - \mathbf{f} + \mathbf{B}^T\lambda = \mathbf{o}. \tag{5}$$

Equation (5) has a solution if and only if $\mathbf{f} - \mathbf{B}^T\lambda \in \mathrm{Im}\mathbf{K}$, which can be expressed by means of a matrix $\mathbf{R}$ the columns of which span the null space of $\mathbf{K}$ as

$$\mathbf{R}^T(\mathbf{f} - \mathbf{B}^T\lambda) = \mathbf{o}. \tag{6}$$

The matrix $\mathbf{R}$ can be formed directly, and $\mathbf{R}^T\mathbf{B}^T$ is non-singular.

Now assume that λ satisfies (6), so that we can evaluate λ from (5) by means of any (left) generalized inverse matrix $\mathbf{K}^+$ which satisfies $\mathbf{K}\mathbf{K}^+\mathbf{K} = \mathbf{K}$. We can verify directly that if $\mathbf{u}$ solves (5), then there is a vector α such that

$$\mathbf{u} = \mathbf{K}^+(\mathbf{f} - \mathbf{B}^T\lambda) + \mathbf{R}\alpha. \tag{7}$$

After eliminating the primal variables $\mathbf{u}$, we can find λ by solving

$$\min\ \theta(\lambda) \quad \text{s.t.} \quad \lambda_I \geq \mathbf{o} \quad \text{and} \quad \mathbf{R}^T(\mathbf{f} - \mathbf{B}^T\lambda) = \mathbf{o}, \tag{8}$$

where

$$\theta(\lambda) = \frac{1}{2}\lambda^T \mathbf{B}\mathbf{K}^+\mathbf{B}^T\lambda - \lambda^T \mathbf{B}\mathbf{K}^+\mathbf{f}. \tag{9}$$

Once the solution $\widehat{\lambda}$ of (8) is known, $\widehat{\mathbf{u}}$ (3) can be evaluated by (7) and

$$\alpha = -(\mathbf{R}^T\widehat{\mathbf{B}}^T\widehat{\mathbf{B}}\mathbf{R})^{-1}\mathbf{R}^T\widetilde{\mathbf{B}}^T\widehat{\mathbf{B}}\mathbf{K}^+(\mathbf{f} - \mathbf{B}^T\widehat{\lambda}), \tag{10}$$

where $\widehat{\mathbf{B}} = [\widehat{\mathbf{B}}_I^T, \mathbf{B}_E^T]^T$, and the matrix $\widehat{\mathbf{B}}_I$ is formed by the rows $\mathbf{b}_i$ of $\mathbf{B}_I$ that correspond to the positive components of the solution $\widehat{\lambda}_I$ characterized by $\widehat{\lambda}_i > 0$. A more effective procedure avoiding manipulation with $\widehat{\mathbf{B}}$ can be found in [9].

To proceed further, let us denote

$$\begin{aligned} \mathbf{F} &= \mathbf{B}\mathbf{K}^+\mathbf{B}^T = \widetilde{\mathbf{B}}\mathbf{S}^+\widetilde{\mathbf{B}}^T, & \widetilde{\mathbf{d}} &= \mathbf{B}\mathbf{K}^+\mathbf{f}, \\ \widetilde{\mathbf{G}} &= \mathbf{R}^T\mathbf{B}^T, & \widetilde{\mathbf{e}} &= \mathbf{R}^T\mathbf{f}, \end{aligned}$$

and let $\mathbf{T}$ denote a matrix that defines orthonormalization of the rows of $\widetilde{\mathbf{G}}$ so that the matrix $\mathbf{G} = \mathbf{T}\widetilde{\mathbf{G}}$ has orthonormal rows. After introducing $\mathbf{e} = \mathbf{T}\widetilde{\mathbf{e}}$, problem (8) reads

$$\min \quad \frac{1}{2}\lambda^T\mathbf{F}\lambda - \lambda^T\widetilde{\mathbf{d}} \quad \text{s.t.} \quad \lambda_I \geq \mathbf{o} \quad \text{and} \quad \mathbf{G}\lambda = \mathbf{e}. \tag{11}$$

