Symmetric Hierarchical Polynomials and the Adaptive h-p-Version

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Abstract

The h-p-version of finite-elements delivers a sub-exponential convergence in the energy norm. A step towards a full adaptive implementation is taken in the context of unstructured meshes of simplices with variable order p in space. Both assumptions lead to desirable properties of shape functions like symmetry, p-hierarchy and simple coupling of elements.

In a first step, it is demonstrated that for standard polynomial vector spaces on simplices not all of these features can be obtained simultaneously. However, this is possible if these spaces are slightly extended or reduced. Thus a new class of polynomial shape functions is derived, which is especially well suited for three dimensional tetrahedra.

The construction is completed by directly minimizing the condition numbers of the arising preconditioned local finite element matrices. The preconditioner is based on two-step domain decomposition techniques using a multigrid solver for the global linear problem $p = 1$, and direct solvers for local higher order problems.

Some numerical results concerning an adaptive (feedback) version of h-p finite elements are presented.

Key words: FEM, h-p-version, shape functions.

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1 Introduction

We choose the simplex as finite element for unstructured grids, which is a tetrahedron in three dimensions, and approximate the solution by a polynomial on each element. We use conforming finite elements in a (self-) adaptive code with efficient iterative solvers, a posteriori error estimators, globally varying polynomial degrees and h-p-adaptation.

On the interval, the one dimensional case, say $[-1, 1]$, the classic orthogonal Legendre polynomials are leading to a kind of optimal set of shape functions for the p- and h-p-version (see [3]) of finite elements for the Laplace equation. In spite of differing suggestions [2, 6, 8, 18, 21, 22], there is no canonical set of polynomials in higher dimensions. For the simplex one has to give up some of the nice characteristics of the Legendre polynomials and a more complicated approach has to be used.

An Analysis leads to some useful properties of shape-functions on the simplex. Only some properties are compatible with each other. Each version of finite elements differs in exploiting these properties for an efficient implementation. This is the first part of the present paper. In the second part we construct vector spaces containing sets of polynomials well-suited for the p- and the h-p-version of finite elements. In the third part we construct shape functions within these spaces which are optimal in the sense of an optimal condition number of the preconditioned linear system. Finally, we present some other ingredients of an adaptive or feedback finite element code in the sense of [10] like error estimation and grid refinement control.

2 Properties of shape functions

2.1 The problem

We consider a linear second order elliptic symmetrical boundary value problem. A suitable set of conforming shape functions $\psi_i \in \mathrm{H}^1(\Omega)$ has to be chosen (displacement functions). These shape functions are formed by local shape functions ϕ_i on each finite element.

We introduce the barycentric coordinates $(b_0, b_1, \ldots, b_d)$ in a d dimensional space with respect to a d-simplex, sometimes called area or volume coordinates or homogeneous coordinates. They may be characterized by an affine transform with coordinates $(0, \ldots, 0, 1, 0, \ldots, 0)$ corresponding

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to a vertex of the simplex. Hence, coordinate $\frac{1}{d}(1,\ldots,1)$ is the centroid of the simplex. Using multi index notation we define the vector space $\mathcal{P}_p^d$ of polynomials of degree p in d variables by the linear span of

$$\mathcal{P}_p^d = \langle \bigcup_{|\alpha|\leq p} b^\alpha \rangle, \quad \alpha \in \mathrm{N}_0^{d+1}$$

Sometimes shape functions are written in terms of $\{x, y, 1-x-y\}$ on a reference triangle. This is equivalent to a function in $\{b_1,\ b_2,\ b_0\}$.

2.2 Hierarchy and orthogonal polynomials

We introduce the concept of p-hierarchy or p-extension.

Definition 2.1 If we have a basis $\mathcal{B}_p$ of shape functions spanning the function space $\mathcal{V}_p$ and we want to reach the space $\mathcal{V}_{p+1}$, we simply can add some shape functions to get the enhanced basis $\mathcal{B}_{p+1} = \mathcal{B}_p \cup \mathcal{B}_{p+1}^{\text{ext}}$.

$$\mathcal{V}_{p+1} = \langle \mathcal{B}_{p+1} \rangle = \langle \mathcal{B}_p \rangle \oplus \langle \mathcal{B}_{p+1} \setminus \mathcal{B}_p \rangle$$

□

P-hierarchy is an integral part of an approximation with varying order p in space. If we choose the order p_1 on one finite-element and a different p_2 on a neighboring element, we can achieve global continuity by linear constraints like [8] or by handling the p-hierarchic excess in a special way (setting it to zero).

An example for p-hierarchic polynomials are the previously mentioned Legendre polynomials. The Legendre polynomials $f_p(x)$ are orthogonal with respect to the scalar product $\langle .. . \rangle$ on $[-1, 1]$. They are hierarchical in their polynomial degree p and symmetrical to the origin. The symmetry behavior is alternately odd and even. To exploit the orthogonality in the case of a one dimensional problem for the Laplace operator one has to use integrated polynomials as shape functions: $\int f_j(t)dt$ [21]. Then, the bilinear form $a(u,v) = \langle \frac{d}{dx}u, \frac{d}{dx}v \rangle$ operates on the same terms as the scalar product does in the previous case. The integrated polynomials are orthogonal with respect to the bilinear form.

Definition 2.2 Here, we associate the term 'orthogonal' polynomials with a sequence of nested sets of polynomials $\mathcal{B}_1 \subset \mathcal{B}_2 \subset \ldots$ for a specific bilinear form. The polynomials have to be linearly independent. A polynomial $f \in \mathcal{B}_i$ is orthogonal with respect to this bilinear form on the vector space generated by the basis $\mathcal{B}_{i-1}$ (no condition for $\mathcal{B}_1$). The vector spaces generated by $\mathcal{B}_i$ are usually the vector spaces of polynomials $\mathcal{P}_{i+1}^d$. The polynomials in $\mathcal{B}_i \setminus \mathcal{B}_{i-1}$ need not be orthogonal onto themselves. □

Orthogonal polynomials are hierarchical in p by definition. Orthogonal polynomials do not necessarily lead to local matrices with condition numbers equal to one, $\kappa_j(A^{\text{loc}}) = 1$, like the Legendre polynomials. However, a basis with this desirable property can be constructed.

