Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Seminar for Applied Mathematics

Exponential convergence of simplicial hp-FEM for H^1-functions with isotropic singularities

Ch. Schwab

Research Report No. 2014-15
June 2014

Seminar für Angewandte Mathematik
Eidgenössische Technische Hochschule
CH-8092 Zürich
Switzerland

Funding ERC: ERC AdG grant STAHDPDE 247277

Exponential convergence of simplicial hp-FEM for H^1-functions with isotropic singularities *

Ch. Schwab

Abstract For functions $u \in H^1(\Omega)$ in a bounded polyhedron $\Omega \subset \mathbb{R}^d$, $d = 2,3$, which are analytic in $\overline{\Omega}\backslash\mathscr{S}$ with point singularities concentrated at the set $\mathscr{S} \subset \overline{\Omega}$ consisting of a finite number of points in $\overline{\Omega}$, we prove exponential rates of convergence of *hp*-version continuous Galerkin finite element methods on families of regular, simplicial meshes in Ω. The simplicial meshes are assumed to be geometrically refined towards $\mathscr{S}$ and to be shape regular, but are otherwise unstructured.

1 Introduction

Many nonlinear PDEs exhibit solutions with are analytic but exhibit isolated point singularities at a set $\mathscr{S}$. We mention only nonlinear Schrödinger equations with self-focusing, density functional models in electron structure calculations (eg. [8, 2, 4] and the references there), nonlinear parabolic PDEs with critical growth (eg. [15] and the references there, or continuum models of crystalline solids with isolated point defects (eg. [16] and the references there).

We prove an exponential convergence result for C^0-conforming *hp*-FEM on regular, simplicial mesh families with *isotropic, geometric refinement* towards the singular point(s) $c \in \mathscr{S}$. These meshes are in addition required to be shape-regular. This type of mesh arises for example in adaptive bisection-tree refinements. Specifically, for singular solutions $u \in H^1(\Omega)$ where $\Omega \subset R^d$, $d = 2,3$ belonging to a countably normed space with radial weights introduced in [6], we construct a continuous, piecewise polynomial interpolant $I^{hp}u$ which exhibits exponential convergence: there exist constants $b, C > 0$ which depend on Ω and on u, in general, such that

$$\|u - I^{hp}u\|_{H^1(\Omega)} \leq C\exp(-bN^{1/(d+1)}) \ . \tag{1}$$

* Work supported by ERC AdG grant STAHDPDE 247277.

Ch. Schwab, SAM, ETH, CH-8092 Zürich, Switzerland, e-mail: schwab@math.ethz.ch

Here, $d = 2,3$ denotes the space dimension and N denotes the number of degrees of freedom in the hp-FE approximation. This rate coincides, in the cases $d = 1,2$, with the bounds obtained in [9, 10] for corner singularities on structured geometric meshes, and in space dimension $d = 3$ generalizes the hp-approximations in [17, Sec. 5.2.2] in the case of vertex singularities to unstructured, tetrahedral meshes with geometric refinement towards $\mathscr{S}$.

The structure of the note is as follows: in Section 2, we introduce a model problem, the geometric assumptions on the singularities, and precise the analytic regularity in countably normed, weighted Sobolev spaces with radial weight functions. In Section 3, we introduce the hp-version FEM; we specify in particular the assumptions on the simplicial, geometric meshes, and on the elemental polynomial degrees, and on the definition of the hp FE spaces. Section 4 contains statement and proof of the exponential convergence bound in $H^1(\Omega)$ on regular, simplicial geometric mesh families.

2 Analytic Regularity

Analytic regularity is characterized in countably normed weighted Sobolev spaces which have been introduced and used in exponential convergence estimates in a number of references; we only mention [9, 10, 1, 11, 12, 6] and the references there. Here, we denote by $\mathscr{S} \subset \overline{\Omega}$ the set of singular points c; we consider solutions $u \in H^1(\Omega)$ which are smooth in $\overline{\Omega}\backslash\mathscr{S}$ so that the singular support of u coincides with $\mathscr{S}$. We work under the following separation assumption on $\mathscr{S}$.

$$\text{The singular set } \mathscr{S} \text{ consist of a finite number of isolated points } c \in \overline{\Omega}. \tag{2}$$

Assumption (2) implies $\varepsilon(\Omega,\mathscr{S}) := \min\{\operatorname{dist}(c,c') : c,c' \in \mathscr{S}, c \neq c'\} > 0$, and allows to partition the set Ω into $|\mathscr{S}|$ many disjoint neighborhoods ω_c of the singularities $c \in \mathscr{S}$. We set $\Omega_{\mathscr{S}} := \bigcup_{c\in\mathscr{S}} \omega_c$ and denote $\Omega_0 := \Omega\backslash\overline{\bigcup_{c\in\mathscr{S}} \omega_c}$.

We characterize analytic regularity of singular solutions by weighted Sobolev spaces. To define these, we introduce distance functions:

$$r_c(x) = \operatorname{dist}(x,c)\ , \qquad x \in \Omega\ , \quad c \in \mathscr{S}\ . \tag{3}$$

With $c \in \mathscr{S}$ we collect all singular exponents $\beta_c \in \mathbb{R}$ in the "multi-exponent"

$$\underline{\beta} = \{\beta_c : c \in \mathscr{S}\} \in \mathbb{R}^{|\mathscr{S}|}\ . \tag{4}$$

We assume ($\underline{\beta} > s$ and $\underline{\beta} \pm s$ understood componentwise for $s \in \mathbb{R}$) [Dist. $2d$ and $3d$]

$$\underline{b} := -1 - \underline{\beta} \in (0,1/2)\ ,\ \text{ie.}\ -1\ > \underline{\beta} >\ -3/2\ . \tag{5}$$

Consider the semi-norms (cp. [6, Definition 6.2 and Equation (6.9)], [1] and [11]),

$$|u|^2_{M^k_{\underline{\beta}}(\Omega)} = |u|^2_{H^k(\Omega_0)} + \sum_{c\in\mathscr{S}} \sum_{\substack{\alpha\in\mathbb{N}_0^d \\ |\alpha|=k}} \left\| r_c^{\beta_c+|\alpha|} \mathsf{D}^\alpha u \right\|^2_{L^2(\omega_c)}, \ k \in \mathbb{N}_0 . \tag{6}$$

We define the norm $\|u\|_{M^m_{\underline{\beta}}(\Omega)}$ by $\|u\|^2_{M^m_{\underline{\beta}}(\Omega)} = \sum_{k=0}^m |u|^2_{M^k_{\underline{\beta}}(\Omega)}$. Here, $|u|_{H^m(\Omega_0)}$ is the usual Sobolev semi-norm of integer order m on Ω_0, and D^α denotes the partial derivative of order $\alpha \in \mathbb{N}_0^d$. The space $M^m_{\underline{\beta}}(\Omega)$ is the weighted Sobolev space obtained as the closure of $C_0^\infty(\Omega)$ with respect to the norm $\|\cdot\|_{M^m_{\underline{\beta}}(\Omega)}$. Under (5), for $\Omega \subset \mathbb{R}^3$ holds $M^2_{\underline{\beta}}(\Omega) \subset H^{1+\theta}(\Omega)$ for some $\theta > 1/2$: choose $\theta(\underline{\beta}) = 1 - \beta_m - \varepsilon$ in [11, Thm. 3.5] with $\beta_m := -1 - \beta_c \in (0, 1/2)$, and $0 < \varepsilon < 1/2 - \beta_m = 3/2 + \beta_c$. In dimension $d = 2$, ie. for $\Omega \subset \mathbb{R}^2$, we find under (5) that $M^2_{\underline{\beta}}(\Omega) \subset H^{1+\theta}(\Omega)$ for some $\theta >$, so that in any case $M^2_{\underline{\beta}}(\Omega) \subset C^0(\overline{\Omega})$ with continuous embedding. With $M^k_{\underline{\beta}}(\Omega)$ in (6), the analytic class in [6, Definition 6.3] reads

$$A_{\underline{\beta}}(\mathscr{S};\Omega) = \left\{ u \in \bigcap_{k\geq 0} M^k_{\underline{\beta}}(\Omega) \,:\, \exists C_u > 0 \text{ s.t. } |u|_{M^k_{\underline{\beta}}(\Omega)} \leq C_u^{k+1} k! \ \forall k \in \mathbb{N}_0 \right\} . \tag{7}$$

Several application problems have solutions in this class, cp. [8] for electron structure models, [1, 6] for elliptic problems in polyhedral domains.

