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PHYSICS-BASED BALANCING DOMAIN DECOMPOSITION BY CONSTRAINTS FOR HETEROGENEOUS PROBLEMS *

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SANTIAGO BADIA^{†‡} AND HIEU NGUYEN[‡]

Abstract. In this work, we present a balancing domain decomposition by constraints method 4 based on an aggregation of elements depending on the physical coefficients. Instead of imposing 5 constraints on purely geometrical objects (faces, edges, and vertices) of the partition interface, we use 6 interface objects (subfaces, subedges, and vertices) determined by the variation of the coefficients. 8 The new method is easy to implement and does not require to solve any eigenvalue or auxiliary 9 problem. When the physical coefficient in each object is constant at every subdomain containing the object, we can show both theoretically and numerically that the condition number does not depend 10 on the contrast of the coefficient. The constant coefficient condition is possible for multi-material 11 12 problems. However, for heterogeneous problems with coefficient varying across a wide spectrum of 13 values in a small spatial scale, such restriction might result in too many objects (a large coarse 14 problem). In this case, we propose a relaxed version of the method where we only require that the maximal contrast of the physical coefficient in each object is smaller than a predefined threshold. 15 The threshold can be chosen so that the condition number is reasonably small while the size of the 1617 coarse problem is not too large. An extensive set of numerical experiments is provided to support 18 our findings.

19 **Key words.** BDDC, heterogeneous problem, adaptive coarse space, parallel solver, parallel 20 preconditioner

AMS subject classifications. 65N55, 65N22, 65F08

22 1. Introduction. Many realistic simulations in science and engineering, such as subsurface flow simulations in a nuclear waste repository or in an oil reservoir, or 23 heat conduction in composites, involve heterogeneous materials. The linear systems 24 resulting from the discretization of these problems are hard to solve. The use of direct 25solvers at a sufficiently fine scale can be prohibitively expensive, even with modern 26supercomputers, due to their high complexity and scalability issues. In addition, the 27high contrast of the physical properties significantly increases the condition number 28 of the resulting linear systems, posing great challenges for iterative solvers. In this 29 work, we will focus on developing a domain decomposition (DD) preconditioner that 30 is robust with the variation of the coefficients of the PDEs. For a different but related approach, to find reasonably accurate heterogeneous solution on a coarse mesh, we 33 refer the interested readers to [19, 1] and references therein.

DD is one of the most popular approaches to solve large-scale problems on parallel 34 35 supercomputers. It splits a problem into weakly coupled subproblems on smaller subdomains and use parallel local solutions on these subdomains to form a parallel 36 preconditioner for the original problem [50, 41]. In DD, the coarse space plays an 37 important role in achieving scalability as well as robustness w.r.t variations in the 38 39 coefficient. Many early DD methods, such as those in [11, 18, 17, 31, 53], work for heterogeneous problems when the subdomain partition is a geometric coarse grid 40 41 that resolves the discontinuities in the properties of the media. This is a strong requirement, since the properties of the media might have complicated variations 42

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43 on many scales and be difficult to capture by a geometric coarse grid. Further, it 44 is impractical, since it would not lead to load-balanced partitions with a reduced 45 interface.

Recently, there have been works on coarse grids that do not resolve the hetero-46geneity in the media [25, 45, 25, 43, 44], and especially automatic coarse spaces that 47adapt to the variation in the properties of the media [22, 23, 42, 47, 15, 49, 48, 28, 48 27, 29, 36, 24]. In the latter, the coarse spaces are constructed from eigenfunctions 49 associated with small eigenvalues (low-frequency modes) of appropriated generalised 50eigenvalue problems. This approach is backed up by rigorous mathematical theory and has been numerically shown to be robust for general heterogeneous problems. However, solving eigenvalue problems is expensive and extra implementation effort is 53 54 required as coarse spaces in DD methods are not naturally formulated as eigenfunctions. Another approach is to use the deluxe scaling technique where local auxiliary Dirichlet problems are solved to compute efficient averaging operators [33, 14, 52]. 56 The approach yields robust DD methods, but extra implementation and computation cost incur due to the auxiliary problems. In this paper, we formulate a new balancing 58 DD by constraints (BDDC) preconditioner that requires no eigenvalue or auxiliary 59 problem and is very robust with the contrast of the coefficient. The main motivation 60 behind this work is to achieve such goal while *maintaining the simplicity* of the BDDC 61 preconditioner. 62 The BDDC method was introduced by Dohrmann in 2003 [12]. It is an improved 63 version of the balancing DD (BDD) method by Mandel [38] and has a close connection 64 65 with the FETI-DP method [21, 20]. In fact, it can be shown that the eigenvalues of the preconditioned operators associated with BDDC and FETI-DP are almost 66 identical [39, 34, 10]. The BDDC method is particularly well-suited for extreme scale 67 simulations, since it allows for a very aggressive coarsening, the computations at 68 different levels can be computed in parallel, the subdomain problems can be solved 69 inexactly [13, 35] by, e.g., one AMG cycle, and it can straightforwardly be extended 7071to multiple levels [51, 40]. All of these properties have been carefully exploited in the series of articles [3, 4, 5, 6] where an extremely scalable implementation of these 72

algorithms has been proposed, leading to excellent weak scalability on nearly half a
 million cores in its multilevel version.

Our new BDDC method is motivated from the fact that non-overlapping DD 75 methods, such as BDDC and FETI-DP, are robust with the variation and contrast 76 77 of the coefficient if it is constant (or varies mildly) in each subdomain [31, 30, 50]. This implies that in order to have robustness for BDDC methods one could use a 78physics-based partition obtained by aggregating elements of the same coefficient value. 79 However, using this type of partition is impractical as the number of the subdomains 80 81 might be too large and can lead to a poor load balancing among subdomains and large interfaces. In order to solve this dilemma, we propose to use a well-balanced 82 partition, e.g., one obtained from METIS [26] an automatic graph partitioner, to 83 distribute the work load among processors. Then, we consider a sub-partition of sub-84 domains based on the physical coefficients, leading to a physic-based (PB) partition. 85 86 Continuity constraints among subdomains will be defined through the definition of objects based on the PB partition. Consequently, the interface objects are adaptively 87 88 defined according to the variation of the coefficient. The resulting BDDC preconditioner with constraints imposed on subfaces, subedges, and vertices will be called 89 PB-BDDC. These ideas can readily be applied to FETI-DP preconditioners. 90

We emphasise that the PB-BDDC method does not require to solve any eigenvalue or auxiliary problems. Its formulation and implementation are very much the same 93 as for the standard BDDC method. The only difference is in identifying and defining

94 BDDC objects to impose constraints. In other words, the simplicity of the standard 95 BDDC method is maintained.

For multi-material problems, e.g., problems with isolated channels or inclusions,

97 it is possible to require the physical coefficient in each PB-subdomain to be constant.

98 In this situation, we are able to prove that the new BDDC method is scalable and its

99 convergence is independent of the contrast of the coefficient.

For heterogeneous problems with a wide spectrum of values in a small spatial 100 scale this restriction is too strong and might result in too many coarse objects (large 101 coarse problem). As a result, we also propose a relaxed definition of the PB partition 102where we only require that the maximal contrast of the physical coefficient in each 103 104 PB-subdomain is smaller than a predefined threshold. The threshold can be chosen so that the condition number is reasonably small while the size of the coarse problem 105is not too large. We empirically show that this relaxed version of PB-BDDC, called 106 rPB-BDDC, is robust and efficient for different difficult distributions of the coefficient. 107

The rest of the paper is organised as follows. In section 2, we introduce the model 108 problem, the domain partitions and the BDDC object classification. In section 3, we 109 present the formulation of the (r)PB-BDDC methods as well as theirs key ingredients, 110 namely coarse degrees of freedom (coarse DOFs), weighting and harmonic extension 111 operators. The convergence analysis is also provided in this section. In section 4, 112 we provide an extensive set of numerical experiments to demonstrate the robustness 113and efficiency of the (r)PB-BDDC methods. We finally draw some conclusions in 114 section 5. 115

2. Problem setting. Let $\Omega \subset \mathbb{R}^d$, with d being the space dimension, be a bounded polyhedral domain. For a model problem, we study the Poisson's equation with non-constant diffusion and homogeneous Dirichlet conditions (the nonhomogeneous case only involves an obvious modification of the right-hand side). Thus, the problem at hand is: find $u \in H_0^1(\Omega)$ such that $-\alpha \Delta u = f$ in $H^{-1}(\Omega)$ sense, with $f \in H^{-1}(\Omega)$ and $\alpha \in L^{\infty}(\Omega)$ strictly positive. The weak form of the problem reads as: find $u^* \in H_0^1(\Omega)$ such that

123 (1)
$$\int_{\Omega} \alpha \nabla u^{\star} \cdot \nabla v \, dx = \int_{\Omega} f v dx, \quad \text{for any } v \in H_0^1(\Omega).$$

Let \mathcal{T} be a shape-regular quasi-uniform mesh of Ω with characteristic size h. It can consist of tetrahedra or hexahedra for d = 3, or triangles or quadrilaterals for d = 2. For simplicity of exposition, we assume that α is constant on each element $\tau \in \mathcal{T}$.