2.3 Coupling

We call the assembly of local finite-element-matrices into a global one coupling, sometimes called 'global assembly'. One line of interpretation is the representation of global FEM ansatz functions, each connected with an degree of freedom, by linear combinations of local shape functions on an element. Coupling means this linear combination, which ideally is a one-to-one relation (local permutation matrix, called 'simple'). This would be the case for so-called compatible shape functions. Many FEM codes use this simple form of global matrix assembly, assuming that the local shape functions are suited for it.

Another bottom-up interpretation is that we have to guarantee we are dealing with globally continuous shape functions $\{\psi_i\}$, which are formed by properly connected local shape functions $\{\phi_i\}$. We introduce two new terms: *simple* and *minimal* coupling.

Definition 2.3 We call the coupling of the shape functions of two connected elements *minimal*, if the number of shape functions involved is minimal. □

This number $n(E, E^*)$ equals twice the dimension of the polynomial vector space on the intersection $\overline{E} \cap \overline{E^*}$ of both elements E, E^*. Coupling coefficients zero corresponding to vanishing shape functions on the intersection do not contribute to n.

We can express the coupling by an under-determined system of linear equations. Taking a coupling matrix C and the sets of shape functions $\{\phi_i\}$ and $\{\phi_i^*\}$, we can write the constraints as

$$C \cdot (\phi_1,\ \phi_2,\ \ldots,\ \phi_1^*,\ \phi_2^*,\ \ldots)^T = 0 \ \text{ on } \ \overline{E} \cap \overline{E^*}.$$

By eliminating columns containing only zeros, eliminating linearly dependent rows and permuting we arrive at a reduced matrix $C \in \mathrm{R}^{n \times 2n}$ of rank n.

We introduce a stronger term of coupling by a special kind of minimal coupling which we call *simple*. The under-determined system of linear equations with (reduced) matrix C should facilitate the conversion between the coefficients of the functions $\{\phi_i\}$ and $\{\phi_i^*\}$. We reduce the matrix C to a smaller matrix $\tilde{C}$ by leaving out columns which are linearly dependent or zero.

Definition 2.4 We define a coupling of shape functions $\{\phi_i\}$ and $\{\phi_i^*\}$ *simple*, if there exists a reduced and permuted matrix $\tilde{C}$ of maximal rank which has block-diagonal form with 1×2 non-zero blocks. □

The reduced matrix looks like this:

$$\tilde{C} = \begin{pmatrix} \tilde{C}_1 & & & \\ & \tilde{C}_2 & & \\ & & \ddots & \\ & & & \tilde{C}_n \end{pmatrix} \text{ with } \tilde{C}_i \in \mathrm{R}^{1\times 2}.$$

Examples 2.1 *We look at the* simple *coupling of two elements E and E^* with 2×2 local matrices A and B and shape functions $\{\phi_1, \phi_2\}$ and $\{\phi_1^*, \phi_2^*\}$. Function ϕ_2 equals function ϕ_1^* on $\overline{E} \cap \overline{E^*}$. No other shape functions of E and E^* are correlated. This leads to a matrix $C = \begin{pmatrix} 0 & 1 & -1 & 0 \end{pmatrix}$, a reduced matrix $\tilde{C} = \tilde{C}_1 = (1 \quad -1)$ and to*

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix}$$

coupled with

$$\begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix}$$

adds up to

$$\begin{pmatrix} a_{11} & a_{12} & 0 \\ a_{12} & a_{22}+b_{11} & b_{12} \\ 0 & b_{12} & b_{22} \end{pmatrix}.$$

Simple coupling may also appear as blocks of $\tilde{C}_i = (1 \ 1)$, in general as $\tilde{C}_i = (1 \ \lambda)$, $\lambda \neq 0$ or as small blocks simply invertible.

The Lagrange polynomials are interpolation polynomials on a set of equidistant points called 'control points' x_i. The polynomials are defined by the orthogonality relation

$$f_i(x_j) = \delta_{i,j}$$

The polynomials of degree p are defined on a d–simplex by the equidistant distribution of $\binom{p+d}{d}$ control points on the simplex, spanning the space $\mathcal{P}_p^d$. The set of Lagrange polynomials implements the interpolation property of the linear shape functions $p = 1$ often used for conforming finite elements. Global continuity can be achieved for a uniform polynomial degree p, identifying shape functions of all elements sharing one geometric control point (coupling of element matrices). Implementation of Dirichlet boundary conditions is easy, too. Shape functions are symmetric/ affine invariant due to symmetry/ affine invariance of the control points.

Remark 2.1 *We conclude that there are shape functions with* minimal *and* simple *coupling. Some are symmetrical, too.*

There are some slight modifications, moving the position of the control points and using points of the numerical integration formula. There are other proposals for unsymmetric modifications of edge shape functions in the inner of a triangle like [11, 7], which are difficult to generalize for tetrahedra [20].

2.4 Symmetry

Definition 2.5 We denote the group of permutations of d elements with S_d and the subset of the alternating group with S_d^+. □

Definition 2.6 We define the action of a group $\mathrm{S} \subset \mathrm{S}_{d+1}$ on a set of polynomials $\mathcal{B}$ in d variables by the set of polynomials resulting from permuting the input variables (by the permutations of the group) in barycentric representation. This covers the definition of the action on a single polynomial and on a whole vector space of polynomials.

$$\mathrm{S}\mathcal{B} = \bigcup_{f\in\mathcal{B}, s\in\mathrm{S}} f\big(s^{-1}(b_0, b_1, \ldots, b_d)\big)$$

□

Definition 2.7 We call a polynomial f, a set of polynomials $\mathcal{B}$ and a vector space $\mathcal{V}$ of polynomials "S-symmetrical", if it is invariant with respect to the action of S

$$f = \mathrm{S}f, \quad \mathcal{B} = \mathrm{S}\mathcal{B} \quad \text{and} \quad \mathcal{V} = \mathrm{S}\mathcal{V}.$$

□

It immediately follows that

- a set of S-symmetrical polynomials is an S-symmetrical set of polynomials and
- a vector space generated by an S-symmetrical set of polynomials is S-symmetrical itself.

