Balancing Domain Decomposition by Constraints algorithms for curl-conforming spaces of arbitrary order

Stefano Zampini, Panayot Vassilevski, Veselin Dobrev and Tzanio Kolev

Abstract We construct Balancing Domain Decomposition by Constraints methods for the linear systems arising from arbitrary order, finite element discretizations of the $H(\mathrm{curl})$ model problem in three-dimensions. Numerical results confirm that the proposed algorithm is quasi-optimal in the coarse-to-fine mesh ratio, and poly-logarithmic in the polynomial order of the curl-conforming discretization space. Additional numerical experiments, including higher-order geometries, upscaled finite elements, and adaptive coarse spaces, prove the robustness of our algorithm. A scalable three-level extension is presented, and it is validated with large scale experiments using up to 16384 subdomains and almost a billion of degrees of freedom.

1 Introduction

We construct Balancing Domain Decomposition by Constraints (BDDC) methods [8] for the linear systems arising from three-dimensional, arbitrary order finite element discretizations of the $H(\mathrm{curl})$ bilinear form

$$\int_{\Omega} \alpha\, \nabla \times \boldsymbol{u} \cdot \nabla \times \boldsymbol{v} + \beta\, \boldsymbol{u} \cdot \boldsymbol{v}\, dx, \quad \alpha \geq 0,\ \beta > 0. \tag{1}$$

The proposed algorithm is quasi-optimal in the coarse-to-fine mesh ratio, and poly-logarithmic in the polynomial order of the finite element discretization space, which is confirmed by the numerical results in Section 3. Our results will be equally valid

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for the Finite Element Tearing and Interconnecting Dual-Primal (FETI-DP) method [12], due to the well known duality between BDDC and FETI-DP [25].

The bilinear form (1) originates from implicit time-stepping schemes of the quasi-static approximation of the Maxwell's equations in the time domain [30]. The coefficient α is the reciprocal of the magnetic permeability, assumed constant, whereas β is proportional to the conductivity of the medium; positive definite anisotropic tensor conductivities can be handled as well. We only present results for essential boundary conditions, but the generalization of the algorithms to natural boundary conditions is straightforward. Magnetostatic problems with $\beta = 0$ are not covered in the present work, and they can be the subject of future research. The same bilinear form appears in block preconditioning techniques for the frequency domain case [13], mixed form of Brinkman (Darcy-Stokes) [39], and in incompressible magneto-hydrodynamics [24].

The operator $\nabla\times$ is the *curl* operator, defined, e.g., in [4]; the vector fields belong to $H(\mathrm{curl})$, the Sobolev space of square-integrable vector fields having a square-integrable curl. The space $H(\mathrm{curl})$ is often discretized using Nédélec elements [26]; those of lowest order use polynomials with continuous tangential components along the edges of the elements. While most existing finite element codes for electromagnetics use lowest order elements, those of higher order have shown to require fewer degrees of freedom (dofs) for a fixed accuracy [31, 13].

The design of solvers for edge-element approximations of (1) poses significant difficulties, since the kernel of the curl operator is non-trivial. An even greater challenge for domain decomposition solvers consists in finding logarithmically stable decompositions in three dimensions, due to the strong coupling that exists between the dofs located on the subdomain edges and those lying on the subdomain faces. Among non-overlapping methods, it is worth citing the wirebasket algorithms [9, 18, 19], Neumann-Neumann [32], and one-level FETI [36, 28]. Overlapping Schwarz methods have also been studied [33, 6].

The edge-element approximation of (1) has also received a lot of attention by the multigrid community; Algebraic Multigrid (AMG) methods have been proposed in [29], [5], and [17]. For geometric multigrid, see [14]. Robust and efficient multigrid solvers can be obtained combining AMG and auxiliary space techniques, that require some extra information on the mesh connectivity and on the dofs [15, 16, 22].

