Goal-adaptive Isogeometric Analysis with hierarchical splines

G. Kuru\textsuperscript{a,∗}, C.V. Verhoosel\textsuperscript{b}, K.G. van der Zee\textsuperscript{b}, E.H. van Brummelen\textsuperscript{b}

\textsuperscript{a}ONERA, The French Aerospace Lab, CFD and Aeroacoustics Department, BP72 - 29 avenue de la Division Leclerc, FR-92322 Châtillon, France
\textsuperscript{b}Multiscale Engineering Fluid Dynamics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

Abstract

In this work, a method of goal-adaptive Isogeometric Analysis is proposed. We combine goal-oriented error estimation and adaptivity with hierarchical B-splines for local $h$-refinement. The goal-oriented error estimate is computed with a $p$-refined discrete dual space, which is adaptively refined alongside the primal space. This discrete dual space is proven to be a strict superset of the primal space. Hierarchical refinements are introduced in marked regions that are formed as the union of chosen coarse-level spline supports from the primal basis. We present two ways of extracting localized refinement indicators suitable for the hierarchical refinement procedure: one based on a partitioning of the dual-weighted residual into contributions of basis function supports and one based on the combination of element indicators within a basis function support. The proposed goal-oriented adaptive strategy is exemplified for the Poisson problem and a free-surface flow problem. Numerical experiments on these problems show convergence of the adaptive method with optimal rates. Furthermore, the corresponding goal-oriented error estimators are shown to be accurate, with effectivity indices in the range of 0.7-1.1.

Keywords: Isogeometric Analysis, Goal-oriented error estimation, Adaptive refinement, Hierarchical splines

1. Introduction

Since the usage of computers has become widespread in engineering design, performing analysis on geometries designed using Computer Aided Design (CAD) software has been a common task. Isogeometric Analysis \cite{1,2}, is a framework for solving (partial) differential equations on domains generated by CAD software. It aims to eliminate or significantly reduce the time required for preparing the designed geometry for analysis, by directly using the CAD representation of the geometry in the analysis step. In addition to the benefits from an engineering management perspective, the exact representation of the design geometries in the analysis step has benefits for applications where the smoothness of the boundary of the domain plays a role, such as flow boundary layers and sliding contact of surfaces \cite{1}. Possibility of having higher order differentiable solutions in Isogeometric Analysis has also proven to be very desirable for many engineering applications where continuity of the solution is a requirement due to the employed formulation, such as binary phase separation \cite{3}, gradient damage models \cite{4} and analysis of shell structures \cite{5,6}. Due to its positive attributes, the interest in Isogeometric Analysis has grown very rapidly after its initial introduction, with applications to many complicated engineering problems in material fracture \cite{7,8}, contact mechanics \cite{9,10}, turbulence computation \cite{11,12}, free-surface flows \cite{13}, fluid-structure interaction \cite{14}, shape optimization \cite{15,16} and many others.

Although Isogeometric Analysis aims to overcome some of the problems often encountered in the engineering design-through-analysis process, the fact that the objects used for geometry representation are often not adequate for attaining a certain accuracy in analysis means that there has to be some sort of a preprocessing step. If this step is done heuristically, it again requires manual labor. To have a truly smooth work flow from design to analysis, adapting the initial design representations based on an automated procedure is essential. Adaptive Isogeometric Analysis methods based on error estimators are vital in performing this task with effectively no intervention by the engineer. Achieving this requires two issues to be addressed: Enriching the approximation space through local refinement of the basis, and finding reliable refinement indicators to assess if and where refinement should take place. The aim of this work is to address these issues by applying goal-oriented error estimation principles to develop an adaptive Isogeometric Analysis method using hierarchical B-splines as the local refinement technique.

In assessing CAD technologies in the context of adaptive Isogeometric Analysis, various qualities are important. Especially locality of the refinement procedure plays an important role, along with the requirement of linear independence and compatibility with the state of the art CAD technologies that are in use in the industry. Hierarchical splines \cite{17} fulfill all of these requirements, yet they are constructed in a simple way. The hierarchical refinement method has been applied to B-splines \cite{17,18} and NURBS \cite{19}. In the field of engineering design, NURBS is the industry standard technology \cite{20,21}. However, B-splines have many properties in common with NURBS and in terms of refinement techniques, virtually every concept can be extended from B-splines to NURBS with relative ease. Therefore, hierarchical B-splines are chosen to be used in this...
Adaptive Isogeometric Analysis with hierarchical splines has already been studied using refinement indicators based on so-called bubble functions [18] and gradients of the approximate solution [22]. In addition to these, hierarchically refined bases are used for Galerkin discretizations for several applications [23, 24]. Adaptive Isogeometric Analysis has also been studied with T-splines [25, 26], PHT-splines [27, 28] and using common Finite Element Method (FEM)-type basis functions with spline parametrizations [29, 30]. Adaptivity with a method of constructing locally refined B-spline elements ensuring up to $C^1$-conformity through a matching procedure had been investigated [31] even before the inception of Isogeometric Analysis.

Next to the techniques of constructing locally refined approximation spaces, an integral element of adaptive refinement is the refinement indicator that is used in deciding where and how a mesh needs to be refined. Refinement indicators are usually based on an a-posteriori estimate of the error. Among the most prominent a-posteriori error estimation methods for Galerkin discretizations are recovery-based methods, residual based methods and goal-oriented methods. For a review of various a-posteriori error estimation techniques, see [32, 33]. The choice of goal-oriented error estimation is motivated by its very nature, i.e., estimating the error in a quantity that is of practical relevance for the application. In mesh adaptivity using estimators that do not take the quantity of interest into account, the refinement aims to resolve features of the solution with equal accuracy over the whole computational domain. In many problems the complicated features of the solution on some parts of the domain might not influence the quantity of interest. Hence, improving the approximate solution based on goal-oriented error estimators is a very natural choice, given that there is a clear quantity of interest.

This work considers the local $h$-refinement of Isogeometric Analysis spaces using hierarchical B-splines, with refinement indicators derived from goal-oriented error estimators. The main contributions of this work are a goal-oriented error estimator using adapted hierarchical B-spline primal spaces that are strictly nested within the proposed dual spaces, the construction of refinement indicators that are suitable for hierarchical refinement, the numerical investigation of these indicators and actual goal-adaptive Isogeometric discretizations of the two example problems.

The proposed methods are applied to the solution of exemplary elliptic problems of Poisson's equation and a prototypical free-surface flow problem. Both problems are posed on 2D domains, yet the methodology is formulated in general dimensions and in an operator-independent way wherever possible. Hence, extension to other elliptic problems should require minimal modifications to the proposed methodology. Furthermore, for problems in 3D, the benefits of local refinement in terms of computational cost would be even more relevant.

Starting with a brief introduction to B-splines, the employed refinement technique using hierarchical B-splines is reviewed in Section 2 in the light of adaptive Isogeometric Analysis. The method of goal-oriented error estimation is introduced in a general setting and an error estimator suitable for adaptive-refinement is proposed in Section 3. Furthermore, in Section 4 two refinement indicators are proposed using this estimator. In Section 4 the error estimator and refinement indicators are studied numerically and the adaptive procedure is tested for two problems. Conclusions and future recommendations are presented in Section 5.

2. Hierarchical refinement of B-splines

Given a bounded open interval $\hat{\Omega} \subset \mathbb{R}$, named the parameter domain, B-splines are piecewise polynomials $N_{i,p} : \hat{\Omega} \rightarrow \mathbb{R}$ of degree $p \in \mathbb{Z}_{\geq 0}$, that form a basis of a globally $C^p$-continuous polynomial space, with $-1 \leq k < p$. The space formed by the B-splines can be characterized by a non-decreasing sequence of knots, named the knot vector. Knots are points in $\hat{\Omega}$, at which the B-splines have reduced continuity, i.e., locations at which the basis functions are not $C^\infty$-continuous. A B-spline curve $C : \hat{\Omega} \rightarrow \Omega$ is a parametrization from the parameter domain $\hat{\Omega} \subset \mathbb{R}$ to the physical domain $\Omega \subset \mathbb{R}^d$, with $d' \geq 1$, using the B-spline basis. The coefficients of the B-splines $B_i \in \mathbb{R}^{d'}$ are referred to as the control points. The B-spline curve is described as:

$$C(\xi) = \sum_{i=0}^{n} N_{i,p}(\xi)B_i$$

where the B-splines $N_{i,p}$ are defined by the Cox-de Boor relation [34, 35], which states for $p = 0$:

$$N_{i,0}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1}, \\ 0 & \text{otherwise} \end{cases}$$ (1a)

and recursively for $p > 0$:

$$N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi)$$ (1b)

For multivariate objects, commonly the tensor product of multiple univariate spline bases is used. For example, the bivariate B-spline surface is constructed as:

$$C(\xi, \zeta) = \sum_{i=0}^{n} \sum_{j=0}^{m} N_{i,p}(\xi)N_{j,q}(\zeta)B_{ij}$$

In the context of Isogeometric Analysis, global $h$-, $p$- and $k$- refinements of the B-spline bases are investigated in [22]. The global $h$-refinement of the B-spline basis corresponds to knot insertion. The $p$-refinement is achieved by order elevation and knot insertions at all knot positions. $k$-refinement is a possibility unique to spline bases, where the order is elevated along with the continuity order, which results in a minimal increase in the number of degrees of freedom to obtain a certain polynomial degree.

