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Comments on combination of vectorized and parallel code for elastic problems

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Abstract

This paper presents some notes on the vectorization and parallelization code for the elasticity problem in Matlab. Leaving aside the solution to the elasticity problem, the most time-consuming operation is the construction of the stiffness matrix. To solve this problem comprehensively, we should combine two approaches. The first approach is to decompose the body using a non-overlapping domain decomposition method (TFETI), which is well parallelizable, and to construct the corresponding objects for each subdomain. The second approach is vectorization to construct a stiffness matrix for each subdomain efficiently. This approach implements in Matlab, and all Matlab codes will be available for download and provide complete finite element implementations in both 2D and 3D.

Keywords: finite element method, vectorization approach, non-overlapping domain decomposition method, parallelization, elasticity problem, Lagrange multipliers

1 Introduction

Elastic problems still represent an essential topic in the continuum mechanics of steel and solids. This paper is focused on the Matlab implementation of elastic problems formulated in terms of displacements.

This approach is based on two previously published papers [1,2] that addressed the problem of elastoplasticity in combination with TFETI domain decomposition and a second paper where we discussed an efficient approach to vectorization, which is a powerful tool in speeding up code in Matlab and other programming languages.

A linear solver considered in this paper is based on a FETI-type domain decomposition method enabling its efficient parallel implementation. The standard FETI method (FETI-1) was initially introduced by Farhat and Roux [3] and theoretically analyzed by Mandel and Tezaur [4]. Using this approach, a body is partitioned into non-overlapping subdomains, an elliptic problem with Neumann boundary conditions is defined for each subdomain, and inter-subdomain field continuity is enforced via Lagrange multipliers. The Lagrange multipliers are efficiently solved from a dual problem by a variant of the conjugate gradient algorithm. The first practical implementations exploited only the favorable distribution of the spectrum of the matrix of the minor problem [5], also known as the dual Schur complement matrix, but the such algorithm was efficient only with a small number of subdomains. Here, we use the Total-FETI (TFETI) [6] variant of the FETI domain decomposition method, where even the Dirichlet boundary conditions are enforced by Lagrange multipliers.

The rest of the paper is organized as follows. Section 2 summarizes the necessary theoretical basis of elastic problems in continuous form. Algebraic formulation and effective assembling of the stiffness matrix are recapitulated in Section 3. The non-overlapping domain decomposition method TFETI is mentioned in Section 4 and finally, the numerical results are introduced in Section 5.

2 Elastic model

Let us consider a deformable body occupying a domain $\Omega \subset \mathbb{R}^3$ with a Lipschitz continuous boundary $\Gamma = \partial\Omega$. We will describe the state of the body during a loading process by the Cauchy stress tensor $\sigma \in S$, the displacement $u \in \mathbb{R}^3$ and the small strain tensor $\varepsilon \in S$. Here $S = \mathbb{R}^{3\times 3}_{sym}$ is the space of all symmetric second order tensors. More details can be found in [7].

The small strain tensor is related to the displacement by the linear relation

$$\varepsilon(u) = \frac{1}{2}\left(\triangledown u + (\triangledown u)^T\right). \tag{1}$$

The equilibrium equation reads

$$-\mathrm{div}(\sigma(x)) = g(x) \quad \forall x \in \Omega, \tag{2}$$

where $g(x) \in \mathbb{R}^3$ represents the volume force acting at the point $x \in \Omega$.

Let the boundary Γ be fixed on a part Γ_U that has a nonzero Lebesgue measure with respect to Γ, i.e., we prescribe the homogeneous Dirichlet boundary condition on Γ_U:

$$u(x) = 0 \quad \forall x \in \Gamma_U. \tag{3}$$

On the rest of the boundary $\Gamma_N = \Gamma \setminus \Gamma_U$, we prescribe the Neumann boundary conditions

$$\sigma(x)n(x) = F(x) \quad \forall x \in \Gamma_N, \tag{4}$$

where $n(x)$ denotes the exterior unit normal and $F(x)$ denotes a prescribed surface forces at the point $x \in \Gamma_N$. Similarly, we can consider other boundary conditions, for example symmetry and periodic conditions.