In this work, we follow the approach proposed by Toselli for three-dimensional FETI-DP with the lowest order Nédélec elements [34], where a stable decomposition is obtained by using a change of basis for the dofs located on the subdomain edges. The same approach has been pursued recently by Dohrmann and Widlund [11], who were able to improve Toselli's results, and obtain sharp and quasi-optimal condition number bounds (in the lowest order case) by using the deluxe variant of BDDC [10]. This is critical for obtaining iteration counts and condition number estimates independent of the jumps of α and β aligned with the subdomain interface. Finally, it has to be noted that BDDC deluxe algorithms for high-order Nédélec elements in two dimensions, and for the lowest order Nédélec elements in three dimensions have been already presented by the first author in [40, 42].

In Section 2, we complement the results in [34, 11] by proposing an algorithm for the change of basis that does not make any assumption on the mesh, the associated discretization space, and the domain decomposition. Inspired by the success of the auxiliary space technique [15], we construct the change of basis by using the so-called *discrete gradient*, a linear operator that maps gradients of scalar functions to their representation in the curl-conforming discretization space. Numerical experiments, provided in Section 3, confirm that the robustness of our approach is not confined to the more standard Nédélec elements, but it also extends to the case of elements with curved boundaries, and to upscaled $H(\mathrm{curl})$ spaces constructed by preserving the de Rham sequence on agglomerations of fine scale elements. Due to page restrictions, we refer the interested reader to [23] for a thorough description of these kind of elements.

2 Design of the algorithm

2.1 Domain decomposition and discrete spaces

We follow the framework of iterative substructuring [37, Chapters 4-6], and we decompose the domain Ω into N non-overlapping open Lipschitz subdomains Ω_i,

$$\overline{\Omega} = \bigcup_{i=1}^{N} \overline{\Omega}_i, \quad \Gamma := \bigcup_{i \neq j} \partial\Omega_j \cap \partial\Omega_i,$$

with Γ the interface between the subdomains. We further assume that Ω and each Ω_i are simply connected (does not contain any holes). We denote by $\mathbf{V}_h(\Omega)$ and $S_h(\Omega)$ the curl- and H^1- conforming finite element spaces of polynomial order p, respectively, together with their subdomain counterparts $\mathbf{V}_h^{(i)} := \mathbf{V}_h(\Omega_i)$ and $S_h^{(i)} := S_h(\Omega_i)$. We denote by $\mathbf{W}$ the global finite element space in which we seek the solution of problems coming from the bilinear form (1), and by $\mathbf{W}^{(i)}$ the corresponding subdomain spaces. We note that $\mathbf{V}_h$ coincides with $\mathbf{W}$ when using Nédélec elements; however, our algorithm covers also the case $\mathbf{V}_h \subset \mathbf{W}$, as it is the case of upscaled finite elements that preserve the de Rham sequence [23], or of three-level extensions of the BDDC algorithm for (1) (see Section 2.4).

The success of the algorithm depends on the analysis of the interface, that leads to the detection of equivalence classes such as the subdomain faces, i.e. sets of connected dofs shared by the same two subdomains, and the subdomain edges, i.e. sets of connected dofs shared by 3 or more subdomains. We assume that a subdivision of Γ in face and edge disjoint subsets has been found; moreover, we assume that each subdomain edge has exactly two endpoints, and none of the edge endpoints lie in the interior of another subdomain edge. As noted in [11, Section 5], this guarantees that the change of basis (defined in the next section) leads to a new well-posed problem.

2.2 BDDC method

The recipe for the construction of a BDDC preconditioner consists in the design of a partially continuous interface space $\widetilde{\mathbf{W}}_\Gamma$, the direct sum of a continuous *primal* space $\mathbf{W}_\Pi$ and a discontinuous *dual* space $\mathbf{W}_\Delta$, and in the choice of an averaging operator E_D for the partially continuous dofs, which drives the analysis and the design of robust primal spaces [25].