Traditional $h$-refinement of B-spline bases via knot insertion can also be done locally in 1D, however in multiple dimensions, the tensor product structure of the basis causes creation of undesired elements, resulting in increased computational cost with arguably little gain in accuracy. This is illustrated graphically.
in Figure 1, along with a more desirable alternative using hierarchical splines. The meshes plotted in Figure 1 are referred to as the Bézier meshes and the lines represent the boundaries of the Bézier elements, across which the polynomial space can admit non-$C^\infty$ solutions.

In the sequel we will introduce hierarchical splines and provide some properties that are relevant to isogeometric analysis, viz. linear independence and nestedness of hierarchically refined spline spaces. The basic results outlined here can be found in slightly different forms in the literature [36,13,37] but we extend the nestedness result to strict nestedness (Proposition 7) which will be used later for the proof of an important result (Theorem 8) that is of specific interest for goal-oriented error estimation with hierarchical splines.

2.1. Hierarchical B-splines

Hierarchical B-splines aim to construct bases on non-tensor product meshes consisting of locally refined portions. This can be seen as an extension of $C^\infty$-continuity preserving local $h$-refinement of elements as seen in Adaptive Finite Element Methods [38] to $C^2$-continuity preserving local $h$-refinement of degree $p > k$ B-spline patches.

The idea of hierarchical refinement is based on combining coarse level B-splines and fine level B-splines at different regions of the domain. The fine level B-splines are generated from coarse level B-splines by global $h$- or $p$-refinement operations and only a subset of the fine level functions are included based on a selected refinement region.

In the definition of hierarchical splines and throughout this text, the open support of a function $f : A \to \mathbb{R}$ will be denoted as $\text{supp}^o f$:

\[
\text{supp}^o f := \{ x \in A : f(x) \neq 0 \}
\]

where $A$ is an open set. Furthermore, $\text{supp} f$ will be used to denote the closure of $\text{supp}^o f$.

**Definition 1** (Hierarchical B-spline basis). Let $(N')_{0 \leq r \leq R}$ be a sequence of $R$ B-spline bases such that $\text{span}(N'^{r+1}) \supset \text{span}(N^r)$. Let $(\hat{\Omega}_y^r)_{0 \leq r \leq R}$ be a sequence of $R + 1$ open sets such that $\hat{\Omega}_y^{r+1} \subseteq \hat{\Omega}_y^r$ with $\hat{\Omega}_y^0 = \hat{\Omega}$ and $\hat{\Omega}_y^R = \emptyset$. The hierarchical B-spline basis at level $R$ is defined as:

\[
\mathcal{H}^R := \bigcup_{r=0}^{R-1} [N^r \in \mathcal{N}^r : \text{supp}^o N^r \subseteq \hat{\Omega}_y^r \land \text{supp}^o N^r \not\subseteq \hat{\Omega}_y^{r+1}] \quad (2)
\]

Definition 1 is equivalent to the definition provided in [18]. It essentially states that the hierarchical B-spline basis is constructed by excluding coarse-level functions whose supports are contained within the refinement region and replacing them by the fine-level functions whose supports are contained within the same region. Although only $h$-refined B-spline spaces are considered here, the properties outlined in the following are generally valid for any sequence of B-spline spaces such that $\text{span}(N'^{r+1}) \supset \text{span}(N^r)$.

A hierarchically $h$-refined basis $\mathcal{H}^2$ is exemplified for a univariate case in the third row of Figure 2 with $\hat{\Omega}_y^1 = (3,5)$ as the marked region of refinement. The B-splines $N^0 \in N^0$ are plotted in the first row and the $h$-refined B-splines $N^1 \in N^1$ are plotted in the second row. To construct $\mathcal{H}^2$, functions from $N^0$ whose supports are not contained within (3,5) and functions from $N^1$ whose supports are contained within (3,5) are included. A further application of the refinement with the selection region corresponding to a single Bézier element $\hat{\Omega}_y^2 = (4,4,5)$ is depicted in Figure 3. This operation...
results in no refinement, since the marked refinement region is too small to fully contain the support of a function from \( N^2 \). This illustrates how element-wise marking common to adaptive finite elements would not be suitable with hierarchical splines.

**Remark 1.** The way the hierarchical B-spline basis is defined makes its properties equally valid for arbitrary-dimensional multivariate spline objects.

B-splines have the property of local linear independence. (see e.g. [39]) This is an important property that will be used in some proofs later on, and is defined as follows:

**Definition 2** (Local linear independence). A set of functions \( \mathcal{M} \), with \( \mathcal{M} \ni N_j : \hat{\Omega} \rightarrow \mathbb{R} \), is said to be locally linearly independent if for any open subset \( A \subset \hat{\Omega} \) there do not exist nonzero coefficients \( d_j \) such that

\[
\sum_{i : N_i \in \mathcal{M}} d_i N_i |_A = 0
\]

where \( N_i |_A \) are the restrictions of \( N_i \) to \( A \).

Global linear independence is defined very similarly, except \( A \) is not taken as an arbitrary open subset, but \( A = \hat{\Omega} \). Using local linear independence property of B-splines, global linear independence of the hierarchical B-splines is demonstrated by the following theorem:

**Theorem 3** (Global linear independence of \( \mathcal{H}^R \)). The hierarchically constructed set of splines as defined in Definition 2 are linearly independent on \( \hat{\Omega} \).

**Proof.** See [13].

**Remark 2.** In general, hierarchical B-splines do not have the property of local linear independence, which is evident from inspecting the number of quadratic polynomials over the interval (4, 5) on the last row of Figure 2. The practical implication of this is that applying hierarchical refinement before a trimming operation can make the mesh unsuitable for analysis: Introducing a cut to the hierarchical splines of Figure 2 at point \( \xi = 4 \) results in linearly dependent functions to the right of the cut. The restriction of the remaining coarse level spline to (4, 5) can be exactly represented by the restrictions of the remaining fine level splines, implying linear dependence for the trimmed geometry. However, it is worth stressing that any trimming would likely be introduced during the design of the object, and subsequent hierarchical refinements on trimmed objects do not give rise to this problem.

In the following proposition, we show that hierarchical refinement produces enriched spaces in which the initial space is nested, which is an important property in view of adaptive algorithms.

**Proposition 4** (Nestedness of hierarchical B-spline spaces). The space spanned by a hierarchical B-spline basis \( \mathcal{H}^R \) is nested within the space spanned by \( \mathcal{H}^{R+1} \) that is obtained by a further refinement of \( \mathcal{H}^R \).

**Proof.** Here we repeat the proof of Vuong et al. [18] in a modified form that is organized into two parts, since we will refer to the individual parts later on:

1. When going from level \( R \) to \( R + 1 \), the discarded functions are denoted \( N^R_{\emptyset} := \{ N \in N^R : \text{supp} N \subseteq \hat{\Omega}^R_1 \} \) and the newly added ones are denoted \( N^{R+1}_{\emptyset} := \{ N \in N^{R+1} : \text{supp} N \subseteq \hat{\Omega}^{R+1}_1 \} \). If \( N^R = \emptyset \), for any other basis \( N^{R+1} \) it holds that \( \text{span}(N^{R+1}_{\emptyset}) \supseteq \text{span}(N^R_{\emptyset}) \). Otherwise, for all \( N \in N^R \) it holds that \( \text{supp} N \subseteq \hat{\Omega}^R_1 \) due to the definition of \( N^R \). Also \( N \in \text{span}(N^{R+1}) \) since \( N \in \text{span}(N^R) \) and \( \text{span}(N^R) \subseteq \text{span}(N^{R+1}) \). Therefore,

\[
\exists d_i \in \mathbb{R} : \quad N = \sum_{i : N_i \in N^{R+1}} d_i N_i^1
\]

which can be split up as:

\[
\exists c_i, d_j \in \mathbb{R} : \quad N = \sum_{i : N_i \in N^{R+1}} c_i N_i^1 + \sum_{j : N_j \in N^{R+1}} d_j N_j^1
\]

