





Parallelization of continuous and discontinuous Galerkin dual-primal Isogeometric tearing and interconnecting methods

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¹ Parallelization of continuous and discontinuous Galerkin

² dual-primal Isogeometric tearing and interconnecting methods

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5 Abstract

In this paper we investigate the parallelization of dual-primal isogeometric tearing and interconnecting (IETI-DP) type methods for solving large-scale continuous and discontinuous Galerkin systems of equations arising from Isogeometric analysis of elliptic boundary value problems. These methods are extensions of the finite element tearing and interconnecting methods to isogeometric analysis. The algorithms are implemented by means of energy minimizing primal subspaces. We discuss how these methods can efficiently be parallelized in a distributed memory setting. Weak and strong scaling studies presented for two and three dimensional problems show an excellent parallel efficiency.

- 6 Keywords: Diffusion problems, Isogeometric analysis, discontinuous Galerkin,
- 7 IETI-DP, parallelization, MPI

⁸ 1. Introduction

Isogeometric Analysis (IgA) is a novel methodology for the numerical solution of partial 9 differential equations (PDE). IgA was first introduced by Hughes, Cottrell and Bazilevs 10 in [24], see also the monograph [7] for a comprehensive presentation of the IgA framework 11 and the recent survey article [3]. The main principle is to use the same basis functions for 12 describing the geometry and to represent the discrete solution of the PDE problem under 13 consideration. The most common choices are B-Splines, Non Uniform Rational B-Splines 14 (NURBS), T-Splines, Truncated Hierarchical B-Splines (THB-Splines), etc., see, e.g., [15], 15 [16] and [2]. One of the strengths of IgA is the capability of creating high-order splines 16 spaces, while keeping the number of degrees of freedom quite small. Moreover, having 17 basis functions with high smoothness is useful when considering higher-order PDEs, e.g., 18 the biharmonic equation. 19

In many cases the domain can not be represented with a single mapping, referred to 20 as *geometrical mapping*. Complicated geometries are decomposed into simple domains, 21 called *patches*, which are topologically equivalent to a cube. The set of patches forming the 22 computational domain is called multipatch domain. The obtained patch parametrizations 23 and the original geometry may not be identical. The result are small gaps and overlaps 24 occurring at the interfaces of the patches, called *segmentation crimes*, see [25], [41] and [23] 25 for a comprehensive analysis. Nevertheless, one still wants to solve PDEs on such domains. 26 To do so, numerical schemes based on the discontinuous Galerkin (dG) method for elliptic 27 PDEs were developed in [20], [22] and [21]. There, the corresponding error analysis is also 28

²⁹ provided. In addition to domains with segmentation crimes, the dG formulation is very ³⁰ useful when considering different B-Splines spaces on each patch, e.g., non-matching grids ³¹ at the interface and different spline degrees. An analysis for the dG-IgA formulation with ³² extensions to low regularity solutions can be found in [37]. For a detailed discussion of ³³ dG for finite element methods, we refer, e.g., to [44] and [8].

In the present paper, we are considering fast solution methods for linear systems arising 34 from the discretization of elliptic PDEs by means of IgA. We investigate non-overlapping 35 domain decomposition (DD) methods of the dual-primal tearing and interconnecting type. 36 This type of methods are equivalent to the so called Balancing Domain Decomposition by 37 Constraints (BDDC) methods, see [39], [45], [42] and references therein. The version based 38 on a conforming Galerkin (cG) discretization, called dual-primal isogeometric tearing and 39 interconnecting (IETI-DP) method was first introduced in [34] and the equivalent IgA 40 BDDC method was analysed in [5]. Further extensions to the analysis are presented 41 in [18]. The version based on the dG formulation, abbreviated by dG-IETI-DP, was 42 introduced in [19], see [12], [13] and [14] for the corresponding finite element counterparts. 43 We also want to mention development in overlapping Schwarz methods, see, e.g., [4] and 44 [6]. The aim of this paper is to present the parallel scalability of the cG and dG IETI-DP 45 methods. We investigate weak and strong scaling in two and three dimensional domains for 46 different B-Spline degrees. The implemented algorithms are based on energy minimizing 47 primal subspaces, which simplifies the parallelization of the solver part, but having more 48 effort in the setup phase (assembling phase). We rephrase key parts of this algorithm 49 and discuss how to realize the communication by means of Message Passing Interface 50 (MPI). In general, FETI-DP and equivalent BDDC methods are by nature well suited 51 for large-scale parallelization and has been widely studied for solving large-scale finite 52 element equations, e.g., in [32], [43], [30] and [27], see also [29] for a hybrid OpenMP/MPI 53 version. Considering a domain decomposition with several ten thousands of subdomains, 54 the influence of the coarse grid problem becomes more and more significant. Especially, 55 its LU-factorization is the bottleneck of the algorithm. The remedy is to reformulate the 56 FETI-DP system in such a way that the solution of the coarse grid problem is not required 57 in the application of the system matrix, but in the preconditioner. This enables the use 58 of inexact methods like geometric or algebraic multigrid, see, e.g., [28], [27], [31], [32] and 59 [33]. Moreover, inexact solvers can also be used in the scaled Dirichlet preconditioner and, 60 if using the saddle point formulation, also for the local solvers, cf., [31], see also [32], [43] 61 and references therein for alternative approaches by means of hybrid FETI. We also want 62 to mention inexact version for the BDDC method, see, e.g., [46], [47], [10], [38] and [48]. 63 FETI-DP methods has also been successfully applied to non-linear problems my means 64 of a non-linear version of FETI-DP. We want to highlight recent advances presented, e.g., 65 in [26], [28] and [27], showing excellent scalability on large-scale supercomputers. 66

In the present paper, we consider the following second-order elliptic boundary value problem in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, with $d \in \{2,3\}$: Find $u : \overline{\Omega} \to \mathbb{R}$ such that

$$-\operatorname{div}(\alpha \nabla u) = f \text{ in } \Omega, \ u = 0 \text{ on } \Gamma_D, \text{ and } \alpha \frac{\partial u}{\partial n} = g_N \text{ on } \Gamma_N, \tag{1}$$

with given, sufficient smooth data f, g_N and α , where the coefficient α is uniformly bounded from below and above by some positive constants α_{min} and α_{max} , respectively. The boundary $\partial\Omega$ of the computational domain Ω consists of a Dirichlet part Γ_D of positive boundary measure and a Neumann part Γ_N . Furthermore, we assume that the Dirichlet boundary Γ_D is always a union of complete patch sides (edges / face in 2D / 3D) which are uniquely defined in IgA. Without loss of generality, we assume homogeneous Dirichlet conditions. This can always be obtained by homogenization. By means of integration by parts, we arrive at the weak formulation of (1) which reads as follows: Find $u \in V_D = \{u \in H^1 : \gamma_0 u = 0 \text{ on } \Gamma_D\}$ such that

$$a(u,v) = \langle F, v \rangle \quad \forall v \in V_D, \tag{2}$$

where γ_0 denotes the trace operator. The bilinear form $a(\cdot, \cdot) : V_D \times V_D \to \mathbb{R}$ and the linear form $\langle F, \cdot \rangle : V_D \to \mathbb{R}$ are given by the expressions

$$a(u,v) := \int_{\Omega} \alpha \nabla u \cdot \nabla v \, dx$$
 and $\langle F, v \rangle := \int_{\Omega} f v \, dx + \int_{\Gamma_N} g_N v \, ds.$

The remainder of the paper is organized as follows: In Section 2, we give a short introduction to isogeometric analysis, providing the basic definitions and notations. Section 3 describes the different discretizations of the model problem obtained the continuous and discontinuous Galerkin methods. In Section 4, we formulate the IETI-DP method for both discretizations and provide implementation details. The way how the algorithm is parallelized is explained in Section 5. Numerical examples are presented in Section 6. Finally we draw some conclusions in Section 7.

77 2. Isogeometric Analysis

In this section, we give a very short overview about IgA. For a more comprehensive study,
we refer to, e.g., [7] and [37].

