Towards optimal shape functions for hierarchical Hermite elements

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Abstract. *In this paper we derive an orthonormal basis for hierarchic higher-order H^2-conforming finite elements in one spatial dimension. This basis is optimal from the point of view of the conditioning of the resulting discrete algebraic problem and from the point of view of the quality of the local interpolation. In addition to its direct application in hp-FEM and hp-adaptivity for Hermite elements in 1D this basis can be used for the design of quality higher-order hierarchic Hermite and Argyris elements in higher spatial dimensions.*

1 Introduction

The Hermite and Argyris elements have not been used very frequently until now because of their rather problematic implementation, although it is well-known that their interpolation and approximation properties are several orders of accuracy superior to various mixed schemes based on standard H^1-conforming elements (see, e.g., [3, 4]). Due to their potential efficiency it is realistic to expect that these elements will become standard for the discretization of fourth-order problems after the algorithmic problems are resolved. To approach this goal, efficient element-by-element assembling procedures for two-dimensional Hermite and Argyris elements, built on top of suitable reference transformations, were recently introduced in [5]. It also makes a good sense to study the extension of the standard lowest-order Hermite and Argyris elements to higher polynomial degrees. As the first step in this direction, in this paper we present a hierarchic basis for higher-order H^2-conforming elements in one spatial dimension that possesses analogous optimality properties to the Lobatto polynomials that are standard for second-order elliptic problems (see, e.g., [1, 2, 6]).

The popularity of the Lobatto polynomials is due to their orthonormality under the H^1_0-product, which is contained in many weak formulations of second-order elliptic problems in 1D. In addition to their optimality for the discretization of the Laplace operator in 1D, the Lobatto shape functions nowadays are the basic ingredient for the research in the design of optimal shape functions for H^1-conforming elements in higher spatial dimensions. The H^2_0-orthonormal basis derived in this paper is expected to play a similar role for the discretization of fourth-order elliptic problems, both in one and higher spatial dimensions.

Since the Hermite and Argyris elements are less standard than the continuous (for example Lagrange) elements, a few comments are in order. First, the Hermite elements conform to the space H^2 (= yield globally smooth approximations) in one spatial dimension only, while in higher spatial dimensions the approximation is smooth only at the vertices (it is continuous in the rest of the domain). Both in 1D and 2D the lowest-order Hermite element is cubic. Globally smooth approximations can be obtained by means of Argyris elements. These elements are the same as Hermite elements in 1D, but in higher spatial dimensions they contain additional degrees of freedom associated with the second derivatives at the vertices and with the normal derivatives across the edges. The lowest-order Argyris element in 2D is quintic ($p = 5$). In the following we will deal with H^2-conforming elements in one dimension, referring to them as Hermite elements.

Model problem

For demonstration purposes let us use the following simple fourth-order problem related to the bending of elastic beams (Euler-Bernoulli model),

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(E(x)I(x)\frac{\mathrm{d}w^2}{\mathrm{d}x^2}\right) = f(x). \tag{1.1}$$

Here $x \in \Omega = (a, b)$, E is the modulus of elasticity, I the area moment of inertia related to the geometry of the beam, f is the tranversely distributed load and the unknown function w is the transverse deflection of the beam. The equation (1.1) is equipped with some combination of *essential* boundary conditions, specifying the deflection w or the derivative $\mathrm{d}w/\mathrm{d}x$ at the endpoints, and *natural* conditions that define either the bending moment $EI\mathrm{d}^2w/\mathrm{d}x^2$ or the shear force $\mathrm{d}/\mathrm{d}x(EI\mathrm{d}^2w/\mathrm{d}x^2)$. For our purposes it is sufficient to assume homogeneous material with both E and I constant in Ω, and we choose the simplest boundary conditions

$$w(a) = w(b) = \frac{\mathrm{d}w}{\mathrm{d}x}(a) = \frac{\mathrm{d}w}{\mathrm{d}x}(b) = 0. \tag{1.2}$$

The weak formulation of (1.1), (1.2) is standard: find a solution $w \in V = H_0^2(\Omega)$ satisfying the integral identity

$$\int_\Omega w''(x)v''(x)\,\mathrm{d}x = \int_\Omega fv\,\mathrm{d}x \qquad \text{for all } v \in V, \tag{1.3}$$

Without loss of generality, the constant EI is included in the load function f.