If \( N^{R+1}_{\emptyset} \cap N^R_{\emptyset} = \emptyset \), the first summation drops. Otherwise, \( \forall N \in N^{R+1}_{\emptyset} \cap N^R_{\emptyset} \), \( \text{supp} N \subseteq \hat{\Omega}^R_1 \), and by the local linear independence of \( N^{R+1}_{\emptyset} \cap N^R_{\emptyset} \) on \( \hat{\Omega} \), all coefficients \( c_i \) are necessarily zero as \( N(\xi) = 0, \forall \xi \in \hat{\Omega} \). This too means that the summation over \( N^{R+1}_{\emptyset} \cap N^R_{\emptyset} \) disappears, hence

\[
\exists d_j \in \mathbb{R} : \quad N = \sum_{j : N_j \in N^{R+1}_{\emptyset}} d_j N_j^1
\]

which implies that \( N \in \text{span}(N^{R+1}_{\emptyset}) \). Since this holds for all \( N \in N^R_{\emptyset} \), it has to hold that

\[
\text{span}(N^{R+1}_{\emptyset}) \supseteq \text{span}(N^R_{\emptyset}) \tag{3}
\]

2. In the refinement operation from level \( \mathcal{H}^R \) to \( \mathcal{H}^{R+1} \), the discarded basis functions of \( \mathcal{H}^R \) are \( \mathcal{H}^R \setminus \mathcal{H}^{R+1} = N^R_{\emptyset} \) and the newly added basis functions of \( \mathcal{H}^{R+1} \) are \( \mathcal{H}^{R+1} \setminus \mathcal{H}^R = N^{R+1}_{\emptyset} \). By [39], we have span(\( \mathcal{H}^R \setminus \mathcal{H}^{R+1} \)) \supseteq \text{span}(\mathcal{H}^R), \text{span}(\mathcal{H}^{R+1}) \supseteq \text{span}(\mathcal{H}^{R+1}), \text{from which it follows that span}(\mathcal{H}^{R+1}) \supseteq \text{span}(\mathcal{H}^R \setminus \mathcal{H}^{R+1}). \text{Furthermore, we have the trivial relation span}(\mathcal{H}^{R+1}) \supseteq \text{span}(\mathcal{H}^{R+1} \cap \mathcal{H}^R) \text{for the functions that remain unchanged by the refinement. Combining the two, we have span}(\mathcal{H}^{R+1}) \supseteq \text{span}(\mathcal{H}^R).
The hierarchical B-spline bases use a sequence of globally refined B-spline bases \( N^r \) for their construction. The main property assumed of these bases is that \( \text{span}(N^r) \subset \text{span}(N^{r+1}) \). This can be satisfied in multiple ways; both \( h \)-refined and \( p \)-refined B-spline bases can be used, possibly with anisotropic refinement. In this work, the elementary case of isotropic \( h \)-refinement is considered.

**Remark 4.** Globally \( h \)-refined B-splines do not satisfy the assumption \( \text{span}(N^r) \subset \text{span}(N^{r+1}) \), hence are not directly usable in hierarchical refinement.

In Finite Element Methods, local refinement is generally done element-wise based on a chosen element indicator. However, in the hierarchical refinement procedure, selection of \( \Omega_1^{r+1} = K_i \), where \( K_i \in \mathbb{T} \) is a single element of the Bézier mesh \( \mathbb{T} \) at level \( r \), could possibly cause no change in the basis, as no basis function support might be contained within a single element. To guarantee refinement, \( \Omega_i^{r+1} \) must at least contain the support of a single basis function \( \text{supp}^r N_i^{r+1} \), \( N_i^{r+1} \in N^{r+1} \) from the higher-level basis. Due to the typically smaller supports of finer level functions, having this as a minimal selection criterion could lead to the addition of fine level functions without excluding any coarse level functions, leading to excessive overlap of functions from different levels. This choice has some disadvantages with respect to e.g. possibility of having a partition of unity basis \([18]\) and the bandwidth of the resulting stiffness matrices. A study of the bandwidth of matrices obtained from Galerkin discretizations employing hierarchical B-spline bases is performed in \([22]\).

**Remark 5.** For the univariate case, the hierarchical B-spline spaces can be spanned by ordinary B-splines that are refined locally by knot insertion. In Appendix \([3]\) these two bases are compared in terms of the condition numbers for the solution of an adaptively discretized Poisson problem, with results slightly favoring hierarchical bases. See \([22, 40]\) for studies of different bases for \( \text{span}(H^R) \).

In this work, the **support condition** proposed by Vuong et al. \([18]\) is employed for the selection of refinement regions. This means \( \Omega_i^{r+1} \supset \text{supp}^r N_i^r \), for a basis function \( N_i^r \in N^r \). With this requirement it is chosen to select functions \( N_i^r \) and construct the refinement region by \( \hat{\Omega}_i^{r+1} = \text{int} \bigcup_{N_i^r} \text{supp} N_i^r \), where \( \text{int} A := A \setminus \partial A \) denotes the interior of a set \( A \).

The following definition of a **globally refined basis** is necessary for proving strict nestedness for the chosen hierarchical refinement strategy:

**Definition 5** (Globally refined basis). Given a basis \( M^0 \), the basis \( M^1 \) is said to be globally refined with respect to \( M^0 \) if and only if for all \( N \in M^0 \)

\[
\# \{N^r_i \in M^1 : \text{supp}^r N^r_i \subset \text{supp}^r N\} > \# \{N_i \in M^0 : \text{supp}^r N_i \subset \text{supp}^r N\}
\]

**Remark 6.** Definition \([5]\) does not imply that \( \text{span}(M^1) \subset \text{span}(M^0) \). However, for the globally \( h \)-refined sequence of B-splines employed in this work, this is indeed the case.

**Lemma 6.** Let \( M^0 \) and \( M^1 \) be sets of locally linearly independent functions on \( \tilde{\Omega} \) such that \( \text{span}(M^1) \supset \text{span}(M^0) \) and \( M^1 \) be globally refined with respect to \( M^0 \). Let \( \hat{\Omega}_a \) be an open subset of \( \tilde{\Omega} \) such that \( \forall N \in M^0 : \text{supp}^r N \subset \hat{\Omega}_a \). For the sets \( M^0_1 := \{N \in M^0 : \text{supp}^r N \subset \hat{\Omega}_a\} \) and \( M^1_1 := \{N \in M^1 : \text{supp}^r N \subset \hat{\Omega}_a\} \) it holds that

\[
\text{span}(M^1_1) \supset \text{span}(M^0_1)
\]

**Proof.** The same approach as the first part of the proof for Proposition \([4]\) is followed, except with \( \#M^1_1 \neq 0 \) due to the restriction on the selection of the refinement region \( \hat{\Omega}_a \). Furthermore, by Definition \([5]\) \( \dim(M^1_1) > \dim(M^0_1) \), whereby \( \text{span}(M^1_1) \supset \text{span}(M^0_1) \). Hence it holds that \( \text{span}(M^1_1) \supset \text{span}(M^0_1) \).

**Proposition 7** (Strict nestedness of hierarchical B-spline spaces). Let \( (N^r)_{0 \leq r \leq R} \) be a sequence of globally refined B-spline bases and let the refinement regions be chosen with the restriction that \( \exists N_i^r \in N^r : \hat{\Omega}_a^{r+1} \supset \text{supp}^r N_i^r \). The space spanned by the resulting hierarchical B-spline basis \( H^R \) is strictly nested within the space spanned by \( H^{R+1} \) that is obtained by a further refinement of \( H^R \).

**Proof.** Again, the proof is similar to that of Proposition \([4]\). The first part is replaced with Lemma \([6]\) to conclude that \( \text{span}(H^{R+1}) \supset \text{span}(H^R \setminus H^{R+1}) \). In the second part, we have \( \text{span}(H^{R+1}) \supset \text{span}(H^R \cap H^{R+1}) \) thanks to the restriction on \( \hat{\Omega}_a \) that guarantees refinement. Combining the two proves that \( \text{span}(H^{R+1}) \supset \text{span}(H^R) \).

**Remark 7.** Limiting refinement regions \( \hat{\Omega}_a \) to unions of basis function supports makes the adaptive algorithm basis dependent. However, in the case of B-splines, this is not an arbitrary choice and relates directly to the spanned polynomial space, since B-splines form a least support basis due to their local linear independence \([41]\).

Refinement of an already refined basis \( H^R \) requires assigning the region \( \tilde{\Omega} \setminus \hat{\Omega}_a \), which is marked based on some indicator, to a level \( i \leq R \). Due to the requirement that \( \hat{\Omega}_a^r \geq \hat{\Omega}_i^r \), when the marked region \( \hat{\Omega}_a \) is added to \( \hat{\Omega}_a \), all lower level selections \( 0 < r < i \) also have to be adjusted such that \( \hat{\Omega}_a^r \geq \hat{\Omega}_i^r \). The selection of level \( i \) is done through inspecting which level \( i \) of the selection \( N_i^r \in H^R \cap H^R_i \) that contributes to the refinement region \( \hat{\Omega}_a \) belongs to. The process of selecting a refinement level from a certain selection of functions \( N_i^r \subset H^R \) and the readjustment of the refinement regions based on this is outlined in Algorithm \([1]\).