Let $\hat{\Omega} := (0,1)^d, d \in \{2,3\}$, be the d-dimensional unit cube, which we refer to as the 80 parameter domain. Let p_{ι} and $M_{\iota}, \iota \in \{1, \ldots, d\}$, be the B-Spline degree and the number 81 of basis functions in x_{ι} -direction. Moreover, let $\Xi_{\iota} = \{\xi_1 = 0, \xi_2, \dots, \xi_{n_{\iota}} = 1\}, n_{\iota} =$ 82 $M_{\iota} - p_{\iota} - 1$, be a partition of [0, 1], called *knot vector*. With this ingredients we are able 83 to define the B-Spline basis $\hat{N}_{i,p}$, $i \in \{1, \dots, M_{\iota}\}$ on [0, 1] via Cox-De Boor's algorithm, 84 cf. [7]. The generalization to $\hat{\Omega}$ is realized by considering a tensor product, again denoted 85 by $\hat{N}_{i,p}$, where $i = (i_1, \ldots, i_d)$ and $p = (p_1, \ldots, p_d)$ are a multi-indices. For notational 86 simplicity, we define $\mathcal{I} := \{(i_1, \ldots, i_d) \mid i_i \in \{1, \ldots, M_i\}\}$ as the set of multi-indices. Since 87 the tensor product knot vector Ξ provides a partition of $\hat{\Omega}$, it introduces a mesh $\hat{\mathcal{Q}}$, and 88 we denote a mesh element by \hat{Q} , called *cell*. 89

The B-Spline basis functions parametrize the computational domain Ω , also called *physical* domain. It is given as image of parameter domain under the geometrical mapping G: $\hat{\Omega} \to \mathbb{R}^d$, defined as

$$G(\xi) := \sum_{i \in \mathcal{I}} P_i \hat{N}_{i,p}(\xi),$$

with the control points $P_i \in \mathbb{R}^d$, $i \in \mathcal{I}$. The image of the mesh $\hat{\mathcal{Q}}_h$ under G defines the mesh on Ω , denoted by \mathcal{Q}_h with cells Q. Both meshes possess a characteristic mesh size \hat{h} and h, respectively. More complicated geometries Ω have to be represented with multiple non-overlapping domains $\Omega^{(k)} := G^{(k)}(\hat{\Omega}), k = 1, \ldots, N$, called *patches*, where each patch is associated with a different geometrical mapping $G^{(k)}$. We sometimes call $\overline{\Omega} := \bigcup_{k=1}^{N} \overline{\Omega}^{(k)}$ a *multipatch domain*. Furthermore, we denote the set of all indices l such that $\Omega^{(k)}$ and $\Omega^{(l)}$ have a common interface $F^{(kl)}$ by $\mathcal{I}_{\mathcal{F}}^{(k)}$. We define the interface $\Gamma^{(k)}$ of $\Omega^{(k)}$ as $\Gamma^{(k)} := \bigcup_{l \in \mathcal{I}_{\mathcal{F}}^{(k)}}^{N} F^{(kl)}$.

We use B-Splines not only for defining the geometry, but also for representing the approximate solution of our PDE. This motivates to define the basis functions in the physical space $N_{i,p} := \hat{N}_{i,p} \circ G^{-1}$ and the corresponding discrete space as

$$V_h := \operatorname{span}\{N_{i,p}\}_{i \in \mathcal{I}}.$$
(3)

Moreover, each function $u_h(x) = \sum_{i \in \mathcal{I}} u_i N_{i,p}(x)$ is associated with the coefficient vector $u = (u_i)_{i \in \mathcal{I}}$. This map is known as *Ritz isomorphism* or *IgA isomorphism* in connection with IgA. One usually writes this relation as $u_h \leftrightarrow u$. In the following, we will use the notation u_h for the function and its vector representations. If we consider a single patch $\Omega^{(k)}$ of a multipatch domain Ω , we will use the notation $V_h^{(k)}, N_{i,p}^{(k)}, \hat{N}_{i,p}^{(k)}, \dots$ with the analogous definitions. To keep notation simple, we will use h_k and \hat{h}_k instead of $h^{(k)}$ and $\hat{h}^{(k)}$, respectively.

¹⁰⁵ 3. Galerkin Methods for Isogeometric Analysis

In this section we rephrase the variational formulation for the continuous and discontin-uous Galerkin method for multipatch IgA systems.

108 3.1. Continuous Galerkin method

We are considering the finite dimensional subspace V_h^{cG} of V_D , where V_h^{cG} is given by

$$V_h^{cG} := \{ v \, | \, v|_{\Omega^{(k)}} \in V_h^{(k)} \} \cap H^1(\Omega).$$

Since, we restrict ourselves to homogeneous Dirichlet conditions, we look for the Galerkin approximate u_h from $V_{D,h}^{cG} \subset V_h^{cG}$, where $V_{D,h}^{cG}$ contains all functions, which vanish on the Dirichlet boundary. The Galerkin IgA scheme reads as follows: Find $u_h \in V_{D,h}^{cG}$ such that

$$a(u_h, v_h) = \langle F, v_h \rangle \quad \forall v_h \in V_{D,h}.$$
(4)

There exists a unique IgA solution $u_h \in V_{D,h}^{cG}$ of (4) that converges to the solution $u \in V_D$ of (2) if h tends to 0. Due to Cea's lemma, the usual discretization error estimates in the H^1 - norm follow from the corresponding approximation error estimates, see [1] or [3].

112 3.2. Discontinuous Galerkin method

In the dG-IgA scheme, we again use the spaces $V_h^{(k)}$ of B-Splines defined in (3), whereas now discontinuities are allowed across the patch interfaces $F^{(kl)}$. The continuity of the function value and its normal fluxes are then enforced in a weak sense by adding additional terms to the bilinear form. We define the dG-IgA space

$$V_h^{dG} := \{ v \, | \, v|_{\Omega^{(k)}} \in V_h^{(k)} \}, \tag{5}$$

where $V_h^{(k)}$ is defined as in (3). A comprehensive study of dG schemes for FE can be found in [44] and [8]. For an analysis of the dG-IgA scheme, we refer to [37]. We define $V_{D,h}^{dG}$ as the space of all functions from V_h that vanish on the Dirichlet boundary Γ_D . Having these definitions at hand, we can define the discrete problem based on the Symmetric Interior Penalty (SIP) dG formulation as follows: Find $u_h \in V_{D,h}^{dG}$ such that

$$a_h(u_h, v_h) = \langle F, v_h \rangle \quad \forall v_h \in V_{D,h}^{dG}, \tag{6}$$

where

$$a_h(u,v) := \sum_{k=1}^N a_e^{(k)}(u,v) \quad \text{and} \quad \langle F,v \rangle := \sum_{k=1}^N \left(\int_{\Omega^{(k)}} fv^{(k)} dx + \int_{\Gamma_N^{(k)}} g_N v^{(k)} ds \right),$$
$$a_e^{(k)}(u,v) := a^{(k)}(u,v) + s^{(k)}(u,v) + p^{(k)}(u,v),$$

and

$$\begin{aligned} a^{(k)}(u,v) &:= \int_{\Omega^{(k)}} \alpha^{(k)} \nabla u^{(k)} \nabla v^{(k)} dx, \\ s^{(k)}(u,v) &:= \sum_{l \in \mathcal{I}_{\mathcal{F}}^{(k)}} \int_{F^{(kl)}} \frac{\alpha^{(k)}}{2} \left(\frac{\partial u^{(k)}}{\partial n} (v^{(l)} - v^{(k)}) + \frac{\partial v^{(k)}}{\partial n} (u^{(l)} - u^{(k)}) \right) ds, \\ p^{(k)}(u,v) &:= \sum_{l \in \mathcal{I}_{\mathcal{F}}^{(k)}} \int_{F^{(kl)}} \frac{\delta \alpha^{(k)}}{h_{kl}} (u^{(l)} - u^{(k)}) (v^{(l)} - v^{(k)}) \, ds. \end{aligned}$$

Here the notation $\frac{\partial}{\partial n}$ denotes the derivative in the direction of the outer normal vector, a positive sufficiently large penalty parameter, and h_{kl} the harmonic average of the adjacent mesh sizes, i.e., $h_{kl} = 2h_k h_l / (h_k + h_l)$.

We equip $V_{D,h}^{dG}$ with the dG-norm

$$\|u\|_{dG}^{2} = \sum_{k=1}^{N} \left[\alpha^{(k)} \left\| \nabla u^{(k)} \right\|_{L^{2}(\Omega^{(k)})}^{2} + \sum_{l \in \mathcal{I}_{\mathcal{F}}^{(k)}} \frac{\delta \alpha^{(k)}}{h_{kl}} \int_{F^{(kl)}} (u^{(k)} - u^{(l)})^{2} ds \right].$$
(7)

Furthermore, we define the bilinear forms

$$d_h(u,v) = \sum_{k=1}^N d^{(k)}(u,v)$$
 where $d^{(k)}(u,v) = a^{(k)}(u,v) + p^{(k)}(u,v),$

116 for later use. We note that $||u_h||_{dG}^2 = d_h(u_h, u_h)$.

Lemma 3.1. Let δ be sufficiently large. Then there exist two positive constants γ_0 and γ_1 , which are independent of $h_k, H_k, \delta, \alpha^{(k)}$ and u_h such that the inequalities

$$\gamma_0 d^{(k)}(u_h, u_h) \le a_e^{(k)}(u_h, u_h) \le \gamma_1 d^{(k)}(u_h, u_h), \quad \forall u_h \in V_{D,h}^{dG}$$
(8)

are valid for all k = 1, 2, ..., N. Furthermore, we have the inequalities

$$\gamma_0 \|u_h\|_{dG}^2 \le a_h(u_h, u_h) \le \gamma_1 \|u_h\|_{dG}^2, \quad \forall u_h \in V_{D,h}^{dG}.$$
(9)

This Lemma is an equivalent statement of Lemma 2.1 in [13] for IgA, and the proof can be found in [19]. A direct implication of (9) is the well posedness of the discrete problem (6) by the Theorem of Lax-Milgram. The consistency of the method together with the interpolation estimates of B-Splines lead to the a-priori error estimate, established in [37].

¹²¹ We note that, in [37], the results were obtained for the Incomplete Interior Penalty (IIP)

scheme. An extension to SIP-dG and the use of harmonic averages for h and/or α are

discussed in Remark 3.1 in [37], see also [36].

