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Fixing Nodes Strategies for the Effective Regularization of the Subdomain Stiffness Matrices Arising in Total FETI

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Abstract

The bottlenecks related to the numerical solution of many engineering problems are very dependent on the techniques used to solve the systems of linear equations that result from their linearizations and finite element discretizations. The large linearized problems can be solved efficiently using the so-called scalable algorithms based on multigrid or domain decomposition method. In cooperation with the Elmer team two variants of the domain decomposition method have been implemented into Elmer: (i) FETI-1 (Finite Element Tearing and Interconnecting) introduced by Farhat and Roux and (ii) Total FETI introduced by Dostal, Horak, and Kucera. In the latter, the Dirichlet boundary conditions are torn off to have all subdomains floating, which makes the method very flexible. In this paper, we review the results related to the efficient solution of symmetric positive semidefinite systems arising in FETI methods when they are applied on elliptic boundary value problems. More specifically, we show three different strategies to find the so-called fixing nodes (or DOFs - degrees of freedom), which enable an effective regularization of the corresponding subdomain system matrices that eliminates the work with singular matrices. The performance is illustrated on an elasticity benchmark computed using ELMER on the French Tier-0 system CURIE.

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1. Introduction

Effective implementation of some efficient FETI methods assumes the application of a direct method for solving a system of linear equations with a symmetric positive semidefinite (SPS) matrix $\mathbf{A}$. To eliminate computations with singular matrices and to enable the use of the standard Cholesky factorizations for nonsingular matrices we apply an effective regularization to $\mathbf{A}$ based on suitably chosen fixing nodes (DOFs) and adding the regularization term to the entries of $\mathbf{A}$ corresponding to these nodes (DOFs). This regularization improves conditioning, stability, and flexibility and eliminates the bottleneck of FETI implementation. The regularization with different strategies for finding fixing nodes have been implemented into Elmer [1] and tested on the French Tier-0 system CURIE.

Elmer is a finite element software for the solution of multiphysic problems. After its inception in 1995 Elmer was developed mainly as a national Finnish project. In 2005 Elmer was published under the GPL, which has increased its international use and development dramatically. Currently it is used perhaps by a few thousand researchers around the world. Of all the user communities, the one working in the area of computational glaciology is perhaps of most significance [13, 14], but there are many other blooming user communities in different application areas that could make use of the improved parallel performance.

2. Effective regularization based on fixing nodes (DOFs) strategies

In the following, we assume that $\mathbf{A}$ is an SPS stiffness matrix of a "floating" 2D or 3D elastic body without a mechanism, such as a subdomain in the TFETI method, and $\mathbf{R}$ is a matrix created columnwise by the kernel basis vectors of $\mathbf{A}$ which are known a priori. If we choose M nodes that are neither near each other nor placed near any line, $M < N$, $M \geq 2$ in 2D, and $M \geq 3$ in 3D, then the submatrix $\mathbf{A}_{\mathcal{J}\mathcal{J}}$ of the stiffness matrix $\mathbf{A}$ defined by the set $\mathcal{J}$ with the indices of the displacements of the other nodes is "reasonably" nonsingular. Of course, this is not surprising, as $\mathbf{A}_{\mathcal{J}\mathcal{J}}$ can be considered as the stiffness matrix of the body that is fixed in the chosen nodes. Using the arguments of mechanics, it is natural to assume that if fixing of the chosen nodes

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makes the body stiff, then $\mathbf{A}_{\mathcal{J}\mathcal{J}}$ is well-conditioned. We call the M chosen nodes *fixing nodes* and denote by $\mathcal{I}$ the set of indices of corresponding displacements.

Our starting point is the following decomposition

$$\mathbf{PAP}^T = \begin{bmatrix} \mathbf{A}_{\mathcal{J}\mathcal{J}} & \mathbf{A}_{\mathcal{J}\mathcal{I}} \\ \mathbf{A}_{\mathcal{I}\mathcal{J}} & \mathbf{A}_{\mathcal{I}\mathcal{I}} \end{bmatrix} \tag{1}$$

of the SPS matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ using the corresponding permutation matrix $\mathbf{P}$.