3 *hp*-Finite Element spaces

For two parameters $0 < \kappa, \sigma < 1$, we consider families $\mathfrak{M}_{\kappa,\sigma} = \{\mathscr{M}^{(\ell)}\}_{\ell\geq 1}$ of geometric meshes $\mathscr{M}^{(\ell)} \in \mathfrak{M}_{\kappa,\sigma}$. The meshes $\mathscr{M} \in \mathfrak{M}_{\kappa,\sigma}$ are regular partitions of the polyhedron Ω into a finite number of open simplices (triangles in space dimension $d = 2$, tetrahedra in space dimension $d = 3$) $T \in \mathscr{M}^{(\ell)}$. Here, regular means that for every $\mathscr{M} \in \mathfrak{M}_{\kappa,\sigma}$, the intersections of closures of any two distinct $T, T' \in \mathscr{M}$ are either empty, a vertex v, an entire edge e or an entire face f. We assume the family $\mathfrak{M}_\sigma$ to be *uniformly κ-shape regular*: for a simplex $T \in \mathscr{M}^{(\ell)}$, we denote by $h_T = \mathrm{diam}(T)$ its diameter and by $\rho_T = \sup\{\rho > 0 | B_\rho \subset T\}$, the radius of the largest ball B_ρ that can be inscribed into T. For a regular, simplicial mesh $\mathscr{M}$, the (nondimensional) shape parameter $\kappa(\mathscr{M}) = \max\{h_T/\rho_T | T \in \mathscr{M}\}$ is well defined. A collection $\{\mathscr{M}^{(\ell)}\}_{\ell\geq 1}$ of regular, simplicial meshes is called *κ-shape regular*, if $\sup_{\ell\geq 1} \kappa(\mathscr{M}^{(\ell)}) \leq \kappa < \infty$.

Each simplex $T \in \mathscr{M}_\ell$ is the image of the reference simplex, defined by $\widehat{T} := \{\hat{x} \in \mathbb{R}^3 : \hat{x}_i > 0, \sum_{i=1}^d \hat{x}_i < 1\}$, under the affine element map F_T, ie.

$$T = F_T(\widehat{T}), \quad T \ni x = F_T(\hat{x}) = B_T\hat{x} + b_T, \ \hat{x} \in \widehat{T} . \tag{8}$$

For a regular, simplicial triangulation $\mathscr{M}$ of Ω with $\kappa(\mathscr{M}) < \infty$, the affine element maps are nondegenerate: the jacobians $B_T = DF_T$ in (8) are nonsingular, and $\|B_T\|_F \leq \kappa(\mathscr{M})$, see, eg., [3, Sec. II]. The reference simplex $\widehat{T}$ is contained in the unit cube $\widehat{K} = (0,1)^d$; with each $T \in \mathscr{M}$, we associate a parallelepiped via $K_T = F_T(\widehat{K})$ and *assume* that $K_T \subset \Omega$. Here, for $T \in \mathscr{M}$ the local polynomial approximation space $\mathbb{P}^p(T) = \text{span}\{x^\alpha : |\alpha| \leq p\}$ is the linear space of all multivariate polynomials on $T \in \mathscr{M}$ whose total degree does not exceed p. The space $\mathbb{P}^p(T)$ is invariant under the affine mapping F_T, i.e. $u \in \mathbb{P}^p(T)$ if and only if $\hat{u} := u \circ F_T \in \mathbb{P}^p(\widehat{T})$.

On parallelepipeds K, the polynomial space $\mathbb{Q}^p(K)$ is the affine image of $\mathbb{Q}^p(\widehat{K})$, $\widehat{K} = \widehat{I}^d$ with $\widehat{I} = (0,1)$, given by

$$\mathbb{Q}^p(\widehat{K}) = \text{span}\{\,\widehat{x}^\alpha : 0 \leq \alpha_i \leq p,\ 1 \leq i \leq d\,\}\ . \tag{9}$$

For each parallelepiped K_T associated with a tetrahedron $T \in \mathscr{M}$ (resp. a triangle if $\Omega \subset \mathbb{R}^2$), with associated affine element mapping $F_T : \widehat{K} \to K_T$ and polynomial degree $p \geq 0$, we set

$$\mathbb{Q}^p(K_T) = \left\{ v \in L^2(K_T) : (v|_{K_T} \circ F_T) \in \mathbb{Q}^p(\widehat{K}) \right\}\ . \tag{10}$$

For polynomial degree $p \geq 1$, and for a family of regular, simplicial triangulations $\mathscr{M}^{(\ell)} \in \mathfrak{M}_{\kappa,\sigma}$ of Ω, we introduce the finite element spaces

$$S^p(\mathscr{M}^{(\ell)}) = \left\{ u \in H^1(\Omega) : u|_T \in \mathbb{P}^p(T), T \in \mathscr{M}^{(\ell)} \right\}\ . \tag{11}$$

hp-FEM are obtained when the level ℓ of geometric mesh refinement is tied to the polynomial degree p.

Mesh layers A key ingredient in exponential convergence proofs of hp-FEM is *geometric mesh refinement* towards the set $\mathscr{S}$ of singularities. We call a regular, simplicial mesh family $\mathfrak{M}_{\kappa,\sigma} = \{\mathscr{M}^{(\ell)}\}_{\ell\geq 1}$ *σ-geometrically refined towards $\mathscr{S} \subset \Omega$* if there exists $0 < \sigma < 1$ such that for every $T \in \mathscr{M}^{(\ell)} : \overline{T} \cap \mathscr{S} = \emptyset$, $\ell = 1,2,\ldots$ holds

$$0 < \sigma < \rho(T;\mathscr{S}) := \frac{\text{diam}(T)}{\text{dist}(T,\mathscr{S})} < \frac{1}{\sigma}\ . \tag{12}$$

We tag members of a σ-geometric family $\mathfrak{M}_{\kappa,\sigma}$ by a subscript σ, i.e. we write $\mathscr{M}_\sigma^{(\ell)}$.

Proposition 1. *Consider a regular, nested and σ-geometrically refined, κ-shape regular simplicial mesh family $\mathfrak{M}_{\kappa,\sigma}$ in Ω. Then, all elements $T \in \mathscr{M}_\sigma^{(\ell)}$ for every $\ell \geq 1$, can be grouped in* mesh-layers*: there exists a partition*

$$\bigcup_{\ell\geq 1} \mathscr{M}_\sigma^{(\ell)} = \mathfrak{L}_1 \mathbin{\dot\cup} \mathfrak{L}_2 \mathbin{\dot\cup} \ldots. \tag{13}$$

and a constant $c(\mathfrak{M}_{\kappa,\sigma}) \geq 1$ with

$$\forall k \geq 1 : \qquad \#(\mathfrak{L}_k) \leq c(\mathfrak{M}_{\kappa,\sigma}) \tag{14}$$

and such that, for every $T \in \mathfrak{L}_k$ and every $k \geq 1$,

$$0 < \frac{1}{c(\mathfrak{M}_{\kappa,\sigma})} \leq \frac{\mathrm{diam}(T)}{\sigma^k} \leq c(\mathfrak{M}_{\kappa,\sigma}) \ . \tag{15}$$

Proof. The proof is by induction over ℓ.