For both the cG and dG formulation, we choose the B-Spline function $\{N_{i,p}\}_{i \in \mathcal{I}_0}$ as basis for the space $V_h^X, X \in \{cG, dG\}$, where \mathcal{I}_0 contains all indices of \mathcal{I} , where the corresponding basis functions do not have a support on the Dirichlet boundary. In the cG case, the basis functions on the interface are identified accordingly to obtain a conforming subspace of V_D . For the remainder of this paper, we drop the superscript $X \in \{cG, dG\}$ and use the symbol V_h for both formulations. Depending on the considered formulation, one needs to use the right space $V_h^X, X \in \{cG, dG\}$. The IgA schemes (4) and (6) are equivalent to the system of linear IgA equations

$$\boldsymbol{K}\boldsymbol{u} = \boldsymbol{f},\tag{10}$$

where $\mathbf{K} = (\mathbf{K}_{i,j})_{i,j\in\mathcal{I}_0}$, $\mathbf{f} = (\mathbf{f}_i)_{i\in\mathcal{I}_0}$ denote the stiffness matrix and the load vector, respectively, with $\mathbf{K}_{i,j} = a(N_{j,p}, N_{i,p})$ or $\mathbf{K}_{i,j} = a_h(N_{j,p}, N_{i,p})$ and $\mathbf{f}_i = \langle F, N_{i,p} \rangle$, and $\mathbf{u}_{i,j}$ is the vector representation of u_h .

127 4. IETI-DP methods and their implementation

¹²⁸ In this section, we recall the main ingredients for the cG-IETI-DP and dG-IETI-DP ¹²⁹ method. We focus mainly on the implementation, since this is the relevant part for ¹³⁰ parallelization.

131 4.1. Derivation of the method

A rigorous and formal definition of the cG-IETI-DP and dG-IETI-DP method is quite technical and not necessary for the parallelization, which is the purpose of this paper. Therefore, we are not going to present the whole derivation of each method. We will give a general description, which is valid for both methods. For a detailed derivation, we refer to [18] and [19].

The first step is to introduce additional dofs on the interface to decouple the local problems and incorporate their connection via Lagrange multipliers λ . This is quite straightforward in the case of the cG formulation, but more involved in the dG case. In any of the two cases, we can equivalently rewrite (10) as: Find $(u, \lambda) \in V_{h,e} \times U$ such that

$$\begin{bmatrix} K_e & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} u \\ \lambda \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix},$$
(11)

where $V_{h,e} \supset V_h$, is the decoupled space with additional dofs and U is the set of Lagrange multipliers. The jump operator B enforces the "continuity" of the solution u in the sense that ker $(B) \equiv V_h$. The matrix K_e is the block diagonal matrix of the patch local stiffness matrices $K^{(k)}$, i.e., $K_e = \text{diag}(K^{(k)})$. Since B only acts on the patch interface dofs, we first can reorder the stiffness matrix in the following way

$$K^{(k)} = \begin{bmatrix} K_{BB}^{(k)} & K_{BI}^{(k)} \\ K_{IB}^{(k)} & K_{II}^{(k)} \end{bmatrix}, \qquad f^{(k)} = \begin{bmatrix} f_B^{(k)} \\ f_I^{(k)} \end{bmatrix}$$

and then consider only the Schur complement representation: Find $(u_B, \lambda) \in W \times U$ such that

$$\begin{bmatrix} S_e & B_B^T \\ B_B & 0 \end{bmatrix} \begin{bmatrix} u_B \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} g \\ 0 \end{bmatrix},$$
(12)

where $S_e = \text{diag}(S_e^{(k)})$, $S_e^{(k)} = K_{BB}^{(k)} - K_{BI}^{(k)}(K_{II}^{(k)})^{-1}K_{IB}^{(k)}$ and $g^{(k)} = f_B - K_{BI}^{(k)}(K_{II}^{(k)})^{-1}f_I^{(k)}$. The space W is the restriction of $V_{h,e}$ to the interface. For completeness, we denote its "continuous" representation as \widehat{W} , i.e., $\ker(B_B) = \widehat{W}$. Equation (12) is valid for the cG-IETI-DP and dG-IETI-DP method, but the matrix K_e has difference entries and the number of boundary dofs (subscript B) is different. Fortunately, this does not change the way how the algorithm is implemented and parallelized. In the following, we will drop the subscript B in u_B and B_B for notational simplicity.

The matrix S_e is not invertible and, hence, we cannot build the Schur complement system of (12). To overcome this, we introduce an intermediate space \widetilde{W} , such that $\widehat{W} \subset \widetilde{W} \subset W$, and S_e restricted to \widetilde{W} , denoted by \widetilde{S} , is invertible. We introduce primal variables as a set $\Psi \subset \widehat{W}^*$ and define the spaces

$$\overline{W} := \{ w \in W : \psi(w^{(k)}) = \psi(w^{(l)}), \forall \psi \in \Psi, \forall k > l \}$$

and

$$W_{\Delta} := \prod_{k=1}^{N} W_{\Delta}^{(k)}, \text{ with } W_{\Delta}^{(k)} := \{ w^{(k)} \in W^{(k)} : \psi(w^{(k)}) = 0 \ \forall \psi \in \Psi \}$$

Moreover, we introduce the space $W_{\Pi} \subset \widehat{W}$ such that $\widetilde{W} = W_{\Pi} \oplus W_{\Delta}$. We call W_{Π} primal

space and W_{Δ} dual space. Typically, the set Ψ corresponds to "continuous" vertex values, edge averages and/or face averages.

Since $\widetilde{W} \subset W$, there is a natural embedding $\widetilde{I} : \widetilde{W} \to W$. Let the jump operator restricted to \widetilde{W} be $\widetilde{B} := B\widetilde{I} : \widetilde{W} \to U^*$. Now we are in the position to reformulate problem (12) in the space \widetilde{W} as follows: Find $(u, \lambda) \in \widetilde{W} \times U$:

$$\begin{bmatrix} \widetilde{S} & \widetilde{B}^T \\ \widetilde{B} & 0 \end{bmatrix} \begin{bmatrix} u \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \widetilde{g} \\ 0 \end{bmatrix},$$
(13)

where $\widetilde{g} := \widetilde{I}^T g$, and $\widetilde{B}^T = \widetilde{I}^T B^T$. Here, $\widetilde{I}^T : W^* \to \widetilde{W}^*$ denotes the adjoint of \widetilde{I} .

By construction, \widetilde{S} is SPD on \widetilde{W} . Hence, we can define the Schur complement F and the corresponding right-hand side as follows:

$$F := \widetilde{B}\widetilde{S}^{-1}\widetilde{B}^T, \quad d := \widetilde{B}\widetilde{S}^{-1}\widetilde{g}.$$

Hence, the saddle point system (13) is equivalent to the Schur complement problem:

Find
$$\lambda \in U$$
: $F\lambda = d$. (14)

Equation (14) is solved by means of the PCG algorithm, but it requires an appropriate preconditioner in order to obtain an efficient solver.

Recalling the definition of $S_e = \text{diag}(S_e^{(k)})_{k=1}^N$, we define the scaled Dirichlet preconditioner $M_{sD}^{-1} := B_D S_e B_D^T$, where B_D is a scaled version of the jump operator B. The scaled jump operator B_D is defined such that the operator enforces the constraints

$$\delta_{j}^{\dagger(l)}(\boldsymbol{u}^{(k)})_{i}^{(k)} - \delta_{i}^{\dagger(k)}(\boldsymbol{u}^{(l)})_{j}^{(k)} = 0 \quad \forall (i,j) \in B_{e}(k,l), \; \forall l \in \mathcal{I}_{\mathcal{F}}^{(k)}$$

and

$$\delta_{j}^{\dagger(l)}(\boldsymbol{u}^{(k)})_{i}^{(l)} - \delta_{i}^{\dagger(k)}(\boldsymbol{u}^{(l)})_{j}^{(l)} = 0 \quad \forall (i,j) \in B_{e}(l,k), \; \forall l \in \mathcal{I}_{\mathcal{F}}^{(k)},$$

where, for $(i, j) \in B_e(k, l)$, $\delta_i^{\dagger(k)} := \rho_i^{(k)} / \sum_{l \in \mathcal{I}_{\mathcal{F}}^{(k)}} \rho_j^{(l)}$ is an appropriate scaling. One can show, that the preconditioned system for the cG version has a quasi-optimal condition number bound with respect to $H/h := \max_k (H_k/h_k)$, i.e.,

$$\kappa(M_{sD}^{-1}F_{|\ker(\widetilde{B}^T)}) \le C(1 + \log(H/h))^2, \tag{15}$$

see [18] and [5]. Moreover, numerical examples show also robustness with respect to jumps in the diffusion coefficient and only a weak dependence on the B-Spline degree p, see, e.g., [19], [18] and [5].