Additionally, we introduce point-symmetry which is *not* covered by the previous definitions.

Definition 2.8 We define a set of polynomials $\mathcal{B}$ to be $\mathrm{S}_{d+1}^{\pm}$-symmetrical in d variables by

$$\forall s \in \mathrm{S}_{d+1} \text{ and } \forall f \in \mathcal{B} \text{ holds } sf \in \mathcal{B} \text{ or } -(sf) \in \mathcal{B}.$$

□

Remark 2.2 *Defining symmetry by* $\forall s \in \mathrm{S}_{d+1}$ *and* $\forall f \in \mathcal{B}$ $\exists \lambda \in \mathrm{R} \setminus \{0\}$ *with* $\lambda(sf) \in \mathcal{B}$ *leads to* $\lambda = \pm 1$*, too.*

Lemma 2.1 *An* $\mathrm{S}^{\pm}$*-symmetrical set* $\mathcal{B}$ *of polynomials is* S^{+}*-symmetrical.*

Remark 2.3 *We conclude that there are* $\mathrm{S}_d^{\pm}$*- and* S_d*-symmetrical shape functions.*

2.5 Symmetry and coupling

Finite Element methods often use a simple set of shape functions defined on a reference element. In the case of simplices, each shape function is transferred to a real element using an affine transformation. There are different possibilities for realizing this transformation. The transformation is unique only modulo permutation of the corner points. Hence, one has to be able to couple any face of one element with any face of another one; where faces can be points, edges, triangles and so on.

One can think of a completely oriented tessellation where the coupling is restricted to only some distinguished combinations of faces. But, in general, there is no such orientation.

Hence, there is no way out of having a deeper look into symmetry and coupling properties.

Theorem 2.1
A set of shape functions for a general conforming tessellation of d-simplices will permit a simple *coupling with blocks* $\tilde{C}_i = (1 \quad -1)$ *if, and only if, the shape functions permit* minimal *coupling and are* S_{j+1}*-symmetrical on each* j*-dimensional face of a simplex.*

We can relax this condition a little by requiring only $\psi_i = \pm\psi_k$ on the common boundary which leads to addition and subtraction of local matrices.

Corollary 2.1
A set of shape functions for a general conforming tessellation of d-simplices will permit a simple *coupling with blocks* $\tilde{C}_i = (1 \quad \pm 1)$ *if the shape functions permit* minimal *coupling and are* $\mathrm{S}_{j+1}^{\pm}$*-symmetrical on each* j*-dimensional face of a simplex.*

Remark 2.4 S_{d+1}*-symmetry is correlated with* simple *coupling of* $(1 \quad -1)$ *and* $\mathrm{S}_{d+1}^{\pm}$*-symmetry is correlated with* simple *coupling of* $(1 \quad \pm 1)$.

2.6 Symmetry and hierarchy

We now want to derive the correlation of symmetry and p-hierarchy. The Legendre polynomials for example are p-hierarchic and $\mathrm{S}_2^{\pm}$-symmetrical, which simply means point and axial symmetry in one dimension. For d dimensions we get the following main result:

Theorem 2.2
There is no p-hierarchical S_{d+1}^{+}*-symmetrical polynomial basis on the d-simplex for* $d > 1$.

Proof We look at the p-hierarchical step from polynomial degree $j(d+1)$ to $j(d+1)+1$ with $j \in \mathrm{N}_0$. Note that the dimension of symmetrizations of the set $\{b_0 - b_1, b_1 - b_2, \ldots, b_{d-1} - b_d\}(b_0 \cdot b_1 \cdots b_d)^j$ is at least $d+1$, but the vector space is of dimension d. □

Corollary 2.2
There is no p-hierarchical $\mathrm{S}_{d+1}^{\pm}$*-symmetrical polynomial basis on the d-simplex for* $d > 1$.

Theorem 2.3
There is no p-hierarchical S_{d+1}*-symmetrical polynomial basis on the d-simplex for* $d \geq 1$.

Corollary 2.3
There are no S_{d+1}^{+}*-symmetrical orthogonal polynomials on the d-simplex for* $d > 1$.

Remark 2.5 *Symmetry and simple coupling on the one hand and p-hierarchy for* $\mathcal{P}_p^d$ *on the other hand exclude each other.*

3 Construction of polynomial Spaces

We want to construct a family of p-hierarchical shape functions for the d-simplex. It has to facilitate a simple coupling which implies symmetry (chapter 2.5). It should be suitable for a p- and h-p-version of finite elements with variable order p which means p-hierarchy, in some sense. Both properties are not possible at the same time (chapter 2.6).

We have to cope with the limitations of theorem (2.2). We shall enlarge the polynomial vector spaces $\mathcal{P}_p^d$ slightly and construct new S_{d+1}-symmetrical vector spaces which avoid the irreducible subspaces of the proof.

3.1 Symmetry S_d

We recursively construct a basis for the new vector space $\mathcal{P}_p^{d,\mathrm{sym}}$ by the span of the vector space $\mathcal{P}_{p-1}^{d,\mathrm{sym}}$ one degree lower and additional functions. These functions are internal functions formed by the product of the "bubble" function $\prod_{j=0}^{d} b_j$ with functions of degree $(p-d-1)$ and boundary functions defined on the faces. The boundary functions are S_{d+1}-permutations (symmetrizations) of such (lower-) i-dimensional functions $(\mathcal{B}_{p-i-1}^{i} \cdot \prod_{j=0}^{i} b_j)$, $i < d$. The only difference to the standard polynomial spaces $\mathcal{P}_p^d$ is the beginning of the recursion. We start with $\{b_0\}$ for $\mathcal{B}_0^0$ which actually has degree 1. If we want to get the standard polynomial spaces $\mathcal{P}_p^d$, we should have taken $\{1\}$. We have enlarged the vector space. This enlargement spreads to the higher dimensions and the higher degrees.

