Some computational results for robust FETI-DP methods applied to heterogeneous elasticity problems in 3D

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1 Introduction

Robust FETI-DP methods for heterogeneous, linear elasticity problems in three dimensions were developed and analyzed in Klawonn and Widlund [2004]. For homogeneous problems or materials with only small jumps in the Young moduli, the primal constraints can be chosen as edge averages of the displacement components over well selected edges; see Klawonn and Widlund [2004] and for numerical experimental work, Klawonn and Rheinbach [2005a]. In the case of large jumps in the material coefficients, first order moments were introduced as additional primal constraints in Klawonn and Widlund [2004], in order to obtain a robust condition number bound. In the present article, we provide some first numerical results which confirm the theoretical findings in Klawonn and Widlund [2004] and show that in some cases, first order moments are necessary to obtain a good convergence rate.

2 Linear elasticity and finite elements

The equations of linear elasticity model the displacement of a linear elastic material under the action of external and internal forces. The elastic body occupies a domain $\Omega \subset \mathbb{R}^3$, which is assumed to be polyhedral and of diameter one. We denote its boundary by $\partial\Omega$ and assume that one part of it, $\partial\Omega_D$, is clamped, i.e., with homogeneous Dirichlet boundary conditions, and that the rest, $\partial\Omega_N := \partial\Omega \setminus \partial\Omega_D$, is subject to a surface force $\mathbf{g}$, i.e., a natural boundary condition. We can also introduce a body force $\mathbf{f}$, e.g., gravity. With $\mathbf{H}^1(\Omega) := (H^1(\Omega))^3$, the appropriate space for a variational formulation is the Sobolev space $\mathbf{H}_0^1(\Omega, \partial\Omega_D) := \{\mathbf{v} \in \mathbf{H}^1(\Omega) : \mathbf{v} = \mathbf{0} \text{ on } \partial\Omega_D\}$. The linear elasticity problem consists in finding the displacement $\mathbf{u} \in \mathbf{H}_0^1(\Omega, \partial\Omega_D)$ of the elastic body Ω, such that

$$\int_{\Omega} G(\mathbf{x})\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{v})d\mathbf{x} + \int_{\Omega} G(\mathbf{x})\,\beta(\mathbf{x})\,\mathrm{div}\mathbf{u}\,\mathrm{div}\mathbf{v}\,d\mathbf{x} = \langle \mathbf{F}, \mathbf{v}\rangle \;\; \forall \mathbf{v} \in \mathbf{H}_0^1(\Omega, \partial\Omega_D).$$
(1)

Here G and β are material parameters which depend on the Young modulus $E > 0$ and the Poisson ratio $\nu \in (0, 1/2]$; we have $G = E/(1+\nu)$ and $\beta = \nu/(1-2\nu)$. In this article, we only consider the case of compressible elasticity, which means that the Poisson ratio ν is bounded away from $1/2$. Furthermore, $\varepsilon_{ij}(\mathbf{u}) := \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})$ is the linearized strain tensor, and

$$\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{v}) = \sum_{i,j=1}^{3} \varepsilon_{ij}(\mathbf{u})\varepsilon_{ij}(\mathbf{v}), \quad \langle \mathbf{F}, \mathbf{v}\rangle := \int_{\Omega} \mathbf{f}^T \mathbf{v}\, d\mathbf{x} \, + \, \int_{\partial\Omega_N} \mathbf{g}^T \mathbf{v}\, d\sigma.$$

For convenience, we also introduce the notation

$$(\varepsilon(\mathbf{u}), \varepsilon(\mathbf{v}))_{L_2(\Omega)} := \int_{\Omega} \varepsilon(\mathbf{u}) : \varepsilon(\mathbf{v})d\mathbf{x}.$$

The bilinear form associated with linear elasticity is then

$$a(\mathbf{u}, \mathbf{v}) = (G\,\varepsilon(\mathbf{u}), \varepsilon(\mathbf{v}))_{L_2(\Omega)} \, + \, (G\,\beta\,\mathrm{div}\mathbf{u}, \mathrm{div}\mathbf{v})_{L_2(\Omega)}.$$