Following Toselli [34], we characterize the primal space $\mathbf{W}_\Pi$ by using two primal constraints per subdomain edge E as given by

$$s_{0,E}(\boldsymbol{w}) := \tfrac{1}{|E|}\int_E \ \boldsymbol{w}\cdot\boldsymbol{t}_E \ ds, \quad \boldsymbol{w}\in\mathbf{V}_h, \tag{2}$$

$$s_{1,E}(\boldsymbol{w}) := \tfrac{1}{|E|}\int_E s\boldsymbol{w}\cdot\boldsymbol{t}_E \ ds, \quad \boldsymbol{w}\in\mathbf{V}_h, \tag{3}$$

where $\boldsymbol{t}_{E_{|e}} := \boldsymbol{t}_e$, with $\boldsymbol{t}_e$ the vector oriented in the direction of a fine mesh edge e belonging to E. For implementation details of the primal space, see Remark 3.

2.3 Change of basis

As in [34, 11], we consider a change of basis for the dofs of $\mathbf{V}_h$ that are located on each subdomain edge E, and we split a finite element function $\boldsymbol{w}$ into a *constant* component $\boldsymbol{\Phi}_E$ and *gradient* components $\nabla\phi_{jE}$ associated with the nodal dofs of S_h lying in the interior of the edge, i.e.

$$\boldsymbol{w}|_E = s_{0,E}(\boldsymbol{w})\boldsymbol{\Phi}_E + \sum_{j=1}^{n_E-1} w_{jE}(\boldsymbol{w})\nabla\phi_{jE} + \boldsymbol{w}_{Ec},$$

with n_E the number of $\mathbf{V}_h$ dofs on E, and $\boldsymbol{w}_{Ec}$ the finite element function (if any) identified by the dofs of $\mathbf{W}$ that lie on E and are not in $\mathbf{V}_h$.

The change of basis in BDDC methods is performed by projection as T^TAT, where the columns of T represents the new basis in terms of the old dofs [21], and A results from the discretization of the bilinear form (1). The structure of T for three-dimensional curl-conforming spaces is as follows [34, 11, 40, 42]

$$T = \begin{bmatrix} I_C & 0 & 0 & \dots & 0 \\ 0 & I_F & T_{FE_1} & \dots & T_{FE_n} \\ 0 & 0 & T_{E_1E_1} & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & T_{E_nE_n} \end{bmatrix},$$

where I_C and I_F are identity matrices of appropriate sizes. Here, F denotes the set of dofs of $\mathbf{V}_h$ that belong to the subdomain faces, and C denotes all the remaining dofs of $\mathbf{W}$ that do not belong to F or to any of the subdomain edge dofs of $\mathbf{V}_h$.

Differently from a conventional change of basis in BDDC, the one used for curl-conforming spaces is not local to the subdomain edges, as it also involves, through the sparse off-diagonal blocks T_{FE_i}, the dofs of F that are located on the fine mesh edges sharing a mesh vertex with any of the E_i.

In our code, we use T^TAT as iteration matrix; however, in order to preserve a one-to-one correspondence between old and new subdomain dofs, we construct the preconditioner using the subdomain matrices $\tilde{A}^{(i)} := R^{(i)}T^TR^{(i)T}A^{(i)}R^{(i)}TR^{(i)T}$, where $A^{(i)}$ is the discretization matrix on $\mathbf{W}^{(i)}$, and $R^{(i)}$ is the usual restriction operator from $\mathbf{W}$ to $\mathbf{W}^{(i)}$. Note that $T^TAT = \sum_{i=1}^N (T^TR^{(i)T})A^{(i)}(R^{(i)}T) \neq \sum_{i=1}^N R^{(i)T}\tilde{A}^{(i)}R^{(i)}$.

The functions $\boldsymbol{\Phi}_E$ and $\nabla\phi_{jE}$ are explicitly constructed in [34, 11]; however, the procedures used therein possess strong limitations, as they need to access the underlying mesh and to understand how the edge dofs are related with the orientation of the fine mesh edges; moreover, they are limited to the lowest order Nédélec space only. In this work, we propose a construction of the change of basis by using the information contained in the discrete gradient operator G, the matrix representation of the mapping $\phi \in S_h \to \nabla\phi \in \mathbf{V}_h$, that is also used by the auxiliary space method, see [15] and [22, Section 4]. We note that, when using Nédélec elements, there are p dofs associated to each fine mesh edge, and that the number of nonzeros per row of G is $p+1$, with p the polynomial order of the finite element space used for S_h. For upscaled elements, the number p_e of dofs of $\mathbf{V}_h$ associated to each fine mesh edge e may vary from one fine mesh edge to another, but the number of nonzeros of the corresponding rows of G is always p_e+1.

