A Domain Decomposition Method Based on Augmented Lagrangian with a Penalty Term in Three Dimensions

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Summary. In our earlier work [4], a dual iterative substructuring method for two dimensional problems was proposed, which is a variant of the FETI-DP method. The proposed method imposes continuity on the interface by not only the pointwise matching condition but also uses a penalty term which measures the jump across the interface. For a large penalization parameter, it was proven that the condition number of the resultant dual problem is bounded by a constant independent of both the subdomain size H and the mesh size h. In this paper, we extend the method to three dimensional problems. For this extension, we consider two things; one is the construction of a penalty term in 3D to give the same convergence speed as in 2D and the other is how to treat the ill-conditioning of the subdomain problems due to a large penalization parameter. To resolve these two key issues, we need to be aware of the difference between 2D and 3D in the geometric complexity of the interface. Based on the geometric observation for the difference, we suggest a modified penalty term and a preconditioner aiming at reducing couplings between functions on the interface.

1 Introduction

We consider the Poisson problem

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{1}$$

where Ω is a bounded polyhedral domain in $\mathbb{R}^3$ and $f \in L^2(\Omega)$.

In our previous work [4], for two dimensional problems, a dual iterative substructuring method was proposed using the augmented Lagrangian method, which is a variant of the FETI-DP method. To the Lagrangian functional of the standard FETI-DP, a penalty term is added, which measures the jump across the interface and includes a positive penalization parameter η. In the same way as in most dual substructuring approaches, the saddle-point problem related to the augmented Lagrangian functional is reduced to a dual problem with Lagrange multipliers as unknowns. Then it is solved by the conjugate gradient method. Differently from the FETI-DP method, it was proven that the dual problem has a constant condition number independently of H and h even though it is not accompanied by any preconditioner.

In this paper, we extend the method to the three dimensional case. For this extension, there are two things to be considered; one is to construct a strong penalty term in 3D to guarantee the same convergence speed as in 2D and the other is how to treat the ill-conditioning of the subdomain problems due to a large penalization parameter. For both issues, we need to be aware of the difference between 2D and 3D in the geometric complexity of an interface. An interface in 3D includes not only faces but also edges which make all nodes on the interface coupled. First, it is noted that the adoption of the same penalty as for two-dimensional problems gives an algorithm which maintains the same performance with respect to the condition number of the dual problem. However, the penalty term makes an unnecessary coupling between functions on face nodes and edges nodes. Since such a coupling causes a considerable decrease on practical efficiency, we suggest a modified penalty term for the three dimensional problem aiming at reducing the coupling between functions on the interface. Next, unlike the FETI-DP method, subdomain problems containing the penalty term are solved iteratively, of which the condition number becomes large as the penalization parameter η increases. The same type of preconditioner as in 2D might be satisfactory for the ill-conditioned problem due to a large η. But, since the preconditioner suggested in [4] contains a coupling among all nodes on the interface in 3D, it is hardly practical in the implementation. Based on such an observation, a more appropriate preconditioner for three-dimension problems is constructed, which is not only optimal with respect to η but also more practical then the one used in 2D.

2 Dual Iterative Substructuring with a Penalty Term

Let $\mathcal{T}_h$ denote a quasi-uniform triangulation on Ω, where the discretization parameter h stands for the maximal mesh size of $\mathcal{T}_h$. For simplicity, we consider a triangulation of hexahedra and the standard trilinear finite element approximate solution of (1): find $u_h \in X_h$ such that

$$a(u_h, v_h) = (f, v_h) \quad \forall v_h \in X_h, \tag{2}$$

where

$$a(u_h, v_h) = \int_\Omega \nabla u_h \cdot \nabla v_h \, dx, \quad (f, v_h) = \int_\Omega f v_h \, dx,$$

and $X_h = \{v_h \in H_0^1(\Omega) \cap \mathcal{C}^0(\overline{\Omega}) \mid \forall \tau \in \mathcal{T}_h,\ v_h|_\tau \in \mathbb{Q}_1(\tau)\}$.