Based on Proposition 1, for ℓ sufficiently large, and for any constant $c_{\mathfrak{T}}(\kappa) > 0$ which is independent of ℓ, every mesh $\mathscr{M}_\sigma^{(\ell)} \in \mathfrak{M}_{\kappa,\sigma}$ may be partitioned into

$$\mathscr{M}_\sigma^{(\ell)} = \mathfrak{O}_\sigma^{(\ell)} \dot{\cup} \mathfrak{T}_\sigma^{(\ell)} \ , \tag{16}$$

where

$$\mathfrak{O}_\sigma^{(\ell)} := \mathfrak{O}_\sigma^{(\ell-1)} \dot{\cup} \mathfrak{L}_\ell = \mathfrak{L}_1 \dot{\cup} \mathfrak{L}_2 \dot{\cup} \ldots \dot{\cup} \mathfrak{L}_\ell \ ,$$

and there exists $c_{\mathfrak{T}} > 0$ being independent of ℓ such that for all ℓ holds

$$\mathscr{S} \subset \bigcup_{T \in \mathfrak{T}_\sigma^{(\ell)}} \overline{T} \ , \qquad \mathrm{dist}(\mathscr{S}, \mathfrak{O}^{(\ell)}) \geq c_{\mathfrak{T}} \sigma^\ell \ . \tag{17}$$

The terminal layers $\mathfrak{T}_\sigma^{(\ell)} \subset \mathscr{M}_\sigma^{(\ell)}$ in (16) satisfy the following properties.

Proposition 2. *There exists a constant $c_{\mathfrak{T}}(\kappa,\sigma) > 0$ such that for every $\mathscr{M}_\sigma^{(\ell)} \in \mathfrak{M}_{\kappa,\sigma}$, the set $\mathfrak{T}_\sigma^{(\ell)}$ has the following properties: for all $\ell \geq 1$ holds* (1) $\#(\mathfrak{T}_\sigma^{(\ell)}) \leq c_{\mathfrak{T}}(\kappa,\sigma)$, (2) $\forall c \in \mathscr{C} : |\mathfrak{T}_\sigma^{(\ell)} \cap \omega_c| \leq c_{\mathfrak{T}}(\kappa,\sigma)\sigma^{d\ell}$, (3) $\forall T \in \mathfrak{T}_\sigma^{(\ell)} : \ h_T \leq c_{\mathfrak{T}}(\kappa,\sigma)\sigma^\ell$.

4 Exponential Convergence

4.1 Statement of the Exponential Convergence Result

Theorem 1. *Let $u \in M^2_{-1-\underline{\beta}}(\Omega)$ with weight vector $\underline{\beta}$ as in* (5) *in a bounded polyhedron $\Omega \subset \mathbb{R}^d$, $d = 2,3$.*

Then, for every sequence $\mathfrak{M}_{\kappa,\sigma}(\mathscr{S})$ of nested, regular simplicial meshes in Ω which are σ-geometrically refined towards $\mathscr{S}$ and which are κ shape-regular, there exist continuous projectors $\Pi^p_{\kappa,\sigma} : M^2_{-1-\underline{\beta}}(\Omega) \to S^p(\mathscr{M}_\sigma^{(p)})$ and constants $b, C > 0$ (depending on κ, C_u, d_u in (7) *and on σ) such that there holds the error bound*

$$\left\| u - \Pi^p_{\kappa,\sigma} u \right\|_{H^1(\Omega)} \leq C \exp(-b \sqrt[d+1]{N}) \ . \tag{18}$$

Here, $N = \dim(S^p(\mathscr{M}_\sigma^{(p)})) = O(p^{d+1})$.

4.2 Proof

The proof of the *approximation result* Theorem 1 is based on constructing the projectors $\Pi^p_{\kappa,\sigma}$; our construction will proceed in several steps and we detail it for $d = 3$, the case $d = 2$ being a (minor) modification. first, we review from [17, Section 5] a family of univariate hp-projections with error bounds which are explicit in the polynomial degree as well as in the regularity of the functions to be approximated. A corresponding family of polynomial projectors on the unit cube $\widehat{K} = (0,1)^3$ with analogous consistency error bounds is then obtained as in [17, Section 5] by tensorization and scaling. We shall use these bounds for a tetrahedron $T \in \mathfrak{O}^{(\ell)}_\sigma \subset \mathscr{M}^{(\ell)}_\sigma \in \mathfrak{M}_{\kappa,\sigma}$ as follows. By Proposition 1, $T \in \mathfrak{L}_k$ for some $1 \le k \le \ell - 1$. The (up to orientation) unique parallelepiped $K_T = F_T(\widehat{K})$ associated with $T \in \mathfrak{L}_k$ has the same scaling properties as T, in particular (15) also holds for K_T. For u belonging to the analytic class (7) with weight vector satisfying (5), $u \in C^0(\overline{\Omega}) \cap C^\infty(\overline{\Omega}\backslash\mathscr{S})$. For $T \in \mathfrak{O}^{(\ell)}_\sigma$, the pullback $\widehat{u}_T = u|_{K_T} \circ F_T$ satisfies on $\widehat{K}$ the same analytic derivative bounds as $u|_T \circ F_T$ on $\widehat{T}$ (with larger constant C_u, depending on κ, but independent of ℓ and of T). The tensorized hp interpolation operator from [17] on $\widehat{K}$ is therefore well-defined and allows to construct a polynomial approximation $\widehat{u}^p_T \in \mathbb{Q}^p(\widehat{K})$ with analytic consistency error bounds on $\widehat{K}$; since $\widehat{T} \subset \widehat{K}$, and since $\mathbb{Q}^p(\widehat{T}) \subset \mathbb{P}^{pd}(\widehat{T})$, the pushforwards of the restrictions $\widehat{u}^p_T|_{\widehat{T}}$ under the affine mapping $F_T : \widehat{T} \to T$ will be local polynomial approximations of degree pd with exponential convergence estimates in $H^1(T)$. Moreover, since the tensorized interpolant is nodally exact in the vertices of $\widehat{K}$, and since the set of vertices of $\widehat{T}$ is a subset of the set of vertices of $\widehat{K}$, *the pushforwards of $\widehat{u}^p_T|_{\widehat{T}}$ under F_T are nodally exact in the vertices of T*. By the continuity of $u \in A_{\underline{\beta}}(\mathscr{S};\Omega)$ on $\Omega\backslash\mathscr{S}$, the resulting global, piecewise polynomial interpolant is nodally exact (and, in particular, continuous) in all vertices of $T \in \mathfrak{O}^{(p)}_\sigma$, but has polynomial jump discontinuities across edges and (in space dimension $d = 3$) faces of $T \in \mathfrak{O}^{(p)}_\sigma$ which we remove by *polynomial trace liftings*, preserving the exponential convergence estimates.

4.2.1 Univariate hp-Projectors and hp Error Bounds

Let $I = (-1,1)$ be the unit interval. For any $k \ge 1$, we write $H^k(I)$ for the usual Sobolev space endowed with norm $\|u\|_{H^k(I)}$. For $q \ge 0$, we denote by $\widehat{\pi}_{q,0} : L^2(I) \to \mathbb{P}^q(I)$ the $L^2(I)$-projection. The following C^{k-1}-conforming and univariate projector has been constructed in [7, Section 8].

Lemma 1. *For any $p,k \in \mathbb{N}$ with $p \ge 2k-1$, there is a projector $\widehat{\pi}_{p,k} : H^k(I) \to \mathbb{P}^p(I)$ that satisfies $(\widehat{\pi}_{p,k}u)^{(k)} = \widehat{\pi}_{p-k,0}(u^{(k)})$, and $(\widehat{\pi}_{p,k})^{(j)}u(\pm 1) := u^{(j)}(\pm 1)$, for any $j = 0,\dots,k-1$.*

Moreover, there holds:

(i) For every $k \in \mathbb{N}$, there exists a constant $C_k > 0$ such that

$$\forall u \in H^k(I)\ ,\forall p \geq 2k-1: \quad \|\widehat{\pi}_{p,k}u\|_{H^k(I)} \leq C_k \|u\|_{H^k(I)}\ . \tag{19}$$

(ii)For integers $p,k \in \mathbb{N}$ with $p \geq 2k-1$, $\kappa = p-k+1$ and for $u \in H^{k+s}(I)$ with any $k \leq s \leq \kappa$ there holds the error bound

$$\|(u-\widehat{\pi}_{p,k}u)^{(j)}\|^2_{L^2(I)} \leq \frac{(\kappa-s)!}{(\kappa+s)!}\|u^{(k+s)}\|^2_{L^2(I)}, \qquad j=0,1,\dots,k. \tag{20}$$

We refer to [7, Proposition 8.4] and [7, Theorem 8.3], respectively, for proofs, and further references.