For each subdomain edge E, we construct the corresponding column block of T as follows. We first extract the matrix $G_{E\mathring{E}}$, where $\mathring{E}$ is the set of dofs of S_h that is associated with those basis functions being nonzero on the nodes in the interior of E; note that $G_{E\mathring{E}}$ has full-column rank, and that $n_E = n_{\mathring{E}} + 1$. We then compute the representation of the subdomain edge constant function $\boldsymbol{\Phi}_E$ in $\mathbf{V}_h$ as the eigenvector corresponding to the nonzero eigenvalue of the orthogonal complement of $G_{E\mathring{E}}$, i.e. $I - G_{E\mathring{E}}(G_{E\mathring{E}}^TG_{E\mathring{E}})^{-1}G_{E\mathring{E}}^T$. The dofs defining $\nabla\phi_{jE}$ are simply given by the columns of G that correspond to $\mathring{E}$. The change of basis block relative to E is

$$\begin{bmatrix} T_{FE} \\ T_{EE} \end{bmatrix} := \begin{bmatrix} 0 & G_{E^c\mathring{E}} \\ \boldsymbol{\Phi}_E & G_{E\mathring{E}} \end{bmatrix},$$

with $E \cup E^c$ the set of row indices corresponding to the nonzero values in the $\mathring{E}$ columns.

Remark 1. The construction of our change of basis just needs sub-matrix extraction operations and the computation of the orthogonal complement of $G_{E\mathring{E}}$, which can be obtained by doing a singular value decomposition of the same matrix, of size $n_E \times n_{\mathring{E}}$: note that n_E is usually very small, on the order of ten, and we can thus efficiently use algorithms for dense matrix storages. After having changed the basis, the sparsity pattern of the local matrices is not spoiled, and optimal nested dissection orderings for the direct solves of the subdomain problems can be found.

Remark 2. For the lowest order Nédélec elements, G has two nonzeros per row; the values are $+1$ or -1 depending on the orientation of the element edge. When hexahedral meshes and box subdomains are considered, our change of basis is the same as that proposed by Toselli [34].

Remark 3. The constraint given in eq. (2) is obtained by selecting the dofs corresponding to each $\boldsymbol{\Phi}_E$ as primal; arithmetic averages for the remaining dofs on the subdomain edges are used to impose the constraint (3), see also [11, Section 2.2].

Remark 4. Our algorithm does not require the user to input the mesh connectivity. From G, we can infer the dofs connectivity which will lead to a well-posed change of basis, since the sparsity pattern of the matrices $G^T G$ and GG^T carry the information of a vertex-to-vertex, and an edge-to-edge mesh connectivity graph, respectively.

2.4 Three-level extension of the algorithm

Three-level extensions of the algorithm [38] are crucial for large scale simulations, as the solution of the coarse problem in BDDC (as with all two-level methods) can become a bottleneck when many subdomains are considered, see [41, Section 3.6] and the references therein for additional details. The minimal coarse space presented in Section 2.2 can be naturally split in two disjoint subsets; the one arising from the constraints given in eq. (2) resembles a lowest-order Nédélec space defined on the coarse element (i.e., the subdomain). The rest of the coarse dofs are instead generated by gradients of scalar functions, and a scalable coarse space can be thus obtained by considering arithmetic averages defined on the coarse subdomain edges.

We thus propose an approximate coarse discrete gradient to obtain a stable decomposition of the coarse dofs generated by eq. (2), obtained by projecting the fine discrete gradient G on the $\boldsymbol{\Phi}_E$ functions. The resulting coarse discrete gradient will have two nonzero entries per row, with entries given by $G^T_{E\partial E}\boldsymbol{\Phi}_E$, with ∂E the indices of the basis functions of S_h associated with the two endpoints of E. We then construct the primal space of the coarse problem as outlined in the previous sections. Numerical results confirm that such an approach provides an optimal coarse space for the second level of the BDDC operator, and leads to scalable three-level algorithms in terms of number of iterations. We note that multilevel extensions, with an arbitrary number of levels, can be obtained by recursion arguments.