After homogenization of the equality constraints and introducing orthogonal projectors, problem (11) turns into

$$\min \quad \overline{\theta}_\varrho(\lambda) \quad \text{s.t.} \quad \mathbf{G}\lambda = \mathbf{o} \quad \text{and} \quad \lambda_I \geq -\widetilde{\lambda}_I, \tag{12}$$

where ϱ is a positive constant, $\mathbf{G}\lambda_I = \mathbf{e}$, and

$$\overline{\theta}_\varrho(\lambda) = \frac{1}{2}\lambda^T\mathbf{H}_\varrho\lambda - \lambda^T\mathbf{P}\mathbf{d}, \quad \mathbf{H}_\varrho = \mathbf{P}\mathbf{F}\mathbf{P} + \varrho\mathbf{Q}, \quad \mathbf{Q} = \mathbf{G}^T\mathbf{G}, \quad \mathbf{P} = \mathbf{I} - \mathbf{Q}.$$

The matrices $\mathbf{P}$ and $\mathbf{Q}$ are the orthogonal projectors onto Ker$\mathbf{G}$ and Im$\mathbf{G}^T$, respectively. It has been proved (see, e.g., Brenner [1] or Pechstein [16]) that there are constants $0 < c < C$ that depend neither on h nor H such that

$$c \leq \lambda_{\min}(\mathbf{H}_\varrho) \leq \max\{CH/h, \varrho\}.$$

5 Connecting subdomains into clusters

The bottleneck of classical FETI methods is the rank d of the projector $\mathbf{Q}$ which is equal to the defect of stiffness matrix $\mathbf{K}$, in our case $d = s$. To reduce the rank of $\mathbf{Q}$, we use the idea of Klawonn and Rheinbach [11] to interconnect some subdomains on the primal level into clusters so that the defect of the stiffness matrix of the cluster is equal to the defect of one of the subdomain stiffness matrices.

For example, to couple adjacent subdomains with common corners $\mathbf{x}, \mathbf{y} \in \overline{\Omega}^i \cap \overline{\Omega}^j$, we can transform the nodal variables associated with $\widetilde{\Omega}^q = \overline{\Omega}^i \times \overline{\Omega}^j$ by the expansion matrix $\mathbf{L}^q$ obtained by replacing two columns of the identity matrix associated with $\mathbf{x}, \mathbf{y}$ by one column obtained as a normalized sum of the columns associated with the displacements of nodes $\mathbf{x}$ and $\mathbf{y}$. Feasible variables $\mathbf{u}^q$ of the cluster are related to global variables $\widetilde{\mathbf{u}}^q$ by $\mathbf{u}^q = \mathbf{L}^q \widetilde{\mathbf{u}}^q$ and the stiffness matrix $\widetilde{\mathbf{K}}^q$ of such cluster in global variables can be obtained by

$$\widetilde{\mathbf{K}}^q = (\mathbf{L}^q)^T \mathrm{diag}(\mathbf{K}^i, \mathbf{K}^j) \mathbf{L}^q.$$

Let us denote by $\mathbf{e}$ and $\overline{\mathbf{e}}$ the vectors with all components equal to 1 and $1/\|\mathbf{e}\|$, respectively. To describe the coupling by averages, we use the transformation of bases proposed by Klawonn and Widlund [12], see also Klawonn and Rheinbach [10] and Li and Widlund [14]. The basic idea is a rather trivial observation that if

$$[\mathbf{C}\ \overline{\mathbf{e}}] = [\mathbf{c}_1, \dots, \mathbf{c}_{p-1}, \overline{\mathbf{e}}], \quad \overline{\mathbf{e}} = \frac{1}{\sqrt{p}} \mathbf{e},$$

denote an orthonormal basis of $\mathbb{R}^p$, then the last coordinate of a vector $\mathbf{x} \in \mathbb{R}^p$ in this basis is given by $x_p = \overline{\mathbf{e}}^T \mathbf{x}$. If we apply the transformation to the variables associated with the interiors of adjacent edges, we can join them by the expansion mapping $\mathbf{L}$ as above.

The procedure can be generalized to specify the feasible vectors of any cluster connected by the edge averages of adjacent edges. Using a proper numbering of variables by subdomains, in each subdomain setting first the variables that are not affected by the interconnecting, then the variables associated with the averages ordered by edges, we get the matrix $\mathbf{Z}$ with orthonormal columns the range of which represents the feasible displacements of the cluster,

$$\mathbf{Z} = \begin{bmatrix} \mathbf{C}\ \mathbf{E} \end{bmatrix}, \ \mathbf{C} = \mathrm{diag}(\mathbf{C}^1, \dots \mathbf{C}^s), \ \mathbf{E} = 1/\sqrt{2} \begin{bmatrix} . & & . & . \\ . & \overline{\mathbf{e}}^{ij} & & . \\ . & & . & . \\ . & \overline{\mathbf{e}}^{ji} & & . \\ . & & . & . \end{bmatrix}, \ (i, j) \in C. \tag{13}$$