Definition 3.1 We recursively construct a basis for the new vector space in barycentric coordinates based on lower dimensions and lower degrees using the group of permutations S_d:

- $\mathcal{B}_0^0 = \{b_0\}$
- $\mathcal{B}_p^0 = \emptyset, \quad p > 0$
- $\mathcal{B}_p^d = \bigcup_{i=0}^{d} S_{d+1}(\mathcal{B}_{p-i-1}^{i} \cdot b_0 \cdot b_1 \cdots b_i), \quad d \geq 1.$

□

Sometimes shape functions are written in a form like $\{x, y, 1-x-y\}$ on a reference triangle. This is equivalent to $\{b_1,\ b_2,\ b_0\}$.

Remark 3.1 *In the previous definition we can substitute the action of* S_{d+1} *by the combinations without repetition of* $i+1$ *elements of the set* $\{b_0, b_1, \ldots, b_d\}$.

Definition 3.2 We now define the new polynomial vector spaces as the span of the basis functions in d dimensions: $\mathcal{P}_p^{d,\mathrm{sym}} = \langle \bigcup_{i=0}^{p} \mathcal{B}_i^d \rangle$ □

Remark 3.2 *The vector spaces* $\mathcal{P}_p^{d,\mathrm{sym}}$ *are* S_{d+1}*-symmetrical. Their bases* $\mathcal{B}_p^{d,\mathrm{sym}}$ *are p-hierarchical, facilitate* minimal *and* simple *coupling with blocks* $(1\ \ -1)$ *and are enlarged* $\mathcal{P}_p^d \subseteq \mathcal{P}_p^{d,\mathrm{sym}} \subseteq \mathcal{P}_{p+1}^d$.

These polynomial spaces are well-suited for the coupling $(1\ \ -1)$, but they have got a high dimension (= too many shape functions). If we relax the coupling to $(1\ \ \pm 1)$, we can reduce this high dimension, but we have to consider the group $S_{d+1}^{\pm}$ (chapter 2.5).

3.2 Symmetry $S_d^{\pm}$

Definition 3.3 We recursively construct a basis for the new $S_{d+1}^{\pm}$-symmetrical vector space, taking the same 0-dimensional space and the action of the alternating group S_d^+ otherwise, modifying the one dimensional basis:

- $\mathcal{B}_0^{0,\pm} = \{b_0\}, \quad \mathcal{B}_p^{0,\pm} = \emptyset, \quad p > 0$
- $\mathcal{B}_0^{1,\pm} = \{b_0,\ b_1\}, \quad \mathcal{B}_1^{1,\pm} = \emptyset, \quad \mathcal{B}_p^{1,\pm} = \{(b_1 - b_0)^p\}, \quad p > 1$
- $\mathcal{B}_p^{d,\pm} = \bigcup_{i=0}^{d} S_{d+1}^{+}(\mathcal{B}_{p-i-1}^{i,\pm} \cdot b_0 \cdot b_1 \cdots b_i), \quad d > 1.$

□

Remark 3.3 *In the previous definition we can substitute the action of* S_{d+1}^{+} *by the even combinations without repetition of* $i+1$ *elements of the set* $\{b_0, b_1, \ldots, b_d\}$. *Watch out for a systematical interpretation of "even"!*

Definition 3.4 We now define the new polynomial vector spaces as the span of the basis functions in d dimensions: $\mathcal{P}_p^{d,\pm} = \langle \bigcup_{i=0}^{p} \mathcal{B}_i^{d,\pm} \rangle$ □

Examples 3.1 *In zero dimension we get the following sequence of polynomials, which are only useful for the construction of higher dimensional ones:*

$\mathcal{P}_0^{0,\pm} = \mathcal{P}_1^{0,\pm} = \mathcal{P}_2^{0,\pm} = \ldots = \langle \{b_0\} \rangle$

Starting with the one dimensional $S_2^{\pm}$*-symmetrical polynomials we get the following sequence:*

$$\begin{aligned}
\mathcal{P}_0^{1,\pm} &= \mathcal{P}_1^{1,\pm} &&= \langle \{b_0,\ b_1\} \rangle \\
\mathcal{P}_2^{1,\pm} &= \langle \mathcal{P}_1^{1,\pm} &&\cup\ \{(b_1 - b_0)^2\} \rangle \\
\mathcal{P}_3^{1,\pm} &= \langle \mathcal{P}_2^{1,\pm} &&\cup\ \{(b_1 - b_0)^3\} \rangle \\
&\vdots
\end{aligned}$$

The spaces $\mathcal{P}_p^{1,\pm}$ *are equal to the former spaces* $\mathcal{P}_p^1$ *for* $p > 0$. *Thus they are smaller than the spaces* $\mathcal{P}_p^{1,\mathrm{sym}}$. *The one dimensional basis is not enlarged any more. Inserting this into the definition for two dimensions we get a sequence of* $S_3^{\pm}$*-symmetrical polynomials:*

$$\begin{aligned}
\mathcal{P}_0^{2,\pm} &= \mathcal{P}_1^{2,\pm} &&= \langle \{b_0,\ b_1,\ b_2\} \rangle \\
\mathcal{P}_2^{2,\pm} &= \langle \mathcal{P}_1^{2,\pm} &&\cup\ \{(b_1 - b_0)^2,\ (b_2 - b_1)^2, \\
&&&\qquad (b_0 - b_2)^2\} \rangle \\
\mathcal{P}_3^{2,\pm} &= \langle \mathcal{P}_2^{2,\pm} &&\cup\ \{(b_1 - b_0)^3,\ (b_2 - b_1)^3, \\
&&&\qquad (b_0 - b_2)^3\} \cup \{b_0(b_0 b_1 b_2), \\
&&&\qquad b_1(b_0 b_1 b_2),\ b_2(b_0 b_1 b_2)\} \rangle \\
\mathcal{P}_4^{2,\pm} &= \langle \mathcal{P}_3^{2,\pm} &&\cup\ \{(b_1 - b_0)^4,\ (b_2 - b_1)^4, \\
&&&\qquad (b_0 - b_2)^4\} \rangle \\
&\vdots
\end{aligned}$$