For a weak formulation of the investigated problems, it is sufficient to introduce the space of kinematically admissible displacements,

$$V = \left\{ v \in [H^1(\Omega)]^3 : \; v = 0 \;\text{ on }\; \Gamma_U \right\}. \tag{5}$$

Then the conditions (2)–(4) can be written in a weak sense by

$$\int_\Omega \langle \sigma, \varepsilon(v) \rangle_F dx = \int_\Omega g^T v dx + \int_{\Gamma_N} F^T v ds \quad \forall v \in V, \; \forall t \in Q. \tag{6}$$

Here $\varepsilon(v)$ is defined by (1), $\langle ., . \rangle_F$ and $\|.\|_F$ denote the Frobenius scalar product and the corresponding norm on the space S, respectively.

We consider the elastic constitutive model given by the Hooke law for isotropic material,

$$\sigma = \mathbb{C}\varepsilon = \lambda \mathrm{tr}(\varepsilon) I + 2\mu\varepsilon \tag{7}$$

with the Lame coefficients λ, μ. For the sake of simplicity, we assume a homogeneous material, i.e., the constant coefficients $\lambda, \mu > 0$. The trace operator of a tensor is denoted by tr$(.)$ and I denotes the identity.

If we substitute (7) into (6), we obtain the weak formulation of the elastic problem. Find $u = u(x) \in V$ such that

$$a_e(u, v) = \int_\Omega g^T v dx + \int_{\Gamma_N} F^T v ds \quad \forall v \in V, \tag{8}$$

where the bilinear form on V reads

$$a_e(w, v) = \int_\Omega \langle \mathbb{C}\varepsilon(w), \varepsilon(v) \rangle_F dx, \quad w, v \in V \tag{9}$$

and $\mathbb{C}$ it the fourth order tensor.

3 Algebraic formulation

For sake of simplicity, let us continue with algebraic formulation. The space of kinematically admissible displacements (5) rewrite into

$$\boldsymbol{V} := \{ \boldsymbol{v} \in \mathbb{R}^n | \boldsymbol{B}_U \boldsymbol{v} = \boldsymbol{o} \},$$

where restriction matrix $\boldsymbol{B}_U \in \mathbb{R}^{m\times n}$ represents the homogeneous Dirichlet boundary condition. Than, we can rewrite the equation (8) as follows: find $\boldsymbol{u} \in \boldsymbol{V}$ such that

$$\boldsymbol{v}^T\left(\boldsymbol{K}\boldsymbol{u} - \boldsymbol{f}\right) = 0 \quad \forall \boldsymbol{v} \in \boldsymbol{V}, \tag{10}$$

where $\boldsymbol{u} \in \mathbb{R}^n$ denotes the unknown displacement vector, $\boldsymbol{f} \in \mathbb{R}^n$ is the vector of external forces, and $\boldsymbol{K} \in \mathbb{R}^{n\times n}$ is corresponding elastic stiffness matrix. For assembling matrix $\boldsymbol{K}$, we adopt the key idea from [2]

$$\boldsymbol{K} = \boldsymbol{S}^T\boldsymbol{D}\boldsymbol{S}, \tag{11}$$

where $\boldsymbol{S}$ is a sparse matrix representing the strain-displacement operator at all integration points and $\boldsymbol{D}$ is block diagonal sparse matrix for elastic problems. For more details how to effectively assamble matrix see [2].

4 TFETI domain decomposition method

We will schematically write the problem in the form:

$$\text{find } \boldsymbol{u} \in \boldsymbol{V}: \quad \tilde{\boldsymbol{K}}\tilde{\boldsymbol{u}} = \tilde{\boldsymbol{f}}, \tag{12}$$

where $\tilde{\boldsymbol{K}}$, $\tilde{\boldsymbol{u}}$, $\tilde{\boldsymbol{f}}$ are the restriction of $\boldsymbol{K},\ \boldsymbol{u},\ \boldsymbol{f}$ with respect to the Dirichlet boundary conditions respectively. Let us note that $\boldsymbol{K}$ is a symmetric and positive semidefinite matrix and $\tilde{\boldsymbol{K}}$ is a symmetric and positive definite matrix. The problem (12) can be equivalently rewritten as a minimization problem:

$$\text{find } \boldsymbol{u} \in \boldsymbol{V}: \quad \boldsymbol{J}(\boldsymbol{u}) \leq \boldsymbol{J}(\boldsymbol{v}),\ \forall \boldsymbol{v} \in \boldsymbol{V}, \tag{13}$$

where

$$\boldsymbol{J}(\boldsymbol{v}) = \frac{1}{2}\boldsymbol{v}^T\boldsymbol{K}\boldsymbol{v} - \boldsymbol{f}^T\boldsymbol{v}, \quad \boldsymbol{v} \in \boldsymbol{V}.$$

To apply the TFETI domain decomposition, we tear the body from the part of the boundary with the Dirichlet boundary condition, decompose it into subdomains, assign each subdomain by a unique number, and introduce new “gluing” conditions on the artificial intersubdomain boundaries and on the boundaries with imposed Dirichlet condition. In particular, the polyhedral domain Ω is decomposed into a system of s disjoint polyhedral subdomains $\Omega^p \subset \mathbb{R}^3$, $p = 1, 2, \ldots, s$.

After the decomposition each boundary Γ^p of Ω^p consists of three disjoint parts Γ_U^p, Γ_N^p, and Γ_G^p, $\Gamma^p = \overline{\Gamma}_U^p \cup \overline{\Gamma}_N^p \cup \overline{\Gamma}_G^p$, where

$$\Gamma_U^p = \Gamma_U \cap \Gamma^p, \ \ \Gamma_N^p = \Gamma_N \cap \Gamma^p, \ \ \Gamma_G^p = \bigcup_{q\in\{1,2,\ldots,s\}\setminus\{p\}} \Gamma_G^{pq},$$

with Γ_G^{pq} being the part of Γ^p which is glued to Ω^q, $p \neq q$.

After that, we can define a vector $\mathbf{v} \in \mathbb{R}^{\mathtt{n}}$, $\mathbf{v} = \left(\boldsymbol{v}_1^T, \boldsymbol{v}_2^T, \ldots, \boldsymbol{v}_s^T\right)^T$, where $\boldsymbol{v}_p \in \mathbb{R}^{n_p}, p \in \{1, 2, \ldots, s\}$, is the vector with dimension $\mathtt{n} = \sum_{p=1}^{s} n_p$ and n_p is number unknown for sumbomain p. Similarly we can find the vector $\mathbf{f} \in \mathbb{R}^{\mathtt{n}}$, $\mathbf{f} = \left(\boldsymbol{f}_1^T, \boldsymbol{f}_2^T, \ldots, \boldsymbol{f}_s^T\right)^T$, $\boldsymbol{f}_p \in \mathbb{R}^{n_p}, p \in \{1, 2, \ldots, s\}$, such that $\boldsymbol{f}_p$ is the algebraic representation of the load restricted on Ω^p and Γ_N^p. Let the matrix $\mathbf{B}_G \in \mathbb{R}^{\mathtt{m}_G \times \mathtt{n}}$ represent the gluing conditions and $\mathbf{B}_U \in \mathbb{R}^{\mathtt{m}_U \times \mathtt{n}}$ the Dirichlet boundary conditions. Both matrices can be combined into one constraint matrix

$$\mathbf{B} = \left[\begin{array}{c} \mathbf{B}_G \\ \mathbf{B}_U \end{array}\right], \quad \mathbf{B} \in \mathbb{R}^{\mathtt{m} \times \mathtt{n}}, \quad \mathtt{m} = \mathtt{m}_G + \mathtt{m}_U. \tag{14}$$

Typically $\mathtt{m}$ is much smaller than $\mathtt{n}$. Let us note that $\mathbf{B}$ can be assembled to have different forms: redundant, non-redundant or orthonormal. For more details see [8–11]. In fact all forms are applicable but due to simplicity of our presentation we use the orthonormal form of $\mathbf{B}$.