Then the following proposition holds (see [16]).

Proposition 1.1 *For given $\varrho > 0$ and $\mathbf{Q} = \mathbf{R}_{\mathcal{I}*}(\mathbf{R}_{\mathcal{I}*}^T \mathbf{R}_{\mathcal{I}*})^{-1}\mathbf{R}_{\mathcal{I}*}^T$, where $\mathbf{R}_{\mathcal{I}*}$ is a restriction of $\mathbf{R}$ to the rows with indices from $\mathcal{I}$, the matrix*

$$\mathbf{A}_\varrho = \mathbf{P}^\top \begin{bmatrix} \mathbf{A}_{\mathcal{J}\mathcal{J}} & \mathbf{A}_{\mathcal{J}\mathcal{I}} \\ \mathbf{A}_{\mathcal{I}\mathcal{J}} & \mathbf{A}_{\mathcal{I}\mathcal{I}} + \varrho\mathbf{Q} \end{bmatrix} \mathbf{P}$$

is symmetric positive definite and $\mathbf{A}_\varrho^{-1}$ is the generalized inverse to $\mathbf{A}$. Thus $\mathbf{A}_\varrho$ can be factorized by any standard Cholesky type factorization method.

To preserve sparsity of the Cholesky factor of $\mathbf{A}_\varrho$ we may use any sparse reordering algorithm such as symmetric approximate minimum degree, symmetric reverse Cuthill-McKee, profile and wavefront reduction, etc. The optimal choice depends on the way in which the sparse matrix is stored and on the problem geometry.

For more details about regularization, we refer to [4] and [16]. To implement the above mentioned observations, it is necessary to have an effective procedure for choosing uniformly distributed fixing nodes to have $\mathbf{A}_{\mathcal{J}\mathcal{J}}$ as stiff (well-conditioned) as possible. Therefore, in the following sections we introduce three different strategies of finding well distributed fixing nodes (DOFs).

2.1. Uniform strategy

Let us first describe a simple but effective method that we use in our research code ([17]) to get M uniformly distributed fixing nodes. The method combines a mesh partitioning algorithm with a method for finding a mesh center. The algorithm reads as follows.

Algorithm 1. Given a mesh and $M > 0$.

1. Split the mesh into M submeshes using the mesh partitioning algorithm.
2. Verify whether the resulting submeshes are connected. If not, a graph post-processing may be used to get connected submeshes.
3. Take a node lying near the center of each submesh.

Step 1 can be carried out by a code for graph decompositions such as METIS. To describe the implementation of Step 3, let us recall that the adjacency matrix of a mesh is a symmetric square matrix $\mathbf{D}$ whose entry d_{ij} is equal to 1 if the corresponding nodes i and j are adjacent in the mesh, and it is equal to zero otherwise. Since we deal with structures (meshes) that contain no loops, the entries on the main diagonal are all equal to zero. Let us also recall that a *walk of length* $k-1$ is a sequence of distinct nodes of the given mesh $(v_1, v_2, \ldots, v_k)$, such that all the edges $v_i v_{i+1}$ are present in the mesh for all $i = 1, 2, \ldots, k-1$. In other words $d_{v_i, v_{i+1}} = 1$ for all $i = 1, 2, \ldots, k-1$. We say the walk starts at v_1 and ends at v_k if the first node in the sequence is v_1 and the last node is v_k. Moreover, we call a walk between nodes v_1 and v_k a (v_1, v_k)*-walk*. We use the following observation.

Lemma 1.1 *Let $\mathbf{D}$ be the adjacency matrix of a given mesh and $\mathbf{e} = [e_i]$, $e_i = 1$, $i = 1, 2, \ldots, n$. Then the number $w(i,k)$ of distinct walks of length k starting at node i is given by*

$$w(i,k) = [\mathbf{D}^k \mathbf{e}]_i.$$

The proof can be obtained by standard arguments ([9]). See also [11]. Since the mesh is approximately regular, we expect that more walks of length k originate from the nodes that are near a center of the mesh than from vertices that are far from it. It simply follows that the node with index i which satisfies

$$w(i,k) \geq w(j,k), j = 1, 2, \ldots, n,$$

for sufficiently large k is in a sense near to the center of the mesh and can be used to implement Step 3 of Algorithm 1.