2.1. Domain partitions. We first consider a partition Θ of Ω into non-overlapping open subdomains. This partition must be driven by computational efficiency in distributed memory platforms, i.e., it should have a reduced interface size and lead to a well-balanced distribution of work load among processors. In a parallel implementation, each subdomain in Θ is generally assigned to a processor. We further assume that every $\mathcal{D} \in \Theta$ can be obtained by *aggregation of elements* in \mathcal{T} and is connected. We denote by $\Gamma(\Theta)$ the interface of the partition Θ , i.e., $\Gamma(\Theta) \doteq (\cup_{\mathcal{D} \in \Theta} \partial \mathcal{D}) \setminus \partial \Omega$.

We also consider a PB subdomain partition. This partition is used latter in the new definition of coarse objects and in the analysis. It is, however, not used for work distribution. Given a subdomain $\mathcal{D} \in \Theta$, we can further consider its partition $\Theta_{\rm pb}(\mathcal{D})$ into a set of "sub-subdomains" with constant α . The minimal set is preferred for efficiency (it will potentially lead to a smaller coarse space) but it is not a requirement (see Remark 5). Clearly, the resulting global PB partitions $\Theta_{\rm pb} \doteq \{\Theta_{\rm pb}(\mathcal{D})\}_{\mathcal{D} \in \Theta}$



FIG. 1. An example of an original partition Θ (left) and a physics-based partition $\Theta_{\rm pb}(right)$ of a square domain where different colors represent different values of α . On the left, we have a $\Theta = \{\Omega_1, \Omega_2, \Omega_3, \Omega_4\}$. On the right, we show the corresponding PB-partition for every subdomains in Θ : $\Theta_{\rm pb}(\Omega_1) = \{\widehat{\Omega}_1, \widehat{\Omega}_2\}, \ \Theta_{\rm pb}(\Omega_2) = \{\widehat{\Omega}_3, \widehat{\Omega}_4\}, \ \Theta_{\rm pb}(\Omega_3) = \{\widehat{\Omega}_5, \widehat{\Omega}_6\}, \ and \ \Theta_{\rm pb}(\Omega_4) = \{\widehat{\Omega}_7, \widehat{\Omega}_8\}.$ The complete PB-partition is $\Theta_{\rm pb} = \{\widehat{\Omega}_1, \dots, \widehat{\Omega}_8\}$. Further, we have $\omega(\widehat{\Omega}_1) = \omega(\widehat{\Omega}_2) = \Omega_1, \ \omega(\widehat{\Omega}_3) = \omega(\widehat{\Omega}_4) = \Omega_2, \ \omega(\widehat{\Omega}_5) = \omega(\widehat{\Omega}_6) = \Omega_3, \ \omega(\widehat{\Omega}_7) = \omega(\widehat{\Omega}_8) = \Omega_4.$

is also a partition of Ω (into PB subdomains). The interface of this partition is $\Gamma(\Theta_{\rm pb}) \doteq (\cup_{\hat{\mathcal{D}}\in\Theta_{\rm pb}}\partial\hat{\mathcal{D}}) \setminus \partial\Omega$. For a subdomain $\mathcal{D} \in \Theta$ (analogously for $\hat{\mathcal{D}} \in \Theta_{\rm pb}$), we denote by $\mathcal{T}_{\mathcal{D}}$ the submesh of \mathcal{T} associated with $\mathcal{D}, \mathcal{T}_{\mathcal{D}} \doteq \{\tau \in \mathcal{T} : \tau \subset \mathcal{D}\} \subset \mathcal{T}$. For any $\hat{\mathcal{D}} \in \Theta_{\rm pb}$, let $\omega(\hat{\mathcal{D}})$ be the only subdomain in Θ that contains $\hat{\mathcal{D}}$. In Figure 1, we show an example of the original partition Θ and the PB partition $\Theta_{\rm pb}$ for a simple problem. The meaning of $\Theta_{\rm pb}(\mathcal{D})$ and $\omega(\mathcal{D})$ is also illustrated.

146 **2.2. Finite element spaces.** Let us perform a discretization of (1) by a con-147 tinuous finite element (FE) space $\bar{\mathbb{V}}$ associated with the mesh \mathcal{T} . The discontinuous 148 Galerkin (DG) case will not be considered in this work, but we refer the reader to 149 [16] for more information.

For every subdomain $\mathcal{D} \in \Theta$, we consider a FE space $\mathbb{V}_{\mathcal{D}}$ associated with the local mesh $\mathcal{T}_{\mathcal{D}}$. Let $H(\mathcal{D})$ be the characteristic length of the subdomain \mathcal{D} and $h(\mathcal{D})$ be the characteristic length of the FE mesh $\mathcal{T}_{\mathcal{D}}$. We define the Cartesian product of local FE spaces as $\mathbb{V} = \prod_{\mathcal{D} \in \Theta} \mathbb{V}_{\mathcal{D}}$. We note that functions in this space are allowed to be discontinuous across the interface $\Gamma(\Theta)$. Clearly, $\overline{\mathbb{V}} \subset \mathbb{V}$.

155 For a subdomain $\mathcal{D} \in \Theta$, we also define the subdomain FE operator $\mathcal{A}_{\mathcal{D}} : \mathbb{V}_{\mathcal{D}} \to$ 156 $\mathbb{V}'_{\mathcal{D}}$ as $\langle \mathcal{A}_{\mathcal{D}}u, v \rangle \doteq \int_{\mathcal{D}} \alpha \nabla u \cdot \nabla v \, dx$, for all $u, v \in \mathbb{V}_{\mathcal{D}}$, and the sub-assembled operator 157 $\mathcal{A}^{\Theta} : \mathbb{V} \to \mathbb{V}'$ as $\langle \mathcal{A}^{\Theta}u, v \rangle \doteq \sum_{\mathcal{D} \in \Theta} \langle \mathcal{A}_{\mathcal{D}}u, v \rangle$, for all $u, v \in \mathbb{V}$.

158 A function $u \in \mathbb{V}_{\mathcal{D}}$ is said to be discrete α -harmonic in \mathcal{D} if

159
$$\langle \mathcal{A}_{\mathcal{D}} u, v \rangle = 0, \text{ for any } v \in \mathbb{V}_{0,\mathcal{D}},$$

160 where $\mathbb{V}_{0,\mathcal{D}} \doteq \{v \in \mathbb{V}_{\mathcal{D}} : v = 0 \text{ on } \partial \mathcal{D}\}$. It should be noted that if u is discrete 161 α -harmonic in \mathcal{D} then it satisfies the energy minimising property, namely

162
$$\langle \mathcal{A}_{\mathcal{D}} u, u \rangle \leq \langle \mathcal{A}_{\mathcal{D}} v, v \rangle, \quad \forall v \in \mathbb{V}_{\mathcal{D}}, \ v|_{\partial \mathcal{D}} = u|_{\partial \mathcal{D}}.$$

163 In addition, we consider the assembled operator $\mathcal{A}: \overline{\mathbb{V}} \to \overline{\mathbb{V}}'$, defined by $\langle \mathcal{A}u, v \rangle =$ 164 $\int_{\Omega} \alpha \nabla u \cdot \nabla v \, dx$, for all $u, v \in \overline{\mathbb{V}}$. This operator is the Galerkin projection of \mathcal{A}^{Θ} onto 165 $\overline{\mathbb{V}}$. We want to compute a FE approximation $u \in \overline{\mathbb{V}}$ of u^* in (1) such that

166 (2)
$$\langle \mathcal{A}u, v \rangle = \langle f, v \rangle$$
, for any $v \in \mathbb{V}$.



FIG. 2. An example of how FE nodes (on the interface of the original partition Θ in Figure 1) are classified in the standard way (left) using neigh_{Θ}, and in the physics-based way (right) using neigh_{Θ pb}. Corner nodes are marked with crosses while nodes in edges are marked with small circles. Using the standard classification, on the left, we obtain $\Lambda(\Theta)$ with one corner and four edges. With the new classification, on the right, we have $\Lambda_{\rm pb}(\Theta)$ with five corners and six edges (eight edges if we only consider connected objects).

167 **2.3. Object classification.** This subsection concerns with objects on subdo-168 main interfaces and their classification. It provides foundations for the definition of 169 coarse DOFs in BDDC methods later on.

Given a subdomain partition Θ , and a point $\xi \in \Gamma(\Theta)$, let us denote by $\operatorname{neigh}_{\Theta}(\xi)$ the set of subdomains in Θ that contain ξ . We can introduce the concept of objects as a classification of points in $\Gamma(\Theta)$. A *geometrical object* is a maximal set λ of points in $\Gamma(\Theta)$ with identical subdomain set. We denote by $\operatorname{neigh}_{\Theta}(\lambda)$ the set of subdomains in Θ containing λ . It should be noted that the set of all geometrical objects, denoted by $\Lambda(\Theta)$, is a partition of $\Gamma(\Theta)$.