In (13), C denotes a set of ordered couples of indices (i, j), $i < j$, s here denotes the number of subdomains in the cluster, and $\overline{\mathbf{e}}^{ij}$ denotes the basis vectors associated with the edge averages. Each couple $(i, j) \in C$ defines the connection of the adjacent edges of Ω^i and Ω^j by averages. The procedure is very similar to that described in the introduction of this section; the only difference is that we replace the expansion matrix $\mathbf{L}^q$ by the basis of feasible displacements of the cluster $\mathbf{Z}^q$. The feasible variables of the cluster are related to global variables $\widetilde{\mathbf{u}}^q$ by

$$\mathbf{u}^q = \mathbf{Z}^q \widetilde{\mathbf{u}}^q$$

and the Schur complement $\widetilde{\mathbf{S}}^q$ of such a cluster in global variables can be obtained by

$$\widetilde{\mathbf{S}}^q = (\mathbf{Z}^q)^T \operatorname{diag}(\mathbf{S}^i, \mathbf{S}^j, \dots, \mathbf{S}^\ell)\mathbf{Z}^q.$$

Assuming that the set of all subdomains is decomposed into c clusters interconnected by the edge averages, we can use the global transformation matrix with orthonormal columns

$$\mathbf{Z} = \operatorname{diag}(\mathbf{Z}^1, \cdots, \mathbf{Z}^c)$$

to connect the groups of $m \times m$ subdomains into clusters to get the stiffness matrix

$$\widetilde{\mathbf{S}} = \mathbf{Z}^T\mathbf{S}\mathbf{Z} = \operatorname{diag}(\widetilde{\mathbf{S}}^1, \cdots \widetilde{\mathbf{S}}^c)$$

and the matrices

$$\widetilde{\mathbf{B}}, \quad \widetilde{\mathbf{R}} = \operatorname{diag}(\widetilde{\mathbf{e}}^1, \dots, \widetilde{\mathbf{e}}^c), \quad \widetilde{\mathbf{G}} = \mathbf{T}\widetilde{\mathbf{R}}^T\widetilde{\mathbf{B}}^T,$$

where $\widetilde{\mathbf{B}}$ denotes a matrix that enforces interconnecting constraints that are not enhanced on the primal level and $\mathbf{T}$ denotes an orthogonalization matrix so that $\widetilde{\mathbf{G}}\widetilde{\mathbf{G}}^T = \mathbf{I}$. It is easy to achieve that

$$\widetilde{\mathbf{B}}\widetilde{\mathbf{B}}^T = \mathbf{I}. \tag{14}$$

Notice that $\widetilde{\mathbf{B}}$ enforces both constraints that connect subdomains into clusters and those connecting the clusters. Moreover, Ker$\widetilde{\mathbf{B}}$ =Ker$\mathbf{BZ}$, but $\mathbf{BZ}$ need not have orthonormal rows. Using the above transformation, we reduced problem (12) to

$$\min \quad \widetilde{\theta}_\varrho(\lambda) \quad \text{s.t.} \quad \widetilde{\mathbf{G}}\lambda = \mathbf{o} \quad \text{and} \quad \lambda_I \geq -\widetilde{\lambda}_I, \tag{15}$$

where ϱ is a positive constant and

$$\widetilde{\theta}_\varrho(\lambda) = \frac{1}{2}\lambda^T\widetilde{\mathbf{H}}_\varrho\lambda - \lambda^T\widetilde{\mathbf{P}}\widetilde{\mathbf{d}}, \tag{16}$$
$$\widetilde{\mathbf{H}}_\varrho = \widetilde{\mathbf{P}}\widetilde{\mathbf{F}}\widetilde{\mathbf{P}} + \varrho\widetilde{\mathbf{Q}}, \quad \widetilde{\mathbf{Q}} = \widetilde{\mathbf{G}}^T\widetilde{\mathbf{G}}, \quad \widetilde{\mathbf{P}} = \mathbf{I} - \widetilde{\mathbf{Q}} \quad \widetilde{\mathbf{F}} = \widetilde{\mathbf{B}}\widetilde{\mathbf{S}}^{+}\widetilde{\mathbf{B}}^T.$$

$\widetilde{\mathbf{P}}$ and $\widetilde{\mathbf{Q}}$ are the orthogonal projectors onto Ker$\widetilde{\mathbf{G}}$ and Im$\widetilde{\mathbf{G}}^T$, respectively.