We decompose Ω into N non-overlapping subdomains $\{\Omega_k\}_{k=1}^N$, where a partition $\{\Omega_k\}_{k=1}^N$ of Ω is assumed to be shape-regular. On each subdomain, the triangulation $\mathcal{T}_{h_k}$ is quasi-uniform with matching grids on the boundaries of neighboring subdomains across the interface Γ. Here the interface Γ is the union of the common interfaces among all subdomains, i.e., $\Gamma = \bigcup_{k<l} \Gamma_{kl}$, where Γ_{kl} denotes the common interface of two adjacent subdomains Ω_k and Ω_l. We define the finite-dimensional subspace X^k on each subdomain Ω_k by

$$X^k = \left\{ v_h^k \in \mathcal{C}^0(\overline{\Omega}_k) \;\middle|\; \forall \tau \in \mathcal{T}_{h_k},\ v_h^k|_\tau \in \mathbb{Q}_1(\tau),\ v_h^k|_{\partial\Omega \cap \partial\Omega_k} = 0 \right\}.$$

By enforcing the continuity at the corner points, we assemble X^k's into X_h^c:

$$X_h^c = \left\{ v = (v_h^k)_k \in \prod_{k=1}^{N} X^k \;\middle|\; v \text{ is continuous at each corner} \right\}.$$

The interface Γ is composed of faces which are shared by two subdomains, edges which are shared by more than two subdomains, and vertices. The geometrical objects on the interface are characterized in more details as

(i) $\mathcal{F}_{kl}$ denotes the common face of Ω_k and Ω_l, which is regarded as an open set.
(ii) $\mathcal{E}_m$, where m is an index of an edge, is an edge shared by neighboring subdomains, which does not include its end points, the vertices.

To enforce the continuity on the interface except vertices, a signed Boolean matrix B is introduced in the same way as in FETI-DP (cf. [1, 2]). Note that we do not allow any redundant continuity constraint on any edges, i.e., in the case where an edge $\mathcal{E}_m$ is shared by four subdomains, there are four different ways to choose three pairs of adjacent subdomains to impose the continuity on the edge nodes.

The finite element problem (2) is reformulated as a minimization problem with constraints imposed by the requirement of continuity across the interface Γ:

$$\min_{v \in X_h^c} \left(\frac{1}{2} \sum_{k=1}^{N} \int_{\Omega_k} |\nabla v|^2 \, dx - (f, v) \right) \quad \text{subject to} \quad Bv = 0.$$

As in the constrained optimization, we introduce a vector μ of Lagrange multipliers in $\mathbb{R}^M$ and define a Lagrangian functional $\mathcal{L} : X_h^c \times \mathbb{R}^M \to \mathbb{R}$ as

$$\mathcal{L}(v, \mu) = \frac{1}{2} \sum_{k=1}^{N} \int_{\Omega_k} |\nabla v|^2 \, dx - (f, v) + \langle Bv, \mu \rangle,$$

where M represents the number of constraints used for the pointwise matching on the interface and $\langle \cdot, \cdot \rangle$ is the Euclidean inner product in $\mathbb{R}^M$. Then, we slightly change the Lagrangian $\mathcal{L}$ by adding a penalty term. It is natural to adopt the same penalty term as suggested for the two dimensional problem in [4]:

$$J_\eta(u, v) = \sum_{k<l} \frac{\eta}{h} \int_{\Gamma_{kl}} (u^k - u^l)(v^k - v^l) \, ds, \quad \eta > 0. \tag{3}$$

To make the 3D algorithm efficient, we should minimize the coupling between the functions associated with face nodes and edge nodes. But, the penalty term in (3) makes face nodes and edge nodes in each part Γ_{kl} of Γ coupled so that all nodes on the interface are tied. By considering the interface as a union of two separate object, faces and edges, we introduce a modified penalty term

$$J_\eta(u,v) = \eta(J_\mathcal{F}(u,v) + J_\mathcal{E}(u,v)), \quad \eta > 0, \tag{4}$$

where

$$J_\mathcal{F}(u,v) = \frac{1}{h}\sum_{k<l}\int_{\mathcal{F}_{kl}} (u^k_{\mathcal{F}_{kl}} - u^l_{\mathcal{F}_{kl}})(v^k_{\mathcal{F}_{kl}} - v^l_{\mathcal{F}_{kl}})\, dx$$

and

$$J_\mathcal{E}(u,v) = \sum_{\mathcal{E}_m}\sum_{(i,j)\in I_{\mathcal{E}_m}}\int_{\mathcal{E}_m} (u^i - u^j)(v^i - v^j)\, ds.$$