176 Remark 1. Since the set of points in the interface is infinite, the previous classi-177 fication of $\Gamma(\Theta)$ into geometrical objects is performed in practice by the classification 178 of vertices, edges, and faces of elements in the mesh \mathcal{T} based on their subdomain set.

Denote by $ndof(\lambda)$ the number of DOFs belonging to λ . We further consider the 179following standard classification of geometrical objects. In the three-dimensional case, 180 $\lambda \in \Lambda(\Theta)$ is a face if $|\text{neigh}_{\Theta}(\lambda)| = 2$ and $\text{ndof}(\lambda) > 1$, is an edge if $|\text{neigh}_{\Theta}(\lambda)| > 2$ and 181 $ndof(\lambda) > 1$, and is a *corner* if $ndof(\lambda) = 1$. In the two-dimensional case, $\lambda \in \Lambda(\Theta)$ 182 is an edge if $|\text{neigh}_{\Theta}(\lambda)| = 2$ and $\text{ndof}(\lambda) > 1$, and is a corner if $\text{ndof}(\lambda) = 1$. In the 183literature, e.g. [31, 50], corners are also referred to as vertices. Analogous definitions 184are also used frequently for FETI-DP methods (see [50]). In Figure 2 (left), an 185186 illustration of this classification is shown for a simple example.

In the next step, we define PB objects, which is the main ingredient of the PB-BDDC methods proposed herein. We consider the set of objects $\Lambda_{\rm pb}(\Theta)$ obtained by applying the previous classification of $\Gamma(\Theta)$ into corners/edges/faces but with neigh_{Θ}(·) replaced by neigh_{Θ pb}(·). In other words, we use sets of subdomains in 191 $\Theta_{\rm pb}$ to classify geometrical objects on $\Gamma(\Theta)$. Figure 2 (right) shows objects in $\Lambda_{\rm pb}(\Theta)$ 192 for a simple example.

193 LEMMA 2. $\Lambda_{pb}(\Theta)$ is a refinement of $\Lambda(\Theta)$.

194 Proof. The statement holds if for every object $\lambda_{\rm pb} \in \Lambda_{\rm pb}(\Theta)$ there exists one and 195 only one object $\lambda \in \Lambda(\Theta)$ containing it. Since all points in $\lambda_{\rm pb}$ belong to the same set 196 of PB subdomains, $\operatorname{neigh}_{\Theta_{\rm pb}}(\lambda)$, they are in the same set of subdomains in Θ , namely 197 $\{\omega(\hat{D})\}_{\hat{D}\in\operatorname{neigh}_{\Theta_{\rm pb}}(\lambda)}$. As a result, all these points belong to the same object in $\Lambda(\Theta)$.

Remark 3. In some cases, the DOF-based classification into corners, edges, and faces might need some modification in order to ensure well-posedness of the BDDC method with corner constraints only. This usually involves the use of a kernel detection mechanism (see, e.g, [46]). A new approach based on perturbations has recently been proposed in [8, 7], where the method is well-posed in all cases.

Remark 4. The PB aggregation (classification) of the interface $\Gamma(\Theta)$ into $\Lambda_{\rm pb}(\Theta)$ 203can be relaxed. As it is currently stated, the PB partition is unique and have the min-204imal number of PB subdomains. However, it might introduces disconnected objects. 205For example, the edge between $\hat{\Omega}_3$ and $\hat{\Omega}_7$ in Figure 2 (right) is disconnected. Alter-206natively, one can require that objects must be connected. This leads to two connected 207 edges between $\hat{\Omega}_3$ and $\hat{\Omega}_7$. We adopt this practice for the numerical experiments in 208 section 4. However, it should be noted that the use of disconnected objects leads to 209a smaller coarse space and can be beneficial in some cases. 210

Remark 5. In practical implementations, one only needs the set of PB geometrical 211objects $\Lambda_{\rm pb}(\Theta)$ to define the PB-BDDC preconditioner. When using the approach 212 with only connected objects (see Remark 4), one does not need to explicitly define 213214the PB partition Θ_{pb} . Only a partition of objects in $\Lambda(\Theta)$ (see Figure 2 (left)) into PB 215objects (see Figure 2 (right)) based on the physical coefficients is required. Therefore, only a (d-1)-dimensional PB partition (of the interface $\Gamma(\Theta)$) is needed. This is 216 what we have actually implemented for our numerical experiments in section 4. We 217only use the PB partition $\Theta_{\rm pb}$ in the analysis in subsection 3.4. In any case, the PB 218partition can easily be implemented if necessary. 219

3. Physics-based BDDC preconditioning. In this section, we present our 220 new PB-BDDC method. The basic idea behind BDDC methods is first to define a 221 sub-assembled operator (no assembling among subdomains), and the global space of 2.2.2 functions that are fully independent ("discontinuous") among subdomains. Secondly, 223 we have to define the under-assembled space (the BDDC space) of functions for which 224 continuity among subdomains is enforced only on a set of coarse DOFs. In order to 225be robust for heterogeneous problems, the PB-BDDC method utilises new definitions 226 227 of the BDDC space (i.e., new coarse DOF continuity among subdomains) and a new weighting operator. 228

3.1. Coarse degrees of freedom. Similarly to other BDDC methods, in the 229PB-BDDC method, some (or all) of the objects in $\Lambda_{\rm pb}(\Theta)$ are associated with a 230*coarse* DOF. We denote this set of objects by Λ_O and call it the set of coarse objects. 231Obviously, $\Lambda_O \subset \Lambda_{\rm pb}(\Theta)$. Typical choices of Λ_O are $\Lambda_O \doteq \Lambda_C$, when only corners 232233 are considered, $\Lambda_O \doteq \Lambda_C \cup \Lambda_E$, when corners and edges are considered, or $\Lambda_O \doteq$ $\Lambda_{\rm pb}(\Theta)$, when corners, edges, and faces are considered. These choices lead to three 234variants of the PB-BDDC method, referred to as PB-BDDC(c), PB-BDDC(ce) and 235PB-BDDC(cef), respectively. Figure 2 (right) actually shows the coarse objects of 236PB-BDDC(ce) for a simple 2D problem. 237

Given an object $\lambda \in \Lambda_O$, we define its coarse DOF as the mean value on λ . The rigorous definition is as follows. Assume $\lambda \in \Lambda_O$ is associated with a subdomain $\mathcal{D} \in \Theta$. We define the coarse DOF $c_{\lambda}^{\mathcal{D}}$ corresponding to λ as

241 (3)
$$c_{\lambda}^{\mathcal{D}}(u_{\mathcal{D}}) \doteq \frac{\int_{\lambda} u_{\mathcal{D}} ds}{\int_{\lambda} 1 ds}, \text{ for } u_{\mathcal{D}} \in \mathbb{V}_{\mathcal{D}}.$$

Clearly, $c_{\lambda}^{\mathcal{D}}$ is a functional in $\mathbb{V}'_{\mathcal{D}}$. When λ is a corner, $c_{\lambda}^{\mathcal{D}}$ is simply the value at that corner. Once we have defined the coarse DOFs, we can define the BDDC space as follows

245 (4)
$$\widetilde{\mathbb{V}} \doteq \{ v \in \mathbb{V} : c_{\lambda}^{\mathcal{D}}(v) = c_{\lambda}^{\mathcal{D}'}(v), \, \forall \lambda \in \Lambda_O, \, \forall \, \mathcal{D}, \mathcal{D}' \in \mathrm{neigh}_{\Theta}(\lambda) \},$$

i.e., the subspace of functions in \mathbb{V} that are continuous "at" coarse DOFs. Clearly, $\overline{\mathbb{V}} \subset \widetilde{\mathbb{V}} \subset \mathbb{V}$.

For BDDC methods, solving the coarse problem is usually the bottleneck (cf. [2, 3, 4, 8]). Therefore, it is of great interest to find a minimal set of coarse objects (the number of the coarse objects is the number of the coarse DOFs and also is the size of the coarse problem), so that BDDC methods can achieve their potential of fast convergence and perfect weak scalability. According to [31, 50], in the case where the physical coefficient in each subdomain is constant, the set of coarse objects only need to guarantee the existence of the so-called *acceptable paths*. We need a similar concept here for the PB-BDDC method.

The definition below is modelled after [50, Definition 6.26], [31] and [32].