**Remark 8.** It is also possible to have coarsening with hierarchical B-splines by choosing a coarsening region and subtracting it from the refinement regions.

3. **Goal-oriented error estimation and adaptivity**

In the adaptive refinement of discretizations, local refinement indicators are used to determine the regions in the computational domain that need a finer discretization. Most often, these
Algorithm 1 Readjustment of selected regions for further refinement

function READJUST(\(\mathcal{R}\))
for all \(N_i \in N_h\) do
\(\mathcal{R}_{e+1} \leftarrow \text{int}(\mathcal{R}_{e+1} \cup \text{supp}(N_i))\)
end for
end function

indicators are based on a method of error measurement and the partitioning of the estimator into localized contributions. Therefore, for an efficient adaptive method it is important to have a good error estimator and reliable local refinement indicators based on this estimator. Many concepts on goal-oriented error estimation from the finite element literature apply directly to Isogeometric Analysis. In this work, the originality in terms of goal-adaptivity is the construction of an error estimator for hierarchical B-spline discretizations, the extraction of suitable local refinement indicators from it, and the study of their properties. The application of goal-oriented error estimation to Isogeometric Analysis can be found in [42] for free boundary problems and in [43] for non-linear rods, where in the latter k-refinement Analysis can be found in [42] for linear problems.

3.1. Goal-oriented error estimation

The aim in goal-oriented error estimation is having a quantitative estimate of the influence of the discretization error on a chosen quantity of interest. Here, we recall the derivation of the goal-oriented error estimation for linear problems and linear quantities of interest. Extension to non-linear cases is possible (see e.g. [44, 38, 45, 46]).

Let a linear problem be given in the abstract form:

Find \(u \in V\) such that:

\[ \mathcal{B}(u, v) = \mathcal{L}(v) \quad \forall v \in V \]  

with continuous linear form \(\mathcal{L}(\cdot)\) and continuous bilinear form \(\mathcal{B}(\cdot, \cdot)\) coercive on \(V\), where \(V\) is a Hilbert space, typically a Sobolev space. The corresponding conforming Galerkin approximation writes:

Find \(u^h \in V^h \subset V\) such that:

\[ \mathcal{B}(u^h, v^h) = \mathcal{L}(v^h) \quad \forall v^h \in V^h \]  

The discretization error is defined as:

\[ e := u - u^h \]  

where \(e \in V\), with \(u \in V\) being the exact solution and \(u^h \in V^h\) being its Galerkin approximation. For Galerkin approximations of linear problems, the following holds for the error:

\[ \mathcal{B}(e, \psi^h) = 0 \quad \forall \psi^h \in V^h \]  

which is called Galerkin orthogonality.

The residual functional \(\mathcal{R}(\cdot) : V \rightarrow \mathbb{R}\) for the Galerkin approximation \(u^h\) is defined as follows:

\[ \mathcal{R}(v) := \mathcal{L}(v) - \mathcal{B}(u^h, v) = \mathcal{B}(u, v) - \mathcal{B}(u^h, v) = \mathcal{B}(v, e) \]  

Our quantity of interest is represented by a linear goal functional \(Q(\cdot) : V \rightarrow \mathbb{R}\) of the solution, whereby the error in the quantity of interest is expressed as:

\[ Q(u) - Q(u^h) = Q(u - u^h) = Q(e) \]  

For finding the error in terms of the goal functional, the following dual problem is introduced:

Find \(z \in V\) such that:

\[ \mathcal{B}(v, z) = Q(v) \quad \forall v \in V \]  

Noticing that \(e \in V\), equation \((10)\) is also valid for \(v = e\). Hence for \(e\) it holds that \(\mathcal{B}(e, z) = Q(e)\). Using this and \((9)\), the exact error in the quantity of interest can be expressed as:

\[ Q(u) - Q(u^h) = \mathcal{B}(e, z) \]  

Due to Galerkin orthogonality \((7)\) it holds that \(\forall \psi^h \in V^h\), \(\mathcal{B}(e, z) = \mathcal{B}(e, z - \psi^h)\). Using this, the expression in \((11)\) can be rewritten as:

\[ Q(u) - Q(u^h) = \mathcal{B}(e, z - \psi^h) = \mathcal{L}(z - \psi^h) - \mathcal{B}(u^h, z - \psi^h) = \mathcal{R}(z - \psi^h) \]  

\(\forall \psi^h \in V^h\), which can be directly evaluated if an approximation \(\hat{z} \approx z\) is found such that \(\mathcal{B}(\hat{z}) \approx Q(v)\), \(\forall v \in V\). Using the approximate dual solution a goal-oriented error estimator is obtained by evaluating the dual-weighted residual for any \(\phi^h \in V^h:\)

\[ Q(u) - Q(u^h) \approx \mathcal{R}(\hat{z} - \psi^h) =: \text{Est} \]  

In FEM, a common way of obtaining \(\hat{z}\) is through Galerkin discretization of the dual problem \((10)\) with \(\hat{z} \in \hat{V} \subset V\). The discretized dual problem is then stated as:

Find \(\hat{z} \in \hat{V}\) such that:

\[ \mathcal{B}(v, \hat{z}) = \mathcal{L}(v) \quad \forall v \in \hat{V} \]  

6
Remark 9. The solution space for the dual problem, $\hat{V}$, should not be in $V^h$, i.e. $\hat{V} \not\subseteq V^h$. Otherwise $B(e, z) = 0$ by (7) and hence $\text{Est} = 0$. $\hat{V}$ is often taken such that $\hat{V} \supseteq V^h$.

With the strategy of refining regions composed of function supports introduced in Section 2, methods of marking regions that comply with this marking restriction are needed. With this ingredient to be addressed later on, the goal-adaptive procedure is outlined in Algorithm 2.

Algorithm 2 Goal-adaptive algorithm with hierarchical splines

\begin{verbatim}
 i ← 0, $\mathcal{H}^i \leftarrow N_0^p$, $\hat{\mathcal{H}}^i \leftarrow N_{p+1}^0$
 while $i \leq h_{\max}$ do
 $u^h \leftarrow \text{solve primal}(\mathcal{H}^i)$, $\hat{z} \leftarrow \text{solve dual}(\mathcal{H}^i)$
 $\hat{\Omega}_{r+1}^i \leftarrow \text{mark supports}(u^h, \hat{z})$
 $\mathcal{H}^{i+1} \leftarrow \text{refine}(\mathcal{H}^i, \hat{\Omega}_{r+1}^i)$, $\hat{\mathcal{H}}^{i+1} \leftarrow \text{refine}(\hat{\mathcal{H}}^i, \hat{\Omega}_{r+1}^i)$,
 $i \leftarrow i + 1$
end while
\end{verbatim}

3.2. The discrete dual problem

The dual problem is also approximated using Galerkin methods with suitable discrete spaces. In the context of Isogeometric Analysis, there are multiple options for the discretization of the dual problem. In classical FEM the goal-oriented estimators are often obtained using discrete dual spaces that result from uniform $h$- or $p$-refinement of the primal basis. In Isogeometric discretizations, due to the additional freedom in adjusting smoothness across elements, there are many more possibilities for the choice of the dual space $\hat{V}$, even with tensor product spaces. In [47], an overview of the choices is provided with dimensions of the dual spaces. An interesting approach that is unique to Isogeometric Analysis is the application of $k$-refinement for the dual discretization, which reduces computational cost compared to the more conventional $h$- and $p$-refinement. Error estimation with $k$-refined dual discretizations has been investigated on uniform meshes in [43].

In this work, we limit ourselves to the rather safe choice of $p$-refined dual discretizations: For an $h, p, k$ approximation of the primal solution, the proposed estimator will be based on an $h, p + 1, k$ approximation of the dual solution. This means that element sizes $h$, inter-element continuities $k$ and geometries of elements match for the dual and primal meshes, but the discrete dual solution will have a degree $p + 1$ polynomial approximation, compared to degree $p$ for the primal solutions. With this choice $\hat{V} \supseteq V^h$ and the dual basis functions have similar supports to the primal basis functions. This is relevant because the adaptive algorithm uses function supports as refinement regions and the refinement of primal and dual meshes are performed in conjunction. The dual basis corresponding to the primal basis of Figure 2 is given in Figure 4.

For the chosen estimator, based on an $h, p + 1, k$ approximation of the dual solution, the dual space has the property that $\hat{V} \supseteq V^h$ on an unrefined B-spline mesh. However, this property is not necessarily valid once $V^h = \text{span}(\mathcal{H}^i)$ has been refined. To have an estimator that behaves similarly after adaptive refinements, it is proposed that dual space $\hat{V} = \text{span}(\mathcal{H}^i)$ is adapted alongside $V^h$ using the same refinement regions $\hat{\Omega}_{r+1}^i$.

