A domain decomposition method based on augmented Lagrangian with an optimized penalty parameter

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1 A Non-overlapping DDM with a Penalty Parameter

A non-overlapping domain decomposition method based on augmented Lagrangian with a penalty term was introduced in the previous works by the authors (Lee and Park [2009, 2012]), which is a variant of the FETI-DP method. In this paper we present a further study focusing on the case of small penalty parameters in terms of condition number estimate and practical efficiency. The full analysis of the proposed method can be found in Lee and Park [2013].

Throughout the paper, we denote by $\lambda_{\min}^A$ and $\lambda_{\max}^A$ the minimum eigenvalue and the maximum eigenvalue of a matrix A, respectively. To avoid the proliferation of constants, we will use $A \lesssim B$ and $A \gtrsim B$ to represent the statements that $A \le (\text{constant})B$ and $A \ge (\text{constant})B$, respectively, where the positive constant is independent of the mesh size, the subdomain size, and the number of subdomains. The statement $A \approx B$ is equivalent to $A \lesssim B$ and $A \gtrsim B$.

We first review the non-overlapping domain decomposition method with a penalty term in the previous works. Then, we state how we can enhance this method in terms of a better choice of a penalty parameter.

We consider the following Poisson model problem with the homogeneous Dirichlet boundary condition

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

where Ω is a bounded polygonal domain in $\mathbb{R}^2$ and f is a given function in $L_2(\Omega)$. Let $\mathcal{T}_h$ denote a quasi-uniform triangulation on Ω and $\hat{X}_h$ the space

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of the conforming $\mathbb{P}_1$ elements associated with $\mathcal{T}_h$. We are concerned with a discretized variational problem of (1) as follows: find $u_h \in \hat{X}_h$ such that

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

where

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

We start with recalling an iterative solver of (2) in Lee and Park [2009, 2012], which is a non-overlapping domain decomposition algorithm based on an augmented Lagrangian. We decompose Ω into non-overlapping subdomains $\{\Omega_j\}_{j=1}^J$ as open sets, where the boundary $\partial\Omega_j$ is aligned with $\mathcal{T}_h$ and the diameter of Ω_j is H_j. On each subdomain, the triangulation $\mathcal{T}_j$ is the triangulation of Ω_j inherited from $\mathcal{T}_h$ and matching grids are taken 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., $\Gamma = \bigcup_{j<k} \Gamma_{jk}$, where Γ_{jk} denotes the common interface of two adjacent subdomains Ω_j and Ω_k.

Based on the non-overlapping subdomain decomposition, a partitioned problem is obtained as follows:

$$\min_{v \in \prod_{j=1}^J X_h^j} \left(\frac{1}{2} \sum_{j=1}^J \int_{\Omega_j} |\nabla v|^2 \, dx - (f, v) \right) \tag{3a}$$

$$\text{subject to } v^j = v^k \text{ on } \Gamma_{jk} \text{ for } \ j < k, \tag{3b}$$

where X_h^j is the restriction of $\hat{X}_h$ on a subdomain Ω_j. To make a localized minimization problem recover the original solution of (2), the continuity constraint (3b) needs to be satisfied on the interface Γ in an appropriate manner (e.g. Burman and Zunino [2006], Farhat et al. [2000], Farhat and Roux [1991], Glowinski and Le Tallec [1990]).

The FETI-DP method, one of the most advanced non-overlapping domain decomposition algorithms, imposes the continuity differently at vertices and the remaining interface nodes except vertices in terms of the choice of finite elements. The continuity at vertices is enforced strongly in a manner that subdomains sharing a vertex have the common value at the vertex while the continuity on the interface except vertices is enforced weakly by introducing Lagrange multipliers. Hence the FETI-DP method starts with the saddle-point problem

$$\mathcal{L}(u_h, \lambda_h) = \max_{\mu_h \in \mathbb{R}^M} \min_{v_h \in X_h^c} \mathcal{L}(v_h, \mu_h), \tag{4}$$

where a Lagrangian functional $\mathcal{L}$ is defined on $X_h^c \times \mathbb{R}^M$ as

$$\mathcal{L}(v,\mu) = \frac{1}{2}\sum_{j=1}^{J}\int_{\Omega_j} |\nabla v|^2\,dx - (f,v) + \langle Bv, \mu\rangle.$$

Here, X_h^c denote the subspace of $\prod_{j=1}^{J} X_h^j$ obtained by enforcing the vertex continuity, B is a signed Boolean matrix which plays a role in making values defined individually on the interface pointwise-matched, M represents the number of constraints used for imposing the pointwise matching on the interface and $\langle\cdot,\cdot\rangle$ is the Euclidean inner product in $\mathbb{R}^M$.