3 Numerical results

Here we present numerical experiments that confirm the robustness of our algorithm; we test the quasi-optimality, the dependence on the polynomial order of the curl-conforming spaces, and the proposed three-levels extension. In addition, we test the case of elements with curved boundaries. We also provide results for adaptive

enrichment (see [41] and the references therein) of the minimal coarse space given by eqs. (2) and (3) in the presence of heterogeneous coefficients. As quality metrics, we consider the experimental condition number (denoted by κ) and the number of conjugate gradient iterations needed to reduce by eight orders of magnitude the initial residual norm, starting from zero initial guess and randomly distributed right-hand side. Unless otherwise stated, the primal space consists of two dofs per subdomain edge as described in Section 2.2, $\alpha = \beta = 1$, and $\Omega = [0,1]^3$.

All the numerical results have been obtained using the discretization packages MFEM [1] (for Nédélec elements and high-order geometries) and ParElag [2] (for upscaled finite elements) developed at Lawrence Livermore National Laboratory, and by using the BDDC implementation developed by the first author in the PETSc library [3, 41]. Irregular decompositions of tetrahedral (TET) or hexahedral (HEX) meshes obtained from the graph partitioner ParMETIS [20] are always considered; deluxe scaling is always used to accommodate for spurious eigenvalues of the preconditioned operator arising from possibly jagged subdomain interfaces [7].

In Figure 1 we report the results of a quasi-optimality test, performed by considering successive uniform refinements of a mesh decomposed in 40 subdomains, and by using Nédélec elements of order $p = 1$ (lowest-order) and $p = 2$. The domain decomposition is kept fixed, in order to fix the value of the maximum subdomain diameter H. The results show a $(1+\log H/h)^2$ dependence in all the cases considered.

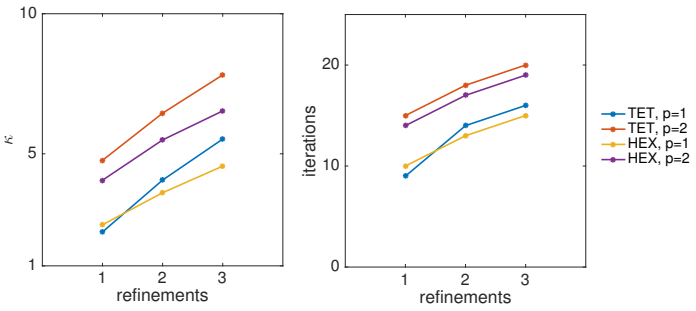


Fig. 1: Quasi-optimality test. κ (left) and number of iterations (right) for successive uniform refinements for Nédélec elements on hexahedra (HEX) and tetrahedra (TET); polynomial orders $p = 1$ and $p = 2$.

We then fix the mesh and the domain decomposition (i.e. H/h), and we increase the polynomial order of the discretization spaces. Figure 2 contains results for the Nédélec elements, going from $p = 1$ to $p = 6$; we note that we obtained the same results when considering statically condensed spaces (relevant when $p > 1$ for the HEX and $p > 2$ for the TET case, data not shown). In the same spirit, Figure 3 contains the results for upscaled curl-conforming elements, obtained by considering two successive levels of structured aggregation (UP1 and UP2 respectively), and with polynomial orders ranging from $p = 1$ to $p = 4$; results for Nédélec elements (NED) on the same mesh are given for comparison. In both cases, Nédélec or up-

scaled elements, our algorithm shows to be robust with the higher degree of the polynomial space, and it leads to a poly-logarithmic convergence rate. The results of this test, together with those related with the quasi-optimality, suggest a condition number bound of the type $(1+\log(p^2H/h))^2$ for the preconditioned operator.

Fig. 2: Polynomial order test. κ and number of iterations as a function of the polynomial order for Nédélec elements on hexahedra (HEX) and tetrahedra (TET).