153 4.2. Implementation of the algorithm

Since F is symmetric and positive definite on \widetilde{U} , we can solve the linear system $F\lambda = d$ by means of the PCG algorithm, where we use M_{sD}^{-1} as preconditioner. The PCG does not require an explicit representation of the matrices F and M_{sD}^{-1} , since we just need their application to a vector. There are different ways to provide an efficient implementation. We will follow the concept of the energy minimizing primal subspaces. The idea is to split the space \widetilde{W} into $\widetilde{W}_{\Pi} \oplus \prod \widetilde{W}_{\Delta}^{(k)}$, such that $\widetilde{W}_{\Delta}^{(k)} \perp_{S} \widetilde{W}_{\Pi}$ for all k, i.e., we choose $\widetilde{W}_{\Pi} := \widetilde{W}_{\Delta}^{\perp_{S}}$, see, e.g., [42] and [9]. By means of this choice, the operators \widetilde{S} and \widetilde{S}^{-1} have the following forms

$$\widetilde{S} = \begin{bmatrix} S_{\Pi\Pi} & 0\\ 0 & S_{\Delta\Delta} \end{bmatrix} \text{ and } \widetilde{S}^{-1} = \begin{bmatrix} S_{\Pi\Pi}^{-1} & 0\\ 0 & S_{\Delta\Delta}^{-1} \end{bmatrix}$$

where $S_{\Pi\Pi}$ and $S_{\Delta\Delta}$ are the restrictions of \widetilde{S} to the corresponding subspaces. We note that $S_{\Delta\Delta}$ can be seen as a block diagonal operator, i.e., $S_{\Delta\Delta} = \text{diag}(S_{\Delta\Delta}^{(k)})$.

¹⁵⁶ The application of F and M_{sD}^{-1} is summarized in Algorithm 1.

157 4.2.1. Constructing a basis for the primal subspace

First we need to provide an appropriate local basis $\{\widetilde{\phi}_j\}_j^{n_{\Pi}}$ for \widetilde{W}_{Π} , where n_{Π} is the number of primal variables. We request from the basis that it has to be nodal with respect to the primal variables, i.e., $\psi_i(\widetilde{\phi}_j) = \delta_{i,j}$, for $i, j \in \{1, \ldots, n_{\Pi}\}$. In order to construct such a basis, we introduce the constraint matrix $C^{(k)} : W^{(k)} \to \mathbb{R}^{n_{\Pi}^{(k)}}$ for each patch $\Omega^{(k)}$ which realizes the primal variables, i. e., $(C^{(k)}v)_j = \psi_{i(k,j)}(v)$ for $v \in W$ and $j \in \{1, \ldots, n_{\Pi}^{(k)}\}$, where $n_{\Pi}^{(k)}$ is the number of primal variables associated with $\Omega^{(k)}$ and i(k, j) the global index of the *j*-th primal variable on $\Omega^{(k)}$. For each patch k, the basis functions $\{\widetilde{\phi}_j^{(k)}\}_{j=1}^{n_{\Pi}^{(k)}}$ of $\widetilde{W}_{\Pi}^{(k)}$ are the solution of the system

$$\begin{bmatrix} K_{BB}^{(k)} & K_{BI}^{(k)} & C^{(k)T} \\ K_{IB}^{(k)} & K_{II}^{(k)} & 0 \\ C^{(k)} & 0 & 0 \end{bmatrix} \begin{bmatrix} \widetilde{\phi}_j^{(k)} \\ \cdot \\ \widetilde{\mu}_j^{(k)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \mathbf{e}_j^{(k)} \end{bmatrix},$$
(16)

where $\mathbf{e}_{j}^{(k)} \in \mathbb{R}^{n_{\Pi}^{(k)}}$ is the *j*-th unit vector. Here we use an equivalent formulation with the system matrix $K^{(k)}$ For each patch *k*, the LU factorization of this matrix is computed and stored. Application of $S_{\Delta\Delta}^{(k)}^{-1}$: The application of $S_{\Delta\Delta}^{(k)}^{-1}$ corresponds to solving a local Neumann problem in the space \widetilde{W}_{Δ} , i.e., $S^{(k)}w^{(k)} = f_{\Delta}^{(k)}$ with the constraint $C^{(k)}w^{(k)} = 0$. This problem can be rewritten as a saddle point problem in the form

$$\begin{bmatrix} K_{BB}^{(k)} & K_{BI}^{(k)} & C^{(k)T} \\ K_{IB}^{(k)} & K_{II}^{(k)} & 0 \\ C^{(k)} & 0 & 0 \end{bmatrix} \begin{bmatrix} w^{(k)} \\ \cdot \\ \cdot \end{bmatrix} = \begin{bmatrix} f_{\Delta}^{(k)} \\ 0 \\ 0 \end{bmatrix}$$

¹⁶¹ From (16), the LU factorization of the matrix is already available.

Application of $\mathbf{S}_{\Pi\Pi}^{(k)}^{(k)^{-1}}$:. The matrix $\mathbf{S}_{\Pi\Pi}$ can be assembled from the patch local matrices $\mathbf{S}_{\Pi\Pi}^{(k)}$. Let $\{\widetilde{\phi}_{j}^{(k)}\}_{j=1}^{n_{\Pi}^{(k)}}$ be the basis of $\widetilde{W}_{\Pi}^{(k)}$. The construction of $\{\widetilde{\phi}_{j}^{(k)}\}_{j=1}^{n_{\Pi}^{(k)}}$ in (16) provides

$$\begin{split} \left(\mathbf{S}_{\Pi\Pi}^{(k)}\right)_{i,j} &= \left\langle S^{(k)}\widetilde{\phi}_{i}^{(k)}, \widetilde{\phi}_{j}^{(k)} \right\rangle = -\left\langle C^{(k)T}\widetilde{\mu}_{i}^{(k)}, \widetilde{\phi}_{j}^{(k)} \right\rangle = -\left\langle \widetilde{\mu}_{i}^{(k)}, C^{(k)}\widetilde{\phi}_{j}^{(k)} \right\rangle \\ &= -\left\langle \widetilde{\mu}_{i}^{(k)}, \mathbf{e}_{j} \right\rangle^{(k)} = -\left(\widetilde{\mu}_{i}^{(k)} \right)_{j}, \end{split}$$

where $i, j \in \{1, ..., n_{\Pi}^{(k)}\}$. Therefore, we can reuse the Lagrange multipliers $\tilde{\mu}_i^{(k)}$ obtained in (16), and can assemble $\mathbf{S}_{\Pi\Pi}^{(k)}$ from them. Once $\mathbf{S}_{\Pi\Pi}$ is assembled, the LU factorization can be calculated and stored.

165 4.2.2. Application of \tilde{I} and \tilde{I}^T

The last building block is the embedding $\widetilde{I}: \widetilde{W} \to W$ and its adjoint $\widetilde{I}^T: W^* \to \widetilde{W}^*$. Recall the direct splitting $W^{(k)} = W_{\Delta}^{(k)} \oplus W_{\Pi}^{(k)}$. Let us denote by $\Phi^{(k)} = [\widetilde{\phi}_1^{(k)}, \ldots, \widetilde{\phi}_{n_{\Pi}^{(k)}}^{(k)}]$ the coefficient representation of the basis for $W_{\Pi}^{(k)}$. Given the primal part \boldsymbol{w}_{Π} of a function in \widetilde{W} , we obtain its restriction to $\widetilde{W}_{\Pi}^{(k)}$ via an appropriately defined restriction matrix $\boldsymbol{R}^{(k)}$, i.e. $\boldsymbol{w}_{\Pi}^{(k)} = \boldsymbol{R}^{(k)} \boldsymbol{w}_{\Pi}$. The corresponding function is then given by $w_{\Pi}^{(k)} = \Phi^{(k)} \boldsymbol{R}^{(k)} \boldsymbol{w}_{\Pi}^{(k)}$.

Following the lines in [42], we can formulate the operator $\widetilde{I}: \widetilde{W} \to W$ as

$$\begin{bmatrix} \boldsymbol{w}_{\Pi} \\ w_{\Delta} \end{bmatrix} \mapsto w := \Phi \boldsymbol{R} \boldsymbol{w}_{\Pi} + w_{\Delta},$$

where Φ and \mathbf{R} are block versions of $\Phi^{(k)}$ and $\mathbf{R}^{(k)}$, respectively. The second function is its adjoint operation $\widetilde{I}^T: W^* \to \widetilde{W}^*$. It can be realized in the following way

$$f \mapsto \begin{bmatrix} \boldsymbol{f}_{\Pi} \\ f_{\Delta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{A} \Phi^T \boldsymbol{f} \\ f - C^T \Phi^T f \end{bmatrix},$$

where A is the corresponding assembling operator to R, i.e., $A = R^{T}$. A more extensive discussion and derivation can be found in [42].