The choice of having $\mathcal{H}^i$ and $\hat{\mathcal{H}}^i$ refined simultaneously, at least guarantees that $\hat{V} \supseteq V^h$, which is a property of the initial B-spline spaces:

**Theorem 8.** Let $\mathcal{H}^0$ be a hierarchically refined basis that uses globally $h$-refined B-spline bases $(N_r^0)^{0 \leq r}$ of degree $p$ with a sequence of refinement regions $(\hat{\Omega}_{r+1}^i)^{0 \leq r}$ such that $\hat{\Omega}_r^i$ contains the support of at least one function from $N_r^0$ and let $\mathcal{H}^i$ be a hierarchically refined basis that uses the same refinement regions $(\hat{\Omega}_{r+1}^i)^{0 \leq r}$ with globally $h$-refined B-spline bases $(N_r^0)^{0 \leq r}$ of degree $p + 1$ with elements matching those of $(N_r^0)^{0 \leq r}$. The following holds for these bases:

$$\text{span}(\mathcal{H}^i) \supseteq \text{span}(\hat{\mathcal{H}}^i)$$

**Proof.** Due to the property that a B-spline space is nested in its $p$-refined space, it holds that:

$$\text{span}(\mathcal{H}^i) \supseteq \text{span}(N_r^0)$$

(14)

For the hierarchically refined basis at a level $r + 1 > 1$, it follows from Definition 1 that:

$$\text{span}(\mathcal{H}^{r+1}) = \left(\text{span}(\mathcal{H}^r) \setminus \text{span}(N_{r-1}^0)\right) \cup \text{span}(N_r^0)$$

(15)

where $N_r^0 = \{ N \in N_r^0 : \text{supp}^p N \subseteq \hat{\Omega}_r^i \}$. Both $N_r^0$ and $\hat{N}_r^0$ are nonempty due to the support restriction on the selection of $\hat{\Omega}_r^i$.

Similar to (15), it also holds that $\text{span}(\hat{\mathcal{H}}^{r+1}) = \left(\text{span}(\hat{\mathcal{H}}^r) \setminus \text{span}(N_{r-1}^0)\right) \cup \text{span}(\hat{N}_r^0)$, which implies $\text{span}(\hat{\mathcal{H}}^{r+1}) \supseteq \text{span}(\hat{N}_r^0)$. Comparing the newly added primal and dual basis functions, by Lemma 5 it should hold that $\text{span}(\hat{N}_r^0) \supseteq \text{span}(N_r^0)$ for a marked region $\hat{\Omega}_r^i \subseteq \hat{\Omega}$, since $\hat{N}_r^0$ is globally $p$-refined with respect to $N_r^0$ and $\text{span}(\hat{N}_r^0) \supseteq \text{span}(N_r^0)$, whereby it is proven that

$$\text{span}(\hat{\mathcal{H}}^{r+1}) \supseteq \text{span}(N_r^0)$$

(16)
For the initial spaces, (14) is valid as they have not undergone any refinement. Thus:

\[
\text{span}(H^1) \subseteq \text{span}(\hat{H}^1) \supseteq \text{span}(\hat{H}^2) \tag{17}
\]

and for the next step

\[
\text{span}(\hat{H}^2) \subseteq \left(\text{span}(H^1) \setminus \text{span}(N_h^i)\right) \cup \text{span}(N_h^i) \tag{18}
\]

Using (16) and the result from the previous step, the same process as in going from (17) to (18) can be repeated to yield \( \text{span}(\hat{H}^3) \supseteq \text{span}(H^3) \).

### 3.3. Refinement indicators for hierarchical B-spline bases

The chosen refinement strategy with hierarchical B-splines is based on marking function supports for refinement, as explained in Section 2. This is somewhat different from the adaptive methods based on marking of elements. In this section, two methods are introduced for obtaining refinement indicators localized to function supports from the global goal-oriented error estimator proposed earlier. The employed marking strategy will also be explained for the two indicators.

#### 3.3.1. A function support refinement indicator

A natural way of obtaining local indicators from error estimation is by partitioning the estimator into local contributions. Since the indicators are meant for function supports, the error is partitioned into basis function contributions. Differently from element partitions, basis function supports in general do not form a disjoint partition of the computational domain, i.e. \( \forall N_i \in H^k, \exists N_j \in H^k : \text{supp}_g N_i \cap \text{supp}_g N_j \neq \emptyset \) if \( p \neq 0 \), with \( H^k \), \( V^h = \text{span}(H^k) \) being the primal basis.

Considering B-splines of degree \( p > 0 \), it holds that \( \hat{\Omega} = \bigcup_{N_i \in H^k} \text{supp}_g N_i \), and with the assumption that the domain parametrization \( T : \hat{\Omega} \rightarrow \Omega \) is a continuous map, it also holds that \( \hat{\Omega} = \bigcup_{N_i \in H^k} \text{supp}_g N_i ^t \), where \( N_i ^t = N_i \circ T^{-1} \). This allows for splitting up any \( C^1(\Omega) \)-continuous function \( f \) in the following way:

\[
f = \sum_{i : N_i \in H^k} f_i \tag{19}
\]

where \( f_i \) are \( C^1(\Omega) \)-continuous partitions of \( f \) local to the support of the basis function \( N_i \); namely, \( f_{i, \text{supp}_g N_i} \in C^1(\text{supp}_g N_i) \) and \( f_{i, \partial \Omega} = 0 \) on \( \partial \Omega \). It can be required that \( f_{i, \text{supp}_g N_i} \|_{\partial \Omega} = 0 \) thanks to the overlap of supports; i.e. all points on \( \partial \text{supp}_g N_i \setminus \partial \Omega \) are interior points of the support of some other basis function \( N_j \in H^k \). This is the approach that is taken in splitting the dual solution, \( \hat{z} \in C^0(\hat{\Omega}) \) with \( 0 \leq k < p \), and its approximation in \( V^h, \psi^h \), that are in the argument of the dual-weighted residual (12). For approximating \( \hat{z} \) with \( \psi^h \in V^h \), \( L^2 \)-orthogonal projection is selected for convenience. Since \( L(.) \) and \( B(\psi^h, \cdot) \) consist only of integrals over the whole domain \( \Omega \) and the boundary \( \Gamma \), the partitioning of \( \hat{z} - \psi^h \) in this way results in integrals over basis function supports \( \text{supp}_g N_i ^t \). With this approach, the error estimator can be rewritten as:

\[
\text{Est} = \mathcal{R}^h(\hat{z} - \psi^h) = \sum_{i : N_i \in H^k} \mathcal{R}^i (\hat{z}_i - \psi_i^h) = \sum_{i : N_i \in H^k} \eta_i^h
\]

with support contributions:

\[
\eta_i^h = \mathcal{R}^i (\hat{z}_i - \psi_i^h) \tag{20}
\]

\( \eta_i^h \) is the support refinement indicator for basis function \( N_i \). With a marking ratio \( \lambda \in [0, 1] \), the marked region using the function support indicator is given as:

\[
\hat{\Omega}_s^\lambda = \bigcup_{N_i \in H^k} \text{supp}_g N_i \in H^k : \eta_i^h = \lambda \max_{N_i \in H^k} |\eta_i^h| \tag{21}
\]

which is essentially a maximum marking strategy for supports.

**Remark 10.** The function support partitioning of the global error estimator results in refinement indicators that are basis dependent.

For the partitioning of \( \hat{z} - \psi^h \), the basis \( \mathcal{H}^k \) of the dual space \( \hat{V} \) can be conveniently made use of. For the proposed indicator, we choose to separate \( \hat{z} - \psi^h \) into locally supported functions in the following way:

\[
\hat{z}_i - \psi_i^h = \sum_{j : N_j \in H^k} \hat{z}_j - \psi_j^h \tag{22}
\]

where \( \mathcal{H}^k = \{ N_i \in H^k : \text{supp}_g N_i \subseteq \text{supp}_g N_i ^t \} \) for a primal basis function \( N_i \in H^k \) and \( \mathcal{H}^k = \{ N_i \in H^k : \text{supp}_g N_i \subseteq \text{supp}_g N_i ^t \} \) for a dual basis function \( N_j \in \mathcal{H}^k \). The constants \( \hat{z}_j \) and \( \psi_j^h \) are the coefficients of the dual basis function \( N_j \). The expression (22) essentially distributes the dual basis function contributions \( \hat{z}_j N_j ^t \) and \( \psi_j^h N_j ^t \) equally to all primal basis functions \( N_j ^t \) whose supports contain \( \text{supp}_g N_i ^t \).

**Remark 11.** By Theorem 8 and the local linear independence of single-level B-spline bases, it can be shown that both sets \( \mathcal{H}^k \) and \( \mathcal{H}^k \) seen in (22) are nonempty.

**Remark 12.** For this particular partition, it is necessary that \( \text{span}(\mathcal{H}^k) = \hat{V} \supset V^h \), whereby it is possible to express any \( \psi^h \in V^h \) in terms of the dual basis as in \( \psi^h = \sum_{j \in H^k} \psi_j^h N_j ^t \).