Here, $u^k_{\mathcal{F}_{kl}}$ is a part of u, which is related to the contribution to u^k on $\mathcal{F}_{kl}$ only from the face nodal basis functions excluding the edge nodal basis functions. We define an augmented Lagrangian $\mathcal{L}_\eta$ with the penalty term J_η

$$\mathcal{L}_\eta(v,\mu) = \mathcal{L}(v,\mu) + \frac{1}{2}J_\eta(v,v).$$

Given the augmented Lagrangian $\mathcal{L}_\eta$, we consider the saddle-point problem:

$$\mathcal{L}_\eta(u_h,\lambda_h) = \max_{\mu_h\in\mathbb{R}^M}\min_{v_h\in X_h^c}\mathcal{L}_\eta(v_h,\mu_h) = \min_{v_h\in X_h^c}\max_{\mu_h\in\mathbb{R}^M}\mathcal{L}_\eta(v_h,\mu_h). \tag{5}$$

It has been established that seeking the solution of (2) is equivalent to finding the saddle-point of (5) (cf. [4]). The problem (5) is represented in the algebraic form

$$\begin{bmatrix} A_\eta & B^T \\ B & 0 \end{bmatrix}\begin{bmatrix} u \\ \lambda \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix},$$

where

$$A_\eta = \begin{bmatrix} A_{\Pi\Pi} & A_{\Pi\Delta} \\ A_{\Pi\Delta}^T & A_{\Delta\Delta} + \eta J \end{bmatrix}, \quad B^T = \begin{bmatrix} 0 \\ B_\Delta^T \end{bmatrix}, \quad u = \begin{bmatrix} u_\Pi \\ u_\Delta \end{bmatrix}, \quad F = \begin{bmatrix} f_\Pi \\ f_\Delta \end{bmatrix}.$$

Here, Π indicates the degrees of freedom (dof) associated with both the interior nodes and the subdomain corners, Δ those related to the face and edge nodes on the interface, and λ the Lagrange multipliers for the continuity constraint across the interface. Eliminating u_Π and u_Δ successively, we have a dual system

$$F_\eta\lambda = d_\eta \tag{6}$$

where

$$F_\eta = B_\Delta S_\eta^{-1} B_\Delta^T, \quad d_\eta = B_\Delta S_\eta^{-1}(f_\Delta - A_{\Pi\Delta}^T A_{\Pi\Pi}^{-1} f_\Pi)$$

with

$$S_\eta = S + \eta J = (A_{\Delta\Delta} - A_{\Pi\Delta}^T A_{\Pi\Pi}^{-1} A_{\Pi\Delta}) + \eta J.$$

Note that F_η is symmetric positive definite.

3 Estimate of Condition Number

By letting the vector v_Δ be partitioned into face and edge dof $v_\Delta = \left[v_f, v_e\right]^T$, the pointwise matching operator B_Δ is represented as

$$B_\Delta = \begin{bmatrix} B_f & 0 \\ 0 & B_e \end{bmatrix}.$$

Let us denote by $D(A)$ a block diagonal matrix such that $D(A) = \text{blockdiag}(A)$. Looking at the connection between the operator B_Δ and the penalty term J_η from their definitions, it is obvious that

$$J = \begin{bmatrix} J_F & 0 \\ 0 & J_E \end{bmatrix} = \begin{bmatrix} B_f^T D(J_{B_f}) B_f & 0 \\ 0 & B_e^T D(J_{B_e}) B_e \end{bmatrix}, \tag{7}$$

where J_{B_f} and J_{B_e} stand for the 2D mass matrix on each face weighted with $1/h$ and the 1D mass matrix on each edge, respectively. We define by Λ the space of vectors of dof associated with the Lagrange multipliers. To analyze the condition number bound for F_η, based on Lemma 3.1 in [6], it is sufficient to specify a suitable norm $\|\cdot\|_\Lambda$ on Λ and to estimate constants satisfying

$$\begin{aligned} c_1\|\lambda\|^2_{\Lambda'} \le \langle\lambda, F_\eta\lambda\rangle \le c_2\|\lambda\|^2_{\Lambda'} \quad \forall\lambda \in \Lambda, \\ c_3\|\mu\|^2_{\Lambda} \le \langle\mu, \mu\rangle \le c_4\|\mu\|^2_{\Lambda} \quad \forall\mu \in \Lambda. \end{aligned} \tag{8}$$