Let the matrix $\mathbf{K} \in \mathbb{R}^{\mathtt{n} \times \mathtt{n}}$, $\mathbf{K} = \mathit{diag}\left(\boldsymbol{K}_1, \boldsymbol{K}_2, \ldots, \boldsymbol{K}_s\right)$ denotes a symmetric positive semidefinite block diagonal matrix, where

$$\boldsymbol{K}_p = \boldsymbol{S}_p^T \boldsymbol{D}_p \boldsymbol{S}_p, \quad \boldsymbol{K}_p \in \mathbb{R}^{n_p \times n_p},$$

and $\boldsymbol{S}_p$, $\boldsymbol{D}_p$ are similar matrices as in (11) but for sumdomain p, $p \in \{1, 2, \ldots, s\}$. The diagonal blocks $\boldsymbol{K}_p$, $p \in \{1, 2, \ldots, s\}$, which correspond to the subdomains Ω^p, are positive semidefinite sparse matrices with known kernels, the rigid body modes.

The algebraical formulation of is following:

$$\left\{\begin{array}{rcl} \text{find } \mathbf{u} \in \mathbf{V} & : & \mathbf{J}(\mathbf{u}) \leq \mathbf{J}(\mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{V}, \\ \mathbf{J}(\mathbf{v}) & := & \frac{1}{2}\mathbf{v}^T \mathbf{K} \mathbf{v} - \mathbf{f}^T \mathbf{v}, \\ \mathbf{V} & := & \left\{\mathbf{v} \in \mathbb{R}^{\mathtt{n}} : \ \mathbf{B}\mathbf{v} = \mathbf{o}\right\}. \end{array}\right. \tag{15}$$

Even though (15) is a standard convex quadratic programming problem, its formulation is not suitable for numerical solution. The reasons are that $\mathbf{K}$ is typically ill-conditioned, singular, and very large.

The complications mentioned above may be essentially reduced by applying the duality theory of convex programming (see, e.g., Dostál [12]), where all the constraints are enforced by the Lagrange multipliers $\boldsymbol{\lambda}$. The Lagrangian associated with problem (15) is

$$L(\mathbf{v}, \boldsymbol{\lambda}) = \mathbf{J}(\mathbf{v}) + \boldsymbol{\lambda}^T \mathbf{B} \mathbf{v}. \tag{16}$$

It is well known [12] that (15) is equivalent to the saddle point problem:

$$\text{find } (\mathbf{u}, \boldsymbol{\lambda}) \in \mathbb{R}^{\mathtt{n}} \times \mathbb{R}^{\mathtt{m}} : \quad L(\mathbf{u}, \boldsymbol{\nu}) \leq L(\mathbf{u}, \boldsymbol{\lambda}) \leq L(\mathbf{v}, \boldsymbol{\lambda}) \quad \forall (\mathbf{v}, \boldsymbol{\nu}) \in \mathbb{R}^{\mathtt{n}} \times \mathbb{R}^{\mathtt{m}} \tag{17}$$

in sense that $\mathbf{u}$ solves (15) if and only if $(\mathbf{u}, \boldsymbol{\lambda})$ solves (17). For more details see [1, 12–14].

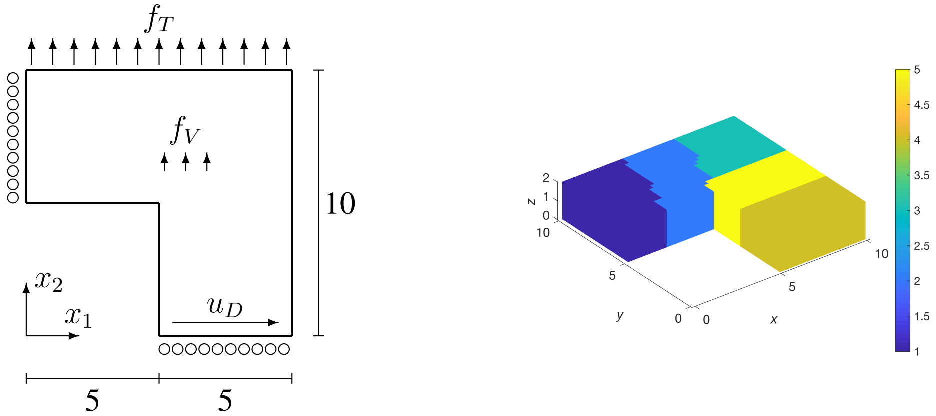

Figure 1: Simplified 2D geometry of the elastic problem (left). The real 3D geometry appears by extrusion in x_3 direction. The corresponding domain decomposition into 5 subdomains (right).