4.2.2 Tensor projector on the unit cube

Based on the univariate projectors $\widehat{\pi}_{p,k}$, we constructed in [17] polynomial projection operators on $I^d = (0,1)^d$ by a) translation and scaling of the projectors $\widehat{\pi}_{p,k}$ to $(0,1)$ and b) by tensorization, as follows: for integers $k \geq 0$ and $d > 1$, we define

$$H^k_{mix}(I^d) = H^k(I) \underbrace{\otimes \cdots \otimes}_{d-\text{times}} H^k(I), \tag{21}$$

where $\otimes$ denotes the tensor-product of separable Hilbert spaces. These spaces are isomorphic to Bochner spaces, ie. $H^k_{mix}(I^d) \simeq H^k(I;H^k_{mix}(I^{d-1})) \simeq H^k_{mix}(I^{d-1};H^k(I))$. In I^d of dimension $d > 1$ and for $p \geq 2k-1$, we define the projector

$$\widehat{\Pi}^d_{p,k} = \bigotimes_{i=1}^{d} \widehat{\pi}^{(i)}_{p,k} : \ H^k_{mix}(I^d) \to \mathbb{Q}^p(I^d) \tag{22}$$

where $\widehat{\pi}^{(i)}_{p,k}$ denotes the univariate projector in Lemma 1, applied in coordinate $1 \leq i \leq d$. For $d,k \geq 1$ there exists a constant $C_{k,d} > 0$ such that for all $p \geq 2k-1$ there holds the stability bound

$$\|\widehat{\Pi}^d_{p,k}v\|_{H^k_{mix}(I^d)} \leq C_{k,d}\|v\|_{H^k_{mix}(I^d)} \tag{23}$$

and

$$\left\| v - \widehat{\Pi}^d_{p,k}v \right\|_{H^k_{mix}(I^d)} \leq C_{k,d} \sum_{i=1}^{d} \|v - \widehat{\pi}^{(i)}_{p,k}v\|_{H^k(I;H^k_{mix}(I^{d-1}))}\ . \tag{24}$$

We choose throughout what follows $k=2$ as in [17], and obtain from (24), (20)

Proposition 3. *[17] Assume that the polynomial degree $p \geq 5$. Then, for any integers $3 \leq s \leq p$, and for $v \in H^{s+5}(\widehat{K})$, there holds*

$$\|v - \widehat{\Pi}^3_{p,2}v\|^2_{H^2_{mix}(\widehat{K})} \lesssim \Psi_{p-1,s-1} \sum_{m=s}^{s+5} |v|^2_{m,\widehat{K}} \tag{25}$$

where the constant implied in $\lesssim$ is independent of s and of p, and where

$$\Psi_{q,r} = 2^{2(r+3)} \frac{\Gamma(q+1-r)}{\Gamma(q+1+r)}, \qquad 0 \le r \le q \; . \tag{26}$$

Moreover, $\widehat{\Pi}^3_{p,2}v$ is nodally exact in the vertices of $\widehat{K} = (0,1)^3$:

$$(\widehat{\Pi}^3_{p,2}v)(x_1,x_2,x_3) = v(x_1,x_2,x_3) \quad \forall x_i \in \{0,1\} \; . \tag{27}$$

4.2.3 Transformation Formula

For $u \in H^k(\Omega)$, and for a simplex $T \in \mathscr{M}_\sigma$, $\hat{u}_T = u|_T \circ F_T \in H^k(\widehat{T})$ for every $k \ge 0$. Quantitative bounds on derivatives under affine transformations F_T in (8) are provided by the *transformation formula* (eg. [3, Section II.6.6]).

Lemma 2. *Let $G \subset \mathbb{R}^d$, $d \ge 2$, denote a bounded polyhedron which is affine equivalent to $\widehat{G}$ via* (8)*, ie. $G = F_T(\widehat{G})$. For $v \in H^k(G)$ and for any $k \in \mathbb{N}$, the pullback $\hat{v}_T := v|_G \circ F_T$ satisfies with $|v|^2_{m,T} = \sum_{|\alpha|=m} \|D^\alpha v\|^2_{L^2(G)}$ and with the Frobeniusnorm $\|B_T\|_F$ of the matrix B_T in* (8) *the bound*

$$|\hat{v}|_{m,\widehat{G}} \le d^m \|B_T\|^m_F |\det(B_T)|^{-1/2} |v|_{m,G} \; . \tag{28}$$

4.2.4 Element Interpolants

For any simplex $T \in \mathfrak{O}^{(\ell)}_\sigma$, the function $u \in A_{\underline{\beta}}(\mathscr{S};\Omega)$ is analytic in the associated parallelepiped $\overline{K_T} \subset \overline{\Omega}$. In $T \in \mathfrak{O}^{(\ell)}_\sigma$, the polynomial approximation of $u|_T$ is obtained by applying Proposition 3 to $\hat{u}_T := u|_{K_T} \circ F_T$:

$$\forall T \in \mathfrak{O}^{(\ell)}_\sigma : \quad u^p_T := \left(\widehat{\Pi}^3_{p,2}(u|_{K_T} \circ F_T) \right) |_{\widehat{T}} \circ F_T^{(-1)} \; . \tag{29}$$

With u^p_T as in (29) we define the *hp-base interpolant* $\tilde{I}^p$ in $\mathfrak{O}^\ell_\sigma$ by

$$\forall T \in \mathfrak{O}^\ell_\sigma \subset \mathscr{M}^{\ell)}_\sigma : \qquad (\tilde{I}^p u)|_T := u^p_T \; . \tag{30}$$

The bound (17) *with $c_{\mathfrak{T}} > 0$ sufficiently large, independent of ℓ* ensures that there exists $c(\kappa,\sigma) > 0$ such that the associated K_T satisfies

$$\forall \ell \in \mathbb{N} \;\; \forall T \in \mathfrak{O}^{(\ell)}_\sigma : \qquad \mathrm{dist}(K_T, \mathscr{S})/\mathrm{diam}(K_T) \ge 1/c \; . \tag{31}$$

4.2.5 Exponential Convergence in Broken Sobolev Norms

Proposition 4. *For $u \in A_{\underline{\beta}}(\mathscr{S};\Omega)$ with* (5)*, there are $b, C > 0$ (depending on u) such that for every $p \ge 1$ and for $\tilde{I}^p$ in* (30) *holds*

$$\|u - \tilde{I}^p u\|_{H^1(\mathfrak{O}_\sigma^{(p)})} \leq C \exp(-bp) \,. \tag{32}$$

Here $C > 0$ depends on u and σ, but is independent of p, and $H^1(\mathfrak{O}_\sigma^{(\ell)})$ denotes the broken H^1 space over $\mathfrak{O}^{(\ell)}$, with corresponding norm.