Taking the structural characteristic of J into consideration, we define the norm $\|\cdot\|_\Lambda$ on Λ by

$$\|\mu\|^2_\Lambda = \mu^T \begin{bmatrix} D(J_{B_f}) & 0 \\ 0 & D(J_{B_e}) \end{bmatrix} \mu, \quad \forall\mu \in \Lambda. \tag{9}$$

The dual norm on Λ is defined by

$$\|\lambda\|_{\Lambda'} = \max_{\substack{\mu \in \Lambda \\ \mu \neq 0}} \frac{|\langle\lambda, \mu\rangle|}{\|\mu\|_\Lambda}, \quad \forall\lambda \in \Lambda.$$

We list useful results in deriving bounds on the extreme eigenvalues of F_η.

Proposition 1. *For $S = A_{\Delta\Delta} - A^T_{\Pi\Delta}A^{-1}_{\Pi\Pi}A_{\Pi\Delta}$, there exists a constant $C = \lambda^S_{\max}/\lambda^J_{\min}$ such that*

$$v^T_\Delta S v_\Delta \le C v^T_\Delta J v_\Delta, \quad \forall v_\Delta \perp \text{Ker}(B_\Delta),$$

where $\lambda^S_{\max}$ and $\lambda^J_{\min}$ are the maximum eigenvalue of S and the minimum nonzero eigenvalue of J, respectively.

Lemma 1. *Let $\lambda^J_{\min}$ be the minimum nonzero eigenvalue of J. Then, we have*

$$\lambda^J_{\min} \ge Ch$$

where the constant C is independent of h and H.

Thanks to Lemma 3.1 in [6], we have the following estimate of the condition number $\kappa(F_\eta)$.

Theorem 1. *For any $\eta > 0$, we have*

$$\kappa(F_\eta) \leq \left(1 + \frac{C}{\eta}\right) C^*$$

where

$$C = \frac{\lambda^S_{\max}}{\lambda^J_{\min}}, \quad C^* = \frac{\max\{\lambda^{J_{B_f}}_{\max}, \lambda^{J_{B_e}}_{\max}\}}{\min\{\lambda^{J_{B_f}}_{\min}, \lambda^{J_{B_e}}_{\min}\}}.$$

Furthermore, the constants C and C^* are independent of the subdomain size H and the mesh size h.

Corollary 1. *For a sufficiently large η, we have*

$$\kappa(F_\eta) \leq C^*,$$

where C^* is the constant estimated in Theorem 1.

Remark 1. The condition number estimate of the augmented FETI-DP (with edge constraints) is $C(1+\log(H/h))^2$; see [3]. In our case, the vertex continuity is enough to make our method have a constant bound for the condition number of the resultant dual system.

4 Computational Issues

For the implementation of the proposed algorithm, we reorder the relevant dof in (6). By rearranging u in order $u = [u_r, u_c]^T$ where u_i, u_f, and u_e are assembled into u_r, we obtain a system in the following form

$$K^\eta_{rr} u_r + K_{rc} u_c + B_r^T \lambda = f_r \tag{10a}$$

$$K^T_{rc} u_r + K_{cc} u_c = f_c \tag{10b}$$

$$B_r u_r = 0 \tag{10c}$$

Note that K^η_{rr} is non-singular and detailed as

$$K^\eta_{rr} = K_{rr} + \eta \tilde{J} = \begin{bmatrix} A_{ii} & A_{i\Delta} \\ A^T_{i\Delta} & A_{\Delta\Delta} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \eta J \end{bmatrix},$$

where

$$A_{\Delta\Delta} = \begin{bmatrix} A_{ff} & A_{fe} \\ A^T_{fe} & A_{ee} \end{bmatrix}, \quad J = \begin{bmatrix} J_F & 0 \\ 0 & J_E \end{bmatrix}.$$