In Mandel and Tezaur [2001], for the FETI-DP method accompanied by the Dirichlet preconditioner it is well-known that the condition number of the resulting dual problem from (4) grows asymptotically as $O(1+\ln(H/h))^2$, where H is the subdomain size and h is the mesh size. It shows that the convergence slows down only due to the increase of H/h, where $(H/h)^2$ are the local problem size. Due to such a scalable property of the FETI-DP method, there seems to be nothing to improve as a parallel algorithm only if parallel machines with infinitely many CPUs or cores are available. But, keeping in mind that most of ordinary users have limited computing resources, the condition number growth with respect to the increase of H/h is unsatisfactory. In this view, Lee and Park [2009, 2012] proposed a dual iterative substructuring method with a penalty term which plays a key role in enhancing the convergence to the extent of the constant condition number bound independent of both H and h. A penalty term $\eta\mathcal{J}$ is considered, which consists of a positive penalty parameter η and a measure of the jump on the interface. The addition of a penalty term $\eta\mathcal{J}$ to the Lagrangian $\mathcal{L}$ yields a saddle-point problem for an augmented Lagrangian functional $\mathcal{L}_\eta$ such as

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

where

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

Here the penalty term $\mathcal{J}$ is a bilinear form on $X_h^c \times X_h^c$ defined as

$$\mathcal{J}(u,v) = \frac{1}{h}\sum_{j<k}\int_{\Gamma_{jk}} (u^j - u^k)(v^j - v^k)\,ds,$$

where $h = \max_{j=1,\cdots,J} h_j$ with the mesh size h_j of $\mathcal{T}_j$.

The problem (5) is expressed in the algebraic form

$$\begin{bmatrix} A_{\Pi\Pi} & A_{\Pi\Delta} & 0 \\ A_{\Pi\Delta}^T & A_{\Delta\Delta} & B_\Delta^T \\ 0 & B_\Delta & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_\Pi \\ \boldsymbol{u}_\Delta \\ \lambda \end{bmatrix} = \begin{bmatrix} f_\Pi \\ f_\Delta \\ 0 \end{bmatrix},$$

where λ indicates the Lagrange multipliers introduced for imposing the continuity constraint across the interface, Π the degrees of freedom associated with both the interior nodes and the subdomain corners, and Δ the remaining part of the degrees of freedom on the interface. The matrix J results from the penalty term $\mathcal{J}$, which is written as

$$J = B_{\Delta}^{T} D_M B_{\Delta}, \tag{6}$$

where D_M is the block diagonal matrix with a diagonal block $\frac{1}{h} M_e$. Here M_e is the 1-D mass matrix on each edge. Eliminating $\boldsymbol{u}_{\Pi}$ and $\boldsymbol{u}_{\Delta}$ successively, we have a dual system

$$F_{\eta} \lambda = d_{\eta} \tag{7}$$

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

$$S_{\eta} = S + \eta J = (A_{\Delta\Delta} - A_{\Pi\Delta}^{T} A_{\Pi\Pi}^{-1} A_{\Pi\Delta}) + \eta J. \tag{8}$$

For the proposed dual iterative substructuring method which results in the dual problem (7), we are concerned with two key properties: one is the convergence of the primal solution u_h of the saddle-point problem (5) from which (7) is originated, to the exact weak solution of (1) and the other is the condition number of F_{η} which determines the convergence rate of dual iterations on (7). In this context, we now discuss the choice of a penalty parameter in the proposed dual iterative substructuring method.

Let us first look over what effect the choice of the penalty parameter has on the convergence of the finite element solution to the weak solution of (1). In finite element formulations based on penalty methods for (3) (cf. Babuška [1973], Burman and Zunino [2006]), the choice of a sufficiently large penalty parameter is required for the stability of a concerning finite element formulation, which is necessary for the convergence of the finite element solution to the exact weak solution of (1). On the other hand, the penalty parameter η plays a different role in the saddle-point formulation (5) based on an augmented Lagrangian functional because Lagrange multipliers as well as a penalty term are introduced to enforce the continuity across the interface. More precisely, such a role difference was confirmed in Lee and Park [2009] by the fact that the primal solution u_h of the saddle-point problem (5) is exactly equal to the finite element solution of (2) regardless of the choice of η. Hence there is no need to consider a right choice of η in the aspect of the convergence of a finite element solution to the solution of (1).