The wellposedness of the linear system (1) follows immediately from the continuity and ellipticity of the bilinear form $a(\cdot, \cdot)$, where the first follows from elementary inequalities and the latter from Korn's first inequality; see, e.g., Ciarlet [1988]. The null space $\mathrm{ker}(\varepsilon)$ of ε is the space of the six rigid body motions. which is spanned by the three translations $\mathbf{r}_i := \mathbf{e}_i, i = 1, 2, 3$, where the $\mathbf{e}_i$ are the three standard unit vectors, and the three rotations

$$\mathbf{r}_4 := \begin{bmatrix} x_2 - \hat{x}_2 \\ -x_1 + \hat{x}_1 \\ 0 \end{bmatrix}, \mathbf{r}_5 := \begin{bmatrix} -x_3 + \hat{x}_3 \\ 0 \\ x_1 - \hat{x}_1 \end{bmatrix}, \mathbf{r}_6 := \begin{bmatrix} 0 \\ x_3 - \hat{x}_3 \\ -x_2 + \hat{x}_2 \end{bmatrix}.$$
(2)

Here $\hat{\mathbf{x}} \in \Omega$ to shift the origin to a point in Ω.

We will only consider compressible elastic materials. It is therefore sufficient to discretize our elliptic problem of linear elasticity (1) by low order, conforming finite elements, e.g., linear or trilinear elements.

Let us assume that a triangulation τ^h of Ω is given which is shape regular and has a typical diameter of h. We denote by $\mathbf{W}^h := \mathbf{W}^h(\Omega)$ the corresponding conforming finite element space of finite element functions. The associated discrete problem is then

$$a(\mathbf{u}_h, \mathbf{v}_h) = \langle \mathbf{F}, \mathbf{v}_h\rangle \quad \forall \mathbf{v}_h \in \mathbf{W}^h.$$
(3)

When there is no risk of confusion, we will drop the subscript h.

Let the domain $\Omega \subset \mathbb{R}^3$ be decomposed into nonoverlapping subdomains $\Omega_i, i = 1, \ldots, N$, each of which is the union of finite elements with matching finite element nodes on the boundaries of neighboring subdomains across the

interface Γ. The interface Γ is the union of three different types of open sets, namely, subdomain faces, edges, and vertices; see Klawonn and Widlund [2004] or Klawonn and Rheinbach [2005a] for a detailed definition. In the case of a decomposition into regular substructures, e.g., cubes or tetrahedra, our definition of faces, edges, and vertices is conform with our basic geometric intuition. In the definition of dual-primal FETI methods, we need the notion of edge averages, and in the case of heterogeneous materials, also of edge first order moments. We note that the rigid body modes $\mathbf{r}_1, \ldots, \mathbf{r}_6$, restricted to a straight edge provide only five linearly independent vectors, since one rotation is always linearly dependent on other rigid body modes. For the following definition, we assume that we have used an appropriate change of coordinates such that the edge under consideration coincides with the x_1-axis and the special rotation is then $\mathbf{r}_6$. The edge averages and first order moments over this specific edge $\mathcal{E}$ are of the form

$$\frac{\int_{\mathcal{E}} \mathbf{r}_k^T \mathbf{u} \, dx}{\int_{\mathcal{E}} \mathbf{r}^T \mathbf{r} \, dx}, \quad k \in \{1, \ldots, 5\}, \mathbf{u} = (u_1^T, u_2^T, u_3^T)^T \in \mathbf{W}^h. \tag{4}$$

3 The FETI-DP algorithm

For each subdomain $\Omega_i, i = 1, \ldots, N$, we assemble local stiffness matrices $K^{(i)}$ and local load vectors $\mathbf{f}^{(i)}$. By $\mathbf{u}^{(i)}$ we denote the local solution vectors of nodal values.

In the dual-primal FETI methods, we distinguish between dual and primal displacement variables by the way the continuity of the solution in those variables is established. Dual displacement variables are those, for which the continuity is enforced by a continuity constraint and Lagrange multipliers $\boldsymbol{\lambda}$ and thus, continuity is not established until convergence of the iterative method is reached, as in the classical one-level FETI methods; see, e.g., Klawonn and Widlund [2001]. On the other hand, continuity of the primal displacement variables is enforced explicitly in each iteration step by subassembly of the local stiffness matrices $K^{(i)}$ at the primal displacement variables. This subassembly yields a symmetric, positive definite stiffness matrix $\widetilde{K}$ which is coupled at the primal displacement variables but block diagonal otherwise. Let us note that this coupling yields a global problem which is necessary to obtain a numerically scalable algorithm.