By eliminating u_r from (10a), we have

$$\begin{bmatrix} F_{cc} & -F_{rc}^T \\ F_{rc} & F_{rr} \end{bmatrix} \begin{bmatrix} u_c \\ \lambda \end{bmatrix} = \begin{bmatrix} d_c \\ d_r \end{bmatrix} \tag{11}$$

where

$$F_{rr} = B_r (K_{rr}^{\eta})^{-1} B_r^T, \quad F_{rc} = B_r (K_{rr}^{\eta})^{-1} K_{rc}, \quad F_{cc} = K_{cc} - K_{rc}^T (K_{rr}^{\eta})^{-1} K_{rc}$$

and

$$d_r = B_r^T (K_{rr}^{\eta})^{-1} f_r, \quad d_c = f_c - K_{rc}^T (K_{rr}^{\eta})^{-1} f_r.$$

Since A_η is invertible, so is F_{cc}. We can therefore eliminate u_c in (11) to get

$$F_\eta \lambda = d_\eta \tag{12}$$

where

$$F_\eta = F_{rr} + F_{rc} F_{cc}^{-1} F_{rc}^T, \quad d_\eta = d_r - F_{rc} F_{cc}^{-1} d_c.$$

Note that the condition number of K_{rr}^{η} grows linearly with η. Hence we need to establish a preconditioner which reduces the effect of η. First, we introduce a preconditioner M_1 as

$$M_1 = \begin{bmatrix} A_{ii} & 0 \\ 0 & A_{\Delta\Delta} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \eta J \end{bmatrix}.$$

Theorem 2. *The condition number of the preconditioned system by M_1 grows asymptotically as*

$$\kappa(M_1^{-1} K_{rr}^{\eta}) := \frac{\lambda_{\max}(M_1^{-1} K_{rr}^{\eta})}{\lambda_{\min}(M_1^{-1} K_{rr}^{\eta})} \lesssim \left(\frac{H}{h}\right)^2.$$

Next, we suggest a preconditioner M_2 as

$$M_2 = \begin{bmatrix} A_{ii} & 0 \\ 0 & \tilde{A}_{\Delta\Delta} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \eta J \end{bmatrix} \quad \text{with} \quad \tilde{A}_{\Delta\Delta} = \begin{bmatrix} A_{ff} & 0 \\ 0 & A_{ee} \end{bmatrix}.$$

Theorem 3. *Two preconditioners M_1 and M_2 are spectrally equivalent, i.e., there are constants c and C independent of h and H such that*

$$c v_r^T M_2 v_r \le v_r^T M_1 v_r \le C v_r^T M_2 v_r, \quad \forall v_r.$$

Therefore, the condition number of the preconditioned system by M_2 grows asymptotically as

$$\kappa(M_2^{-1} K_{rr}^{\eta}) \lesssim \left(\frac{H}{h}\right)^2.$$

Finally, by eliminating the coupling between all pairs of faces and edges, we establish a preconditioner M_3 as

$$M_3 = \begin{bmatrix} A_{ii} & 0 \\ 0 & \overline{A}_{\Delta\Delta} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \eta J \end{bmatrix} \quad \text{with} \quad \overline{A}_{\Delta\Delta} = \begin{bmatrix} \overline{A}_{ff} & 0 \\ 0 & \overline{A}_{ee} \end{bmatrix}.$$

Here, the matrices $\overline{A}_{ff}$ and $\overline{A}_{ee}$ are block diagonal with a block for each face and for each edge, respectively. Also we rewrite A_{ff} and A_{ee} as block matrices of the same structure as $\overline{A}_{ff}$ and $\overline{A}_{ee}$.

Theorem 4. *Assume that on each subdomain Ω_k, a triangulation $\mathcal{T}_{h_k}$ satisfies*

$$Volume(T_c) \le \min\{Volume(T_c^a)\},$$

where $T_c \in \mathcal{T}_{h_k}$ is a hexahedron containing a subdomain corner as one of its vertices and T_c^a is an adjacent hexahedron to T_c. Then, the condition number of the preconditioned system by M_3 grows asymptotically as

$$\kappa(M_3^{-1} K_{rr}^{\eta}) \lesssim \left(\frac{H}{h}\right)^2 .$$

Remark 2. The condition number of the subdomain problem in FETI-DP also depends on the ratio H/h, more presisely, $\kappa(K_{rr}) \le C(H/h)^3$. In FETI-DP, the subdomain problems are usually solved by direct methods. However, in the case of subdomain problems of relatively large size, iterative solvers are used (cf. [5]).

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