257 DEFINITION 6 (Acceptable path). Let Θ_{pb}^{∂} be the set of PB subdomains $\hat{\mathcal{D}} \in \Theta_{pb}$ 258 touching the interface $\Gamma(\Theta)$, i.e., $\partial \hat{\mathcal{D}} \cap \Gamma(\Theta) \neq \emptyset$. For two subdomains $\hat{\mathcal{D}}_a, \hat{\mathcal{D}}_b \in \Theta_{pb}^{\partial}$ 259 that share an edge λ but no face in $\Lambda_{pb}(\Theta)$ or share a corner λ but no edge in $\Lambda_{pb}(\Theta)$, 260 an acceptable path is a sequence { $\hat{\mathcal{D}}_a = \hat{\mathcal{D}}_1, \hat{\mathcal{D}}_2, \dots, \hat{\mathcal{D}}_n = \hat{\mathcal{D}}_b$ } of PB subdomains in 261 Θ_{pb}^{∂} , which satisfy the following properties:

262 *i)* they all share the common object $\lambda \in \Lambda_{pb}(\Theta)$

ii) subdomains $\hat{\mathcal{D}}_k$ and $\hat{\mathcal{D}}_{k+1}$, $k = 1, ..., \hat{n} - 1$, must share, apart from λ , an object in Λ_O and the type of the shared object (face, edge or corner) must be the same for the whole sequence

266 *iii*) their (constant) coefficients satisfy

TOL
$$\alpha_k \ge R(k, \lambda) \min(\alpha_a, \alpha_b), \quad 1 \le k \le r$$

where TOL is some predefined tolerance and $R(k,\lambda) = 1$ if λ is an edge and $R(k,\lambda) = h(\hat{\mathcal{D}}_k)/H(\hat{\mathcal{D}}_k)$ if λ is a corner.

- Assumption 7. We assume that the set of BDDC objects Λ_O satisfies the following properties:
- 1. In the three dimensional case, for each face on $\Gamma(\Theta)$, there is at least one edge that is part of its boundary and belongs to Λ_O .
- 274 2. For all pairs of subdomains $\hat{\mathcal{D}}_a, \hat{\mathcal{D}}_b \in \Theta_{pb}^{\partial}$, which have an edge but not a face 275 in $\Lambda_{pb}(\Theta)$ in common, or a corner but not an edge in $\Lambda_{pb}(\Theta)$ in common, 276 there exists an acceptable path for a predefined tolerance TOL.

277 Remark 8. In Definition 6, if the shared object λ belongs to the set of BDDC 278 objects Λ_O , then there exists a trivial acceptable path $\{\hat{\mathcal{D}}_a, \hat{\mathcal{D}}_b\}$ with TOL = 1 and 279 n = 2. Thus, BDDC(ce) and BDDC(cef) always satisfy Assumption 7 for TOL = 1.

3.2. Injection operators. Let us define the projection $\mathcal{Q}: \mathbb{V} \to \overline{\mathbb{V}}$ as some 280 weighted average of interface values together with an α -harmonic extension to sub-281domain interiors (see, e.g., [39]). We define these ingredients as follows. 282

For $u \in \mathbb{V}$ and $\xi \in \Gamma(\Theta)$, the weighting operator is defined as 283

284 (5)
$$\mathcal{W}u(\xi) \doteq \sum_{\mathcal{D}\in \operatorname{neigh}_{\Theta}(\xi)} \delta_{\mathcal{D}}^{\dagger}(\xi) u_{\mathcal{D}}(\xi), \text{ with } \delta_{\mathcal{D}}^{\dagger}(\xi) \doteq \frac{\sum_{\tau \in \mathcal{T}_{\mathcal{D}}, \tau \ni \xi} \alpha_{\tau} |\tau|}{\sum_{\tau \in \mathcal{T}, \tau \ni \xi} \alpha_{\tau} |\tau|},$$

285 where $|\tau|$ denotes the volume (area if in 2D) of the element τ .

The α -harmonic extension operator \mathcal{E} taking data on the interface $\Gamma(\Theta)$ and α -286harmonically extending it to each subdomain $\mathcal{D} \in \Theta$ is formally defined as 287

$$\mathcal{E}u \doteq (1 - \mathcal{A}_0^{-1} \mathcal{A})u,$$

where \mathcal{A}_0 is the Galerkin projection of \mathcal{A} onto the bubble space $\mathbb{V}_0 \doteq \{v \in \mathbb{V} : v = v\}$ 289 0 on $\Gamma(\Theta)$. 290

We finally define $\mathcal{Q} = \mathcal{E}\mathcal{W}$. 291

3.3. PB-BDDC preconditioner. In this subsection, we present the PB-BDDC 292 preconditioner, and describe its set-up and formulation. The PB-BDDC precondi-293tioner is a BDDC preconditioner in which the set of coarse DOFs enforce continuity 294on a set of PB coarse objects, thus modifying the BDDC space being used. Once one 295has defined the set of PB coarse objects Λ_{O} , the rest of ingredients of the PB-BDDC 296preconditioner are identical to the ones of a standard BDDC preconditioner. In any 297case, the definition of the weighting operator introduced in (5) is new. 298

The BDDC preconditioner is a Schwarz-type preconditioner that combines interior 299 corrections with corrections in the BDDC space (see, e.g., [9, 50]). In case of the PB-300 BDDC preconditioner, the BDDC correction is expressed as $\mathcal{Q}(\tilde{\mathcal{A}}^{\Theta})^{-1}\mathcal{Q}^{T}$, where $\tilde{\mathcal{A}}^{\Theta}$ is 301 the Galerkin projection of \mathcal{A}^{Θ} onto $\widetilde{\mathbb{V}}$. More specifically, the PB-BDDC preconditioner 302 reads as follows: 303 $^{1}+\mathcal{Q}(\tilde{\mathcal{A}}^{\Theta})^{-1}\mathcal{Q}^{T}.$

$$\mathcal{B} = \mathcal{A}_{0}^{-1} + \mathcal{O}(\tilde{\mathcal{A}}^{\in})$$

Apart from the task of identifying and defining coarse objects, the implementation 305 of the PB-BDDC method is identical to that of the standard BDDC method. We 306 refer the interested reader to [12, 13, 40, 9] for more details on the formulation of 307 BDDC methods and to [2, 4, 6] for an efficient implementation of BDDC methods on 308 distributed memory machines, which requires much further elaboration. 309

3.4. Condition number estimates. In order to prove condition number esti-310 mates for the PB-BDDC preconditioner, we first need to introduce \mathcal{B} , an auxiliary 311 BDDC preconditioner. The definition of this preconditioner follows verbatim that 312 313 of the PB-BDDC preconditioner above but the PB subdomain partition Θ_{pb} is used instead of Θ . 314

Given the FE mesh \mathcal{T} , the FE space type, and the subdomain partition Θ_{pb} , one 315 can similarly build the FE spaces and operators as in subsection 2.2, leading to the 316 sub-assembled space \mathbb{V}^{pb} and operator $\mathcal{A}^{\Theta_{\mathrm{pb}}}$. Further, we can define the injection 317 operator $\widehat{\mathcal{Q}}$ using the definitions in subsection 3.2 with Θ is replaced by $\Theta_{\rm pb}$ for the 318 weighting $\widehat{\mathcal{W}}$ and harmonic extension $\widehat{\mathcal{E}}$ operators. 319

LEMMA 9. For any PB subdomain $\widehat{\mathcal{D}} \in \Theta_{pb}$, the function $\delta_{\widehat{\mathcal{D}}}^{\dagger}(\cdot)$ is constant on 320 each PB object λ associated with it. i.e. 321

322 (6)
$$\delta_{\widehat{\mathcal{D}}}^{\dagger}(\xi) = \delta_{\widehat{\mathcal{D}}}^{\dagger}(\xi'), \quad \forall \xi, \xi' \in \lambda.$$

323 In addition, the following important inequality, cf. [50, 6.19], holds

324 (7)
$$\alpha_{\widehat{\mathcal{D}}_a} \left(\delta_{\widehat{\mathcal{D}}_b}^{\dagger}(\xi) \right)^2 \leq C_{\delta^{\dagger}} \min \left(\alpha_{\widehat{\mathcal{D}}_a}, \alpha_{\widehat{\mathcal{D}}_b} \right), \quad \forall \widehat{\mathcal{D}}_a, \widehat{\mathcal{D}}_b \in \operatorname{neigh}_{\Theta_{\mathrm{pb}}}(\xi)$$

where $C_{\delta^{\dagger}} \lesssim \max\left(1, \frac{N_{\max}-1}{4}\right)$ with N_{\max} is the maximal number of elements in \mathcal{T} sharing at least one point.

227 Proof. The identity (6) follows from (5), the fact that α is constant in each sub-228 domain in $\Theta_{\rm pb}$ and $\operatorname{neigh}_{\Theta_{\rm pb}}(\xi) = \operatorname{neigh}_{\Theta_{\rm pb}}(\xi') = \operatorname{neigh}_{\Theta_{\rm pb}}(\lambda)$.