Notice that the vector

$$\mathbf{p} = \lim_{k\to\infty} \|\mathbf{D}^k \mathbf{e}\|^{-1} \mathbf{D}^k \mathbf{e}$$

is a unique nonnegative eigenvector which corresponds to the largest eigenvalue of $\mathbf{D}$. It is also known as the Perron vector of $\mathbf{D}$. It can be approximated by a few steps of the power or Lanczos methods ([15]).

2.2. *Geometrical strategy*

Geometrical strategy is the simplest one and is based on finding fixing nodes using simple geometrical and combinatorial arguments: choose M mesh nodes that are mutually as far apart as possible and that are not placed near any line.

2.3. *Kernel strategy*

If the kernel of $\mathbf{A}$ is known, then we can use it to identify a submatrix $\mathbf{A}_{\mathcal{J}\mathcal{J}}$ of $\mathbf{A}$ of a maximal order. Since the Schur complement of $\mathbf{A}_{\mathcal{J}\mathcal{J}}$ is the zero matrix, the solution of a consistent system with $\mathbf{A}$ reduces to the Cholesky decomposition of $\mathbf{A}_{\mathcal{J}\mathcal{J}}$. The following estimate proved in [10] indicates that we can use information obtained from the kernel of $\mathbf{A}$ to identify suitable zero pivots.

Proposition 1.2 *Let* $\mathbf{A} \in \mathbb{R}^{n\times n}$ *denote a symmetric matrix whose kernel is spanned by the full column rank matrix* $\mathbf{R} \in \mathbb{R}^{n\times d}$ *with orthonormal columns, so that* d *is the defect of* $\mathbf{A}$*. Let* $\mathcal{I} = \{i_1, \dots, i_d\}$, $\quad 1 \le i_1 < i_2 < \dots < i_d \le n$, *denote a set of indices, and let* $\mathcal{J} = \mathcal{N} - \mathcal{I}$, $\quad \mathcal{N} = \{1, 2, \dots, n\}$.

Then

$$\lambda_{\min}(\mathbf{A}_{\mathcal{J}\mathcal{J}}) \ge \overline{\lambda}_{\min}(\mathbf{A})\, \sigma^4_{\min}(\mathbf{R}_{\mathcal{I}*}), \tag{2}$$

where $\overline{\lambda}_{\min}(\mathbf{A})$ *and* $\sigma_{\min}(\mathbf{R}_{\mathcal{I}*})$ *denote the least nonzero eigenvalue of* $\mathbf{A}$ *and the least singular value of* $\mathbf{R}_{\mathcal{I}*}$.

The heuristic that we propose reads as follows. We start with a suitable column transformations with complete pivoting to reduce $\mathbf{R}$ into the form

$$\mathbf{RG} = \mathbf{P}\begin{bmatrix} \mathbf{D} \\ \mathbf{B} \end{bmatrix},$$

where $\mathbf{G} \in \mathbb{R}^{d\times d}$ is suitable nonsingular matrix, such as a product of Gauss transformations or Householder reflections [15], $\mathbf{D} \in \mathbb{R}^{d\times d}$ is the diagonal matrix with the pivots on the diagonal, $\mathbf{P} \in \mathbb{R}^{n\times n}$ is suitable permutation matrix, and $\mathbf{B} \in \mathbb{R}^{(n-d)\times d}$. In the first step of complete pivoting, we choose the pivot as the largest entry in absolute value of $\mathbf{R}$ and add suitable multiples of the column with the pivot to the other columns to generate zeros in the row corresponding to the pivot. In the next steps, we repeat the procedure to the modified $\mathbf{R}$, but choose the pivots only from the columns that do not contain any pivot chosen before. The positions of the zero rows or columns of the factors in the decomposition of $\mathbf{A}$ are just the positions of the nonzero components of $\mathbf{P}_{*\mathcal{I}}$, $\mathcal{I} = \{1, \dots, d\}$.