¹⁷³ 5. Parallelization of the building blocks

Here we investigate how the single operations can be executed in parallel in a distributedmemory setting. The parallelization of the method is performed with respect to the

Algorithm 1 Algorithm for calculating $\boldsymbol{\nu} = F\boldsymbol{\lambda}$ and $\boldsymbol{\nu} = M_{sD}^{-1}\boldsymbol{\lambda}$ for given $\boldsymbol{\lambda} \in U$

procedure $F(\lambda)$ Application of $B^T : \{f^{(k)}\}_{k=1}^N = B^T \boldsymbol{\lambda}$ Application of $\widetilde{I}^T : \{\mathbf{f}_{\Pi}, \{f_{\Delta}^{(k)}\}_{k=1}^N\} = \widetilde{I}^T \left(\{f^{(k)}\}_{k=1}^N\right)$ Application of \widetilde{S}^{-1} : $\mathbf{\bar{w}}_{\Pi} = \mathbf{S}_{\Pi\Pi}^{-1} \mathbf{f}_{\Pi}$ $w_{\Delta}^{(k)} = S_{\Delta\Delta}^{(k)}{}^{-1} f_{\Delta}^{(k)} \quad \forall k = 1, \dots, N$ End Begin Application of \widetilde{I} : $\{w^{(k)}\}_{k=1}^N = \widetilde{I}\left(\{\mathbf{w}_{\Pi}, \{w_{\Delta}^{(k)}\}_{k=1}^N\}\right)$ Application of $B: \boldsymbol{\nu} = B\left(\{w^{(k)}\}_{k=1}^{N}\right)$ end procedure procedure $M_{sD}^{-1}(\boldsymbol{\lambda})$ Application of $B_D^T : \{w^{(k)}\}_{k=1}^N = B_D^T \boldsymbol{\lambda}$ Application of S_e : Begin Solve $K_{II}^{(k)} x^{(k)} = -K_{IB}^{(k)} w^{(k)}$ $\forall k = 1, \dots, N$ $v^{(k)} = K_{BB}^{(k)} w^{(k)} + K_{BI}^{(k)} x^{(k)}$. $\forall k = 1, \dots, N$ End Application of $B_D: \boldsymbol{\nu} = B_D\left(\{v^{(k)}\}_{k=1}^N\right)$ end procedure

patches, i.e., one or several patches are assigned to a processor. The required communication has to be understood as communication between patches, which are assigned to
different processors. The majority of the used MPI methods are performed in its nonblocking version. We aim at overlapping computations with communications wherever
possible.

181 5.1. Parallel version of PCG

We solve $F\lambda = d$ with the preconditioned CG method. This requires a parallel imple-182 mentation of CG, where we follow the approach presented in Section 2.2.5.5 in [42], see 183 also [11]. This approach is based on the concept of accumulated and distributed vectors. 184 We say a vector $\boldsymbol{\lambda}_{acc} = [\boldsymbol{\lambda}_{acc}^{(q)}]$ is an *accumulated* representation of $\boldsymbol{\lambda}$, if $\boldsymbol{\lambda}_{acc}^{(q)}(k_q(i)) = \boldsymbol{\lambda}(i)$, where *i* is the global index corresponding to the local index $k_q(i)$ on processor *q*. On the 185 186 contrary, $\lambda_{dist} = [\lambda_{dist}^{(q)}]$ is a *distributed* representation of λ , if the sum of all processor 187 local contributions give the global vector, i.e., $\lambda_{dist}(i) = \sum_{q} \lambda_{dist}^{(q)}(k_q(i))$. Hence, each 188 processor only holds the part of λ , which belongs to its patches, either in a distributed or 189 accumulated description. The Lagrange multipliers and the search direction of the CG are 190 represented in the accumulated setting, whereas the residual is given in the distributed 191 representation. In order to achieve the accumulated representation, information exchange 192 between the neighbours of a patch is required. This is done after applying the matrix and 193 the preconditioner, respectively and implemented via MPI_Send and MPI_Recv operations. 194

The last aspect in the parallel CG implementation is the realization of scalar products. Given a distributed representation u_{dist} of u and an accumulated representation of v_{acc} of *v*, the scalar product $(u, v)_{l^2}$ is then given by $(u, v)_{l^2} = \sum_q (u_{dist}^{(q)}, v_{acc}^{(q)})_{l^2}$, i.e., first the local scalar products are formed, globally added, and distributed with MPI_Allreduce.

199 5.2. Assembling

- ²⁰⁰ The assembling routine of the IETI-DP algorithm consists of the following steps:
- 1. Assemble the patch local stiffness matrices and right hand side,
- 202 2. assemble the system matrix in (16) and calculating its LU-factorization,
- $_{203}$ 3. assemble $S_{\Pi\Pi}$ and calculating its LU-factorization,
- 4. calculate the LU-factorization of $K_{II}^{(k)}$,
- 5. calculate the right hand side $\{g_{\Pi}, g_{\Delta}\} = \widetilde{g} \in \widetilde{W}^*$, with $g^{(k)} = f_B K_{BI}^{(k)} (K_{II}^{(k)})^{-1} f_I^{(k)}$.

²⁰⁶ Most of the tasks are completely independent of each other and, hence, can be performed ²⁰⁷ in parallel. Only the calculation of $S_{\Pi\Pi}$ and $\tilde{g} = \tilde{I}^T g$ require communication, which will ²⁰⁸ be handled in Section 5.3.

The LU-factorization of $S_{\Pi\Pi}$ is only required at one processor, since it has to be solved only once per CG iteration. According to [29], it is advantageous to distribute this matrix to all other processors in order to reduce communication in the solver part, see [32] and references therein for improving scalability based on a different approach. In the current paper, we investigate cases, where one, several and all processor hold the LU-factorization of $S_{\Pi\Pi}$. Therefore, each processor is assigned to exactly one holder of $S_{\Pi\Pi}$. This relation is implemented by means of an additional MPI communicator.

We note that, for extremely large scale problems with $\geq 10^5$ subdomains, one has to consider different strategies dealing with $S_{\Pi\Pi}^{-1}$. Most commonly one uses AMG and solves $S_{\Pi\Pi}u_{\Pi} = f_{\Pi}$ in an inexact way, see, e.g., [27] and [31]. When considering a moderate number of patches, i.e., $10^3 - 10^4$, the approach using the LU-factorization of $S_{\Pi\Pi}$ is the most efficient one. In this paper, we restrict ourselves to this case.

The patch local matrix $S_{\Pi\Pi}^{(k)}$ is obtained as a part of the solutions of (16) and the assembling of the global matrix $S_{\Pi\Pi}$ is basically a MPI_gatherv operation. In the case where all processors hold $S_{\Pi\Pi}$ we use MPI_allgatherv. If several processors hold the LU factorization, we just call MPI_gatherv on each of these processors. A different possibility would be to first assemble $S_{\Pi\Pi}$ on one patch, distribute it to the other holders and then calculate the LU-factorization on each of the processors.

227 5.3. Solver and Preconditioner

More communication is involved in the solver part. According to Algorithm 1, we have to perform the following operations:

- 230 1. application of B and B^T and its scaled versions
- 231 2. application of \tilde{I} and \tilde{I}^T
- ²³² 3. application of \tilde{S}^{-1}
- 4. application of S^{-1}

The only operations which require communication are \tilde{I} and \tilde{I}^T . To be more precise, the communication is hidden in the operators A and R, see Section 4.2, all other operations are block operations, where the corresponding matrices are stored locally on each processor. In principle, their implementation is given by accumulating and distributing
values. The actual implementation depends on how many processors hold the coarse grid
problem.

In order to implement \tilde{I} , we need the distribution operation R. If all processors hold $S_{\Pi\Pi}$, this operations reduces to just extracting the right entries. Hence it is local and no communication is required. Otherwise, each holder of $S_{\Pi\Pi}$ reorders and duplicates the entries of w_{Π} in such a way, that all entries corresponding to the patches of a single slave are in a contiguous block of memory. Then we utilize the MPI_scatter method to distribute only the necessary data to all slave processors. See Figure 1 for an illustration.

We arrive at the implementation of \tilde{I}^T . Each processor stores the values of $\boldsymbol{w}_{\Pi}^{(k)}$ in a vector $\tilde{\boldsymbol{w}}_{\Pi}^{(k)}$ of length n_{Π} already in such a way, that $\sum_{k=1}^{N} \tilde{\boldsymbol{w}}_{\Pi}^{(k)} = \boldsymbol{w}_{\Pi}$. Storing the entries in this way enables the use the MPI reduction operations to efficiently assemble the local 246 247 248 contributions. If only one processor holds the coarse problem, we use the MPI_Reduce 249 method to perform this operation. Similarly, if all processors hold $S_{\Pi\Pi}$, we utilize the 250 MPI_Allreduce method. If several processors have the coarse grid problem, we use a 251 two level approach. First, each master processor collects the local contributions from 252 its slaves using the MPI_Reduce operation. In the second step, all the master processors 253 perform an MPI_Allreduce operation to accumulate the contributions from each group 254 and simultaneously distribute the result under them. This procedure is visualized in 255 Figure 1. 256

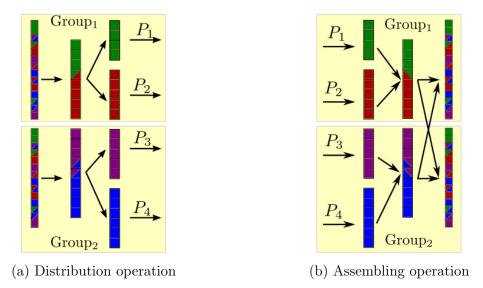


Figure 1: Distribution and assembling operation, illustrated for four processors, partitioned into two groups corresponding to two $S_{\Pi\Pi}^{-1}$ holder.

²⁵⁷ 6. Numerical examples

We consider the model problem (1) in the two dimensional computational domain $\Omega = (0,1)^2$ formed by $32 \times 32 = 1024$ patches. Each of them is a square arranged in a uniform grid. For the three dimensional case we consider the domain $\Omega = (0,1)^2 \times (0,2)$, partitioned into $8 \times 8 \times 16$ regular cubes. Note that, in IgA framework, we cannot choose the number of subdomains as freely as in the finite element case since they are fixed by the geometry. Therefore, the number of 1024 subdomains stays constant throughout the tests. Since we are interested in the parallel scalability of the proposed algorithms, we assume for simplicity homogeneous diffusion coefficients $\alpha \equiv 1$. In all tests we consider the smooth right hand side $f(x, y) = 20\pi^2 \sin(4\pi(x+0.4)) \sin(2\pi(y+0.3))$, corresponding to the exact solution $u(x, y) = \sin(4\pi(x+0.4)) \sin(2\pi(y+0.3)) + x + y$. For the discretization, we use tensor B-Spline spaces V_h of different degree p. We increase the B-Spline degree in such a way that the number of knots stay the same, i.e., the smoothness of V_h increases.