On the triangle the polynomial sets for a degree p which is not divisible by 3 *are identical to* $\mathcal{P}_p^2$, *all other vector spaces are generated by* $\mathcal{P}_p^2$ *and* 2 *additional polynomials.*

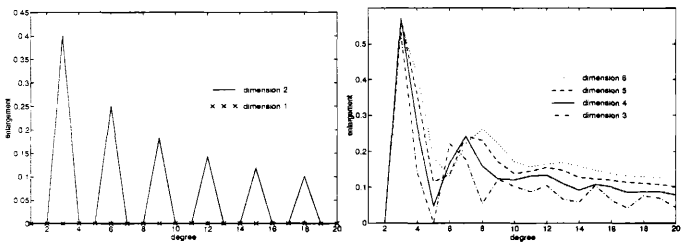

Figure 1: Enlargement of $\mathcal{P}_p^{d,\pm}$: values of $(dim\mathcal{P}_p^{d,\pm} - dim\mathcal{P}_p^d)/(dim\mathcal{P}_{p+1}^d - dim\mathcal{P}_p^d)$

Remark 3.4 *The usual linear Lagrange polynomials are contained in both $\mathcal{B}_1^d$ and $\mathcal{B}_1^{d,\pm}$. The associated hierarchical quadratic polynomials are contained in $\mathcal{B}_2^{d,\pm}$, too.*

Remark 3.5 *The linear Lagrange polynomials can be interpreted as symmetrization of the canonical basis of $\mathcal{P}_1^d$: $\{1\} \cup \{b_1, b_2, \ldots, b_d\}$.*

Remark 3.6 *The bases $\mathcal{B}_p^{d,\pm}$ are $S_{d+1}^{\pm}$-symmetrical, p-hierarchical and facilitate* minimal *and* simple *coupling with blocks* $(1 \quad \pm 1)$. *The spanned vector spaces $\mathcal{P}_p^{d,\pm}$ are only slightly enlarged ($\mathcal{P}_p^d \subseteq \mathcal{P}_p^{d,\pm} \subseteq \mathcal{P}_p^{d,\mathrm{sym}} \subseteq \mathcal{P}_{p+1}^d$) and have got an even lower dimension than $\mathcal{P}_p^{d,\mathrm{sym}}$.*

3.3 The enlargement

We saw that the enlarged polynomial spaces fulfill

$$\mathcal{P}_p^d \subseteq \mathcal{P}_p^{d,\pm} \subseteq \mathcal{P}_{p+1}^d$$

which limits the enlargement of $\mathcal{P}_p^{d,\pm}$ (note 3.6). Actually, we can show that with $p \to \infty$ this enlargement vanishes in the following sense:

$$(1) \qquad \frac{dim\mathcal{P}_p^{d,\pm} - dim\mathcal{P}_p^d}{dim\mathcal{P}_{p+1}^d - dim\mathcal{P}_p^d} \leq O(p^{-1}) \quad \text{for fixed } d$$

We prove this also giving the dependence on d by

Lemma 3.1

$$dim\mathcal{P}_p^{d,\pm} - dim\mathcal{P}_p^d \leq d\binom{p+d-2}{p}$$

Proof $dim\mathcal{P}_p^d$ may also be written by the recursive equation of $dim\mathcal{P}_p^{d,\pm}$ obtained from definition of $\mathcal{P}_p^{d,\pm}$. The difference obeys the same equation. It can be majorized by a recursion of $d \cdot dim\mathcal{P}_p^{d-2}$. □

d	dim $\mathcal{P}_5^d$	dim $\mathcal{P}_5^{d,\pm}$	dim $\mathcal{P}_{10}^d$	dim $\mathcal{P}_{10}^{d,\pm}$
1	6	6	11	11
2	21	21	66	66
3	56	56	286	294
4	126	130	1001	1045
5	252	276	3003	3192
6	462	546	8008	8757

Table 1: Dimensions of $\mathcal{P}_p^d$ and $\mathcal{P}_p^{d,\pm}$

p	reduced S	reduced $S^{\pm}$	reduced $S^{\pm}_{\mathrm{surf}}$	original $\mathcal{P}_p^3$	extended $S^{\pm}_{\mathrm{surf}}$	extended $S^{\pm} = \mathcal{P}_p^{3,\pm}$	extended S
1	4	4	4	4	4	4	4
2	4	10	10	10	10	10	16
3	16	16	16	20	28	28	28
4	28	34	35	35	35	38	44
5	44	56	56	56	56	56	68
6	68	80	80	84	92	92	104
7	104	116	120	120	120	128	140
8	140	164	165	165	165	168	192

Table 2: Dimensions of $\mathcal{P}_p^3$ in R^3, of extended and reduced spaces, S-symmetric, $S^{\pm}$-symmetric and $S^{\pm}_{\mathrm{surf}}$-symmetric on the surface of the tetrahedron only

With $dim\mathcal{P}_p^d = \binom{p+d}{p}$ the proof of formula (1) is completed. Figure (1) shows the actual values of the quotient. $\mathcal{P}_p^{1,\pm}$ is not enlarged and $\mathcal{P}_p^{2,\pm}$ is enlarged by 2 polynomials only for every third p. It indicates, in conjunction with the actual numbers in table 1, that the values decrease asymptotically with p^{-1}.

In table 2 we have added the dimensions for extended and reduced symmetric polynomial spaces obtained by the recursion. Reduction in this context results in incomplete polynomial spaces due to the symmetrization analog of the previous extension of spaces. The spaces of polynomials with symmetry on the boundary of the element only do not differ much from symmetry for all polynomials, including the inner functions. The $S^{\pm}$-symmetric reduced polynomials are an attractive lower dimensional counterpart of the $S^{\pm}$-symmetric full polynomials $\mathcal{P}_p^{d,\pm}$ and the S-symmetric reduced polynomials are connected with full S-symmetric polynomials $\mathcal{P}_p^d$. We also remark the drop-out of full symmetric reduced polynomials at degree $p = 2$ and via recursion inherited minor drop-outs. In the future we will use the polynomials $\mathcal{P}_p^{d,\pm}$ only.