2 Hierarchic higher-order elements

Consider a reference domain $K_a = (-1, 1)$. The lowest-order cubic Hermite element is determined via four degrees of freedom associated with the values and first derivatives at the endpoints of K_a. The corresponding four vertex functions have the form

$$\begin{aligned}
\omega_0(x) &= \frac{1}{2} - \frac{3}{4}x + \frac{1}{4}x^3, \\
\omega_1(x) &= \frac{1}{2} + \frac{3}{4}x - \frac{1}{4}x^3, \\
\omega_2(x) &= \frac{1}{4} - \frac{1}{4}x - \frac{1}{4}x^2 + \frac{1}{4}x^3, \\
\omega_3(x) &= -\frac{1}{4} - \frac{1}{4}x + \frac{1}{4}x^2 + \frac{1}{4}x^3.
\end{aligned} \tag{2.4}$$

This element can be extended to higher polynomial orders $p \geq 4$ either in the *nodal* or *hierarchic* fashion. The nodal Hermite elements are constructed in a standard way, assuming a suitable set of nodal points (such as, e.g., the Chebyshev or Gauss-Lobatto points) of the order $p - 2$. Some examples of higher-order nodal Hermite elements can be found in [4].

The idea of hierarchic shape functions is standard, fully analogous to the H^1-conforming elements (see, e.g., [6]). The lowest-order basis $\mathcal{B}_3$ for the biharmonic operator consists of the four cubic Hermite vertex functions

$$\mathcal{B}_3 = \{\omega_0, \omega_1, \dots, \omega_3\}, \tag{2.5}$$

and the basis $\mathcal{B}_{p+1}$ for the polynomial order $p+1 \geq 4$ is defined as $\mathcal{B}_{p+1} = \mathcal{B}_p \cup \{\omega_{p+1}\}$, where ω_{p+1} is a suitable polynomial of the order $p+1$, that vanishes at the boundary of K_a together with its first derivative. Since these shape functions vanish on the boundary of K_a in all external degrees of freedom, they are called *bubble functions*. Obviously, such definition of bubble functions leaves us a lot of freedom that can be used, for example, to optimize their conditioning properties.

Recall that the optimality of the Lobatto hierarchic bubble functions $l_2, l_3, \dots$ for the discretization of the Laplace operator in one dimension (see, e.g., [6]), is due to their orthogonality in the H_0^1-product

$$(u, v)_{H_0^1(K_a)} = \int_{-1}^{1} u'(x)v'(x)\, \mathrm{d}x, \quad u, v \in H_0^1(K_a). \tag{2.6}$$

Based on (2.6), the Lobatto shape functions are defined as primitive functions to the Legendre polynomials $L_1, L_2, \dots$ Let us extend this idea to the biharmonic operator with the weak form

$$\int_{-1}^{1} u''(x)v''(x)\, \mathrm{d}x,$$

that naturally corresponds to the H_0^2-product

$$(u, v)_{H_0^2(K_a)} = \int_{-1}^{1} u''(x)v''(x)\, \mathrm{d}x, \quad u, v \in H_0^2(K_a). \tag{2.7}$$