We will use subscripts I, Δ, and Π, to denote the interior, dual, and primal displacement variables, respectively, and obtain for the local stiffness matrices, load vectors, and solution vectors of nodal values

$$K^{(i)} = \begin{bmatrix} K_{II}^{(i)} & K_{\Delta I}^{(i)T} & K_{\Pi I}^{(i)T} \\ K_{\Delta I}^{(i)} & K_{\Delta\Delta}^{(i)} & K_{\Pi\Delta}^{(i)T} \\ K_{\Pi I}^{(i)} & K_{\Pi\Delta}^{(i)} & K_{\Pi\Pi}^{(i)} \end{bmatrix}, \mathbf{u}^{(i)} = \begin{bmatrix} \mathbf{u}_I^{(i)} \\ \mathbf{u}_\Delta^{(i)} \\ \mathbf{u}_\Pi^{(i)} \end{bmatrix}, \mathbf{f}^{(i)} = \begin{bmatrix} \mathbf{f}_I^{(i)} \\ \mathbf{f}_\Delta^{(i)} \\ \mathbf{f}_\Pi^{(i)} \end{bmatrix}.$$

We also introduce the notation

$$\mathbf{u}_B = [\mathbf{u}_I \ \mathbf{u}_\Delta]^T, \mathbf{f}_B = [\mathbf{f}_I \ \mathbf{f}_\Delta]^T, \mathbf{u}_B^{(i)} = [\mathbf{u}_I^{(i)} \ \mathbf{u}_\Delta^{(i)}]^T, \text{ and } \mathbf{f}_B^{(i)} = [\mathbf{f}_I^{(i)} \ \mathbf{f}_\Delta^{(i)}]^T.$$

Accordingly, we define

$$K_{BB} = \text{diag}_{i=1}^N(K_{BB}^{(i)}), \quad K_{BB}^{(i)} = \begin{bmatrix} K_{II}^{(i)} & K_{\Delta I}^{(i)T} \\ K_{\Delta I}^{(i)} & K_{\Delta\Delta}^{(i)} \end{bmatrix}, \quad K_{\Pi B} = [K_{\Pi B}^{(1)} \dots K_{\Pi B}^{(N)}].$$

We note that K_{BB} is a block diagonal matrix. By subassembly in the primal displacement variables, we obtain

$$\widetilde{K} = \begin{bmatrix} K_{BB} & \widetilde{K}_{\Pi B}^T \\ \widetilde{K}_{\Pi B} & \widetilde{K}_{\Pi\Pi} \end{bmatrix},$$

where a tilde indicates the subassembled matrices and where

$$\widetilde{K}_{\Pi B} = [\widetilde{K}_{\Pi B}^{(1)} \cdots \widetilde{K}_{\Pi B}^{(N)}].$$

Introducing local assembly operators $R_\Pi^{(i)}$ which map from the local primal displacement variables $\mathbf{u}_\Pi^{(i)}$ to the global, assembled $\widetilde{\mathbf{u}}_\Pi$, we have

$$\widetilde{K}_{\Pi B}^{(i)} = R_\Pi^{(i)} K_{\Pi B}^{(i)}, \quad \widetilde{\mathbf{u}}_\Pi = \sum_{i=1}^N R_\Pi^{(i)} \mathbf{u}_\Pi^{(i)}, \quad \widetilde{K}_{\Pi\Pi} = \sum_{i=1}^N R_\Pi^{(i)} K_{\Pi\Pi}^{(i)} R_\Pi^{(i)T},$$

for $i = 1, \dots, N$. Due to the subassembly of the primal displacement variables, Lagrange multipliers have to be used only for the dual displacement variables $\mathbf{u}_\Delta$ to enforce continuity. We introduce a discrete jump operator $B = [O \ B_\Delta]$ such that the solution $\mathbf{u}_\Delta$, associated with more than one subdomain, coincides when $B\mathbf{u}_B = B_\Delta\mathbf{u}_\Delta = 0$ with $\mathbf{u}_B = [\mathbf{u}_I^T, \mathbf{u}_\Delta^T]^T$. Since we assume pointwise matching grids across the interface Γ, the entries of the matrix B are $0, 1,$ and -1. However, we will otherwise use all possible constraints and thus work with a fully redundant set of Lagrange multipliers as in [Klawonn and Widlund, 2001, Section 5]; cf. also Rixen and Farhat [1999]. Thus, for an edge node common to four subdomains, we will use six constraints rather than choosing as few as three.