We investigate the scaling behaviour of the cG-IETI-DP and dG-IETI-DP method. Al-270 though, we consider also the dG variant, we restrict ourselves to matching meshes. Oth-271 erwise, it would not be possible to compare the two methods. Moreover, some patches 272 would have a significant larger number of dofs, which leads to load imbalances and affects 273 the scaling in a negative way. The domain is refined in a uniform way by inserting a 274 single knot for each dimension on each knot span. We denote by H_k the patch diameter 275 and by h_k the characteristic mesh size on $\Omega^{(k)}$. The set of primal variables is chosen by 276 continuous patch vertices and interface averages for the two dimensional setting. For the 277 three dimensional examples, we choose only continuous edge averages in order to keep the 278 number of primal variables small. 279

The preconditioned conjugate gradient method is used to solve (14) with the scaled Dirichlet preconditioner M_{sD}^{-1} . We choose zero initial guess and a relative reduction of the residual of 10^{-8} . For solving the local systems and the coarse grid problem, a direct solver is used.

The algorithm is realized in the isogeometric open source C++ library G+SMO [40], 284 which is based on the Eigen library [17]. We utilize the PARDISO 5.0.0 Solver Project 285 [35] for performing the LU factorizations. The code is compiled with the gcc 4.8.3 286 compiler with optimization flag -03. For the communication between the processors, we 287 use the MPI 2 standard with the OpenMPI 1.10.2 implementation. The results are obtain 288 on the RADON1 cluster at Linz. We use 64 out of 68 available nodes, each equipped with 289 2x Xeon E5-2630v3 "Haswell" CPU (8 Cores, 2.4Ghz, 20MB Cache) and 128 GB RAM. 290 This gives the total number of 1024 available cores. 291

We investigate two quantities, the assembling phase and the solving phase. In the assembling phase, we account for the time used for

• assembling the local matrices and right hand sides,

• LU-factorization of K_{II} ,

• LU-factorization of
$$\begin{bmatrix} K & C^T \\ C & 0 \end{bmatrix}$$

• calculation of $\widetilde{\Phi}$ and $\widetilde{\mu}$,

2

• assembling the coarse grid matrix $S_{\Pi\Pi}$ and calculation of its LU factorization.

As already indicated in Section 5, $S_{\Pi\Pi}$ is only assembled on certain processors. The solving phase consists of the CG algorithm for (14) and the back-substitution to obtain the solution from the Lagrange multipliers. The main ingredients are

• application of F,

• application of M_{sD}^{-1} .

In Section 6.1 and Section 6.2, we study the weak and strong scaling behaviour for the cG-IETI-DP and the dG-IETI-DP method. In this two sections, we assume that only one processor holds the coarse grid matrix $S_{\Pi\Pi}$. The comparison of having a different number of $S_{\Pi\Pi}$ holders is done in Section 6.3.

308 6.1. Weak scaling

In this subsection we investigate the weak scaling behaviour, i.e., the relation of problem size and number of processors is constant. In each refinement step we multiply the number of used cores by $2^d, d \in \{2, 3\}$. The ideal behaviour would be a constant time for each refinement.

First, we consider the two dimensional case. We apply three initial refinements and start 313 with a single processor and perform up to additional 5 refinements with maximum 1024 314 processors. We choose as primal variables continuous vertex values and edge averages. 315 The results for degree $p \in \{2, 3, 4\}$ are illustrated in Figure 2. The first row of figures 316 corresponds to the cG-IETI-DP method, and the second one corresponds to the dG-317 IETI-DP method. The left column of Table 1 summarizes timings and the speedup for 318 the cG-IETI-DP method, whereas the right column presents the results for the dG-IETI-319 DP method. For each method, we investigate the weak scaling for the assembling and 320 solution phase. As in Figure 2, we present the scaling and timings for $p \in \{2, 3, 4\}$. 321

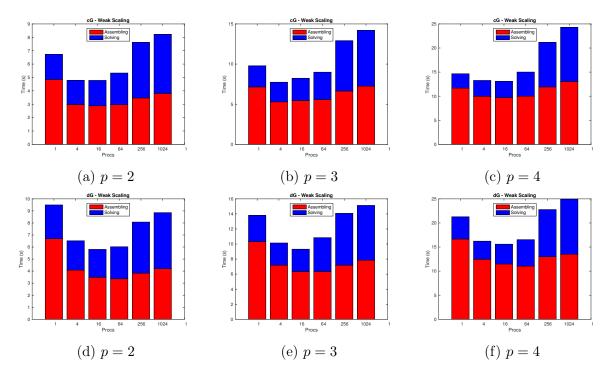


Figure 2: Weak scaling of the cG-IETI-DP (first row) and dG-IETI-DP (second row) method for B-Spline degrees $p \in \{2, 3, 4\}$ in two dimensions. Each degree corresponds to one column.

We observe that the time used for the assembling stays almost constant, hence shows quite optimal behaviour. However, the time for solving the system increases when refining and increasing the number of used processors. Especially, when considering the largest number of processors, we see a clear increase of the solution time. One reason is that the number of iterations slightly increases when increasing the system size. This is due to the quasi optimal condition number bound of the IETI-DP type methods, cf. (15).

	cG-IETI	-DP	p = 2			dG-IETI	-DP	p = 2			
	// 1 . C	Т	Ass.	Solv.	Total	// 1.0	T.	Ass.	Solv.	Total	
# procs	#dofs	Iter.	Time	Time	Time	#dofs	Iter.	Time	Time	Time	
1	99104	7	4.8	1.9	6.7	133824	8	6.7	2.8	9.5	
4	328224	8	3.0	1.8	4.8	394688	9	4.1	2.4	6.5	
16	1179680	9	2.9	1.9	4.8	1309632	10	3.5	2.3	5.8	
64	4455456	10	3.0	2.4	5.4	4712384	11	3.4	2.7	6.1	
256	17298464	11	3.5	4.2	7.7	17809344	11	3.8	4.2	8.0	
1024	68150304	11	3.8	4.4	8.2	69169088	12	4.2	4.7	8.9	
	cG-IETI	-DP		p = 3		dG-IETI	-DP	p = 3			
//	// dofa	Iton	Ass.	Solv.	Total	// dofa	Itom	Ass.	Solv.	Total	
# procs	#dofs	Iter.	Time	Time	Time	#dofs	Iter.	Time	Time	Time	
1	120576	8	7.2	2.6	9.8	159264	8	10.3	3.5	13.8	
4	366080	9	5.3	2.4	7.7	436512	9	7.2	3.0	10.2	
16	1250304	10	5.5	2.8	8.3	1384224	10	6.3	3.0	9.3	
64	4591616	10	5.6	3.4	9.0	4852512	11	6.4	4.5	10.9	
256	17565696	11	6.6	6.3	12.9	18080544	12	7.2	6.9	14.1	
1024	68679680	12	7.3	7.0	14.3	69702432	12	7.9	7.3	15.2	
	cG-IETI	-DP		p = 4		dG-IETI-DP		p=4			
//	// dofa	Iton	Ass.	Solv.	Total	// dofa	Itom	Ass.	Solv.	Total	
# procs	#dofs	Iter.	Time	Time	Time	#dofs	Iter.	Time	Time	Time	
1	144096	8	11.7	3.0	14.7	186752	9	16.7	4.6	21.3	
4	405984	9	10.0	3.3	13.3	480384	10	12.4	3.8	16.2	
16	1322976	10	9.7	3.4	13.1	1460864	11	11.5	4.1	15.6	
64	4729824	11	10.0	5.0	15.0	4994688	11	11.0	5.5	16.5	
256	17834976	12	11.9	9.3	21.2	18353792	12	13.0	9.8	22.8	
1024	69211104	13	13.0	11.3	24.3	70237824	13	13.5	11.4	24.9	

Table 1: Weak scaling results for the two dimensional testcase for the cG and dG IETI-DP method. Left column contains results for the cG variant and the right column for the dG version. Each row corresponds to a fixed B-Spline degree $p \in \{2, 3, 4\}$

Secondly, as already pointed out in Section 5, the solving phase consists of more communication between processors, which cannot be completely overlapped with computations.
Moreover, one also has to take in account global synchronization points in the conjugate
gradient method.