5 Results

The proposed algorithms were implemented in new library developed in Matlab and parallelized using Matlab Distributed Computing Server and Matlab Parallel Toolbox. The numbers of subdomains are chosen to keep the number of nodes per subdomain approximately constant except for the coarsest mesh level. In our code we allow multiple subdomains per processor which is discussed for example in [15].

All the calculations were done on a MacBook Pro with a 2.4 GHZ quad-core Intel Core i5 and 16GB of memory. Parallel jobs from two to four processors were run in Matlab software.

We consider a body that occupies the domain depicted in Figure 1 (left) in $x_1 - x_2$ plane. The corresponding 3D geometry appears by extrusion in x_3 direction. The size of the body in this direction is equal to one if the 3D problem is considered. On the left and bottom sides of the depicted domain, the symmetry boundary conditions are prescribed, i.e., $\mathbf{u} \cdot \mathbf{n} = 0$ where $\mathbf{n}$ is a normal vector to the boundary. On the bottom, we also prescribe nonhomogeneous Dirichlet boundary condition $u_D = 0.5$ in the direction x_1. Further, the constant traction of density $f_t = 200$ is acting on the upper side in the normal direction The material parameters are set as follows: $E = 206900$ (Young's modulus) and $\nu = 0.29$ (Poisson's ratio). The body is discretized into 9600 elements and 11529 nodes.

For the spatial discretization of Ω, let us consider hexahedral meshes generated by our code decomposed into 5 subdomains using Metis. An example of such decomposition is depicted in Figure 1.

For the computations in our implementation, we used the iterative PCGP algorithm, which is suitable for use with the Dirichlet preconditioner, and the value of the stopping criterion sets to 1e-9.

The total displacement and distributions of the HMH stress are depicted in Figures 2 left and 2 right, respectively.

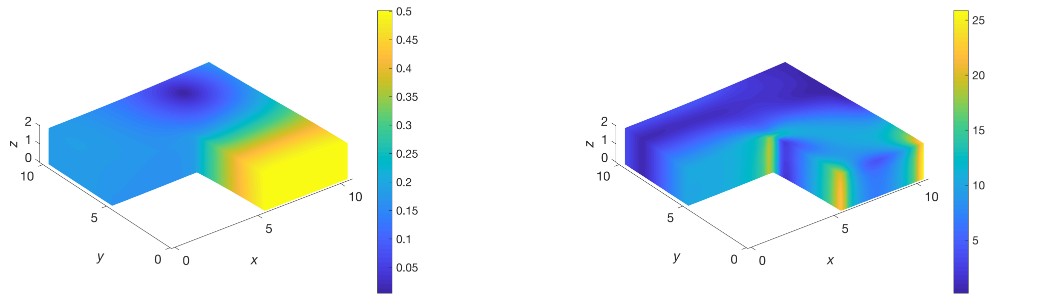

Figure 2: The total displacement on deformed body (left) and the HMH stress on deformed body (right).

6 Concluding remarks

The paper is focused on an efficient and flexible implementation of elastic problems. We have mainly proposed an innovative combination of vectorized and parallel approaches. The vectorized approach was used for assembling stiffness matrices, and the parallel approach was used for solving more significant benchmarks and the faster solution. We used the TFETI domain decomposition method, and the corresponding problem was solved by dual formulation. The algorithms were implemented in Matlab and were run in parallel by Matlab Parallel Toolbox. The performance of our algorithms was demonstrated on the 3D elastic L-shape body. We plan to apply this combination of approaches also to elastoplastic problems.

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