Now we need to verify (7). Since α is constant in each PB subdomain, we can rewrite and bound $\delta_{\widehat{T}}^{\dagger}(\xi)$ as follows

331 (8)
$$\delta_{\widehat{\mathcal{D}}_{b}}^{\dagger}(\xi) = \frac{\alpha_{\widehat{\mathcal{D}}_{b}}A_{\widehat{\mathcal{D}}_{b}}}{\sum_{\widehat{\mathcal{D}}\in \operatorname{neigh}_{pb}(\xi)}\alpha_{\widehat{\mathcal{D}}}A_{\widehat{\mathcal{D}}}} < \frac{\alpha_{\widehat{\mathcal{D}}_{b}}A_{\widehat{\mathcal{D}}_{b}}}{\alpha_{\widehat{\mathcal{D}}_{a}}A_{\widehat{\mathcal{D}}_{a}} + \alpha_{\widehat{\mathcal{D}}_{b}}A_{\widehat{\mathcal{D}}_{b}}},$$

where $A_{\widehat{\mathcal{D}}} > 0$ denotes the volume (area) of the patch of elements in $\widehat{\mathcal{D}}$ containing ξ . Clearly, $\delta^{\dagger}_{\widehat{\mathcal{D}}}(\xi) \leq 1$. Therefore, $\alpha_{\widehat{\mathcal{D}}_a}(\delta^{\dagger}_{\widehat{\mathcal{D}}_b}(\xi))^2 \leq \alpha_{\widehat{\mathcal{D}}_a}$. Now we need to prove that

334 (9)
$$\alpha_{\widehat{\mathcal{D}}_a}\left(\delta_{\widehat{\mathcal{D}}_b}^{\dagger}(\xi)\right)^2 \le C_{\delta^{\dagger}} \alpha_{\widehat{\mathcal{D}}_b}.$$

335 Using (8), it is sufficient to show

336 (10)
$$\alpha_{\widehat{\mathcal{D}}_a} \alpha_{\widehat{\mathcal{D}}_b} A_{\widehat{\mathcal{D}}_b}^2 \le C_{\delta^{\dagger}} (\alpha_{\widehat{\mathcal{D}}_a} A_{\widehat{\mathcal{D}}_a} + \alpha_{\widehat{\mathcal{D}}_b} A_{\widehat{\mathcal{D}}_b})^2.$$

Since the mesh \mathcal{T} is quasi-uniform, elements sharing at least a point have roughly the same volume (area). Consequently, $A_{\widehat{\mathcal{D}}_b} \lesssim (N_{\max} - 1) A_{\widehat{\mathcal{D}}_a}$ (the worst case scenario is when $\widehat{\mathcal{D}}_b$ has $N_{\max} - 1$ elements and $\widehat{\mathcal{D}}_a$ has 1 element). Using this, we have

$$340 \qquad \alpha_{\widehat{\mathcal{D}}_{a}}\alpha_{\widehat{\mathcal{D}}_{b}}A_{\widehat{\mathcal{D}}_{b}}^{2} \lesssim \left(\mathbf{N}_{\max}-1\right)\alpha_{\widehat{\mathcal{D}}_{a}}\alpha_{\widehat{\mathcal{D}}_{b}}A_{\widehat{\mathcal{D}}_{a}}A_{\widehat{\mathcal{D}}_{b}} \leq \frac{\mathbf{N}_{\max}-1}{4}\left(\alpha_{\widehat{\mathcal{D}}_{a}}A_{\widehat{\mathcal{D}}_{a}}+\alpha_{\widehat{\mathcal{D}}_{b}}A_{\widehat{\mathcal{D}}_{b}}\right)^{2}.$$

 $_{341}$ This implies (10) and we finish the proof.

The definition of the set of coarse objects of $\hat{\mathcal{B}}$ requires further elaboration. The set of objects $\Lambda(\Theta_{\rm pb})$ obtained by applying the classification in subsection 2.3 for the PB subdomain partition $\Theta_{\rm pb}$ provides a classification of $\Gamma(\Theta_{\rm pb}) \supset \Gamma(\Theta)$. We have the following relation between the PB objects $\Lambda_{\rm pb}(\Theta)$ and the (standard) objects of the PB partition $\Lambda(\Theta_{\rm pb})$.

347 LEMMA 10. All the objects in
$$\Lambda_{\rm pb}(\Theta)$$
 are also in $\Lambda(\Theta_{\rm pb})$, i.e., $\Lambda_{\rm pb}(\Theta) \subset \Lambda(\Theta_{\rm pb})$

Proof. Let us consider an object $\lambda_{\rm pb} \in \Lambda_{\rm pb}(\Theta)$. In both object partitions $\Lambda_{\rm pb}(\Theta)$ 348 and $\Lambda(\Theta_{\rm pb})$, we are using the same criteria, i.e., $\operatorname{neigh}_{\Theta_{\rm pb}}(\cdot)$, to classify points. The 349 350 difference is that $\Lambda_{\rm pb}(\Theta)$ is the result of a classification of points in $\Gamma(\Theta)$ whereas $\Lambda(\Theta_{\rm pb})$ is obtained from a classification of points in $\Gamma(\Theta_{\rm pb})$. Since $\Gamma(\Theta) \subset \Gamma(\Theta_{\rm pb})$, all points in $\lambda_{\rm pb}$ belong to the same object $\lambda' \in \Lambda(\Theta_{\rm pb})$. Since $\lambda_{\rm pb}$ is on the in-352 terface $\Gamma(\Theta)$, there exist at least two subdomains $\hat{\mathcal{D}}, \hat{\mathcal{D}}' \in \operatorname{neigh}_{\Theta_{\mathrm{pb}}}(\lambda_{\mathrm{pb}})$ such that 353 $\omega(\hat{\mathcal{D}}) \neq \omega(\hat{\mathcal{D}}')$. Let us assume there is a point $\xi \in \lambda'$ such that $\xi \notin \lambda_{\rm pb}$. Then, 354 $\xi \in \Gamma(\Theta_{\rm pb}) \setminus \Gamma(\Theta)$, i.e., it only belongs to one subdomain in Θ . As a result, $\omega(\mathcal{D})$ is 355 the same for all $\hat{\mathcal{D}} \in \operatorname{neigh}_{\Theta_{nb}}(\xi)$. Thus, we have a contradiction, since $\operatorname{neigh}_{\Theta_{nb}}(\xi)$ 356cannot be the same as neigh_{Θ_{pb}} (λ_{pb}). 357

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With the theoretical support from Lemma 10, we can define the set of coarse objects $\widehat{\Lambda}_O$ of $\widehat{\mathcal{B}}$ as a classification of $\Gamma(\Theta_{\rm pb})$ as follows. On $\Gamma(\Theta)$, we consider the same set of objects Λ_O used in the PB-BDDC preconditioner, i.e., Λ_C , or $\Lambda_C \cup$ Λ_E , or $\Lambda_{\rm pb}(\Theta)$. For the rest of the interface $\Gamma(\Theta_{\rm pb}) \setminus \Gamma(\Theta)$, we enforce *full continuity* among PB subdomains. It can be understood as treating all FE nodes on $\Gamma(\Theta_{\rm pb}) \setminus \Gamma(\Theta)$ as corners. Denote this set of objects by $\widehat{\Lambda}^*$, we have $\widehat{\Lambda}_O = \Lambda_O \cup \widehat{\Lambda}^*$. Figure 3 illustrates the partitions and coarse objects of \mathcal{B} and $\widehat{\mathcal{B}}$ when $\Lambda_O = \Lambda_C \cup \Lambda_E$.

Remark 11. By construction, the BDDC space $\widetilde{\mathbb{V}}^{\text{pb}}$ of the auxiliary BDDC preconditioner $\widehat{\mathcal{B}}$ is identical to the BDDC space $\widetilde{\mathbb{V}}$, defined in (4), of the PB-BDDC preconditioner.



FIG. 3. Partitions and coarse objects of the PB-BDDC preconditioner \mathcal{B} (left) and the auxiliary BDDC preconditioner $\widehat{\mathcal{B}}$ (right) when $\Lambda_O = \Lambda_C \cup \Lambda_E$: corner objects are labeled with crosses while nodes of other objects are labeled with circles.

LEMMA 12. The condition number $\kappa(\mathcal{BA})$ of the PB-BDDC preconditioned operator is bounded by

371 (11)
$$\kappa(\mathcal{B}\mathcal{A}) \leq \max_{v \in \widetilde{\mathbb{V}}^{\mathrm{pb}}} \frac{\langle \mathcal{A}^{\Theta_{\mathrm{pb}}} \widehat{\mathcal{Q}}v, \widehat{\mathcal{Q}}v \rangle}{\langle \mathcal{A}^{\Theta_{\mathrm{pb}}}v, v \rangle}.$$

372 *Proof.* According to [39, Theorem 15], $\kappa(\mathcal{BA})$ is bounded by

373 (12)
$$\kappa(\mathcal{BA}) \le \max_{v \in \widetilde{\mathbb{V}}} \frac{\langle \mathcal{A}^{\Theta} \mathcal{Q}v, \mathcal{Q}v \rangle}{\langle \mathcal{A}^{\Theta}v, v \rangle}.$$

Now we only need to bound the right-hand-side in (12) by the one in (11).