Proof. Since $\mathscr{S}$ consists of finitely many singular points c, by localization and superposition, we may assume wlog. $\mathscr{S} = \{c\}$ and denote by $\beta = \beta_c > -2$. For $1 \leq k \leq \ell < p$, consider a simplex $T \in \mathfrak{L}_k \cap \omega_c \subset \mathfrak{M}_\sigma^{(p)}$ and the associated parallelepiped $K_T = F_T(\widehat{K}) \supset T$. It satisfies $0 < \sigma < r_c(x)|_{K_T}/\sigma^k < 1/\sigma$. By assumption, $K_T \subset \Omega$ and, by (17), $\mathrm{dist}(K_T, \mathscr{S}) \geq c_{\mathfrak{T}} \sigma^\ell$. Then, for $u \in A_{\underline{\beta}}(\mathscr{S};\Omega)$ and for this $T \in \mathfrak{L}_k$, $\hat{u}_T := u|_{K_T} \circ F_T$ is analytic in $\overline{\widehat{K}}$ and satisfies, by (28) with $G = K_T$ and $\widehat{G} = \widehat{K}$,

$$\forall m \in \mathbb{N} : \quad |\hat{u}_T|_{m,\widehat{K}} \leq d^m \|B_T\|_F^m |\det(B_T)|^{-1/2} |u|_{m,K_T} \,.$$

For $u \in A_{\underline{\beta}}(\mathscr{S};\Omega)$ and $T \in \mathfrak{L}_k$, we obtain for $|u|_{m,K_T}$ using (12) and (15)

$$\begin{aligned} |u|^2_{m,K_T} &= \|D^m u\|^2_{L^2(K_T)} \lesssim \|r_c^{\beta+m} \sigma^{-k(\beta+m)} D^m u\|^2_{L^2(K_T)} \\ &\leq \sigma^{-2k(\beta+m)} \|r_c^{\beta+m} D^m u\|^2_{L^2(K_T)} \leq \sigma^{-2k(\beta+m)} C_u^{2(m+1)} (m!)^2 \,. \end{aligned}$$

We define $u_T^p \in \mathbb{Q}^p(T) \subset \mathbb{P}^{pd}(T)$ as in (29). From (25), for every integer $3 \leq s \leq p$ and with $\Psi_{q,r}$ as in (26) and for $j = 0,1,2$,

$$\|D^j(\hat{u} - \hat{u}_T^p)\|^2_{L^2(\widehat{T})} \leq \|D^j(\hat{u} - \hat{u}_T^p)\|^2_{L^2(\widehat{K})} \leq \Psi_{p-1,s-1} \sum_{m=s}^{s+5} |\widehat{u}_T|^2_{m,\widehat{K}} \,.$$

Using the κ-shape regularity of $T \in \mathfrak{L}_k \subset \mathscr{M}_\sigma^{(p)} \in \mathfrak{M}_{\kappa,\sigma}$, we find $\|B_T\|_F \leq \kappa h_T$ (eg. [3, (Chap. II, (6.9)]) and, by (15) and (28), that $h_T \lesssim \kappa \sigma^k$ so that for every $m \in \mathbb{N}$

$$|\widehat{u}_T|^2_{m,\widehat{K}} \leq \frac{(\kappa d \sigma^k)^{2m}}{|\det(B_T)|} |u|^2_{m,K_T} \leq \frac{(\kappa d \sigma^k)^{2m}}{|\det(B_T)|} \sigma^{-2k(\beta+m)} C_u^{2(m+1)} (m!)^2 \,.$$

We obtain for $j = 0,1,2$ the bound

$$\|\widehat{D}^j(\hat{u} - \hat{u}_T^p)\|^2_{L^2(\widehat{T})} \leq \Psi_{p-1,s-1} \sum_{m=s}^{s+5} \frac{(\kappa d \sigma^k)^{2m}}{|\det(B_T)|} \sigma^{-2k(\beta+m)} C_u^{2(m+1)} (m!)^2 \,.$$

Transporting to $T = F_T(\widehat{T}) \in \mathfrak{L}_k$, we find for $\beta_c = -1 - b_c$ and $j = 0,1,...$

$$\begin{aligned} \|D^j(u - u_T^p)\|^2_{L^2(T)} &\lesssim \Psi_{p-1,s-1} \sum_{m=s}^{s+5} (\kappa d \sigma^k)^{2(m-j)} \sigma^{-2k(\beta+m)} C_u^{2(m+1)} (m!)^2 \\ &\lesssim \Psi_{p-1,s-1} (\kappa d C_u)^{2s} \sigma^{2k(1+b_c-j)} \Gamma(s+6)^2 \,. \end{aligned} \tag{33}$$

For $T \in \mathfrak{O}^{(\ell)}$, we define the piecewise polynomial interpolant $\tilde{I}^p u|_T$ by (29). Then $\tilde{I}^p u$ coincides with u in the vertices of all $T \in \mathfrak{O}^{(\ell)}$ and is in particular continuous in these vertices; it is, however, in general discontinuous across edges and faces.

Using the finite cardinality (14), and summing the bound (33) with $j = 0, 1$ over layers $\mathfrak{L}_1, ..., \mathfrak{L}_p$, we obtain with $\bar{C} := C_u \kappa d$ and $\beta_c = -1 - b_c$, $0 < b_c < 1$

$$\|u - \tilde{I}^p u\|_{H^1(\mathfrak{O}^{(p)})} \leq C(\kappa, \sigma) \sum_{k=1}^{p} \Psi_{p-1,s-1} \bar{C}^{2s} \sigma^{2kb_c} \Gamma(s+6)^2 \ . \tag{34}$$

Using [17, Lemma 5.9], we find that there exist $b, C > 0$ (depending on $\bar{C} > 0$ and on κ and d) such that for every $p \geq 1$ holds

$$\min_{1 \leq s \leq p} \left\{ \Psi_{p-1,s-1} \bar{C}^{2s} \Gamma(s+6)^2 \right\} \leq C^2 \exp(-2bp) \ . \tag{35}$$

Inserting this bound into (34), summing the geometric series and absorbing a linear factor of p into the exponential completes the proof.

4.2.6 Polynomial Trace Lifting in $\mathfrak{O}_\sigma^{(p)}$

By the nodal exactness (27), the hp base interpolant $\tilde{I}^p$ constructed in (30) of Proposition 4 is continuous in vertices of simplices $T \in \mathfrak{O}_\sigma^{(p)}$, but has in general discontinuities across interelement edges $E \in \mathscr{E}_T$ of simplices $T \in \mathfrak{O}_\sigma^{(p)}$ (in dimensions $d = 2, 3$) and across interelement faces $F \in \mathscr{F}_T$ of simplices $T \in \mathfrak{O}_\sigma^{(p)}$ (in dimension $d = 3$) with polynomial trace jumps $[\![\tilde{I}^p]\!]_E$ and $[\![\tilde{I}^p]\!]_F$.

For each $T \in \mathfrak{O}_\sigma^{(p)}$, the nodal exactness (27) of $\tilde{I}^p u$ implies for each $E \in \mathscr{E}_T$ that $[\![\tilde{I}^p u]\!]_E \in \mathbb{P}_0^{pd}(E) := (\mathbb{P}^{pd} \cap H_0^1)(E)$, $d = 2, 3$, and, for $d = 3$ and each $F \in \mathscr{F}_T$, $[\![\tilde{I}^p u]\!]_F \in \mathbb{P}^{pd}(F)$. We lift successively these polynomial trace jumps first for all interelement edges $E \in \mathscr{E}_T$ and, second, in dimension $d = 3$ also for all interelement faces $F \in \mathscr{F}_T$, for every $T \in \mathfrak{O}_\sigma^{(p)}$. Since $T \in \mathfrak{O}_\sigma^{(p)} \subset \mathscr{M}_\sigma^{(p)} \in \mathfrak{M}_{\kappa,\sigma}$ is κ shape-regular, so are all $F \in \mathscr{F}_T$. For $E \in \mathscr{E}_T$, let $F_E \in \mathscr{F}_T$ denote any face in $\mathscr{F}_T$ with $E \subset \partial F$.