#### 3.3.2. An element-based refinement indicator

Apart from creating refinement indicators specifically meant for function supports, it is also possible to use element refinement indicators for marking and subsequently to extend the marked elements to function supports by including neighboring elements.

Given a partial differential equation expressed in the form \( L u = f \) in \( \Omega \), with a differential operator \( L \) of order at most \( k + 1 \), appropriate boundary conditions on \( \partial \Omega \) and an approximate solution \( \psi^h \in V^h \subset C^0(\Omega) \); the element indicators are defined as:

\[
\eta_i = \int_{K_i} (f - Lu^h)(\hat{z} - \psi^h) \text{d}x + \int_{\partial K_i \cap \partial \Omega} G(\hat{z} - \psi^h) \text{d}s \tag{23}
\]

with \( G(\cdot) \) denoting the integrand of any integrals over \( \partial \Omega \) present in the expression for \( \mathcal{R}^h(\cdot) \).
Remark 13. Indicators of the form (23) can be obtained by elementwise integration by parts of the dual-weighted residual (12). The absence of interior boundary terms is due to the discrete solution having continuous \( k \)th derivatives; the boundary terms resulting from the elementwise integration by parts cancel across the interior element edges, affirming that \( \text{Est} = \sum_{i:K_i \in \mathcal{T}_h} \eta_i \) also when they are discarded from the element contributions. In Section 4.1 this is exemplified for the \( C^1 \) discretizations of the Laplace operator.

It must be noted that the indicator \( \eta_i \) given in (23) is the refinement indicator of an individual element. In the proposed element-based method, the marking decision is done based on the element indicator \( \eta_i \)

\[
\mathcal{T}_h^\ast = \{ K_i \in \mathcal{T}_h : |\eta_i| \geq \lambda \max_{K \in \mathcal{T}_h} |\eta_K| \}
\]

using a marking ratio \( \lambda \in (0, 1) \). Afterwards, a marked element \( K_i \in \mathcal{T}_h^\ast \) is extended to a function support \( \text{supp}^\ast N_i \supseteq K_i \) by taking the combinations of indicators for neighboring elements which yield the highest refinement indicator:

\[
\hat{\Omega}_h^\ast = \text{supp}^\ast N_i \quad \text{with} \quad N_i = \arg \max_{K \in \mathcal{H}_h^\ast} \left| \sum_{\eta_K \in \Omega_h} \eta_K \right| \quad (24)
\]

where \( \mathcal{H}_h^\ast = \{ N \in \mathcal{H}_h : \text{supp}^\ast N \supseteq K \} \) is the set of basis functions that have some support over \( K_i \) and \( \text{supp}^\ast N = \{ K \in \mathcal{T}_h : K \supseteq \text{supp}^\ast N \} \) is the set of elements that are within the support of basis function \( N \). The refinement region is then the union of all such regions for every marked element:

\[
\hat{\Omega}_h^\ast = \text{int} \bigcup_{i:K_i \in \mathcal{T}_h} \overline{\hat{\Omega}_h^\ast} \quad (25)
\]

Remark 14. This process of combining elements to obtain suitable refinement regions as required by the hierarchical refinement algorithm (Algorithm 6) is analogous to the completion procedures in traditional adaptive methods, which are used for obtaining conforming discrete spaces after a bisection operation.

4. Numerical simulations

In this section we first consider the Poisson problem to study the quality of the proposed error estimators under uniform mesh refinement and its adaptive discretization on an L-shaped domain. The effectivity of the refinement indicators in combination with the proposed adaptivity approach is then studied. Finally the adaptive discretization of a prototypical free-surface flow problem is demonstrated. For both problems two-dimensional domains are considered.

4.1. The Poisson problem

We consider the Poisson problem over a domain \( \Omega \) with homogeneous Dirichlet conditions over the boundary \( \Gamma_D \), and general Neumann boundary conditions over the boundary \( \Gamma_N \). Note that \( \Gamma_D \cup \Gamma_N = \partial \Omega \) and \( \text{int}(\Gamma_D) \cap \text{int}(\Gamma_N) = \emptyset \). The weak form problem is given by Problem 4 with

\[
\mathcal{B}(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad \mathcal{L}(v) = \int_{\Omega} f v \, dx + \int_{\Gamma_N} g v \, ds \quad (26)
\]

and

\[
V = \{ v \in H^1(\Omega) : v|_{\partial \Omega} = 0 \} \quad (27)
\]

where \( f \) and \( g \) represent the source term and Neumann data, respectively. The corresponding dual problem is given by problem 10 using the same bilinear form \( \mathcal{B}(\cdot, \cdot) \), a linear goal functional \( Q(u) \), and the dual space \( V = H^1_0(\Omega) \).

For this problem, the function support indicator (20) as introduced in Section 3.3.1 substantiates as

\[
|\eta_i^\ast| = \left| \int_{\text{supp}^\ast \text{supp}^\ast N_i} g(z - \psi^h) \, ds \right| - \left| \int_{\text{supp}^\ast \text{supp}^\ast N_i} \nabla u^h \cdot \nabla (z - \psi^h) - (z - \psi^h) f \, dx \right| \quad (28)
\]

The element-based refinement indicator (23) as introduced in Section 3.3.2 follows as

\[
|\eta_i| = \left| \int_{\text{supp}^\ast \text{supp}^\ast \Omega_h} (g - \nabla u^h \cdot \mathbf{n})(z - \psi^h) \, ds \right| + \left| \int_{\Omega_h} (\Delta u^h + f)(\hat{z} - \psi^h) \, dx \right| \quad (29)
\]

For both indicators, \( \psi^h \in V^h \) is taken as the orthogonal \( L^2 \)-projection of \( \hat{z} \) onto \( V^h \).

4.1.1. Effectivity of the error estimators

Effectivity of an estimator is defined as the ratio of the actual error and the estimated error:

\[
\eta_{\text{eff}} = \frac{\text{Est}}{Q(u) - Q(u^h)}
\]

To assess the effectivity of the proposed error indicators, we first consider the convergence of their corresponding error estimators under uniform refinement. We consider the domain \( \Omega = (-0.5, 0.5) \times (-0.5, 0.5) \) with homogeneous Dirichlet conditions over \( \Gamma_D = \partial \Omega \) and the source term that satisfies (26) when the exact solution is given by \( u(x, y) = (x - 1/2)^2(y - 1/2)(y - 1/2)/((x + 2/3)(y + 3/4)) \). The quantity of interest is taken as the average value of the solution over the whole domain, i.e. \( Q(u) = \int_{\Omega} u \, dx \).

The primal and dual problems are discretized on uniformly \( h \)-refined meshes with \( C^{p+1} \)-continuous B-splines of degree \( p \) and \( p + 1 \), respectively. In Figure 5, the actual and estimated errors are plotted against the dimension of the discrete primal space, \( n \), along with their effectivity indices. The observed optimal convergence rates for the errors, i.e. \(-2p/d\) of the exact error by the theory of ordinary adaptive FEM [48], and the effectivity indices approach 1 demonstrate that the error estimator adequately reflects the error in the quantity of interest.
Figure 5: Study of the estimator under uniform refinement

In Figure 5 the sum of the absolute value of refinement indicators is plotted for both localizations of the estimated error. The observed optimal rates of convergence for both indicators suggest that the proposed refinement indicators are asymptotically equivalent to the actual error in the quantity of interest.

4.1.2. Adaptive discretization on an L-shaped domain

We next consider the adaptive discretization of the homogeneous Poisson problem (i.e. $f = 0$) on the L-shaped domain as shown in Figure 5. Homogeneous Dirichlet conditions are assumed over the boundary $\Gamma_D$ and the Neumann data over $\Gamma_N$ is given by

$$g(x, y) = \begin{cases} 
g_1(x, y) & x > y \text{ and } (x, y) \in \Gamma_N \\
g_2(x, y) & x \leq y \text{ and } (x, y) \in \Gamma_N \\
-g_2(x, y) & x > y \text{ and } (x, y) \in \Gamma_N \\
-g_1(x, y) & x \leq y \text{ and } (x, y) \in \Gamma_N 
\end{cases}$$

(30)

Figure 6: Convergence of the refinement indicators under uniform mesh refinement
Figure 7: Description of the L-shaped domain

with \( \Gamma_{N_1} \) and \( \Gamma_{N_2} \) as described in Figure 7 and

\[
g_1(x, y) = 2 \left[ x \sin \left( \frac{2\theta(x, y)\pi}{3} \right) - y \cos \left( \frac{2\theta(x, y)\pi}{3} \right) \right] \frac{3(x^2 + y^2)^{2/3}}{3\sqrt{2}}
\]

\[
g_2(x, y) = 2 \left[ y \sin \left( \frac{2\theta(x, y)\pi}{3} \right) + x \cos \left( \frac{2\theta(x, y)\pi}{3} \right) \right] \frac{3(x^2 + y^2)^{2/3}}{3\sqrt{2}}
\]

where \( \theta(x, y) \) is the clockwise angle between the \( x \)-axis and the line connecting points \((0, 0)\) and \((x, y)\). We choose the quantity of interest as:

\[
Q(u) = u(1, -1) = \int_\Omega u(x, y) \delta(1 - x) \delta(-1 - y) \, dx \tag{31}
\]

where \( \delta \) is the Dirac distribution. For the exact solution \( Q(u) = \sqrt{2}/2 \). It is to be noted that in this case both the primal problem and the dual problem incur singularities, near \((0, 0)\) and \((1, -1)\), respectively.