On the one hand, using the fact that $\widetilde{\mathbb{V}} = \widetilde{\mathbb{V}}^{\mathrm{pb}}$, we have $\langle \mathcal{A}^{\Theta} v, v \rangle = \langle \mathcal{A}^{\Theta_{\mathrm{pb}}} v, v \rangle$ for all $v \in \widetilde{\mathbb{V}}$ because any $v \in \widetilde{\mathbb{V}}$ is continuous in each subdomain of Θ . On the other hand, let us prove that the weighting operator $\widehat{\mathcal{W}}$ defined by (5) for Θ_{pb} restricted to \mathbb{V} is identical to the weighting operator \mathcal{W} defined by (5) for Θ . Let us consider a subdomain $\mathcal{D} \in \Theta$ and its PB partition $\Theta_{\mathrm{pb}}(\mathcal{D})$. We have

$$\delta^{\dagger}_{\mathcal{D}}(\xi) = \sum_{\hat{\mathcal{D}} \in \Theta_{\mathrm{pb}}(\mathcal{D}), \, \hat{\mathcal{D}} \ni \xi} \delta^{\dagger}_{\hat{\mathcal{D}}}(\xi),$$

10

by the definition in (5). For an arbitrary function $v \in \mathbb{V} \subset \mathbb{V}^{\text{pb}}$, we find that 375

376
$$\mathcal{W}v(\xi) = \sum_{\mathcal{D}\in \text{neigh}_{\Theta}(\xi)} \delta^{\dagger}_{\mathcal{D}}(\xi) v_{\mathcal{D}}(\xi) = \sum_{\mathcal{D}\in \text{neigh}_{\Theta}(\xi)} \sum_{\hat{\mathcal{D}}\in\Theta_{\text{pb}}, \hat{\mathcal{D}}\ni\xi} \delta^{\dagger}_{\hat{\mathcal{D}}}(\xi) v_{\mathcal{D}}(\xi)$$
377
$$= \sum_{\hat{\mathcal{D}}\in\Theta_{\hat{\mathcal{D}}}, \hat{\mathcal{D}}\in\Theta_{\hat{\mathcal{D}}}, \hat{\mathcal{D}}, \hat{\mathcal{D}}\in\Theta_{\hat{\mathcal{D}}}, \hat{\mathcal{D}}, \hat{\mathcal$$

377
$$= \sum_{\hat{\mathcal{D}} \in \text{neigh}_{\Theta_{pb}}(\xi)} \delta_{\hat{\mathcal{D}}}^{\mathsf{T}}(\xi) v_{\hat{\mathcal{D}}}(\xi) = \mathcal{V}$$

378

Therefore, $\widehat{\mathcal{Q}}v$ and $\mathcal{Q}v$ are identical on $\Gamma(\Theta)$ and $\widehat{\mathcal{Q}}v$ is continuous across $\Gamma(\Theta_{\rm pb})$. In 379 addition, Qv is discrete α -harmonic in each $\mathcal{D} \in \Theta$ and have minimal energy norm 380 w.r.t \mathcal{A}^{Θ} . As a consequence, 381

$$\langle \mathcal{A}^{\Theta} \mathcal{Q} v, \mathcal{Q} v \rangle = \sum_{\mathcal{D} \in \Theta} \langle \mathcal{A}_{\mathcal{D}}^{\Theta} \mathcal{Q} v, \mathcal{Q} v \rangle$$

$$\leq \sum_{\mathcal{D}\in\Theta} \langle \mathcal{A}_{\mathcal{D}}^{\Theta} \widehat{\mathcal{Q}} v, \widehat{\mathcal{Q}} v \rangle = \sum_{\hat{\mathcal{D}}\in\Theta_{\mathrm{pb}}} \langle \mathcal{A}_{\hat{\mathcal{D}}}^{\Theta_{\mathrm{pb}}} \widehat{\mathcal{Q}} v, \widehat{\mathcal{Q}} v \rangle = \langle \mathcal{A}^{\Theta_{\mathrm{pb}}} \widehat{\mathcal{Q}} v, \widehat{\mathcal{Q}} v \rangle$$

This finishes the proof. 385

We could stop here and derive the estimate for $\kappa(\mathcal{BA})$ knowing that the condition 386number of the auxiliary BDDC preconditioned operator $\hat{\mathcal{B}}\mathcal{A}$ is estimated by an upper 387 bound of the last quantity on the right of (12). However, we will go a bit further to 388 389 obtain a stronger result.

LEMMA 13. Assume that Λ_O is such that Assumption 7 holds. Then we have the 390 following inequality: 391

392 (13)
$$\max_{v \in \widetilde{\mathbb{V}}^{\mathrm{pb}}} \frac{\langle \mathcal{A}^{\Theta_{\mathrm{pb}}} \widehat{\mathcal{Q}}v, \widehat{\mathcal{Q}}v \rangle}{\langle \mathcal{A}^{\Theta_{\mathrm{pb}}}v, v \rangle} \leq C \max\{1, \mathrm{TOL}\} \max_{\mathcal{D} \in \Theta^{\partial}_{\mathrm{pb}}} \left(1 + \log\left(\frac{H(\mathcal{D})}{h(\mathcal{D})}\right)\right)^2,$$

where the constant C is independent of the number of subdomains, $H(\hat{D})$, $h(\hat{D})$ and 393 the physical coefficient α . 394

Proof. By triangle inequality, we have 395

396 (14)
$$\max_{v \in \widetilde{\mathbb{V}}^{\mathrm{pb}}} \frac{\langle \mathcal{A}^{\Theta_{\mathrm{pb}}} \widehat{\mathcal{Q}} v, \widehat{\mathcal{Q}} v \rangle}{\langle \mathcal{A}^{\Theta_{\mathrm{pb}}} v, v \rangle} \le 1 + \max_{v \in \widetilde{\mathbb{V}}^{\mathrm{pb}}} \frac{\langle \mathcal{A}^{\Theta_{\mathrm{pb}}} (\widehat{\mathcal{Q}} v - v), (\widehat{\mathcal{Q}} v - v) \rangle}{\langle \mathcal{A}^{\Theta_{\mathrm{pb}}} v, v \rangle}$$

Let $w = \widehat{\mathcal{Q}}v - v$. Given a FE function $u \in \mathbb{V}_{\hat{\mathcal{D}}}$, we denote by $\theta_{\lambda}^{\hat{\mathcal{D}}}(u) \in \mathbb{V}_{\hat{\mathcal{D}}}$ the FE 397 function that is discrete α -harmonic in $\hat{\mathcal{D}}$ and agrees with u at the FE nodes in the 398 object λ and vanishes at all the other nodes on $\partial \hat{\mathcal{D}}$. Since $\Lambda(\Theta_{pb})$ is a partition of 399 $\Gamma(\Theta_{\rm pb})$, we can split w into object and subdomain contributions as follows: 400

401 (15)
$$w = \sum_{\lambda \in \Lambda(\Theta_{\rm pb})} \sum_{\hat{\mathcal{D}} \in {\rm neigh}_{\Theta_{\rm pb}}(\lambda)} \theta_{\lambda}^{\hat{\mathcal{D}}}(w).$$

By the construction of the set of object $\widehat{\Lambda}_O = \Lambda_O \cup \widehat{\Lambda}^*$ and the definition of $\widetilde{\mathbb{V}}^{\mathrm{pb}}$, w 402 vanishes at all coarse objects in $\widehat{\Lambda}^*$, i.e., at all FE nodes in $\Gamma(\Theta_{\rm pb}) \setminus \Gamma(\Theta)$. Consequently, 403 (15) can be simplified as follows: 404

405 (16)
$$w = \sum_{\lambda \in \Lambda_{\rm pb}(\Theta)} \sum_{\hat{\mathcal{D}} \in \Theta_{\rm pb}^{\partial}} \theta_{\lambda}^{\hat{\mathcal{D}}}(w).$$

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When Λ_O satisfies Assumption 7, the set of objects in $\widehat{\Lambda}_O$ also fulfils [50, Assumption 6.27]. Consequently, using Lemma 9, we can perform an analysis similar to that in the proof [50, Lemma 6.36] (see also [31, Lemma 10]) to obtain

409
$$\langle \mathcal{A}_{\hat{\mathcal{D}}}^{\Theta_{\mathrm{pb}}} \theta_{\lambda}^{\hat{\mathcal{D}}}(w), \theta_{\lambda}^{\hat{\mathcal{D}}}(w) \rangle$$

410 411 $\leq C \max\{1, \text{TOL}\} \left(1 + \log\left(\frac{H(\hat{\mathcal{D}})}{h(\hat{\mathcal{D}})}\right)\right)^2 \sum_{\hat{\mathcal{D}} \in \text{neigh}_{\Theta_{\text{pb}}}(\lambda)} \langle \mathcal{A}_{\hat{\mathcal{D}}}^{\Theta_{\text{pb}}} v, v \rangle$

for any $\hat{\mathcal{D}} \in \Theta_{\text{pb}}^{\partial}$ and $\lambda \in \Lambda(\Theta_{\text{pb}})$. Here the constant C is proportional to $C_{\delta^{\dagger}}$ in Lemma 9, but is otherwise independent of $H(\hat{\mathcal{D}})$, $h(\hat{\mathcal{D}})$ and the physical coefficient α . Adding up the estimate for all subdomain $\hat{\mathcal{D}} \in \Theta_{\text{pb}}$, we find that

415 (17)
$$\langle \mathcal{A}^{\Theta_{\mathrm{pb}}} w, w \rangle \leq C \max\{1, \mathrm{TOL}\} \max_{\hat{\mathcal{D}} \in \Theta_{\mathrm{pb}}^{\partial}} \left(1 + \log\left(\frac{H(\hat{\mathcal{D}})}{h(\hat{\mathcal{D}})}\right)\right)^2 \langle \mathcal{A}^{\Theta_{\mathrm{pb}}} v, v \rangle.$$

416 This finishes the proof.

417 Combining results in Lemma 12 and Lemma 13, we have the final bound for 418 the PB-BDDC preconditioner, which is both weakly scalable and independent of the 419 coefficient α .