We recapitulate from [14, Lemma 15, Thm. 1] the required lifting and the stability estimates. Consider the reference simplex $\widehat{T} \subset \mathbb{R}^d$, $d = 2, 3$. Given a piecewise polynomial function $\hat{g}_p$ of degree p on each $\widehat{F} \in \mathscr{F}_{\widehat{T}}$ that is continous on $\partial\widehat{T}$, in [14, Lemma 15, Thm. 1], a polynomial trace lifting $\hat{v}_p = \mathscr{L}_{\widehat{T},\partial\widehat{T}}(\hat{g}_p) \in \mathbb{P}^p(\widehat{T})$ is constructed which satisfies on the reference simplex $\widehat{T}$ in space dimension $d = 2, 3$ the bound $\|\hat{v}_p\|_{H^1(\widehat{T})} \leq \widehat{C} \|\hat{g}_p\|_{H^{1/2}(\partial\widehat{T})}$ (with $\hat{C} > 0$ independent of p). As $H^{1/2}(\widehat{T}) = (L^2(\widehat{T}), H^1(\widehat{T}))_{1/2}$, we have the interpolation inequality $\|\hat{g}_p\|_{H^{1/2}(\partial\widehat{T})} \leq \widehat{C} \|\hat{g}_p\|_{L^2(\partial\widehat{T})}^{1/2} \|\hat{g}_p\|_{H^1(\partial\widehat{T})}^{1/2}$. With the polynomial inverse inequality on each face $\widehat{F} \subset \partial\widehat{T}$ we get (with a possibly different constant $\hat{C} > 0$ which is independent of p)

$$\|\hat{v}_p\|_{H^1(\hat{T})} \le \widehat{C} p \|\hat{g}_p\|_{L^2(\partial\hat{T})} \,. \tag{36}$$

Squaring this and scaling $\widehat{T}$ to $T = F_T(\hat{T}) \in \mathfrak{O}_\sigma^{(p)}$ we find

$$\|\mathscr{L}_{T,\partial T}(g_p)\|^2_{L^2(T)} + h_T^2 \|D^1 \mathscr{L}_{T,\partial T}(g_p)\|^2_{L^2(T)} \le C(\kappa) p^2 h_T \|g_p\|^2_{L^2(\partial T)} \,. \tag{37}$$

Iterating (36) twice, from $\hat{E} \subset \partial\hat{F}$ to $\hat{F} \subset \partial\hat{T}$ to $\hat{T}$, we obtain for $\widehat{g}_p \in \mathbb{P}_0^p(\widehat{E})$ a polynomial edge lifting $\widehat{\mathscr{L}_{\widehat{T},\widehat{E}}}(\widehat{g}_p) \in \mathbb{P}^p(\widehat{T})$ on the reference simplex $\widehat{T} \subset \mathbb{R}^3$ with

$$\|\hat{\mathscr{L}}_{\hat{T},\hat{E}}(\hat{g}_p)\|_{H^1(\hat{T})} \le \widehat{C} p^2 \|\hat{g}_p\|_{L^2(\hat{E})} \,. \tag{38}$$

Squaring (38) and scaling to $T = F_T(\hat{T}) \in \mathfrak{O}_\sigma^{(p)}$ yields for $g_p \in \mathbb{P}_0^p(E)$ on $E \in \mathscr{E}_T$

$$h_T^{-2} \|\mathscr{L}_{T,E}(g_p)\|^2_{L^2(T)} + \|D^1 \mathscr{L}_{T,E}(g_p)\|^2_{L^2(T)} \le C(\kappa) p^4 \|g_p\|^2_{L^2(E)} \,. \tag{39}$$

Let now $d = 3$ and let $F, F' \in \mathscr{F}_T$ be two distinct faces which share edge $\bar{E} = \overline{F} \cap \overline{F'}$. Using (36) in dimension $d = 2$ and scaled to T, we lift $g_p = [\![\tilde{I}^p u]\!]_E \in \mathbb{P}_0^{pd}(E)$ twice, once into F and once into F', resulting in a $v_p \in C^0(\overline{F \cup F'})$, $v_p \in \mathbb{P}^{pd}(F) \cup \mathbb{P}^{pd}(F')$, and $v_p\,|_{\partial\overline{F \cup F'}} = 0$ which satisfies (37) with F in place of T. We may therefore extend this continuous, piecewise polynomial function v_p from $\overline{F \cup F'}$ by zero to a function $\tilde{v}_p \in C^0(\partial T)$ which is, on each $F \in \mathscr{F}_T$, a polynomial of total degree at most pd. There exists a lifting $\mathscr{L}_{T,F}(\tilde{v}_p) \in \mathbb{P}^{pd}(T)$ such that for each $F \in \mathscr{F}_T$ we have $\mathscr{L}_{T,F}(\tilde{v}_p)\,|_F = v_p\,|_F$ on $F \in \mathscr{F}_E$, $(\mathscr{L}_{T,F}(\tilde{v}_p)\,|_F)\,|_E \equiv g_p$ on E and such that (39) holds. For each edge E in $\mathfrak{O}_\sigma^{(p)}$, we lift the polynomial jump in this way into all $T \in \mathfrak{O}_\sigma^{(p)}$ for which $E \in \mathscr{E}_T$ by the *edge-lifting operator*

$$\mathscr{L}_E(g_p) := \sum_{T : E \in \mathscr{E}_T} \mathscr{L}_{T,E}(g_p) \,. \tag{40}$$

By κ shape regularity, $\#\{T \in \mathfrak{O}_\sigma^{(p)} : E \in \mathscr{E}_T\}$ is bounded independently of p and of the particular edge E by an absolute constant depending only on κ. With $\tilde{I}^p$ in (30), we define

$$\check{I}^p u := \tilde{I}^p u - \sum_E \mathscr{L}_E([\![\tilde{I}^p u]\!]_E) \,. \tag{41}$$

Then, $\check{I}^p u$ is continuous across edges $E \in \mathscr{E}_T$ for every $T \in \mathfrak{O}_\sigma^{(p)}$, and $[\![\check{I}^p u]\!]_F \in \mathbb{P}_0^{pd}(F) := (\mathbb{P}^{pd} \cap H_0^1)(F)$ for all $F \in \mathscr{F}_T$.

We next lift, for each face $F \in \mathscr{F}_T$, the face jump $[\![\check{I}^p u]\!]_F \in \mathbb{P}_0^{pd}(F)$ by extending first by zero to all other faces $F' \in \mathscr{F}_T \backslash \{F\}$, then lift polynomially by referring to [14, Theorem 1]. By construction, this lifting $\mathscr{L}_{T,F}([\![\check{I}^p u]\!]_F) \in \mathbb{P}^p(T)$ will vanish on all $F' \in \mathscr{F}_T : F' \neq F$. For each face F, we repeat this lifting at most twice for $T, T' \in \mathfrak{O}_\sigma^{(p)}$ such that $F \in \mathscr{F}_T \cap \mathscr{F}_{T'}$. We define the continuous interpolant

$$\begin{aligned} I^p u &:= \check{I}^p u - \sum_{F\in\mathscr{F}_T: T\in\mathfrak{O}_\sigma^{(p)}} \mathscr{L}_{T,F}([\![\check{I}^p u]\!]_F) \\ &= \tilde{I}^p u - \sum_{E\in\mathscr{E}_T: T\in\mathfrak{O}_\sigma^{(p)}} \mathscr{L}_E([\![\tilde{I}^p u]\!]_E) - \sum_{F\in\mathscr{F}_T: T\in\mathfrak{O}_\sigma^{(p)}} \mathscr{L}_{T,F}([\![\check{I}^p u]\!]_F)\ . \end{aligned} \tag{42}$$

To verify exponential convergence in submesh $\mathfrak{O}_\sigma^{(p)}$, we estimate in (42)

$$\begin{aligned} \|u - I^p u\|_{H^1(\mathfrak{O}_\sigma^{(p)})} \leq \|u - \tilde{I}^p u\|_{H^1(\mathfrak{O}_\sigma^{(p)})} &+ \left\| \sum_{E\in\mathscr{E}_T: T\in\mathfrak{O}_\sigma^{(p)}} \mathscr{L}_E([\![\tilde{I}^p u]\!]_E) \right\|_{H^1(\mathfrak{O}_\sigma^{(p)})} \\ &+ \left\| \sum_{F\in\mathscr{F}_T: T\in\mathfrak{O}_\sigma^{(p)}} \mathscr{L}_{T,F}([\![\check{I}^p u]\!]_F) \right\|_{H^1(\mathfrak{O}_\sigma^{(p)})} . \end{aligned} \tag{43}$$

The first term was bound in Prop. 4. We bound the second term.