4 Construction of shape functions

4.1 Preconditioning

In the context of the iterative solution of the linear systems another tool comes into play. It is the convergence rate of the iteration. It can be estimated for some classic iterations like conjugate gradients and Richardson-iteration in terms of the condition number. But, for the sake of efficiency linear systems are often preconditioned, so we have to consider the condition number of the preconditioned matrix instead. There are two similar approaches for preconditioning linear systems of p-version [13, 1] and [17, 16], both leading to estimates independent from h and with a rather mild increase in $\log^2 p$.

It is well known from domain decomposition, that any construction of a preconditioner as splitting into a linear or piecewise constant global function space and several higher order local spaces leads to such an h-independence under the condition of *minimal coupling*. Coupling comes into play localizing the global higher order function spaces. Hence we construct our preconditioner as the splitting into the global linear space and additional local spaces. To keep them local, we have to separate spaces for each edge, triangle, tetrahedron etc. Now we can interpret this preconditioner B as a block-diagonal version of the stiffness-matrix A. Calculating the preconditioned condition number $\kappa(B^{-1}A)$, we can see that it is majorized by the maximum of the local condition numbers $\tilde{\kappa}$ $(\frac{\max\lambda}{\min\lambda\neq 0})$ of the generalized eigenvalue problem $B_{\text{loc}}x = \lambda A_{\text{loc}}x$. $\tilde{\kappa}$ is calculated from the generalized eigenvalues orthogonal to the common eigenfunction of the eigenvalue 0. This means that we only have to optimize and calculate local condition numbers and the condition number is independent from h with the aid of a good preconditioner for the linear h-version problem.

4.2 Condition numbers

We want to construct the final version of our shape functions by using the polynomial vector spaces $\mathcal{P}_p^{d,\text{sym}}$ and $\mathcal{P}_p^{d,\pm}$ of chapter (2.5). The set of functions should maintain the symmetry and coupling properties of the original basis $\mathcal{B}_p^d$ and $\mathcal{B}_p^{d,\pm}$. P-hierarchy is guaranteed by the nesting of the vector spaces. The only missing property is a low condition number of the preconditioned system.

We make a general approach to optimization of the local condition numbers. The optimal polynomials are in a linear vector space $\mathcal{V} = \langle f_1, f_2, \ldots\rangle$. Every optimized polynomial v_k has a representation of

$$v_k := \sum_{i=1}^{k} q_{ki} f_i, \qquad k = 1, \ldots$$

We have to determine the coefficients q_{ki} that v_k has the desired properties. We used some direct procedures for minimization of the condition numbers.

All optimization procedures have in common the necessity of a correct management of the polynomials, their symmetry and their coupling properties. This includes the construction of the appropriate basis functions for each optimized shape function set. The optimized shape functions are a linear combination of the basis functions. The combination itself depends on the optimization. The actual basis functions $\tilde{f}_i$ are in some cases (optimized) shape functions v_k of previous optimization steps, and in some cases symmetrizations of them.

We now compare the resulting local condition numbers. We choose the Laplace operator on the equilateral simplex. The condition numbers shown in table 3 are evaluated numerically.

d	$p=2$	$p=3$	$p=4$	$p=5$	$p=6$	$p=7$	$p=8$
2	6.00	19.2	20.8	45.6	54.5	56.2	57.4
3	12.3	125.	127.	194.	361.		
4	21.1	336.	467.	882.			

Table 3: Condition numbers of the preconditioned stiffness matrix for $\mathcal{P}_p^{d,\pm}$

We were not able to prove a special kind of asymptotics in p but we simply present the actual numbers of interest. We think that a hard prove would not only be intricated because of the structure of the function spaces $\mathcal{P}_p^{d,\pm}$, but also of less practical worth for real-problem p.

Nevertheless, we obtain low local condition numbers; hence, an additional acceleration of an iterative solver would be obsolete. But, our main result still is the new polynomial spaces $\mathcal{P}_p^{\text{sym}}$ and $\mathcal{P}_p^{\pm}$, including their properties.

5 FEM framework

5.1 Error estimation

Putting this new shape functions into a framework of an adaptive or feedback finite element code, we have to consider some other details. We use an a posteriori error estimator to indicate those elements and regions to refine in

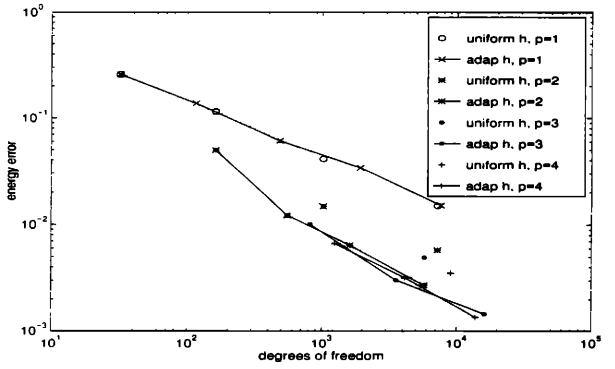

Figure 2: Uniform and adaptive h-version.

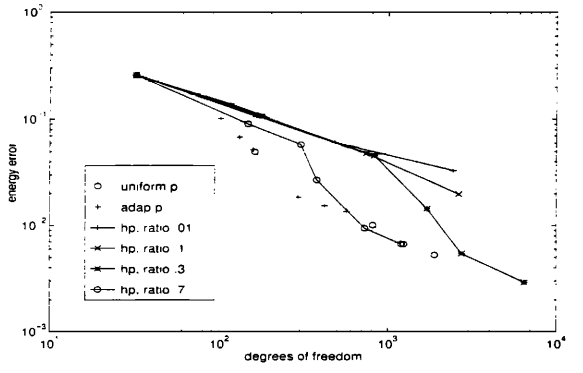

Figure 3: P-version and adaptive h-p-version.

the next step of the adaptive procedure. Assuming that our initial grid is fine enough, we can use an error estimator similar to [10]. See [5, 15] for different choices. With a suitable saturation condition fulfilled, the edge wise local p-extensions of [10] can be proven to be a good error estimator. We extend this to higher order elements by considering an edge p-extension of one degree higher than used for the solution. This enables cheap error estimation even in the case of nonuniform p. We call this error the p-error.