For the discretization of the primal problem a series of hierarchically refined B-spline spaces \( V_h = \text{span}(H^\prime) \cap V \subset C^1(\bar{\Omega}) \) constructed from a hierarchy of continuously differentiable \( h \)-refined second order B-spline bases \( N_r \). For the discretization of the dual problem, a series of discrete spaces \( \hat{V} = \text{span}(\hat{H}^\prime) \cap V \) constructed from a hierarchy of \( C^1 \)-continuous \( h \)-refined third order B-spline bases \( \hat{N}_r \) is chosen. To ensure \( C^1 \)-continuity throughout the interior of the domain, the L-shaped geometry is parametrized using repeating control points at the corners \((0, 0)\) and \((1, 1)\), as also been done e.g. in [1, Fig. 17]. The refinement indicators used for this problem are expressed in (28) and (29).

For the marking strategy three ratios \( \lambda \in \{0.95, 0.5, 0.25\} \) are used, meaning all regions with indicator \( |\eta| \geq \lambda |\eta_{\text{max}}| \) are marked for refinement. The solutions of the primal and the dual problems after 50 refinement steps with \( \lambda = 0.95 \) are plotted in Figure 8. The Bézier meshes after 15, 30 and 60 refinement steps using both indicators are plotted in Figure 9 for the case \( \lambda = 0.95 \). As would be expected, refinement with both indicators is generally concentrated around the singularities of the primal and the dual solutions, namely near the re-entrant corner at the origin and the location of the quantity of interest, \((1, -1)\). Overall, the element-based indicator appears to mark less per refinement step. This behavior can be attributed to the fact that, with the support indicator, a single element that has a large er-
error can result in the marking of multiple basis functions whose supports contain that element.

The exact and estimated errors are plotted versus the number of degrees of freedom in Figure 10 for the three marking ratios. Due to the singularities in the primal and dual solutions, the uniform-refinement approximation converges at a suboptimal rate of $-3/2$. The adaptive approximation recovers the optimal convergence rate of $-2$, for both the support indicator and the element-based indicator. Furthermore, the accuracy of the adaptive discretizations is not very sensitive to how liberally marking is performed, as described by the parameter $\lambda$. This is beneficial in limiting the number of intermediate solves in the adaptive algorithm. Both indicators show similar behavior in terms of the improvement of accuracy per added degree of freedom, with the support indicator performing only slightly better.

The effectivities of the error estimators (Figure 11) stay in similar regions for adaptive discretizations using the two indicators. Although the actual error is underestimated by the estimator in both cases, they are in close agreement with the error for most part, at a level above or around 70% of the actual error. The adaptive discretizations using the element indicator slightly outperforms those with the support indicator in terms of the accuracy of the estimated error.

In Table 1 we give a general indication of the total computational cost of the proposed adaptive algorithm, for various values of the marking parameter $\lambda$. In all cases investigated here except for the adaptive refinement based on the element indicator with the impractical marking ratio of $\lambda = 0.95$, the total cost of the adaptive algorithm is smaller than a single solve of the uniformly refined case. For the adaptive discretizations, $n$ denotes the number of degrees of freedom after the last refinement step. Cholesky (LDLT) decomposition is used for all linear solves. The underperformance of the element-based indicator in terms of the total CPU time can be attributed to the fact that for a given $\lambda$, the support indicator marks much more liberally; whereby the same error level is reached with a much smaller number of refinement steps. Lastly, it is worth noting

Figure 10: Errors in the quantity of interest under adaptive discretization of the Poisson problem on the L-shaped domain, with various marking ratios

Figure 11: Effectivity indices under adaptive discretization of the Poisson problem on the L-shaped domain, with $\lambda = 0.95$
Table 1: CPU times with various values of the marking parameter $\lambda$

| Discretization | $n$ | $|Q(u) - Q(u^h)|$ | CPU time |
|----------------|-----|-----------------|----------|
| Uniform        | 2244| 5.72972 · 10^{-3}| 155 s    |
| Supp. ind., $\lambda = 0.25$ | 294 | 5.47364 · 10^{-5} | 13 s     |
| Supp. ind., $\lambda = 0.5$  | 325 | 4.91581 · 10^{-5} | 19 s     |
| Supp. ind., $\lambda = 0.95$ | 315 | 5.48413 · 10^{-5} | 44 s     |
| Elem. ind., $\lambda = 0.25$ | 314 | 5.63982 · 10^{-5} | 135 s    |
| Elem. ind., $\lambda = 0.5$  | 301 | 6.19853 · 10^{-5} | 150 s    |
| Elem. ind., $\lambda = 0.95$ | 301 | 6.19853 · 10^{-5} | 232 s    |

Figure 12: Description of the notched channel domain for the free-surface flow problem

that the CPU times are obtained with no effort on optimizing the implementation of the adaptive algorithm.

4.2. Free-surface flow

We consider the Bernoulli free-boundary problem (22) over the domain depicted in Figure 12 as a prototypical free-surface problem for a flow through a notched channel. This problem is particularly of interest to B-spline discretizations, since the dual problem contains the curvature of the free surface for which higher-continuity discrete geometries are preferred. Laplace’s equation, i.e., $\Delta u = 0$, is solved over the domain $\Omega$ while Dirichlet boundary conditions are prescribed over the fixed part of the boundary, homogeneous over $\Gamma_D$ and nonhomogeneous over $\Gamma_D^b$, according to $u = u_D = y$. Over the free boundary $\Gamma$, both Neumann and Dirichlet conditions are prescribed as $u = u_D = 1$ and $\frac{\partial u}{\partial n} = g = 1$.

In order to satisfy both boundary conditions, the boundary $\Gamma$ has to attain a specific shape, which makes the Bernoulli problem a free-boundary problem. Since the solution to the boundary value problem depends on the position of the free-surface and vice versa, this problem is inherently non-linear. We employ the explicit Neumann update scheme (42) to solve the free boundary problem. Alternatively, a Newton scheme can be found in (51).

As a reference configuration, a free surface $\Gamma_0$ is assumed (i.e., a horizontal surface at $y = 1$). The displacement of the free boundary is parametrized with respect to this reference configuration using the displacement field $\theta : \Gamma_0 \rightarrow \mathbb{R}^2$. The boundary in the current configuration is denoted by $\Gamma_\theta$. The corresponding domain $\Omega_\theta$ is defined with respect to the initial domain $\Omega_0$, where the deformation is found through the solution of an auxiliary vector Laplacian problem with $\theta$ as the Dirichlet condition on $\Gamma_0$ and homogeneous Dirichlet conditions on $\Gamma_D$.

In the Neumann scheme, based on the iteratively approximated free-boundary $\theta^\epsilon$ and the approximate domain $\Omega_\theta^\epsilon$, the weak problem (41) is solved with

$$B_{\theta^\epsilon}(u, v) = \int_{\Omega_\theta^\epsilon} \nabla u \cdot \nabla v \, dx \quad \mathcal{L}_{\theta^\epsilon}(v) = \int_{\Gamma_\theta^\epsilon} gv \, ds$$

and

$$U_{\theta^\epsilon} = \{ u \in H^1(\Omega_\theta^\epsilon) : u|_{\Gamma_D^b} = u_D \} \quad V_{\theta^\epsilon} = \{ v \in H^1(\Omega_\theta^\epsilon) : v|_{\Gamma_D} = 0 \}$$

For the discretization of this problem $C^1$-continuous, second order hierarchically refined spline spaces are constructed on an approximate current configuration $\Omega_\theta^\epsilon$. To ensure $C^1$-continuity in the interior and the free boundary, the kinks in the geometry of the notch are parametrized by repeating control points.

Once the free-surface problem is solved, a dual problem linearized around the approximate free boundary $\Gamma_\theta^\epsilon$ can be solved over the deformed domain $\Omega_\theta^\epsilon$. The derivation of the shape-linearized dual problem can be found in (52). Here we consider the elevation $\alpha^\theta(x)$ of the free boundary $\Gamma_\theta^\epsilon$ at point $x = 2 + \sqrt{2}$ as the goal functional

$$Q_\theta(u) = \int_{\Gamma_0} q_{bd}^\theta \alpha^\theta \, ds \quad \text{and} \quad q_{bd}^\theta(x) = \delta(x - 2 - \sqrt{2})$$

where the elevation is measured from $\Gamma_0$. A reference value for this quantity of interest is obtained from (42) as 0.02269.