For $T \in \mathfrak{O}_\sigma^{(p)}$, we write, using $[\![u]\!]_E = 0$ for $E \in \mathscr{E}_T$

$$\begin{aligned} & h_T^{-2} \|\mathscr{L}_{T,E}([\![\tilde{I}^p u]\!]_E)\|^2_{L^2(T)} + \|D^1 \mathscr{L}_{T,E}([\![\tilde{I}^p u]\!]_E)\|^2_{L^2(T)} \\ \leq \quad & C(\kappa) p^4 \|[\![\tilde{I}^p u]\!]_E\|^2_{L^2(E)} = C(\kappa) p^4 \|[\![u - \tilde{I}^p u]\!]_E\|^2_{L^2(E)}\ . \end{aligned} \tag{44}$$

The multiplicative trace inequality implies for a κ-shape regular simplex $T \subset \mathbb{R}^d$ with diameter h_T that for every $F \in \mathscr{F}_T$ and for every $\varphi \in H^1(T)$ holds

$$\|\varphi|_F\|^2_{L^2(F)} \leq C(\kappa) \left(h_T^{-1} \|\varphi\|^2_{L^2(T)} + h_T \|D^1\varphi\|^2_{L^2(T)} \right)\ . \tag{45}$$

Iterating this for $T \in \mathfrak{O}_\sigma^{(p)}$ from $E \in \mathscr{E}_T$ to $F \in \mathscr{F}_T$ gives, for $\varphi \in H^2(T)$,

$$\|\varphi|_E\|^2_{L^2(E)} \lesssim h_T^{-2} \|\varphi\|^2_{L^2(T)} + \|D^1\varphi\|^2_{L^2(T)} + h_T^2 \|D^2\varphi\|^2_{L^2(T)} \tag{46}$$

where the implied constant depends only on κ.

Using (46) with $\varphi = (u - \tilde{I}^p u)|_T = u|_T - u_T^p \in H^2(T)$ for $T \in \mathfrak{O}_\sigma^{(p)}$ in (44) gives

$$h_T^{-2} \|\mathscr{L}_{T,E}([\![\tilde{I}^p u]\!]_E)\|^2_{L^2(T)} + \|D^1 \mathscr{L}_{T,E}([\![\tilde{I}^p u]\!]_E)\|^2_{L^2(T)} \lesssim p^4 \sum_{j=0}^{2} h_T^{2(j-1)} \|D^j (u - u_T^p)\|^2_{L^2(T)}\ .$$

Using (33) and that $h_T \sim \sigma^k$ for $T \in \mathfrak{L}_k$ we obtain

$$\|\mathscr{L}_{T,E}([\![\tilde{I}^p u]\!]_E)\|^2_{H^1(T)} \lesssim p^4 \Psi_{p-1,s-1}(\kappa d C_u)^{2s} \Gamma(s+6)^2 \sigma^{2kb_c}\ . \tag{47}$$

Finally, we bound the third term in (43), ie. $\|\mathscr{L}_{T,F}([\![\check{I}^p u]\!]_F)\|_{H^1(T)}$ for $F \in \mathscr{F}_T$. Since $\mathscr{L}_{T,F}([\![\check{I}^p u]\!]_F) = 0$ on $\partial T \backslash F$, by the Poincaré inequality in $\{v \in H^1(T) : v|_{\partial T \backslash F} = 0\}$ it suffices to bound $\|D^1 \mathscr{L}_{T,F}([\![\check{I}^p u]\!]_F)\|_{L^2(T)}$. Since $[\![u]\!]_F = 0$, using (41) we obtain

$$h_T^{-1}\|\mathscr{L}_{T,F}([\![\check{I}^p u]\!]_F)\|_{L^2(T)} \lesssim \|D^1\mathscr{L}_{T,F}([\![\check{I}^p u]\!]_F)\|_{L^2(T)} = \|D^1\mathscr{L}_{T,F}([\![u-\check{I}^p u]\!]_F)\|_{L^2(T)} .$$

We estimate further, using the stability of the lifting $\mathscr{L}_{T,F}$ and (45),

$$\begin{aligned}\|D^1\mathscr{L}_{T,F}([\![u-\check{I}^p u]\!]_F)\|_{L^2(T)}^2 &\lesssim p^2\|u-\check{I}^p u\|_{L^2(F)}^2 \\ &\lesssim p^2(h_T^{-1}\|u-\check{I}^p u\|_{L^2(T)}^2 + h_T\|D^1(u-\check{I}^p u)\|_{L^2(T)}^2) .\end{aligned} \tag{48}$$

Recalling (41), we bound for $j=0,1$

$$\begin{aligned}\|D^j(u-\check{I}^p u)\|_{L^2(T)}^2 &= \|D^j(u-\tilde{I}^p u + \textstyle\sum_E \mathscr{L}_{T,E}([\![\tilde{I}^p u]\!]_E))\|_{L^2(T)}^2 \\ &\lesssim \|D^j(u-\tilde{I}^p u)\|_{L^2(T)}^2 + \textstyle\sum_E \|D^j(\mathscr{L}_{T,E}([\![\tilde{I}^p u]\!]_E))\|_{L^2(T)}^2 .\end{aligned}$$

We use (33) for the first term, and (47) for the second term to conclude for $j=0,1$

$$\|D^j(u-\check{I}^p u)\|_{L^2(T)}^2 \lesssim p^4\Psi_{p-1,s-1}(\kappa d C_u)^{2s}\Gamma(s+6)^2\sigma^{2k(1+b_c-j)} .$$

Using again that $T\in\mathfrak{L}_k$ satisfies $h_T\sim\sigma^k$, we insert into (48) and arrive at

$$\|D^1\mathscr{L}_{T,F}([\![u-\check{I}^p u]\!]_F)\|_{L^2(T)}^2 \lesssim p^6\Psi_{p-1,s-1}(\kappa d C_u)^{2s}\Gamma(s+6)^2\sigma^{2kb_c} .$$

Inserting this and the bound (47) into (43), we obtain for $\|u-I^pU\|_{H^1(\mathfrak{O}_\sigma^{(p)})}$ exactly once more the bound (34) (with a slightly higher power of p). Absorbing the polynomial factor into the exponential, we conclude the exponential error bound

$$\|u-I^p u\|_{H^1(\mathfrak{O}_\sigma^{(p)})} \le C\exp(-bp) \tag{49}$$

for the continuous *hp*-interpolant $I^p u$ defined in (42) in $\mathfrak{O}_\sigma^{(p)}$ using again (35).

4.2.7 Approximation in $\mathfrak{T}_\sigma^{(\ell)}$

Under (5), for $\Omega\subset\mathbb{R}^3$ holds $M_{\underline{\beta}}^2(\Omega)\subset H^{1+\theta}(\Omega)$ for some $\theta>(d-2)/2$, $d=2,3$. From Proposition 2 items (1)-(3), the collections $\{T\in\mathfrak{T}_\sigma^{(p)} : T\in\omega_c\}$, $c\in\mathscr{S}$ have uniformly bounded (w.r. to p) cardinality and shape regularity. Then $u\in H^{1+\theta}(\Omega)$ and for a Clément-type, continuous, piecewise linear quasiinterpolant $\Pi_{\mathfrak{T}}^{(p)}u$ in $\mathfrak{T}_\sigma^{(p)}\cap\omega_c$

$$\|u-\Pi_{\mathfrak{T}}^{(p)}u\|_{H^1(\mathfrak{T}_\sigma^{(p)}\cap\omega_c)} \le c(\kappa,\sigma)\sigma^{\theta p} = C\exp(-b'p) . \tag{50}$$

Combining (49) and (50) and applying a bounded (uniformly w.r. to p by Prop. 2, item (1)) number of further polynomial edge- and face liftings at the interface of $\mathfrak{O}_\sigma^{(p)}$ and $\mathfrak{T}_\sigma^{(p)}$ completes the construction of I^{hp} in (1) and, hence, the proof.