Notice that the number of the rows of $\mathbf{G}$ is m^2 times larger that that of $\widetilde{\mathbf{G}}$, so that the cost of $(\mathbf{G}^T\mathbf{G})^{-1}$ is about m^4 times larger than that of $(\widetilde{\mathbf{G}}\widetilde{\mathbf{G}})^{-1}$.

6 Bounds on the spectrum of $\widetilde{\mathbf{H}}_\varrho$ and optimality

Using that Im$\widetilde{\mathbf{P}}$ and Im$\widetilde{\mathbf{Q}}$ are invariant subspaces of $\widetilde{\mathbf{H}}_\varrho$, it is easy to check that

$$\min\{\overline{\lambda}_{\min}(\widetilde{\mathbf{P}}\widetilde{\mathbf{F}}\widetilde{\mathbf{P}}), \varrho\} \leq \lambda_i(\widetilde{\mathbf{H}}_\varrho) \leq \max\{\|\widetilde{\mathbf{F}}\|, \varrho\}. \quad (17)$$

Applying standard arguments (see, e.g., [5, Lemma 3.1]), it is easy to reduce the problem of finding bounds on the spectrum of $\widetilde{\mathbf{H}}_\varrho$ to the problem of finding bounds on the spectrum of $\widetilde{\mathbf{S}}_i$. Some bounds were proved recently (see [5]):

Theorem 1 *For each integer $m > 1$, let $\widetilde{\mathbf{S}}$ denote the Schur complement of the cluster with the side-length H_c comprising $m \times m$ square subdomains of the side-length $H_s = H_c/m$. Let the subdomains be discretized by a regular grid with the step-length h and interconnected by the edge averages. Let $\overline{\lambda}_{\min}(\mathbf{S})$ denote the smallest nonzero eigenvalue of*

$$\mathbf{S} = \mathrm{diag}(\mathbf{S}^1, \ldots, \mathbf{S}^{m^2}),$$

where $\mathbf{S}^i$ denote the Schur complements of the subdomain stiffness matrices $\mathbf{K}^i$, $i = 1, \ldots, m^2$, with respect to the interior variables. Then

$$\|\mathbf{S}\| = \lambda_{\max}(\mathbf{S}) \geq \lambda_{\max}(\widetilde{\mathbf{S}}), \quad (18)$$

$$\overline{\lambda}_{\min}(\mathbf{S}) \geq \overline{\lambda}_{\min}(\widetilde{\mathbf{S}}) \geq \frac{2n_e}{n_s}\overline{\lambda}_{\min}(\mathbf{S}) \sin^2\left(\frac{\pi}{2m}\right) \approx \frac{1}{2}\overline{\lambda}_{\min}(\mathbf{S}) \left(\frac{\pi}{2m}\right)^2. \quad (19)$$

The spectrum of $\mathbf{S}$ can be bounded in terms of the decomposition and discretization parameters H_s and h, respectively – there are positive constants c, C such that

$$ch/H_s \leq \lambda_{\min}(\mathbf{S}) \leq \|\mathbf{S}\| \leq C. \quad (20)$$

For the proof, see Pechstein [16, Lemma 1.59] or Brenner [1]. Since there are algorithms that can solve (15) with the rate of convergence that depends on the bounds on the spectrum of $\widetilde{\mathbf{H}}_\varrho$, we can formulate the following theorem.

Theorem 2 *Let $\varrho \approx \|\widetilde{\mathbf{F}}\|$ and let the parameters H_s, m, and h specify problem* (15)*. Then there are constants $c, C > 0$ independent of H_s, m, h such that*

$$c \leq \lambda_{\min}(\widetilde{\mathbf{H}}_\varrho) \leq \|\widetilde{\mathbf{H}}_\varrho\| \leq CmH_s/h. \quad (21)$$

Moreover, there is a constant $M_{\max}$ such that if $C_1 > 2$ is an arbitrary constant and

$$mH_s/h \leq C_1,$$

then the SMALBE-M algorithm [6, Chap. 9] with the inner loop implemented by MPRGP [6, Chap. 8] can find an approximate solution of any problem (15) *generated with the parameters H_s, m, h in at most $M_{\max}$ matrix–vector multiplications.*

The proof is similar to the proof of optimality of TFETI for a variational inequality [6, Sect. 10.8] or contact problems [6, Sect. 11.10].