After integrating the Lobatto bubble functions $l_2, l_3, \dots$,

$$\bar{l}_k(\xi) = \int_{-1}^{\xi} l_{k-2}(\zeta)\, \mathrm{d}\zeta, \quad 5 \leq k, \tag{2.8}$$

we see that

$$\begin{aligned} \bar{l}_k(-1) &= \int_{-1}^{-1} l_{k-2}(\zeta)\, \mathrm{d}\zeta = 0, \\ \bar{l}'_k(-1) &= l_{k-2}(-1) = 0, \\ \bar{l}'_k(1) &= l_{k-2}(1) = 0, \end{aligned} \tag{2.9}$$

which agrees with our needs. However, at the same time

$$\bar{l}_k(1) = \int_{-1}^{1} l_{k-2}(\zeta)\, \mathrm{d}\zeta \neq 0 \tag{2.10}$$

for all even $k > 5$, which obviously prevents $\bar{l}_k(\xi)$ from being a bubble function. Hence, only for all odd $k \geq 5$ the bubble functions ω_k can be defined directly as

$$\omega_k(\xi) = \bar{l}_{k-2}(\xi), \quad 5 \leq k. \tag{2.11}$$

For even polynomial orders, the bubble functions $\omega_k(\xi)$ are obtained from the H_0^2-orthogonality requirement via an algebraic system consisting of several linear equations

$$(\omega_j, \omega_k)_{H_0^2} = 0 \qquad \text{for } 4 \le k,\ 4 \le j < k$$

(some of which are satisfied automatically when imposing additional symmetry requirements) and one quadratic equation,

$$(\omega_k, \omega_k)_{H_0^2} = 1 \qquad \text{for } 4 \le k.$$

For reference, the formulae of $\omega_4, \omega_5, \ldots, \omega_{12}$ are as follows:

$$\begin{aligned}
\omega_4(x) &= \sqrt{\frac{5}{128}}\left(1-x^2\right)^2, \\
\omega_5(x) &= \sqrt{\frac{7}{128}}\left(1-x^2\right)^2 x, \\
\omega_6(x) &= \frac{1}{6}\sqrt{\frac{9}{128}}\left(1-x^2\right)^2\left(-7x^2+1\right), \\
\omega_7(x) &= \frac{1}{2}\sqrt{\frac{11}{128}}\left(1-x^2\right)^2\left(3x^2-1\right)x, \\
\omega_8(x) &= \frac{1}{16}\sqrt{\frac{13}{128}}\left(1-x^2\right)^2\left(33x^4-18x^2+1\right), \\
\omega_9(x) &= \frac{1}{48}\sqrt{\frac{15}{128}}\left(1-x^2\right)^2\left(143x^4-110x^2+15\right)x, \\
\omega_{10}(x) &= \frac{1}{32}\sqrt{\frac{17}{128}}\left(1-x^2\right)^2\left(143x^6-143x^4+33x^2-1\right), \\
\omega_{11}(x) &= \frac{1}{32}\sqrt{\frac{19}{128}}\left(1-x^2\right)^2\left(221x^6-273x^4+91x^2-7\right)x, \\
\omega_{12}(x) &= \frac{1}{384}\sqrt{\frac{21}{128}}\left(1-x^2\right)^2\left(4199x^8-6188x^6+2730x^4-364x^2+7\right).
\end{aligned} \tag{2.12}$$

Fortunately, the bubble functions $\omega_4, \omega_5, \ldots$ are orthogonal under the H_0^2-product (2.7) not only to each other, but also to the vertex functions $\omega_0, \omega_1, \ldots, \omega_3$. Thus the presented set of hierarchic shape functions possesses an optimality property analogous to the Lobatto shape functions for the Laplace operator. The bubble shape functions $\omega_4, \omega_5, \ldots, \omega_{11}$ are shown in Fig. 1.

2.1 Conditioning comparison

It is well-known that good conditioning of the shape functions is crucial for higher-order finite elements, and the Hermite elements are not an exception. A simple but very useful comparison can be performed using a one-element mesh $\mathcal{T}_{h,p} = \{K_a\}$. In this case the stiffness matrix $\boldsymbol{S}_0$ is obtained by leaving out the four rows and four columns corresponding to the vertex functions from the master element stiffness matrix $\boldsymbol{S}_{K_a} = \{\int_{-1}^{1} \omega''(x)_i \omega''(x)_j \,\mathrm{d}x\}_{i,j}$.