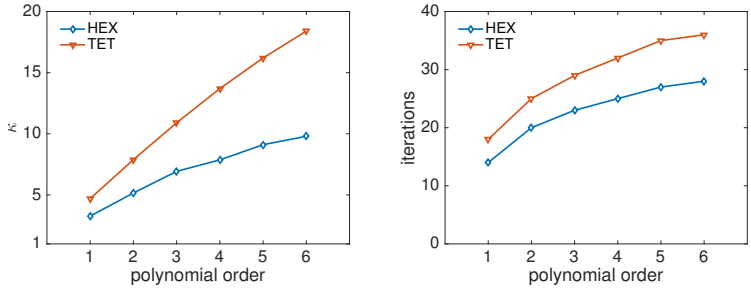
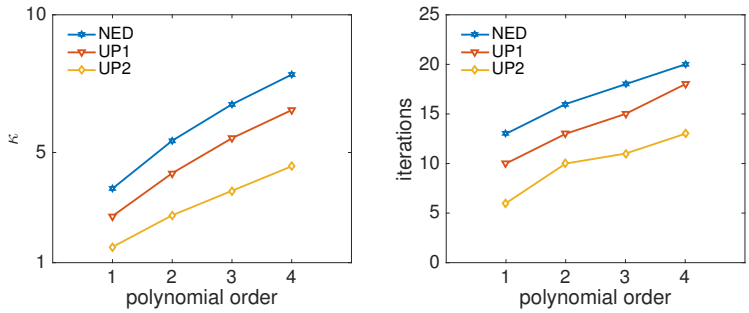


Fig. 3: Polynomial order test. κ and number of iterations as a function of the polynomial order for Nédélec elements (NED), and upscaled curl-conforming elements. UP1 one level of element aggregation with structured coarsening, UP2 two levels.



Further numerical evidence for the robustness of our approach is given by the results shown in Table 1, where condition numbers and number of iterations are reported by testing against third-order geometries, in combination with Nédélec elements of order $p = 1,2$. The meshes used to run the tests have been obtained from 2 levels of uniform refinements of those shown in Figure 4, and they are available with the MFEM source code as `escher-p3.mesh` and `fichera-q3.mesh`. The number of subdomains considered is 40.

Fig. 4: Third-order meshes used for the results in Table 1.

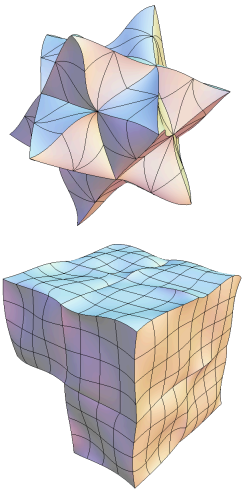


Table 1: High-order geometry test. Size of linear systems (dofs), condition number, (κ) and number of iterations (it) for Nédélec elements of degree 1 and 2 with the meshes shown in Figure 4.

TET, $p=1$, TET, $p=2$		
dofs	27K	144K
κ	11.8	23.7
it	26	37

HEX, $p=1$, TET, $p=2$		
dofs	12K	92K
κ	5.7	8.4
it	21	26

We next consider the case of heterogeneous coefficients; we fix $\alpha = 1$, and vary the distribution of β as pictured in Figure 5. For this test, we adaptively enrich the minimal coarse space by means of the adaptive selection of constraints algorithm described in [41, 40]; results have been obtained using either tetrahedral or hexahedral meshes, 40 subdomains, and with Nédélec elements of order $p = 1$ and $p = 2$. The number of dofs in the tetrahedral case is approximately 200 thousand (K) for $p = 1$, and 1.2 million (M) for $p = 2$; in the hexahedral case, the number of dofs are 330K and 3.5M, respectively. Results are reported in Table 2, together with the adaptive threshold used (λ), and the ratio between the number of generated coarse dofs and the number of interface dofs (C/Γ).

Fig. 5: Heterogeneous β distribution used for testing adaptive coarse spaces.