420 THEOREM 14. The condition number of the PB-BDDC preconditioned operator 421 $\kappa(\mathcal{BA})$ is bounded by

422
$$\kappa(\mathcal{BA}) \le C \max\{1, \text{TOL}\} \max_{\hat{\mathcal{D}} \in \Theta_{\text{pb}}^{\partial}} \left(1 + \log\left(\frac{H(\hat{\mathcal{D}})}{h(\hat{\mathcal{D}})}\right)\right)^2$$

423 where the constant C is independent of the number of subdomains, $H(\hat{D})$, $h(\hat{D})$ and 424 the physical coefficient α .

425 Remark 15. As seen in the Lemma 13 and Theorem 14, the condition number 426 associated with the PB-BDDC method depends only on the characteristic size and 427 mesh size of PB subdomains touching the original interface $\Gamma(\Theta)$. Further, the con-428 vergence of the PB-BDDC is independent of variations of the coefficient. The main 429 target of this work is achieved.

3.5. Relaxed physics-based BDDC. The definition of the coarse objects for the PB-BDDC preconditioner, based on the requirement that the coefficient has to be constant in each PB subdomain, can result in a large coarse space. That is the case for heterogeneous problems where the physical coefficient varies across a wide spectrum of values in a small spatial scale.

In order to deal with a more general class of problems, we propose the relaxed PB-BDDC preconditioner (rPB-BDDC) where we only require that the maximal contrast in each PB subdomain is less than some predefined tolerance r. We consider a relaxed PB partition Θ^{pb} such that

439 (18) $\max_{\tau,\tau' \subset \hat{\mathcal{D}}} \frac{\alpha_{\tau}}{\alpha_{\tau'}} \le r, \quad \text{for any } \hat{\mathcal{D}} \in \Theta^{\text{pb}}.$

440 Here the threshold r is equal or greater than 1. This way, we can control the size of

441 the coarse problem and the condition number bounds with the choice of r.

442 As the coefficient is no longer constant in each PB subdomain, we need to use 443 a weighted-constraint in the definition of coarse DOFs. More specifically, instead of 444 using (3), we use

445 (19)
$$c_{\lambda}^{\mathcal{D}}(u) \doteq \frac{\int_{\lambda} \bar{\alpha} \, u \, ds}{\int_{\lambda} \bar{\alpha} \, 1 \, ds}, \quad \text{where } \bar{\alpha}(\xi) \doteq \max_{\tau \in \mathcal{T}, \tau \ni \xi} \alpha_{\tau}.$$

446

447 Remark 16. The larger r becomes the smaller the size of the coarse problem of the rPB-BDDC preconditioner is and the larger its condition number grows to. When 448 r = 1 the rPB-BDDC preconditioner becomes the PB-BDDC preconditioner. By 449 tuning the threshold r, one can obtain a right balance between the time spent on 450451 setting up the preconditioner (especially in forming the coarse space) and the time spent on applying the preconditioner in a Krylov solver. The optimal threshold is of 452course problem dependent. However, finding a good threshold is not tricky. This is 453illustrated in section 4. 454

Remark 17. The rPB-BDDC preconditioner makes use of a threshold. This is similar to the adaptive coarse space approach where only eigenfunctions associated with eigenvalues below a predefined threshold are included in the coarse space. However, the rPB-BDDC preconditioner does not involve any eigenvalue or auxiliary problems and is far simpler and cheaper.

460 **4. Numerical experiments.** In this section, we test the robustness and effi-461 ciency of the PB-BDDC and rPB-BDDC preconditioners for the system matrix asso-462 ciated with (2) for different types of variation in the coefficient α , which are similar 463 but generally harder than the ones in [42, 28, 36].

464 Due to the difficulty of heterogeneous problems, in PB-BDDC and rPB-BDDC 465 methods, we tend to use a large number of objects. Many of them are not corners. In 466 all tested cases, these objects are enough to make the local Neumann problems and 467 global coarse problem well-posed and we can optionally drop corner objects. No corner 468 detection mechanism (see, e.g, [46]) has been needed in any tested case. Alternatively, 469 one might want to consider the perturbed formulation introduced in [7, 8]. However, 470 this approach has not been extended to heterogeneous problems yet.

In all of the experiments, we consider the physical domain $\Omega = (0, 1)^2$. Unless stated otherwise, we use the uniform triangular meshes of size h = 1/72 and the regular 3×3 subdomain partition. In all cases, we report the dimension of the coarse space, denoted by dim, and the number of iterations required for the conjugate gradient method to reduce the residual norm by a factor of 10^6 . We also provide the condition number κ in most examples.

477 **4.1. Two channels.** In this test case, we consider two channels of high α cutting 478 through vertical subdomain edges (see Figure 4). The coefficient in the channels α_{max} 479 takes the values $\{10^2, 10^4, 10^6, 10^8\}$, while the coefficient in the rest of the domain is 480 equal to 1.

From Table 1, we can see that the condition number and the number of iterations for the standard BDDC preconditioner (BDDC(ce)) definitely increase with α_{max} , whereas they remain practically constant for both variants of the PB-BDDC preconditioners (PB-BDDC(ce) and PB-BDDC(e)). In other words, the convergence of the PB-BDDC method is independent of the contrast and the PB-BDDC method is perfectly robust for this test case. Figure 4 shows the coarse objects of PB-BDDC(ce) on the interface of the partition.

$\dim \rightarrow$	BDDC(ce) 16		P	PB-BDDC(ce) 64			PB-BDDC(e) 36		
α_{\max}	# it.	κ	#	it.	κ	#	it.	κ	
10^{2}	21	2.12e3	1	.0	5.47e0	1	3	1.20e1	
10^{4}	28	2.87e5	1	.0	$5.31\mathrm{e0}$	14	4	1.21e1	
10^{6}	44	2.89e7	1	.0	$5.31\mathrm{e0}$	1!	5	$1.21\mathrm{e}1$	
10^{8}	64	3.88e9	1	0	$5.31\mathrm{e0}$	1!	5	$1.21\mathrm{e}1$	

 $\begin{array}{c} \text{TABLE 1}\\ \text{Comparison of the iteration count and condition number in the two channels test case.} \end{array}$



FIG. 4. Distribution of the coefficient in the two-channels test case when $\alpha_{max} = 10^6$. The coarse objects of PB-BDDC(ce) are shown on the interface with corners labeled by stars and DOFs in edges labeled by circles.

488 **4.2. Channels and inclusions.** In this test case, we consider both channels 489 and inclusions of high coefficient. First, the three channels include all the elements 490 whose centroids are less than $2 \cdot 10^{-2}$ from one of the following three lines:

- 491 $L1: x_1 x_2 0.2 = 0,$
- 492 $L2: x_1 + x_2 0.7 = 0,$

$$433 L3: x_1 - 0.7x_2 - 0.7 = 0$$

The coefficient α_{max} in these channels takes the values $\{10^2, 10^4, 10^6, 10^8\}$. Secondly, the inclusions are defined as the regions of elements whose all vertices x satisfy

497
$$mod(floor(10x_i), 2) = 1, \text{ for } i = 1, 2.$$

For an element τ that belongs to one of the inclusions and is not in the channels, its coefficient is defined as

500 (20) $\alpha|_{\tau} = (\alpha_{\max}/10)^{1/5*\text{floor}(0.5*\text{floor}(10x_1(c_{\tau}))+1)}$, where c_{τ} is the centroid of τ .



FIG. 5. Distribution of the coefficient for the channels and inclusions test case when $\alpha_{\text{max}} = 10^6$. The coarse objects of PB-BDDC(ce) are shown on the interface with corners labeled by stars and DOFs in edges labeled by circles.

501 The coefficient in (20) is: a) constant in each inclusion b) increasing from left to right 502 c) increasing as α_{max} increases and d) always belongs to $(1, \alpha_{\text{max}})$. For the rest of the 503 domain, we set $\alpha = 1$. The maximal contrast ratio in this experiment is 10^8 .