Fig. 2 (left) shows the conditioning in the H_0^2-product of the nodal higher-order shape functions on the equidistant, Chebyshev and Gauss-Lobatto points, together with the hierarchic shape functions (2.12). Since more general fourth-order problems may contain the Laplace operator explicitly, the conditing of the shape functions in the H_0^1-product is presented in the right part of Fig. 2.

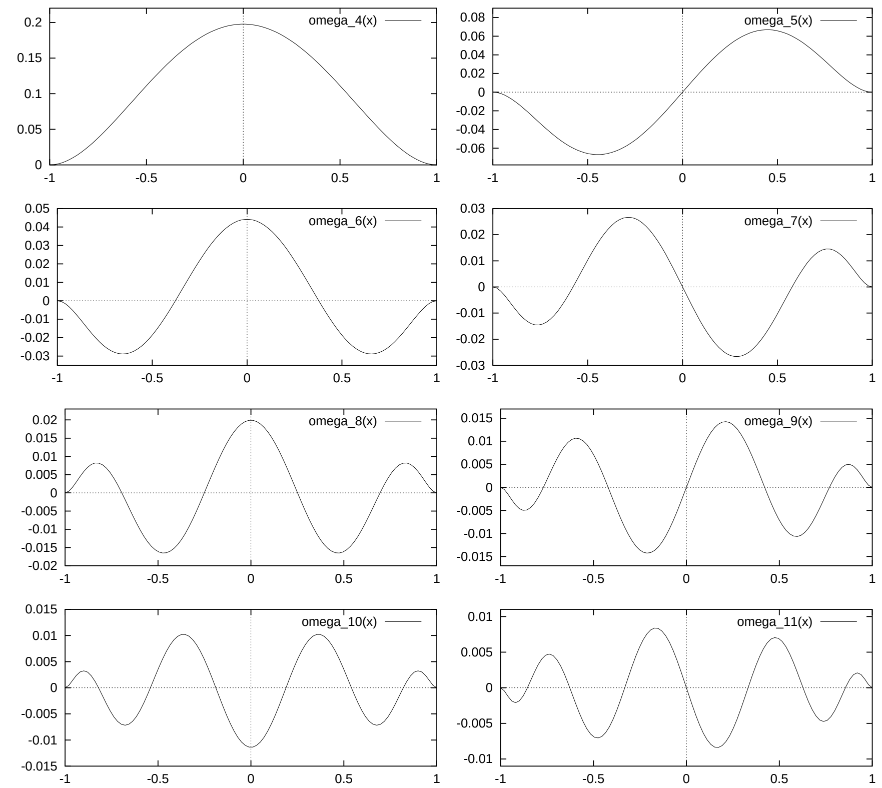

Figure 1: Hierarchic shape functions $\omega_4, \omega_5, \ldots, \omega_{11}$.

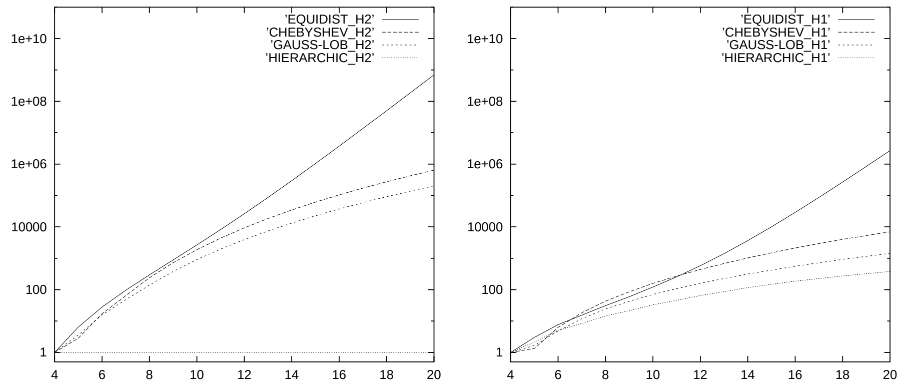

Figure 2: Conditioning of various sets of bubble functions in the H_0^2-product, with the polynomial order $p = 4, 5, \ldots, 20$ on the horizontal axis.