The weak form dual problem is given by (10) with

$$B_{\theta^\epsilon}(z, v) = \int_{\Omega_\theta^\epsilon} \nabla v \cdot \nabla z \, dx + \int_{\Gamma_\theta^\epsilon} \frac{\partial g}{\partial n} + k^\theta g \frac{\partial g}{\partial n} \frac{\partial z}{\partial n} \, ds$$

and

$$\mathcal{L}_{\theta^\epsilon}(v) = - \int_{\Gamma_\theta^\epsilon} \frac{\partial^2 g}{\partial n} v \, ds$$

where $k^\theta : \Gamma_\theta^\epsilon \rightarrow \mathbb{R}$ is the approximate additive curvature of the boundary. Due to the curvature term, a $C^1$ B-spline parametrization of the free boundary is instrumental for the goal-adaptive discretization of this problem.

The dual solution is computed on the approximate domain $\Omega_\theta^\epsilon$ with a discrete space constructed using $C^1$-continuous, cubic hierarchical B-spline basis $H^\epsilon$. For this problem the proposed refinement indicators have the same form as in (28) and (29), but they are computed on the approximate domain $\Omega_\theta^\epsilon$ and the approximate boundary $\Gamma_\theta^\epsilon$.

The goal-adaptive discretization of the Bernoulli problem using $C^1$-continuous second order hierarchically refined splines for the primal problem and $C^1$-continuous third order splines for the dual problem after 60 refinement steps yields the solutions plotted in Figure 13. The Bézier meshes for the two indicators are given in Figure 14. As expected, most refinement is performed in the regions of the tip of the notch and the vicinity of the quantity of interest. The two indicators produce largely similar meshes, with the element-based indicator again marking less densely than the support indicator per refinement step. Furthermore, the change in mesh density seems to be faster with the element-based indicator.
The estimated error and the error with respect to the reference solution are plotted for adaptive refinement using both indicators in Figure 15 with marking ratios $\lambda \in \{0.95, 0.5, 0.25\}$. Adaptive refinement with both indicators result in optimal convergence of the error in $Q(u)$, with the support indicator again slightly outperforming overall. For the investigated range of marking ratios from $\lambda = 0.25$ to $\lambda = 0.95$, the adaptive discretizations produce virtually indistinguishable errors for a given number of degrees of freedom. The similarity of the adaptive methods is also seen in their effectivity indices, as plotted in Figure 16. The effectivity indices of the estimator on meshes adapted using both indicators improve rapidly in the first few adaptivity iterations as the free boundary takes a shape around which the linearized dual is accurate. The element indicator seems to reach the point at which the linearization errors are negligible more rapidly. After this point, both adaptive strategies give good estimations of the error, being over 70% of the actual error.

5. Conclusions and recommendations

A goal-adaptive Isogeometric Analysis procedure is proposed, where the local refinement of the initial geometry spaces is achieved using hierarchical B-splines. Local $h$-refinement of B-spline bases of degree $p$ with refinement indicators derived from a goal-oriented error estimator is considered. For the error estimator, a Galerkin approximation with hierarchically $h$-refined B-spline bases of degree $p + 1$ is proposed. The proposed discrete dual space is proven to be a strict superset of...
the discrete primal space. To comply with the refinement region requirements of the hierarchical refinement strategy, two novel refinement indicators are constructed to be used in the marking of function supports for refinement. These indicators are the support indicator, which is directly used for the marking of basis function supports, and the element-based indicator, which uses combinations of element indicators to decide which support to refine.

Based on investigations with a model problem, it is concluded that the proposed error estimator converges with optimal rates under uniform refinement. Furthermore, the estimated error is assessed to stay sharp under uniform refinement, with effectivity indices generally in the range of 0.9-1 for the considered case. The local error indicators specifically devised for the hierarchical refinement procedure are shown to converge with the same optimal rates under uniform refinement, which is judged to be a strong indication of sound adaptivity potential.

The studied individual ingredients are combined in an adaptive procedure whose performance is demonstrated with two steady example problems: Poisson’s equation on an L-shaped domain and free-surface flow through a notched channel. Adaptive refinement using both indicators result in optimal convergence rates in terms of the quantity of interest for both example problems, despite the low regularity of the solutions. From the apparent rates of convergence of the adaptive solutions it is concluded that both indicators are suitable for the hierarchical refinement procedure. Furthermore, the effectivity indices of the error estimator on adapted approximation spaces stay in the range 0.7-1 for the most part, showing that the proposed error estimator remains accurate under adaptive refinement as well, even for problems with significant non-linearities arising from free boundaries.

The aim of goal-adaptive refinement of spline spaces is shown to be achievable with some new ideas on the localization of the error estimator and the flexibility of refinement that is provided by hierarchical splines. For the ultimate goal of unifying design and analysis practices in engineering, this result can be seen as a step in eliminating some of the necessities of manual interventions that prevent a large scale implementation of the design-through-analysis methodology proposed by Isogeometric Analysis.

It has been remarked that there are possibilities other than the ones explored here. In particular, the possibility of local $h$- and $p$-refinement offered by hierarchical splines could be combined to permit $hp$-adaptive Isogeometric Analysis, with some effort to modify the procedure. Same modifications would likely enable anisotropic refinements as well. Therefore, the extension of the hierarchical refinement procedures to anisotropic $hp$-refinement is a natural direction to follow. Furthermore, it was suggested that Isogeometric Analysis permits many different options for the discretization of the dual problem. A study of error estimators based on other discrete duals may result in indicators suitable for adaptivity purposes that are cheaper to compute. Lastly, the application of the adaptive procedure to hierarchical NURBS, as already explored in [22] with a different error estimator, is an important step for analysis in the industrial context. As the critical properties of B-splines used here are also shared by NURBS, the proposed estimator and the refinement indicators introduced here are generalizable to adaptivity with hierarchical NURBS.

**Acknowledgements**

The research of G. Kuru is partially funded by the European Commission FP7 ANADE (PITN-GA-289428) project. The research of K.G. van der Zee and C.V. Verhoosel is funded by the Netherlands Organisation for Scientific Research (NWO), VENI scheme.

**A. Comparison of hierarchical and knot insertion bases in 1D**

With hierarchical splines, functions from multiple levels can have overlapping supports. This results in slightly higher bandwidth for the resulting matrix equations and possibly can affect the conditioning adversely. In the univariate case, it is possible to obtain ordinary B-spline bases, locally refined by knot insertion, that span the same discrete space as hierarchical splines. In the following, the hierarchical spline bases will be compared to the knot insertion bases in terms of the condition number for the solution of matrix equations arising from a 1D Poisson problem.

Given the open interval $\Omega = (-1, 1)$, the problem in its strong form is:

$$\begin{align*}
\frac{d^2 u}{dx^2} &= f & \text{in} & \Omega \\
u &= u_0 & \text{on} & \partial \Omega
\end{align*}$$

(36)
Figure 17: Adapted bases spanning the same discrete space at step 15, hierarchical B-spline basis (left) and knot-insertion B-spline basis (right)

with

\[ f(x) = \frac{2a^3 x}{(1 + a^2 x^2)^2}, \quad u_D(x) = \arctan(ax) \]

and \( a > 0 \) a scaling coefficient. It can be shown that \( u = \arctan(ax) \) is the solution to problem (36).

The weak form of problem (36) is discretized by choosing finite dimensional \( h \)-refined quadratic hierarchical spline spaces as the trial and test spaces of the Galerkin method. The hierarchical basis that spans this space is denoted \( H^\theta \) and the knot insertion basis that spans the same space is denoted \( N^\theta \).

Since the exact solution \( u = \arctan(ax) \) is known, element-wise \( H^1 \) norms of the true error, \( \eta_K = ||u_h - u||_{H^1(K)} \), are used as element indicators to drive the refinement procedure, a thresholding-type marking [48], accompanied with a completion step as with the element-based indicator explained in Section 3. With parameters \( a = 1000 \) for the forcing and \( \lambda = 0.9 \) for the marking fraction, the condition numbers \( \sigma_{\text{max}}/\sigma_{\text{min}} \), defined as the ratio of the maximum and the minimum singular values of the stiffness matrix, are plotted against degrees of freedom in Figure 18. An example of the resulting bases at refinement step 15 is given in Figure 17 along with the sparsity pattern of the resulting stiffness matrix (Figure 19) to give an indication of the influence of the increased overlap on the bandwidth.

The results show that having lower and higher level functions together results in increased condition numbers for both bases. However, the condition number is less severe for the hierarchically refined basis, with the employed choice of having refinement regions defined by the union of basis function supports.

References