We can see from Table 2 that as α_{max} becomes larger the condition number and the number of iterations associated with the standard BDDC(ce) method increases significantly. In contrast, both variant of the PB-BDDC methods, PB-BDDC(ce) and PB-BDDC(e), are perfectly robust with respect to the changes of the coefficient in the channels and in the inclusions. Especially, PB-BDDC(e) maintains its robustness with a reasonably small coarse space.

$\dim \rightarrow$	BDDC(ce) 16		PB-BI	DDC(ce) 89	$\begin{array}{c} PB-BDDC(e)\\ 39 \end{array}$		
α_{\max}	# it.	κ	# it.	ĸ	# it.	κ	
10^{2}	23	1.48e3	13	1.01e1	14	5.71e1	
10^{4}	45	8.33e4	13	8.93e0	15	8.08e1	
10^{6}	82	6.02e6	13	8.79e0	15	8.15e1	
10^{8}	97	5.30e8	13	8.76e0	15	8.15e1	

TABLE 2

Comparison of the iteration count and condition number in the channels and inclusions test case.

510 **4.3. Complex channels.** In this test case, we demonstrate the importance of 511 having acceptable paths. We consider a distribution with multiple channels of high 512 coefficient α_{max} taking values in $\{10^2, 10^4, 10^6, 10^8\}$ (see Figure 6 for the case when 513 $\alpha_{\text{max}} = 10^6$).

514 From Table 3, we can see that PB-BDDC(ce) is perfectly robust. On the other 515 hand, the condition number and number of iterations of the PB-BDDC(e) preconS. BADIA AND H. NGUYEN



FIG. 6. Distribution of the coefficient in the complex channels test case. The coarse objects of PB-BDDC([c]e) are shown on the interface with corners labeled by stars and DOFs in edges labeled by circles. Only few corners are required to guarantee perfect robustness (to have acceptable paths).

ditioner increase significantly as α_{max} increases. The reason is that there are some pairs of channels share a corner but not an edge. In PB-BDDC(e), none of these corners are selected as a coarse objects. Consequently, there is no acceptable path with TOL independent of the contrast between the associated paired of channels (PB subdomains) and Assumption 7 does not hold. By including a small number of these critical corners (represented by stars in Figure 6) in order to satisfy Assumption 7, the resulting preconditioner, labeled PB-BDDC([c]e), is perfectly robust w.r.t changes in

523 the contrast of the coefficient (see Table 3).

 TABLE 3

 Comparison of the iteration count and condition number in the complex channels test case.

OC([c]e)
3
(κ)
21e1)
27e1)
27e1)
27e1)

524 **4.4. Sinusoidal variation.** In this experiment, we consider a coefficient that 525 varies like a sinusoid. We use a finer uniform triangular mesh of size h = 1/144. For 526 an element $\tau \in \mathcal{T}$, the coefficient α_{τ} is defined by

527
$$\log_{10}(\alpha_{\tau}) = \kappa \sin(w\pi(x_1(c_{\tau}) + x_2(c_{\tau}))) + \alpha_{\text{shift}},$$

where $\kappa = 3$, w = 14, and c_{τ} is the the centroid of τ . We note that when κ and/or w become larger the problem is more difficult. The distribution when $\alpha_{\text{shift}} = 0$ is



FIG. 7. Distribution of the coefficient mimicking sin function. The coarse objects of rPB-BDDC(ce) with $r = 10^3$ are shown on the interface with corners labeled by stars and DOFs in edges labeled by circles.

shown in Figure 7. It is as if there are many channels going through subdomain edgesat the same time.

In this test case, the coefficient varies very rapidly. We test the standard BDDC method and the rPB-BDDC method introduced in subsection 3.5, by allowing the upper bound r for the maximal contrast in each PB subdomain to vary among $\{10^1, 10^2, 10^3\}$. Only iteration counts are reported as the condition number estimation becomes too expensive for the mesh being used.

This is a difficult problem and the standard BDDC(ce) method requires almost a hundred iterations to converge (see Table 4). The relaxed physics-based methods, 538 rPB-BDDC(ce) and rPB-BDDC(e), are able to significantly reduce the number of 539 iterations. That comes with the cost of solving larger coarse problems. However, by 540 using a suitable threshold r, we can obtain a decent preconditioner, e.g. rPB-BDDC(e) 541542with $r = 10^3$, which requires only 11 iterations using a reasonably small coarse space of size 64. In addition, the rPB-BDDC method is also perfectly robust with shifting 543in the value of the coefficient. The iteration count does not change when α_{shift} takes 544values in $\{0, 6\}$. 545

		BDDC(ce)	rPB-BDDC(ce)		r	rPB-BDDC(e)			
	r	10	10	10^{2}	10^{3}	1	0	10^2	10^{3}
	dım	16	474	292	188	2	12	116	64
$\alpha_{\rm shift}=0$	# it.	92	7	10	11	1	0	12	11
$\alpha_{\rm shift} = 6$	# it.	99	7	10	11	1	0	12	11

TABLE 4Comparison of the iteration count in the continuous sin test case.



FIG. 8. Distribution of the coefficient in the log-normal test case. The coarse objects of rPB-BDDC(ce) with $r = 10^2$ are shown on the interface with corners labeled by stars and DOFs in edges labeled by circles.

4.5. Log-Normal. In this test case, we test the performance of the rPB-BDDC method for a log-normal distribution of the coefficient. This type of distribution is particularly important for geoscience and petroleum engineering applications. We consider $\alpha_{\text{cont}}(x, w) = 10^{Z(x,w)}$, where Z(x, w) is a Gaussian random field with zero mean and Gaussian covariance

551
$$C(x,y) = \sigma^2 \exp\left(-\frac{\|x-y\|^2}{\ell^2}\right)$$
, with $\sigma = 1.5, \ \ell^2 = 1e-3$

For this experiment, a uniform triangular mesh of size h = 1/128 is utilized. Using the spectral decomposition method described in [37], we are able to obtain a realization of $\alpha_{\text{cont}}(x, w)$ at mesh vertices. The piecewise coefficient α_{τ} on an element τ is then defined as the average of $\alpha_{\text{cont}}(x, w)$ at the three vertices. The distribution of α with a partition obtained from METIS [26] is shown in Figure 8. The contrast ratio in this test case is nearly 10¹⁰. The coarse objects of rPB-BDDC(ce) when $r = 10^2$ are also illustrated.

In Table 5, we can see that, compared to the standard BDDC(ce) method, rPB-BDDC(ce) and rPB-BDDC(e) preconditioners require much fewer iterations to converge. They, however, have a larger coarse space. By adjusting the threshold for the maximal contrast in each object, we can reduce the size of the coarse space while maintaining a reasonably fast convergence. This is clearly illustrated in Table 5.

5. Conclusions. In this work, we have proposed a novel type of BDDC pre-564565 conditioners that are robust for heterogeneous problems with high contrast. The 566underlying idea is to modify the continuity constraints enforced among subdomains 567 making use of the knowledge about the physical coefficients. In order to do that, we rely on a physically motivated partition of standard coarse objects (corners, edges, and 568 faces) into coarse sub-objects. The motivation for that is the well-known robustness 569 of DD methods when there are only jumps of physical coefficients across the interface 570571 between subdomains. All these ideas can also be used in the frame of FETI methods.

	BDDC(ce)	rPI	rPB-BDDC(ce)			rPB-BDDC(e)		
rdim	49	$\begin{array}{c} 10\\ 488 \end{array}$	$ \begin{array}{r} 10^2 \\ 284 \end{array} $	$5 \cdot 10^3$ 239	$\begin{array}{c} 10\\ 204 \end{array}$	$10^2 \\ 127$	$\begin{array}{c} 5\cdot 10^3 \\ 105 \end{array}$	
# it.	77	16	25	28	25	29	33	

 TABLE 5

 Comparison of the iteration count in the log-normal test case.

In cases where the physical coefficient is constant in each coarse sub-object, we are able to prove that the associated condition number can be bounded independent of the number of the subdomains and the contrast of the physical coefficient. In other words, the new preconditioner is scalable and robust for heterogeneous problems.

Apart from the new set of coarse objects and a new weighting operator, the (r)PB-576 BDDC preconditioners are very much the same as the standard BDDC preconditioner. 577 As a result, the implementation of the new preconditioners involve a very simple 578modification of the standard BDDC implementation. In all of our experiments, the 579new preconditioners deliver fast, robust and contrast-independent convergence while 580 581 maintaining the simplicity of BDDC methods at a reasonable computational cost. Compared to the other robust DD solvers for heterogeneous problems currently avail-582able, such as the ones in [25, 45, 25, 43, 44, 22, 23, 42, 47, 15, 49, 48, 28, 27, 29, 36, 24], 583 our new methods do not involve any type of eigenvalue or auxiliary problems. 584

For further work, we want to implement the new preconditioners in the extremely scalable BDDC code in FEMPAR [3, 4, 5, 6]. The multilevel extension and the taskoverlapping implementation are particularly interesting in the (r)PB-BDDC case due to generally larger coarse problem. With such extremely scalable implementation, we are interested in applying our new preconditioners to realistic 3D problems, e.g., in geoscience applications.

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