7 Numerical experiments

We carried out some numerical experiments to check the bounds and compare H-TFETI-DP with TFETI for both linear and non-linear problems. In all experiments, we use the relative precision stopping criterion with $\varepsilon = 10^{-4}$.

7.1 Comparing estimate and experiments

To compare estimates (19) with the real values, we have computed [5] the bounds on the extreme nonzero eigenvalues of the Schur complements of $m \times m$ clusters joined by edge averages using $m \in \{2, 4, 8, 16\}$, $H_c = 1$, $H_s = 1/m$, and $h = 1/64$. Some of the results are in Table 1. The results comply with those carried out by Klawonn and Rheinbach [11] and Lee [13].

Table 1: Regular condition number and extreme nonzero eigenvalues – edge averages

m	2	4	8	16
H_s/h	32	16	8	4
$\overline{\lambda}_{\max}(\widetilde{\mathbf{S}})$	2.8235	2.8098	2.7638	2.6843
$\overline{\lambda}_{\min}(\widetilde{\mathbf{S}})$	0.0173	0.093	0.047	0,0022
$\overline{\lambda}_{\min}^{\mathrm{est}}(\widetilde{\mathbf{S}})$	0.0104	0.059	0.029	0.0012

7.2 Comparing linear unpreconditioned H-TFETI-DP and TFETI

We compared H-TFETI-DP with standard TFETI on the unit square Poisson benchmark discretized by Q1 finite elements on regular grid with parameters h and H_s, $H_s/h = 100$ [5]. We used the ESPRESO (ExaScale PaRallel FETI SOlver) package [15] developed at the Czech National Supercomputing Center in Ostrava. The domain was decomposed into $n_c \times n_c$ clusters, $n_c = 6, 18, 54$, each cluster comprising 15×15 square subdomains joined by edge averages. Notice that H-TFETI-DP outperforms TFETI due to the small coarse problem and cheap iterations.

Table 2: Billion variables Poisson - unpreconditioned H-TFETI-DP and TFETI, m=15, see [5]

Clusters	Subdomains	Cores	Unknowns	H-TFETI-DP (iter/sec)	TFETI (iter/sec)
36	8,100	108	81,018,001	117/26.0	45/14.5
324	72,900	972	729,054,001	118/27.7	42/40.2
2,916	656,100	8.748	6,561,162,001	116/28.0	41/61.0

7.3 Model variational inequality and elastic body on rigid obstacle

We used the above procedure to get the discretized H-TFETI-DP QP problem (12) that we solved by a combination of the SMALBE-M (semimonotonic augmented Lagrangian) [6, Chap. 9] algorithm with the inner loop resolved by MPRGP (modified proportioning with reduced gradient projection) [6, Chap. 8]. We implemented both algorithms in the PETSc based package PERMON [7] developed at the Department of Applied Mathematics of the VSB-Technical University of Ostrava and the Institute of Geonics of the Czech Acadamy of Science.

Table 3: Semicoercive variational inequality, primal dimension 20,480,000, inequalities 3169

m=	1	2	4	8
outer iter	52	25	16	12
matrix × vector	243	252	186	218
coarse problem dimension	2048	512	128	32

Our final benchmark is a clamped cube over a sinus-shape obstacle as in Fig. 3, loaded by own weight, decomposed into $4 \times 4 \times 4$ clusters, $H_s/h = 14$, using the ESPRESO [15] implementation of H-TFETI-DP for contact problems. We can see that TFETI needs a much smaller number of iterations, but H-TFETI-DP is still faster due to 64-times smaller coarse space and better exploitation of the node-core memory organization. In general, if we use $m \times m \times m$ clusters, the hybrid strategy reduces the dimension and the cost of the coarse problem by m^3 and m^6, respectively.

Table 4: Clamped elastic cube over the sinus-shaped obstacle, $m = 4$, $H_s/h = 14$

Clusters	Subdomains	Cores	Unknowns (10^6)	H-TFETI-DP (iter/sec)	TFETI (iter/sec)
64	4,096	192	13	169/23.9	117/24.9
512	72,900	1536	99	208/30.2	152/115.1
1,000	656,100	3000	193	206/42.6	173/279.9

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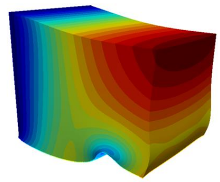

Fig. 3: Displacements of a clamped elastic cube over the sinus-shaped obstacle

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