While the nodal shape functions on equidistant points perform very poorly in both cases (as expected), it is interesting to see that the Gauss-Lobatto points are significantly better than the Chebyshev points. The hierarchic bubble functions are superior in both cases, and in particular they are optimal in the H_0^2-product, with the condition number $\kappa(\boldsymbol{S}_0) = 1$ for all $p \geq 4$.

3 Interpolation on Hermite elements

The interpolation on higher-order finite elements in Hilbert spaces is much more interesting than the interpolation on lowest-order elements, since the orthogonal projection can be employed on various levels. Consider a function $g \in V \setminus V_{h,p}$. There are at least three basic options for the calculation of its interpolant $g_{h,p} \in V_{h,p}$ with different quality and cost:

1. The *best approximation* based on the global orthogonal projection. Let us write $g_{h,p} = \sum_{j=1}^{N} y_j v_j$, where $v_1, v_2, \ldots, v_N$ are some basis functions of $V_{h,p}$, and $y_1, y_2, \ldots, y_N$ the unknown coefficients. The orthogonal projection $g_{h,p}$ is uniquely defined via the orthogonality condition $(g - g_{h,p}) \perp V_{h,p}$, that can be rewritten as a system of linear algebraic equations

$$\sum_{j=1}^{N} y_j (v_j, v_i)_V = (g, v_i)_V, \qquad i = 1, 2, \ldots, N.$$

   This interpolant obviously is optimal in the norm $\| \cdot \|_V$, however the cost of its calculation is proportional to solving the whole finite element problem.

2. The *projection-based interpolation* combines the standard vertex interpolation on the level of lowest-order elements with the orthogonal projection on the higher-order polynomial spaces locally in the element interiors. Because of this, it is optimal among all interpolants that match vertex values and derivatives of g at grid vertices. When used in combination with orthogonal higher-order bubble functions, its efficiency is similar to the explicit nodal interpolant. These assertions will be proven below.

3. The traditional explicit *nodal interpolation* does not employ the orthogonal projection at all. It is fastest but least accurate, and it introduces the additional nontrivial problem of optimal interpolation points.

3.1 Projection-based interpolation

In order to reduce the CPU cost of the projection, the orthogonal projection can be localized to element interiors. Analogously to the H^1-conforming case (see, e.g., [6]), the interpolant $g_{h,p}$ is sought in two steps: as a sum of the vertex and bubble interpolants

$$g_{h,p} = g^v_{h,p} + g^b_{h,p}. \tag{3.13}$$

Vertex interpolant:

The vertex interpolant is defined as the elementwise cubic function $g^v_{h,p} \in C^1(\Omega)$ satisfying

$$g^v_{h,p}(x_i) = g(x_i), \ \left(g^v_{h,p}\right)'(x_i) = g'(x_i), \qquad i = 0, 1, \ldots, M. \tag{3.14}$$

Bubble interpolant:

The bubble interpolant $g^b_{h,p}$ is only constructed on elements K_i with $p_i \geq 4$. Since the residual $g - g^v_{h,p}$ vanishes at all grid points x_i together with its first derivative, on every element K_i, $i = 1, 2, \ldots, M$, it belongs to the space $H^2_0(K_i)$. Consider the polynomial subspace

$$P_{00}^{p_i}(K_i) = \{v \in P^{p_i}(K_i);\ v(x_{i-1}) = v(x_i) = v'(x_{i-1}) = v'(x_i) = 0\} \subset H_0^2(K_i) \tag{3.15}$$

of the dimension $p_i - 3$. It follows from the Poincaré-Friedrichs' inequality that in the space $H_0^2(K_i)$ one can use either the full H^2-product,

$$(u, v)_{2,2,K_i} = \int_{K_i} u(x)v(x) + u'(x)v'(x) + u''(x)v''(x)\,\mathrm{d}x, \tag{3.16}$$

or equivalently the H_0^2-product,

$$(u, v)_{H_0^2(K_i)} = \int_{K_i} u''(x)v''(x)\,\mathrm{d}x. \tag{3.17}$$

Let us stay with the latter for simplicity. The bubble interpolant $g^b_{h,p}$ on the element K_i is uniquely determined by the orthogonality condition

$$(g - g_{h,p}) \perp P_{00}^{p_i}(K_i).$$

Using the bubble functions $v^b_{i,k} \circ x^{-1}_{K_i}$ that generate the space $P_{00}^{p_i}(K_i)$, this requirement is equivalent to

$$\left(g - g^v_{h,p} - g^b_{h,p}, v^b_{i,k}\right)_{H_0^2(K_i)} = 0, \qquad k = 4, 5, \ldots, p_i. \tag{3.18}$$

Expressing further

$$g^b_{h,p}|_{K_i} = \sum_{m=4}^{p_i} \alpha_m^{(i)} v^b_{i,m},$$

and inserting this linear combination into (3.18), one obtains a system of $p_i - 3$ linear algebraic equations,

$$\int_{K_i} \left(g - g^v_{h,p} - \sum_{m=4}^{p_i} \alpha_m^{(i)} v^b_{i,m}\right)''(x)\ \left(v^b_{i,k}\right)''(x)\,\mathrm{d}x = 0, \quad k = 4, 5, \ldots, p_i, \tag{3.19}$$

for the unknown coefficients $\alpha_m^{(i)}$. Transformed to the reference domain K_a, this reads

$$\sum_{m=4}^{p_i} \alpha_m^{(i)} \underbrace{\int_{K_a} \omega''_m(\xi)\omega''_k(\xi)\,\mathrm{d}\xi}_{\delta_{mk}} = \int_{K_i} (\tilde{g} - \tilde{g}^v_{h,p})''(\xi)\omega''_k(\xi)\,\mathrm{d}\xi. \tag{3.20}$$

Hence, by the orthogonality of the hierarchic shape functions (2.12) in the H_0^2-product, the matrix of the linear system is diagonal, and the unknown coefficients are given by

$$\alpha_k^{(i)} = \int_{K_i} (\tilde{g} - \tilde{g}^v_{h,p})''(\xi)\omega''_k(\xi)\,\mathrm{d}\xi, \qquad k = 4, 5, \ldots, p_i. \tag{3.21}$$

We use the symbols $\tilde{g}(\xi) = g(x_{K_i}(\xi))$ and

$$\begin{aligned}\tilde{g}^v_{h,p}(\xi) &= (g^v_{h,p}(x_{K_i}(\xi)) \\ &= \omega_0(\xi)g(x_{i-1}) + \omega_1(\xi)g(x_i) + J_{K_i}\omega_2(\xi)g'(x_{i-1}) + J_{K_i}\omega_3(\xi)g'(x_i).\end{aligned}$$

By this result the orthogonal bubble functions clearly demonstrate their usefulness. The nodal bubble functions may be used in place of ω_4, ω_5, …, ω_{p_i}, but the lack of orthogonality does not allow the simplification (3.21), and a system of $p_i - 3$ linear algebraic equations of the form (3.20) has to be solved on every element K_i. After obtaining the coefficients $\alpha_k^{(i)}$, $k = 4, 5, \ldots, p_i$, for every element K_i, $i = 1, 2, \ldots, M$, the construction of the projection-based interpolant $g_{h,p} = g^v_{h,p} + g^b_{h,p}$ is accomplished.