5 Concluding Remarks

We have proved the exponential convergence rate (18) for continuous *hp*-FE approximations κ shape-regular, simplicial meshes with geometric refinement tof analytic functions with isolated point singularities at a set $\mathscr{S}$ in a bounded domain $D \subset \mathbb{R}^d$, $d = 1,2,3$. Apart from κ-shaperegularity and σ-geometric mesh refinement the proof did not assume further structural assumptions on the triangulations. In particular, simplicial partitions which are obtained by successive bisection tree refinement in the course of adaptive subdivisions are admissible. The approximation results imply the exponential convergence rate $\exp(-b\sqrt[3]{N})$ for second order, elliptic PDEs in polygons $D \subset \mathbb{R}^2$ (where $\mathscr{S}$ denotes the set of corners of D) which are considered, for example, in [1, 7, 12]. Theorem 1 also implies the exponential convergence rate $\exp(-b\sqrt[4]{N})$ for *hp*-approximations of electron densities in DFT, due to the quasioptimality of Galerkin approximations shown, for example, in [2, 4] and the references there. In this application, $\mathscr{C}$ denotes the set of nuclei, whose centers $c \in \mathscr{S}$ are assumed known. Unlike other approaches such as plane waves, *hp*-approximations do not, apriori, impose any specific functional form of the electron densities. Due to the locality of approximation and the separation (2) of the points $c \in \mathscr{S}$, we may apply Theorem 1 in each neighborhood ω_c implying that the total number of degrees of freedom to achieve accuracy $\varepsilon > 0$ in the norm $H^1(D)$ scales as $O(\#(\mathscr{S})|\log\varepsilon|^4)$, ie. *linear scaling* in the number $\#(\mathscr{S})$ of nuclei and *polylogarithmic scaling* in the target accuracy ε. This is analogous to what is reported recently for discontinuous Galerkin discretizations in [13], where Proposition 4 can be used a starting point of proof of an exponential convergence result on tetrahedral meshes; for geometric meshes of hexahedra, analogous results can be found in [17, Sec. 5.2.2]. Exponentially convergence quadrature algorithms for the (singular) electron-pair integrals are available in [5]. The results in the present note are confined to space dimension $d \leq 3$. The approach generalizes, however, directly to *hp*-approximations of point singularities in any dimension d with exponential rate $\exp(-b\sqrt[d+1]{N})$. Likewise, the result will remain true for *linear polynomial degree vectors* and, more generally, for degree vectors of bounded variation as introduced in [17]. The details will be reported elsewhere.

References

1. I. Babuška and B. Q. Guo. Regularity of the solution of elliptic problems with piecewise analytic data. I. Boundary value problems for linear elliptic equation of second order. *SIAM J. Math. Anal.*, 19(1):172–203, 1988.
2. G. Bao, G. Hu, D. Liu, An *h*-adaptive Finite Element solver for the calculation of the electronic structures, J. Comp. Phys. 231 (2012) 4967-4979.
3. D. Braess. Finite Elements (5th. Ed.) Cambridge Univ. Press (2011)
4. E. Cances, R. Chakir and Y. Maday, Numerical analysis of the planewave discretization of some orbital-free and Kohn-Sham models, ESAIM: ESAIM: Mathematical Modelling and Numerical Analysis, 46(02), 341-388, 2012.

5. A. Chernov, T. von Petersdorff and Ch. Schwab, Exponential Convergence of *hp* Quadrature for integral operators with Gevrey kernels ESAIM: ESAIM: Mathematical Modelling and Numerical Analysis, 45, 387-422, 2011.
6. M. Costabel, M. Dauge, and S. Nicaise. Analytic regularity for linear elliptic systems in polygons and polyhedra. *Math. Models Methods Appl. Sci.*, 22(8), 2012.
7. M. Costabel, M. Dauge, and C. Schwab. Exponential convergence of *hp*-FEM for Maxwell's equations with weighted regularization in polygonal domains. *Math. Models Methods Appl. Sci.*, 15(4):575–622, 2005.
8. S. Fournais, T.O. Sørensen, M. Hoffmannn-Ostenhof, and T. Hoffmann-Ostenhof, Non-isotropic cusp conditions and regularity of the electron density of molecules at the nuclei. Ann. Inst. Henri Poincaré **8** (2007) pp. 731-748.
9. W. Gui and I. Babuška. The *h*, *p* and *h*-*p* versions of the finite element method in 1 dimension. II. The error analysis of the *h*- and *h*-*p* versions. *Numer. Math.*, 49(6):613–657, 1986.
10. B. Q. Guo and I. Babuška, *The hp-version of the finite element method. Part I: The basic approximation results*, Part II: General results and applications. Computational Mechanics **1** (1986) 21-41 and 203-220.
11. B. Q. Guo and I. Babuška. Regularity of the solutions for elliptic problems on nonsmooth domains in $\mathbb{R}^3$. I. Countably normed spaces on polyhedral domains. *Proc. Roy. Soc. Edinburgh Sect. A*, 127(1):77–126, 1997.
12. B. Q. Guo and C. Schwab. Analytic regularity of Stokes flow on polygonal domains in countably weighted Sobolev spaces. *J. Comp. Appl. Math.* **119** (2006) 487–519.
13. L. Lin, L. Ying and W. E. Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation Journ. Comp. Phys. (2013)
14. R. Munoz-Sola. Polynomial liftings on a tetrahedron and applications to the *hp*-FEM in three dimensions. SIAM J. Numer. Anal. **34**(1997) pp. 282-314.
15. Samarskii, Alexander A. and Galaktionov, Victor A. and Kurdyumov, Sergei P. and Mikhailov, Alexander P. Blow-up in quasilinear parabolic equations de Gruyter Expositions in Mathematics, **19** (1995) (Translated from the 1987 Russian original by Michael Grinfeld and revised by the authors), Walter de Gruyter & Co., Berlin.
16. M. Luskin and C. Ortner, Atomistic-to-continuum coupling, Acta Numerica, **22** (2013) 397-508.
17. D. Schötzau, C. Schwab, and T. P. Wihler. *hp*-dGFEM for elliptic problems in polyhedra. II: Exponential convergence. SIAM J. Numer. Anal., 51/4 (2013), pp. 2005-2035 (extended version in Technical Report 2009-29, Seminar for Applied Mathematics, ETH Zürich).

Recent Research Reports

Nr.	Authors/Title
2014-05	X. Claeys and R. Hiptmair and C. Jerez-Hanckes and S. Pintarelli Novel Multi-Trace Boundary Integral Equations for Transmission Boundary Value Problems
2014-06	X. Claeys and R. Hiptmair Integral Equations for Acoustic Scattering by Partially Impenetrable Composite Objects
2014-07	P. Grohs and S. Keiper and G. Kutyniok and M. Schaefer Cartoon Approximation with α -Curvelets
2014-08	P. Grohs and M. Sprecher and T. Yu Scattered Manifold-Valued Data Approximation
2014-09	P. Grohs and U. Wiesmann and Z. Kereta A Shearlet-Based Fast Thresholded Landweber Algorithm for Deconvolution
2014-10	P. Grohs and S. Vigogna Intrinsic Localization of Anisotropic Frames II: α-Molecules
2014-11	S. Etter and P. Grohs and A. Obermeier FFRT - A Fast Finite Ridgelet Transform for Radiative Transport
2014-12	A. Paganini Approximate Shape Gradients for Interface Problems
2014-13	E. Fonn and P. Grohs and R. Hiptmair Polar Spectral Scheme for the Spatially Homogeneous Boltzmann Equation
2014-14	J. Dick and F.Y. Kuo and Q.T. Le Gia and Ch. Schwab Multi-level higher order QMC Galerkin discretization for affine parametric operator equations