Let us next discuss the choice of the penalty parameter in terms of the condition number of F_{η}. The convergence study for dual iterations in Lee and Park [2009, 2012] shows that the dual system (7) has a constant condition number bound independent of H and h where a sufficiently large penalty parameter is taken. On the contrary, we have observed through numerical results that there might be an estimated parameter $\eta^{*} < 10$ with which the proposed dual iterative algorithm is almost optimal in terms of its condition number. Based on such observation, we shall focus on the case of small penalty parameters throughout the following sections.

2 Condition Number Estimate

In this section, we find the relationship between the standard FETI-DP operator and the proposed dual operator in algebraic form. Based on the relationship, we carry out convergence analysis in terms of the condition number of the dual system F_η without size limitation of the penalty parameter. As results, it is confirmed why a fast convergence of the dual iteration is attained even if a small η is taken.

We first have the following condition number estimate of the concerned dual system based on a key relationship between two matrices F_η and F, where F is the standard FETI-DP operator as $F = B_\Delta S^{-1} B_\Delta^T$.

Theorem 1. *For any $\eta > 0$, the condition number $\kappa(F)$ is estimated as*

$$\kappa(F_\eta) \leq \frac{C_{F,D_M}}{\eta + C_{F,D_M}} \kappa(F) + \frac{\eta}{\eta + C_{F,D_M}} \kappa(D_M), \tag{9}$$

where $C_{F,D_M} = (\lambda_{\max}^F \lambda_{\min}^{D_M})^{-1}$.

Remark 1. Theorem 1 shows the change of $\kappa(F_\eta)$ with respect to a choice of η as well as the connection of $\kappa(F_\eta)$ with $\kappa(F)$. In particular, $\kappa(F_\eta)$ becomes close to $\kappa(F)$ as η decreases to zero. In addition, it follows from (9) that

$$\kappa(F_\eta) \leq \kappa(D_M) + \frac{C_{F,D_M}(\kappa(F) - \kappa(D_M))}{\eta + C_{F,D_M}}, \tag{10}$$

which implies that the result shown in Figure 1 in Lee and Park [2009] is in agreement with (10) when $\kappa(F) > \kappa(D_M)$.

Then the extreme eigenvalues of matrices F and D_M can be estimated as

$$\begin{aligned} &\lambda_{\min}^{D_M} \gtrsim 1, \quad \lambda_{\max}^{D_M} \lesssim 1 \\ &\lambda_{\min}^{F} \gtrsim 1, \quad \lambda_{\max}^{F} \lesssim \max_{j=1,\cdots,J} \left(\frac{H_j}{h_j} \left(1 + \ln \frac{H_j}{h_j} \right) \right), \end{aligned}$$

which imply that

$$\begin{aligned} &\kappa(D_M) \lesssim 1 \\ &\kappa(F) \lesssim \max_{j=1,\cdots,J} \left(\frac{H_j}{h_j} \left(1 + \ln \frac{H_j}{h_j} \right) \right). \end{aligned}$$

Hence it is noted that either $\kappa(F) \leq \kappa(D_M)$ or $\kappa(F) > \kappa(D_M)$ holds according to the size of H/h. First, in the case of small H/h such that

$$\kappa(F) \leq \kappa(D_M),$$

it follows from Theorem 1 that, for any $\eta > 0$,

$$\kappa(F_\eta) \leq \kappa(D_M) \lesssim 1. \tag{11}$$

Next, in the following theorem we will see the case of large H/h such that

$$\kappa(F) > \kappa(D_M).$$

Using the estimated extreme eigenvalues of D_M and F, we can characterize bounds of the condition number of the concerned dual system as follows.

Theorem 2. *For any H/h such that*

$$\kappa(F) > \kappa(D_M),$$

there is a positive constant C_{opt} independent of H and h such that

$$\kappa(F_\eta) < \kappa(D_M) + C_{opt} \quad \textit{for any } \eta \geq C_{opt},$$

where $C_{opt} \approx 1$.

Remark 2. The convergence studies in Lee and Park [2009, 2012] for a dual iterative substructuring method with a penalty term were limited to the case when a sufficiently large penalty parameter η is used. The estimate (11) and Theorem 2 show why a faster convergence of the dual iteration in the proposed method is attained in comparison with the FETI-DP method even if a relatively small η is taken while Theorem 1 for a large η is identical to the previous results in Lee and Park [2009, 2012].

Remark 3. Due to length limitation, this paper is focused on the convergence analysis for the case of small penalty parameters in 2-D. More works for 3-D extension and computational issues such as the preconditioning of the subdomain problems can be found Lee and Park [2013].