We compute a similar error by an hierarchic h-extension which means a local subdivision of an edge. The local linear system on the edge delivers an error estimation which we call the h-error. The h-error usually is of lower quality. Hence. for refinement decision, the p-error is used.

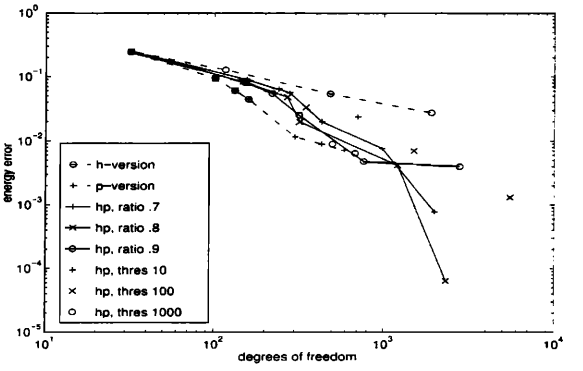

Figure 4: Adaptive h-version, adaptive p-version and adaptive h-p-version.

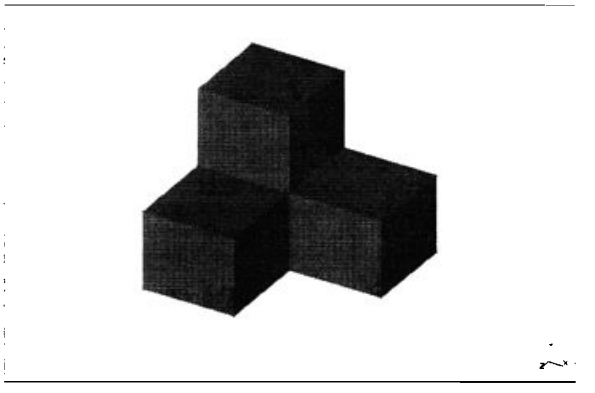

Figure 5: Computational domain

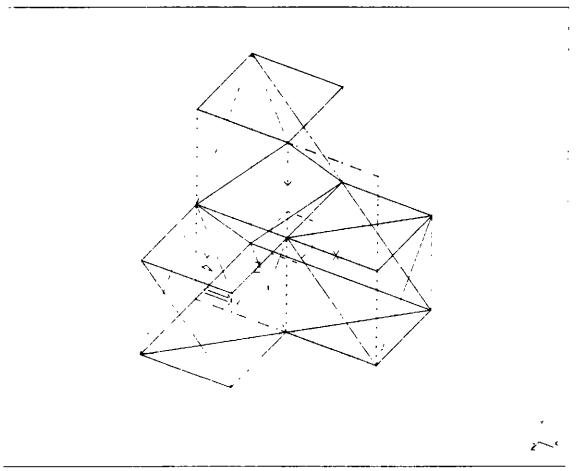

Figure 6: Initial coarse grid

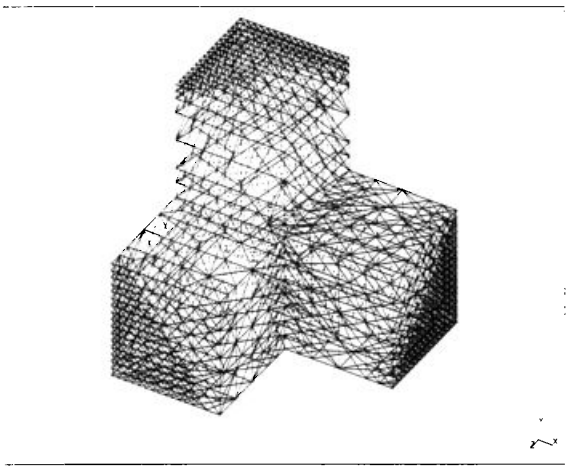

Figure 7: Adaptively refined grid, h-version

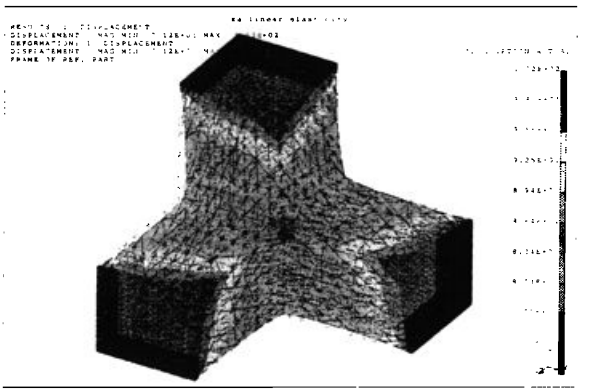

Figure 8: Computed displacement on refined grid

5.2 Feedback grid control

The refinement decision uses a maximum criterion of element errors with a minimum percentage guaranteed [10]. Elements for refinement are marked. They are refined in adaptive h version and p version. For h-p version afterwards a decision for each element is made whether to refine in h-direction (subdivide element) or in p-direction (increase polynomial degree). This decision depends on the ratio of h-error/p-error which is compared to a threshold. The threshold is sometimes fixed for the whole computation or chosen as a fixed percentage of the maximum ratio. Some experiments with history of estimated errors (usually short) or measures of computational work spend for each decision were not convincing enough to justify the additional complexity of implementation and behavior. For other considerations about h-p grid generation see [12, 14, 19].

We present some numerical experiments concerning the performance of different finite element versions. Depicted is the error measured in energy norm versus the number of unknowns in the linear system of equations. The examples show that the uniform p-version is faster than the uniform h-version; different behavior of the adaptive versions and performance of the h-p adaption for some threshold parameters is shown. For a detailed explanation see [3].