We can now reformulate the finite element discretization of (3) as

$$\begin{bmatrix} K_{BB} & \widetilde{K}_{\Pi B}^T & B^T \\ \widetilde{K}_{\Pi B} & \widetilde{K}_{\Pi\Pi} & O \\ B & O & O \end{bmatrix} \begin{bmatrix} \mathbf{u}_B \\ \widetilde{\mathbf{u}}_\Pi \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_B \\ \widetilde{\mathbf{f}}_\Pi \\ \mathbf{0} \end{bmatrix}. \tag{5}$$

Elimination of the primal variables $\widetilde{\mathbf{u}}_\Pi$ and of the interior and dual displacement variables $\mathbf{u}_B$ leads to a a reduced linear system of the form

$$F\boldsymbol{\lambda} = \mathbf{d},$$

where the matrix F and the right hand side $\mathbf{d}$ are formally obtained by block Gauss elimination. Let us note that the matrix F is never built explicitly but that in every iteration appropriate linear systems are solved; see Farhat et al. [2000], Klawonn and Widlund [2004] or Klawonn and Rheinbach [2005a] for further details.

To define the FETI-DP Dirichlet preconditioner M^{-1}, we introduce a scaled jump operator B_D; this is done by scaling the contributions of B associated with the dual displacement variables from individual subdomains. We define

$$B_D = [B_D^{(1)}, \ldots, B_D^{(N)}],$$

where the $B_D^{(i)}$ are defined as follows: each row of $B^{(i)}$ with a nonzero entry corresponds to a Lagrange multiplier connecting the subdomain Ω_i with a neighboring subdomain Ω_j at a point $x \in \partial\Omega_{i,h} \cap \partial\Omega_{j,h}$. We obtain $B_D^{(i)}$ by multiplying each such row of $B^{(i)}$ with $1/|\mathcal{N}_x|$, where $|\mathcal{N}_x|$ denotes the multiplicity of the interface point $x \in \Gamma$. This scaling is called multiplicity scaling and is suitable for homogeneous problems; see Klawonn and Widlund [2004] or Klawonn and Rheinbach [2005a] for a scaling suitable for heterogeneous materials. Our preconditioner is then given in matrix form by

$$M^{-1} = B_D R_\Gamma^T S R_\Gamma B_D^T = \sum_{i=1}^N B_D^{(i)} R_\Gamma^{(i)T} S^{(i)} R_\Gamma^{(i)} B_D^{(i)T}. \tag{6}$$

Here, $R_\Gamma^{(i)}$ are restriction matrices that restrict the degrees of freedom of a subdomain to its interface and $R_\Gamma = \mathrm{diag}_i(R_\Gamma^{(i)})$.

We have to decide how to choose the primal displacement variables. The simplest choice is to select them as certain primal vertices of the subdomains; see Farhat et al. [2001], where this approach was first considered; this version has been denoted by Algorithm A. Unfortunately, this choice does not always lead to good convergence results in three dimensions. To obtain better convergence for three dimensional problems, a different coarse problem was suggested by introducing additional constraints. These constraints are averages or first order moments over selected edges or faces, which are enforced to have the same values across the interface. For further details, see Farhat et al. [2000], Klawonn and Widlund [2004], or Klawonn and Rheinbach [2005a]. To obtain robust condition number bounds for highly heterogeneous materials, additional first order moments over selected edges have to be used; cf. Klawonn and Widlund [2004]. There are different ways of implementing these additional primal constraints. One is to use additional, optional Lagrange multipliers, see Farhat et al. [2000] or Klawonn and Widlund [2004], another one is to apply a transformation of basis, see Klawonn and Widlund [2004] and Klawonn and Rheinbach [2005a]. In this article, we will use the approach with a transformation of basis. Let us note that this approach leads again to a mixed linear system of the form (5) and that the same algorithmic form as for Algorithm A can be used; see Klawonn and Widlund [2004], Klawonn and

Rheinbach [2005a], and Klawonn and Rheinbach [2005b] for further details. For our FETI-DP algorithm, using a well selected set of primal constraints of edge averages or first order moments and in some very difficult cases also of primal vertices, we have the estimate, cf. Klawonn and Widlund [2004],

Theorem 1. *The condition number satisfies*

$$\kappa(M^{-1}F) \leq C\,(1 + \log(H/h))^2.$$

Here, $C > 0$ is independent of h, H, and the values of the coefficients G_i.

A more general result can be shown if the concept of acceptable paths is introduced; cf. Klawonn and Widlund [2004] for more details.