3. Numerical examples

The performance of our strategies is illustrated on the stiffness matrix $\mathbf{A}$ of the elastic three-dimensional body made of steel and discretized by trilinear bricks with the Neumann boundary conditions (see Fig. 1). In Fig. 1, we illustrate the resulting configurations of fixing nodes (DOFs) found by different strategies: (i) no, (ii) kernel, (iii) geometrical, (iv) uniform.

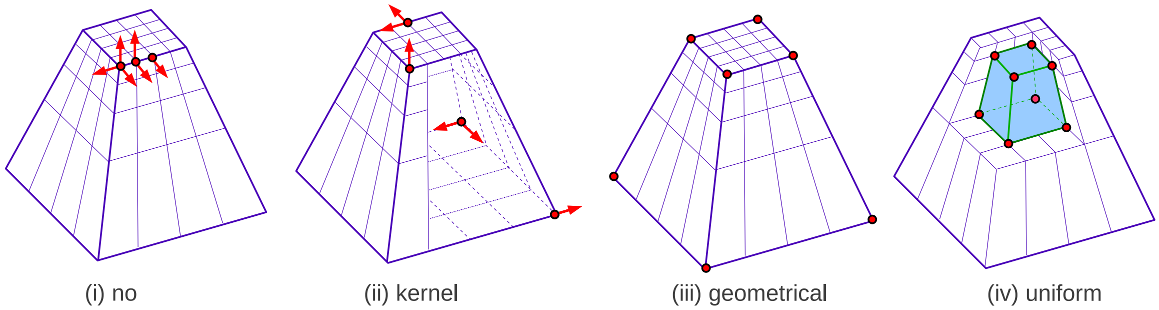
(i) no (ii) kernel (iii) geometrical (iv) uniform

Fig. 1. Fixing nodes (DOFs) strategies.

In Table 1, we report the condition number of the nonsingular part $\mathbf{A}_{\mathcal{J}\mathcal{J}}$ with respect to the chosen strategy. The results of experiments agree with the intuitive rule that fixing nodes distributed in a more regular pattern improves the conditioning of $\mathbf{A}_{\mathcal{J}\mathcal{J}}$. Comparing the results, we conclude that all the proposed strategies are effective.

To show the scalability behavior of our ELMER FETI implementation we take a 3D elastic cube and decompose it into identical boxes. Then each box is discretized by 8000 bricks. In Table 2, we report the numbers of unknowns, cores and iterations, and the computational time achieved on the French Tier-0 system CURIE. For large decompositions the so-called coarse problem solution starts to dominate. Therefore we plan to replace the standard FETI method by its hybrid version which eliminates this drawback.

Table 1. Conditioning of the nonsingular part $\mathbf{A}_{\mathcal{J}\mathcal{J}}$.

strategy	no	kernel	geometrical	uniform
cond($\mathbf{A}_{\mathcal{J}\mathcal{J}}$)	9.4e18	9371	900	518

Table 2. Scalability results.

unknowns	cores (subdomains)	time	CG iterations
192,000	8	5.57	17
648,000	27	10.52	26
3,000,000	125	9.27	31
8,232,000	343	10.26	32
24,000,000	1000	19.88	33
81,000,000	3375	31.52	35

4. Summary

We have introduced the concept of fixing nodes and used it to the effective regularization of singular subdomain stiffness matrices arising in FETI methods. This regularization with all mentioned strategies of finding fixing nodes (DOFs) improves stability and flexibility and eliminates the bottleneck of previous ELMER FETI implementation. Particularly, it improves conditioning and enables factorization using any standard Cholesky type decomposition method for nonsingular matrices. This completely removes working with singular matrices. The scalability behavior has been shown up to thousands of cores on the French Tier-0 system CURIE. Indeed for large decompositions the so-called coarse problem solution starts to dominate. This drawback can be eliminated by the so-called hybrid FETI method which we plan to implement into Elmer. The proposed algorithms were also successfully applied to the solution of large contact problems discretized using TFETI to more than 11 millions of nodal variables ([11]).

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