Next, we consider the weak scaling for the three dimensional case. As already indicated 332 in the introduction of this section, we choose only continuous edge averages as primal 333 variables. We perform the tests in the same way as for the two dimensional case. However, 334 we already start with two processors and perform two initial refinements. Multiplying 335 the number of used processors by 8 with each refinement, we end up again with 1024336 processors on the finest grid. The two algorithms behave similar to the two dimensional 337 case, where the assembling phase gives quite good results and the solver phase shows 338 again an increasing time after each refinement. The results are visualized in Figure 3 and 339 summarized in Table 2. Note, for the dG-IETI-DP method with p = 4 and ~ 54 Mio. 340 dofs, we exceeded the memory capacity of the cluster. 341

342 6.2. Strong scaling

Secondly, we are investigating the strong scaling behaviour. Now we fix the problem size and increase the number of processors. In the optimal case, the time used by a certain quantity reduces in the same way as the number of used processors increases. We use

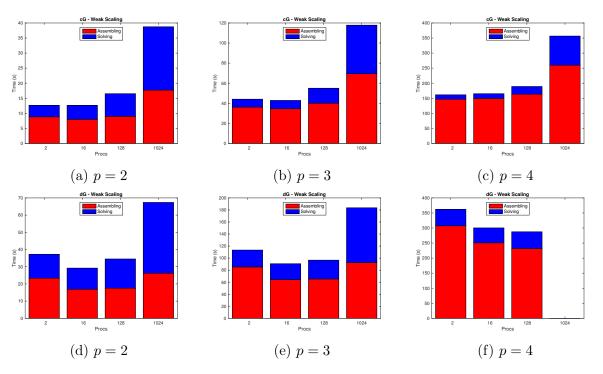


Figure 3: Weak scaling of the cG-IETI-DP (first row) and dG-IETI-DP (second row) method for B-Spline degrees $p \in \{2, 3, 4\}$ in three dimensions. Each degree corresponds to one column. No timings are obtained in the case of 1024 cores in (f) due to memory limitations

the same primal variables for the strong scaling studies as in the weak scaling studies in Section 6.1.

Again as in Section 6.1, we begin with the two dimensional example. We perform 7 initials refinements and end up with 17 Mio. dofs on 1024 subdomains. We start already with 4 processors in the initial case and do 8 refinements until we reach 1024 cores. Similar to Section 6.1, the results for $p \in \{2, 3, 4\}$ are illustrated in Figure 4 and summarized in Table 3.

We observe that the assembling phase has a quite good scaling performance, as already 353 observed for the weak scaling results in Section 6.1. Moreover, the higher the B-Spline 354 degree, the better the parallel performance behaves. This holds due to increased computa-355 tional costs for the parallel part. Similar to the weak scaling results, the solver phase does 356 not provide such an excellent scaling as the assembling phase. Still, we obtain a scaling 357 from around 500 when using 1024 processors. We note that the degree of the B-Splines 358 does not seem to have such a significant effect on the scaling for the solver phase as for 359 the assembling phase. 360

In the three dimensional example we perform four initial refinements and obtain around 361 5 Mio. dofs. The presentation of the results is done in the same way as in the previous 362 examples, see Figure 5 and Table 4. Also in three dimensions the cG-IETI-DP algorithms 363 behaves very similarly to the two dimensional case, showing excellent scaling results. 364 However, the dG version of the algorithm shows a good scaling but not as promising as 365 cG version. Especially, when considering p = 2, we observe degraded scalability for the 366 assembling phase. Having a closer look at the timings, we observe that this originates 367 from small load imbalances in the interior domains, due to the additional layer of dofs 368 and the larger number of primal variables. The latter one leads to an increased time in 369

	cG-IETI	-DP	p = 2			dG-IETI-	dG-IETI-DP			p = 2			
# proof	#dofa	Iter.	Ass.	Solv.	Total	#dofa	Iter.	Ass.	Solv.	Total			
# procs	#dofs	mer.	Time	Time	Time	#dofs	nter.	Time	Time	Time			
2	220896	16	8.8	3.8	12.6	396932	26	23.3	14.0	37.3			
16	1023200	17	8.0	4.7	12.7	1551400	27	16.9	12.3	29.2			
128	5969376	17	9.0	7.5	16.5	7730288	28	17.5	17.0	34.5			
1024	40238048	19	17.7	21.0	38.7	46577920	28	26.2	41.2	67.4			
	cG-IETI	-DP	p = 3			dG-IETI-	DP	p = 3					
# proof	#dofs	Iter.	Ass.	Solv.	Total	#dofa	Iter.	Ass.	Solv.	Total			
# procs	#dois	ner.	Time	Time	Time	#dofs		Time	Time	Time			
2	350840	17	36.2	7.9	44.1	598405	29	85.3	28.1	113.4			
16	1361976	18	34.5	8.4	42.9	2005737	30	64.2	26.5	90.7			
128	7020728	18	40.0	15.0	55.0	8985265	30	65.4	31.3	96.7			
1024	43894200	21	69.4	48.4	117.8	50613825	31	92.6	91.0	183.6			
	cG-IETI	-DP		p = 4		dG-IETI-	DP	p = 4					
//	// dofa	Itom	Ass.	Solv.	Total	// dofa	Itom	Ass.	Solv.	Total			
# procs	#dofs	Iter.	Time	Time	Time	#dofs	Iter.	Time	Time	Time			
2	523776	18	146.6	14.8	161.4	853878	32	307.3	55.1	362.4			
16	1768320	18	149.2	15.9	165.1	2538650	32	250.7	49.8	300.5			
128	8188800	20	163.6	25.6	189.2	10367970	34	232.0	55.4	287.4			
1024	47765376	22	259.7	96.9	356.6	~ 54000000	х	х	х	х			

Table 2: Weak scaling results for the three dimensional testcase for the cG and dG IETI-DP method. Left column contains results for the cG variant and the right column for the dG version. Each row corresponds to a fixed B-Spline degree $p \in \{2, 3, 4\}$. No timings are available for the dG-IETI-DP method with p = 4 on 1024 cores due to memory limitations.

solving (16), due to a larger number of right hand sides on the interior subdomains. One
can further optimize the three dimensional case, by considering different strategies for
the primal variables, where one aims for smaller and more equally distributed numbers of
primal variables.

374 6.3. Study on the number of $S_{\Pi\Pi}^{-1}$ holders

In this last section of the numerical experiments, we want to investigate the influence of 375 the number of holders of $S_{\Pi\Pi}^{-1}$ on the scaling behaviour. As already indicated in Section 5.3, 376 if more processors hold the LU-factorization of the coarse grid matrix, it is possible to 377 decrease the communication effort after applying $S_{\Pi\Pi}^{-1}$, while having more communication 378 before the application. The advantage of this strategy is to be able to have a better 379 overlap of communication with computations. However one has to take into account, that 380 this also increases the communication in the assembling phase, since the local contribution 381 $S_{\Pi\Pi}^{(k)}$ has to be sent to all the master processors. 382

We only consider the two dimensional domain, where we perform 7 initials refinements, 383 but on a decomposition with 4096 subdomains and end up with around 70 Mio. dofs. 384 This gives a comparable setting as in Section 6.1 having the most refined domain. In order 385 to better observe the influence of the number of $S_{\Pi\Pi}^{-1}$ holders, we increase the number of 386 subdomains, leading to a larger coarse grid problem. We only investigate the case of using 387 1024 processors and the number of $S_{\Pi\Pi}$ holders given by $2^n, n \in \{0, 1, \ldots, 10\}$. Hence, we 388 obtain the number of master processors ranging from 1 to 1024, such that each master 389 has the same number of slaves. The results are summarized in Figure 6 and Table 5. 390

³⁹¹ We observe that choosing several holders of the coarse grid problem in the cG version

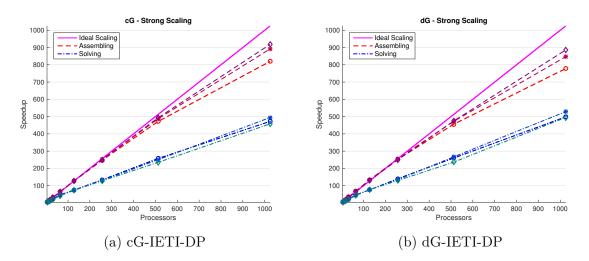


Figure 4: Strong scaling of the cG-IETI-DP (left column) and dG-IETI-DP (right column) method for B-Spline degrees $p \in \{2, 3, 4\}$ in two dimensions. The markers $\{\circ, *, \diamond\}$ as well as different shades of red (assembling phase) and blue (solver phase) correspond to the degrees $\{2, 3, 4\}$.

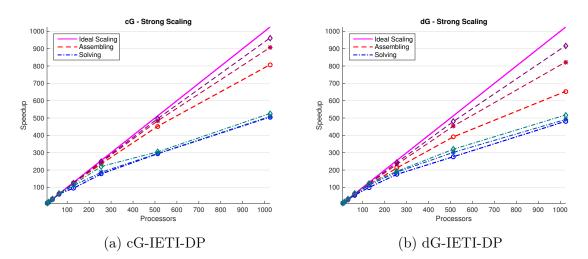


Figure 5: Strong scaling of the cG-IETI-DP (left column) and dG-IETI-DP (right column) method for B-Spline degrees $p \in \{2, 3, 4\}$ in three dimensions. The markers $\{\circ, *, \diamond\}$ as well as different shades of red (assembling phase) and blue (solver phase) correspond to the degrees $\{2, 3, 4\}$.

does not really have a significant effect. However, in the dG version, due to an increased number of primal variables, the use of several holders actually increases the performance of the solver by around 10%. Nevertheless, what is gained in the solving part does not pay off with the additional effort in the assembling phase. Considering the total computation time in Table 5, the best options is still either using only a single coarse grid problem on one processor or making a redundant factorization on each processor.