4 Numerical results

We first consider a model problem, where two subdomains are surrounded by subdomains with much smaller stiffnesses, i.e., Young moduli. Furthermore, we assume that these two special subdomains share only an edge; cf. Figure 1. In Klawonn and Widlund [2004] it was shown that a well selected set of primal constraints, which has five linearly independent primal constraints related to that special edge shared by the two stiffer subdomains and otherwise six linearly independent edge constraints for each face, is sufficient to prove a condition number bound as in Theorem 1. In that article, the five linearly independent constraints are chosen as three edge averages and two properly chosen first order moments; cf. also (4). Here, the six linearly independent constraints for each face can be chosen as edge averages (and moments) over appropriately chosen edges of the considered face. In a set of experiments, we have tested
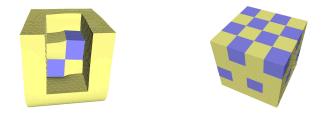

Fig. 1. Left: Two stiff cubic subdomains sharing an edge surrounded by softer material. Cubic domain Ω cut open in front and on top.
Right: Alternating layers of a heterogeneous material distributed in a checkerboard pattern and a homogeneous material.

different combinations of edge constraints on the specific edge shared by the two stiffer subdomains; cf. Table 1. In the case of three constraints only edge averages are used, in the case of five, additionally two first order moments are

Table 1. Comparison of different number of edge constraints on the edge shared by the two stiffer subdomains; $3 \times 4 \times 4 = 48$ brick-shaped subdomains of $1\,536$ d.o.f. each, $55\,506$ total d.o.f. Stopping criterion: Relative residual reduction of 10^{-10}.

# edge constraints	0		3		5	
E_1/E_2	Iter.	Cond.	Iter.	Cond.	Iter.	Cond.
10^0	29	9.21	28	9.10	**28**	**9.09**
10^3	47	4.36×10^2	37	7.51×10^1	**30**	**9.03**
10^6	70	4.24×10^5	47	7.16×10^4	**30**	**9.03**

applied. On all other edges, an edge average over each displacement component is used to define the primal constraints. We see that using no constraints or only edge average constraints on the specific edge leads to a large condition number. Applying all five constraints leads to a good condition number which is bounded independently of the jump in the Young moduli. Since we only have one difficult edge in this example, the iteration count is not increased accordingly; the eigenvalues are still well clustered except for two outliers in the case of three edge averages, see Klawonn and Rheinbach [2005b]. Next, we analyze a more involved example, where we will see that additional first order moments not only improve the condition number but are absolutely necessary to obtain convergence. We consider a linear elasticity model problem with a material consisting of different layers as shown on the right side in Figure 1. The ratio of the different Young moduli is $E_2/E_1 = 10^6$ with $E_2 = 210$ and a Poisson ratio of $\nu = 0.29$ for both materials. Here, in addition to three edge averages on each edge, we have also used two first order moments as primal constraints; see Klawonn and Widlund [2004] and Klawonn and Rheinbach [2005b] for more details. The results clearly show that the additional first order moments help to improve the convergence significantly; see Klawonn and Widlund [2004] for theoretical results. In Table 3 the parallel scalability is shown for a cube of eight layers; cf. Figure 1. All computations were carried out using PETSc; see Balay et al. [2005]. The numerical results given in Tables 2 and 3 were obtained on a 16 processor (2.2 Ghz Opteron 248; Gigabit Ethernet) computing cluster in Essen. A more detailed numerical study is current work in progress; cf. Klawonn and Rheinbach [2005b].

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Table 2. Heterogeneous linear elasticity: Comparison of FETI-DP algorithm using edge averages vs. edge averages and first order moments; 1 728 cubic subdomains of 5 184 d.o.f. each, 7 057 911 total d.o.f. Stopping criterion: Relative residual reduction of 10^{-10}.

edge averages			edge averages + first order moments		
Cond.	Iter.	Time	Cond.	Iter.	Time
2.14×10^5	$> \mathbf{1\,000}$	$> 6\,686$s	5.19	**24**	629s

Table 3. FETI-DP: Parallel scalability using edge averages and first order moments. Stopping criterion: Relative residual reduction of 10^{-7}.

Proc.	$\frac{\text{Subdom.}}{\text{Proc.}}$	$\frac{\text{d.o.f.}}{\text{Subdom.}}$	Total d.o.f.	Iter.	Cond.	Time
1	512	5 184	2 114 907	17	5.18	**1 828s**
2	256	5 184	2 114 907	17	5.18	**842s**
4	128	5 184	2 114 907	17	5.18	**428s**
8	64	5 184	2 114 907	17	5.18	**215s**
16	32	5 184	2 114 907	17	5.18	**122s**

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