3 Numerical Results

In this section, computational results are presented, which are in agreement with the theoretical bound estimated in Sect. 2. We consider the model problem (1) with the exact solution

$$u(x,y) = \begin{cases} y(1-y)\sin(\pi x) & \text{in 2-D} \\ \sin(\pi x)\sin(\pi y) z(1-z) & \text{in 3-D} \end{cases}$$

for $\Omega = (0,1)^d, d = 2,3$. We use the conjugate gradient method with a constant initial guess ($\lambda_0 \equiv 1$). The stop criterion is the relative reduction of the initial residual by a chosen TOL

$$\frac{\|r_k\|_2}{\|r_0\|_2} \leq \mathrm{TOL},$$

where r_k is the dual residual error on the kth CG iteration and $\mathrm{TOL} = 10^{-8}$. Here, discretization parameters h, H, and J are used, which stand for the mesh size, the subdomain size, and the number of subdomains, respectively. Through numerical tests, Ω in 2-D is decomposed into J square subdomains with $J = 1/H \times 1/H$. Each subdomain is partitioned into $2 \times H/h \times H/h$ uniform triangular elements. In 3-D, Ω is decomposed into J cubic subdomains with $J = 1/H \times 1/H \times 1/H$ while each subdomain is partitioned into $H/h \times H/h \times H/h$ uniform cubic elements.

In Table 1 for the two-dimensional problem, the condition numbers of the dual system are presented in the cases with η in $[0, 10]$. In addition, for comparison with the case with a large η, the result for $\eta = 10^6$ is presented. For each $\eta > 0$, the condition number $\kappa(F_\eta)$ is bounded by a constant even if H/h increases. In Table 1, any penalty parameter chosen in $(1/2, 10)$ improves the condition number regardless of the increase of H/h. In addition, the condition numbers for the case with $\eta \in (1/2, 10)$ are less than that for the case with a large η. According to the condition number and the iteration count, $\eta = 2$ is regarded as an optimal one. Table 2 for 3-D shows similar results in 2-D; $\eta = 1$ seems to be optimal as H/h increases.

Table 1 Condition number of F_η for a small η where $J = 4 \times 4$ in 2-D

η	$\frac{H}{h} = 4$		$\frac{H}{h} = 8$		$\frac{H}{h} = 16$		$\frac{H}{h} = 32$	
	$\kappa(F_\eta)$	iter. #	$\kappa(F_\eta)$	iter. #	$\kappa(F_\eta)$	iter. #	$\kappa(F_\eta)$	iter. #
0	7.2033	14	2.2901e+1	23	5.9558e+1	33	1.4707e+2	48
0.2	3.7811	12	5.6829	15	6.4744	18	6.7436	19
0.4	2.6637	10	3.3617	13	3.5166	13	3.6410	14
0.6	2.0733	9	2.3969	10	2.5127	11	2.5753	12
0.8	1.6990	8	1.9367	9	1.9974	10	2.0247	10
1	1.5030	7	1.6468	8	1.6801	9	1.6957	9
2	1.1304	5	1.1067	5	1.1053	5	1.1050	5
4	1.3353	6	1.4469	7	1.4625	8	1.4477	8
6	1.5050	7	1.7008	9	1.7470	9	1.7378	9
8	1.6130	7	1.8691	9	1.9404	10	1.9387	10
10	1.6875	7	1.9945	10	2.0799	11	2.0868	11
10^6	2.0938	3	2.7170	7	2.9243	13	2.9771	14

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Table 2 Condition number of F_η for a small η where $J = 4 \times 4 \times 4$ in 3-D

η	$\frac{H}{h} = 4$		$\frac{H}{h} = 8$		$\frac{H}{h} = 16$		$\frac{H}{h} = 32$	
	$\kappa(F_\eta)$	iter. #	$\kappa(F_\eta)$	iter. #	$\kappa(F_\eta)$	iter. #	$\kappa(F_\eta)$	iter. #
0	8.1805e+1	73	3.0183e+2	107	1.1892e+3	153	4.6946e+3	218
0.2	6.9551	22	6.8882	22	6.7708	21	6.6486	21
0.4	4.4201	18	4.6965	18	4.8197	18	4.8325	17
0.6	3.8658	16	4.3214	16	4.4810	17	4.4959	16
0.8	3.5613	15	4.0772	16	4.2515	16	4.2834	16
1	3.3611	15	3.9076	15	4.0901	15	4.1292	15
2	3.1992	14	4.0118	16	4.3020	16	4.3345	16
4	3.6343	15	4.8935	17	5.3381	18	5.4422	19
6	3.8905	15	5.4275	17	5.9726	19	6.1152	20
8	4.0564	15	5.7842	18	6.4011	20	6.5659	21
10	4.1740	15	6.0390	19	6.7099	21	6.8890	21
10^6	4.8585	7	7.5658	14	8.5609	16	8.8699	18

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