398 7. Conclusion

We have investigated the parallel scalability of the cG-IETI-DP and dG-IETI-DP method, respectively. Numerical tests showed a very good scalability in the strong and weak scaling for the assembling phase for both methods. We reached a speedup of approximately 900 when using 1024 cores. Although the speedup of the solver phase is not as good as the one for the assembler phase, we still reached a speedup of around 500 when using 1024

2d		<i>p</i> =	= 2			<i>p</i> =	= 3		p = 4			
	assembling solving			ng	assem	bling	solving		assembling		solving	
cG-IETI-DP	pha		pha		pha	se	pha		pha		pha	se
# procs	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.
4	190.8	4	138.2	4	364.5	4	202.6	4	653.7	4	279.1	4
8	94.8	8	88.8	6	181.2	8	141.8	6	325.9	8	202.7	6
16	47.1	16	45.9	12	89.9	16	71.9	11	162.3	16	102.6	11
32	23.1	32	22.9	24	44.5	32	35.7	23	80.4	32	51.3	22
64	11.6	65	11.8	46	22.4	65	18.5	44	40.2	64	26.3	42
128	5.9	127	7.3	75	11.3	128	11.1	73	20.4	128	14.8	75
256	3.0	247	4.1	133	5.7	251	6.1	131	10.4	250	8.7	128
512	1.6	471	2.1	257	2.9	487	3.2	250	5.3	493	4.7	235
1024	0.9	819	1.1	472	1.6	891	1.6	494	2.8	917	2.4	456
	assem	oling	solving		assembling s		solvi	lving assemb		bling solvin		ing
dG-IETI-DP	pha	se	pha	se	phase		phase		phase		phase	
# procs	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.
4	216.6	4	144.0	4	402.2	4	225.5	4	711.8	4	294.2	4
8	106.9	8	92.9	6	199.5	8	156.8	5	352.6	8	210.6	5
16	52.5	16	47.9	12	98.1	16	80.4	11	174.3	16	106.4	11
32	25.1	34	25.7	22	47.5	33	42.2	21	84.9	33	55.2	21
64	12.7	68	12.2	47	23.9	67	20.4	44	42.9	66	27.0	43
128	6.5	132	7.6	75	12.0	134	11.6	77	21.7	131	15.1	77
256	3.4	252	4.1	140	6.2	255	6.6	135	11.4	249	9.0	129
512	1.9	455	2.2	260	3.4	472	3.3	267	6.0	474	4.9	236
1024	1.1	777	1.1	498	1.9	846	1.7	528	3.2	885	2.3	494

Table 3: Strong scaling results: Time (s) and Speedup for $p \in \{2, 3, 4\}$ in two dimensions having approximately 17 Mio. dofs. First row shows results for the cG variant of the IETI-DP method, whereas the second row contains results for the dG version. Each column corresponds to a degree p.

404 cores. One can even increase the parallel performance of the solver part by increasing 405 the number of processors, which are holding the coarse grid problem. However, numer-406 ical examples have shown that this does not really pay off in the total time, due to an 407 increased assembling time. To summarize, we saw that the proposed methods are well 408 suited for large scale parallelization of assembling and solving IgA equations in two and 409 three dimensions.

410 Acknowledgements

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meshes. *Math. Models Methods Appl. Sci.*, 16(7):1031–1090, 2006.

3d	p = 2				p = 3				p = 4			
	asseml	oling	solvi	solving		assembling		solving		assembling		ng
cG-IETI-DP	pha	se	pha	se	phase		phase		phase		phase	
# procs	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.
8	140.4	8	93.7	8	624.8	8	205.3	8	2565.7	8	382.6	8
16	70.5	16	47.7	16	312.8	16	103.4	16	1285.6	16	182.5	17
32	35.2	32	25.0	30	157.0	32	53.7	31	643.3	32	93.7	33
64	17.5	64	11.9	63	78.6	64	27.2	60	322.5	64	46.6	66
128	9.0	125	7.9	95	40.2	124	14.9	110	163.0	126	26.4	116
256	4.8	236	4.2	178	20.4	245	8.8	187	82.1	250	13.9	221
512	2.5	452	2.6	294	10.3	483	5.6	296	41.4	496	10.0	305
1024	1.4	807	1.5	506	5.5	906	3.2	509	21.4	961	5.8	526
	assem	oling	solving		assembling		solving		assembling		solving	
dG-IETI-DP	pha	se	pha	se	phase		phase		phase		phase	
# procs	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.	Time	Sp.
8	249.6	8	210.8	8	985.8	8	433.2	8	3588.1	8	854.8	8
16	126.2	16	106.6	16	498.6	16	217.1	16	1792.9	16	405.7	17
32	65.0	31	56.6	30	255.4	31	110.3	31	913.5	31	205.0	33
64	33.1	60	30.5	55	128.5	61	58.2	60	460.0	62	105.9	65
128	17.4	115	17.0	99	65.5	120	30.7	113	234.3	123	56.4	121
256	9.4	212	9.6	175	33.8	233	18.4	188	117.8	244	35.4	193
512	5.1	391	6.1	277	17.4	453	11.5	302	59.9	479	21.4	320
1024	3.1	653	3.5	481	9.6	822	7.1	491	31.3	917	13.2	517

Table 4: Strong scaling results: Time (s) and Speedup for $p \in \{2, 3, 4\}$ in three dimensions having approximately 5 Mio. dofs. First row shows results for the cG variant of the IETI-DP method, whereas the second row contains results for the dG version. Each column corresponds to a degree p.

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cG-IETI-DP	p = 2				p = 3		p = 4			
$\# S_{\Pi\Pi}^{-1}$	Assemble	Solving	Total	Assemble	Solving	Total	Assemble	Solving	Total	
Holder	Time	Time	Time	Time	Time	Time	Time	Time	Time	
1	3.61	3.66	7.27	6.50	5.52	12.02	11.23	8.30	19.53	
2	4.49	3.58	8.07	7.97	5.57	13.54	13.83	8.02	21.85	
4	4.53	3.82	8.35	7.65	5.40	13.05	13.60	8.09	21.69	
8	4.46	3.63	8.09	7.72	5.76	13.48	13.32	8.15	21.47	
16	4.34	3.49	7.83	7.64	5.61	13.25	13.16	7.93	21.09	
32	4.33	3.73	8.06	7.74	5.39	13.13	13.15	8.78	21.93	
64	4.34	3.59	7.93	7.62	5.45	13.07	13.10	8.04	21.14	
128	4.49	4.06	8.55	7.60	6.05	13.65	13.06	8.47	21.53	
256	4.31	4.64	8.95	7.63	6.43	14.06	13.02	8.81	21.83	
512	4.34	3.61	7.95	7.55	5.71	13.26	13.23	8.09	21.32	
1024	3.73	3.80	7.53	6.56	5.77	12.33	11.19	8.26	19.45	
dG-IETI-DP		p=2			p = 3		p = 4			
$\# S_{\Pi\Pi}^{-1}$	Assemble	Solving	Total	Assemble	Solving	Total	Assemble	Solving	Total	
Holder	Time	Time	Time	Time	Time	Time	Time	Time	Time	
1	4.57	5.09	9.66	7.28	7.16	14.44	12.44	10.01	22.45	
2	5.23	4.16	9.39	9.10	6.26	15.36	15.02	9.01	24.03	
4	5.25	4.18	9.43	9.12	6.58	15.70	14.93	8.73	23.66	
8	5.19	4.28	9.47	8.97	6.29	15.26	14.95	9.30	24.25	
16	5.26	4.20	9.46	8.78	6.41	15.19	14.79	9.16	23.95	
32	5.11	4.64	9.75	8.82	6.29	15.11	14.96	9.05	24.01	
64	5.35	4.75	10.1	9.06	6.87	15.93	14.85	9.37	24.22	
128	5.07	6.06	11.13	8.88	8.25	17.13	14.61	10.65	25.26	
256	5.07	5.89	10.96	8.66	7.77	16.43	14.52	11.32	25.84	
512	5.03	6.15	11.18	8.66	8.29	16.95	14.43	11.16	25.59	
1024	4.70	5.33	10.03	7.45	7.68	15.13	12.89	10.60	23.49	

Table 5: Influence of the number of processors having an LU-factorization of $S_{\Pi\Pi}$. Timings in seconds for 1024 Processors on a domain with around 70 Mio. dofs and 2048 subdomains.

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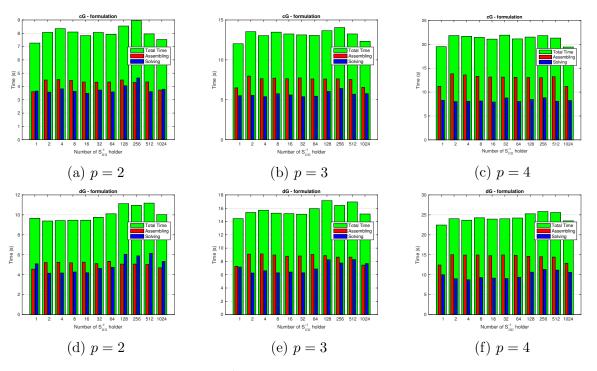


Figure 6: Influence of the number of $S_{\Pi\Pi}^{-1}$ holders on the scaling. First row corresponds to cG-IETI-DP, second row to dG-IETI-DP. Each column has a fixed degree $p \in \{2, 3, 4\}$. Figures (a-c) summarizes the cG version and Figures (d-f) the dG version, respectively.

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