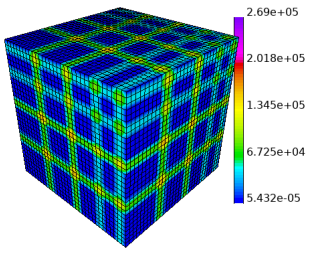


Table 2: Adaptive coarse spaces. Condition number (κ), number of iterations (it) and coarse-to-fine ratio (C/Γ) for different eigenvalue thresholds λ.

TET, $p=1$

λ	-	10	5	2.5
κ	150.2	7.5	4.6	2.2
it	54	15	12	8
C/Γ	0.01	0.05	0.06	0.09

TET, $p=2$

λ	-	10	5	2.5
κ	413.3	5.9	4.3	2.3
it	113	15	12	9
C/Γ	0.01	0.02	0.02	0.04

HEX, $p=1$

λ	-	10	5	2.5
κ	203.4	5.8	3.2	2.0
it	62	13	10	7
C/Γ	0.02	0.05	0.06	0.09

HEX, $p=2$

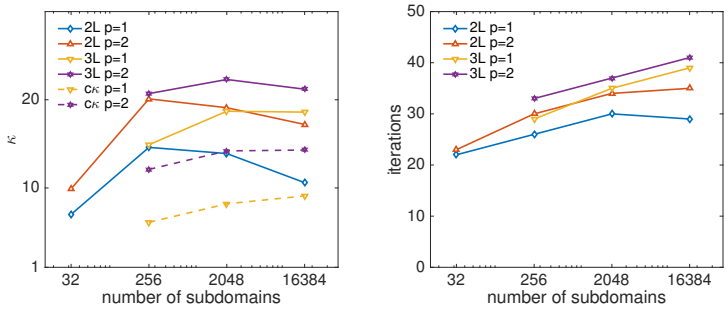
λ	-	10	5	2.5
κ	330.8	5.1	3.4	2.0
it	97	14	11	8
C/Γ	0.01	0.01	0.02	0.04

Without adaptive coarse spaces, the algorithm performs poorly (as expected) since the jumps in β are not aligned with the (irregular) subdomain boundaries;

on the other hand, the number of iterations and the condition numbers are consistently (and constantly) reduced when considering adaptive coarse spaces associated with smaller and smaller tolerances λ. The ratio of coarse-to-fine dofs remain bounded for all the tolerance values considered; interestingly, the coarsening procedure is more effective for $p = 2$ than for $p = 1$, as also observed experimentally with Raviart-Thomas vector fields [27, 43].

We close this section by reporting the results of a weak scalability test. Since we consider unstructured domain decompositions, we obtain subdomain problems of approximately the same size by using uniform refinements of an hexahedral mesh; at each level of refinement, we multiply by eight the number of subdomains used. As a consequence, we cannot guarantee that the shape of the subdomains remains the same. The total number of dofs in the test ranges from 186K to 94M with Nédélec elements of degree $p = 1$, and from 1.5M to 742M for $p = 2$. In Figure 6, we compare the results using a standard two-level BDDC algorithm (2L) and a three-level approach (3L), where the coarse subdomains have been obtained by aggregating 32 fine subdomains using ParMETIS; the condition number of the coarse BDDC preconditioned operator is also provided (κ_c, left panel, dashed lines). The number of iterations are scalable up to 16384 subdomains in both cases; condition numbers and number of iterations are slightly larger for the 3L case, but the algorithm preserves the convergence properties of the 2L case.

Fig. 6: Weak scalability test. κ and number of iterations as a function of the number of subdomains for two-level (2L) and three-level BDDC (3L). Coarse condition number (κ_c) is also shown.



4 Conclusions

We have constructed BDDC methods for arbitrary order, finite element discretizations of the $H(\mathrm{curl})$ model problem. Numerical results have shown that the proposed algorithm leads to a poly-logarithmic condition number bound, with a mild dependence on the polynomial order of the approximation space, of the type $(1+\log(p^2H/h))^2$. The robustness of our approach has been confirmed for various cases, including high-order geometries, upscaled curl-conforming finite elements,

and heterogeneous distributions of the coefficients. A scalable, three-level extension of the method has also been proposed; large scale parallel experiments using up to 16384 subdomains and almost a billion of dofs have been provided to validate the algorithm.

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