Lemma 3.1 (Local optimality) *Suppose $\Omega = (a, b) \subset \mathbb{R}$ be covered with a finite element mesh $\mathcal{T}_{h,p}$ consisting of M Hermite finite elements $K_i = (x_{i-1}, x_i)$ equipped with the polynomial orders $3 \le p_i = p(K_i)$. Let $g \in H^2(\Omega)\cap C^0(\overline{\Omega})$, $g_{h,p} \in V_{h,p}$ its projection-based interpolant (3.13) and $\tilde{g}_{h,p} \in V_{h,p}$ an arbitrary other interpolant satisfying*

$$\tilde{g}_{h,p}(x_j) = g(x_j), \quad \tilde{g}'_{h,p}(x_j) = g'(x_j) \qquad \text{for all } j = 0, 1, \ldots, M.$$

Then

$$|g - g_{h,p}|_{2,2,K_i} \le |g - \tilde{g}_{h,p}|_{2,2,K_i} \qquad \text{for all } i = 1, 2, \ldots, M, \tag{3.22}$$

and therefore also

$$|g - g_{h,p}|_{2,2,\Omega} \le |g - \tilde{g}_{h,p}|_{2,2,\Omega}. \tag{3.23}$$

Proof The fact that the bubble interpolant $g^b_{h,p}$ is defined as the orthogonal projection of $g - g^v_{h,p} \in H^2_0(K_i)$ onto $P^{p_i}_{00}(K_i)$ implies that

$$\begin{aligned}|g - g_{h,p}|_{2,2,K_i} &= |(g - g^v_{h,p}) - g^b_{h,p}|_{2,2,K_i} \\ &= \min_{v\in P^{p_i}_{00}(K_i)} |(g - g^v_{h,p}) - v|_{2,2,K_i} \\ &\le |(g - g^v_{h,p}) - (\tilde{g}_{h,p} - g^v_{h,p})|_{2,2,K_i} \\ &= |g - \tilde{g}_{h,p}|_{2,2,K_i}.\end{aligned}$$

The integral $|g - g_{h,p}|^2_{2,2,\Omega}$ can be written as a sum

$$|g - g_{h,p}|^2_{2,2,\Omega} = \sum_{i=1}^{M} |g - g_{h,p}|^2_{2,2,K_i}.$$

The inequality (3.22) finally yields

$$\sum_{i=1}^{M} |g - g_{h,p}|^2_{2,2,K_i} \le \sum_{i=1}^{M} |g - \tilde{g}_{h,p}|^2_{2,2,K_i} = |g - \tilde{g}_{h,p}|^2_{2,2,\Omega}.$$

Everything works in the same way when the H^2_0-product is replaced with the full H^2-product.

As a consequence, the projection-based interpolant is better or equally good as any other interpolant that preserves the values and first derivatives at the mesh vertices (including any Hermite nodal interpolant).

4 Conclusion and outlook

We presented (to our best knowledge) a new set of hierarchic shape functions for higher-order Hermite elements in one dimension, consisting of four vertex functions ω_0, ω_1, ..., ω_3, and $p-3$ bubble functions $\omega_4, \omega_5, \ldots, \omega_p$, which are orthonormal in the H_0^2-product. The bubble functions are further orthonormal to the vertex functions in the H_0^2-product. This makes the basis optimal for the discretization of the biharmonic operator in one dimension, in the same way the Lobatto shape functions are optimal for the Laplace operator.

The orthogonal bubble functions $\omega_4, \omega_5, \ldots$ were used to define an efficient projection-based interpolation technique operating fully explicitly, without the need to solve any system of linear algebraic equations. This interpolation technique turned out to be locally optimal (Theorem 3.1).

Our next steps will lead to the generalization of these results to hierarchic Hermite and Argyris finite elements in higher spatial dimensions.

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