The first example is a nearly quadratic one,

$$\Delta u(x) = 1, \quad x \in [-1.1]^3$$

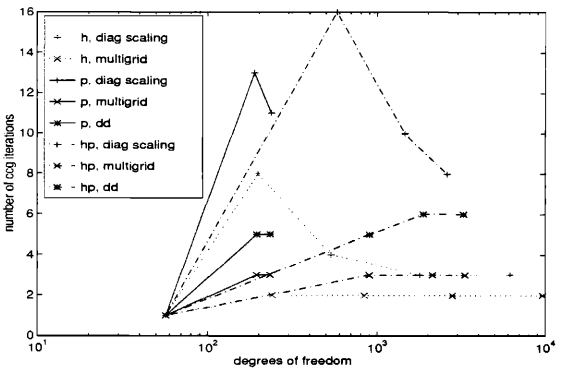

Figure 9: Adaptive FEM iteration counts for diagonal scaling, multigrid preconditioner and domain decomposition preconditioner (different final precision).

with homogeneous Dirichlet boundary conditions. The results are in figures 2 and 3 (computational domain only $1/8$). Figure 2 shows a comparison of h-versions with different order p. For linear elements $p = 1$ adaptivity does not pay off whereas adaptivity is preferable for higher p. The solution is very well approximated by quadratic elements and every linear approximation remains poor. Next, figure 3 shows the performance of the related h-p versions. The biggest part of p refined elements compared to h refined delivers best performance, approaching original p version.

The next example is an analytic one, also preferring higher order approximations:

$$\Delta u(x) = \cos x_1 \cos x_2 \cos x_3, \quad x \in [-\pi/2, \pi/2]^3$$

with homogeneous Dirichlet boundary conditions. The results are contained in figure 4 (computational domain only $1/8$, different scaling). Different h-p versions are compared to an adaptive h-version and an adaptive p-version. The .8 threshold h-p version performs best, whereas h-p versions with higher or lower h/p ratio are better in a middle phase.

5.3 Iterative solvers

We already have presented an iterative two-level domain decomposition solver while constructing an optimal set of shape functions similar to [13, 1]. We now compare it with another approach due to [9] only exploiting the history of refined grids called ccg. Optimal convergence has been proven for linear elements in [4]. We choose a multigrid $V_{2,2}$ solver with 3×3 block symmetric Gauss-Seidel smoother for the global system arising in domain decomposition and present some iteration counts and residuum reduction rates. The ccg algorithm is originally equipped with a diagonal scaling.

The last example is from linear elasto mechanics. The Lamé equations are solved with a three dimensional displacement approach. A Poisson ratio of .29 is used. There are no interior forces and most of the surface is free. Only three outer squares have a prescribed displacement pointing from the center to the outside. The elastic body and its initial grid are shown in figures 5 and 6. Figure 7 shows a h refined grid during computation and figure 8, finally, shows the deformed body.

Figure 9 shows the behavior of both solvers for an adaptive h-p version. For diagonal scaling it shows the typical behavior a of decreasing number of iterations after a high peak at a low number of unknowns. The total work adds up to a small constant depending on asymptotical behavior. Preconditioning leads to constant lower numbers of iterations, but each iteration itself is more expensive. Pure multigrid Gauss-Seidel, in conjunction with our optimized shape functions, seems to be faster than more additional domain decomposition with multigrid.

6 Conclusion

We have presented a framework for adaptive h-p finite element methods for second order boundary value problems. Aiming an efficient computational code with fully automatic control, we have chosen the h-p version of finite elements ensuring (sub-) exponential convergence in contrast to the standard algebraic one. To generate the full convergence order, well-adapted grids had to be generated by the code.

The demands for efficiency in conjunction with unstructured grids (because of geometry constraints and adaptation), varying polynomial degrees (in space and in adaptation history) and some concerns on robustness required new shape functions. The different polynomial degrees call for the concept of p-hierarchy of the shape functions. The easy assembly of the global stiffness matrix and the load vector on unstructured grids of simplices clearly lead to the requirements of symmetry of the shape functions on the boundary of each individual element. Finally, independence of orientation demands symmetry of the shape functions on the whole element.

However, it was proved that no families of shape functions in dimensions higher than $d = 1$ could have both properties, p-hierarchy and symmetry, at once for standard polynomial spaces. Hence, the spaces of polynomi-

als spanned by the shape functions were slightly modified and p-hierarchic and symmetric shape functions were constructed.

Therefore, a domain decomposition preconditioner for h-p grids based on a standard multilevel iterative solver for h grids was developed. This construction implied an orthogonalization of shape functions by means of optimization of the resulting condition numbers of the preconditioner. The optimization procedure delivered the uniqueness (modulo symmetry) of the shape functions.

With suitable error estimators and refinement strategies some numerical experiments were performed, demonstrating the superior convergence properties of pre-asymptotic p-version and the global convergence of h-p-version finite elements, which agrees with the theory. This was shown both for the characteristic 3D singularities of the Laplacian and for some 3D examples of linear elasto mechanics.

References

[1] I. Babuška, A. Craig, J. Mandel, and J. Pitkäranta. Efficient preconditioning for the p-version finite element method in two dimensions. *SIAM J. Numer. Anal.*, 28(3):624–661, 1991.

[2] I. Babuška, M. Griebel, and J. Pitkäranta. The problem of selecting the shape functions for a p-type element method. *Internat. J. Numer. Methods Engrg.*, 28:1891–1908, 1989.

[3] I. Babuška and M. Suri. The p and h-p-versions of the finite element method, basic principles and properties. *SIAM Rev.*, 36(4):578–632, 1994.

[4] F. A. Bornemann and P. Deuflhard. Cascadic multigrid method for elliptic problems. *Numer. Math.*, 1995. to appear.

[5] F. A. Bornemann, B. Erdmann, and R. Kornhuber. A posteriori error estimates for elliptic problems in two and three space dimensions. *SIAM J. Numer. Anal.*, 1993. to appear.

[6] P. Carnevali, R. B. Morris, Y. Tsuji, and G. Taylor. New basis functions and computational procedures for p-version finite element analysis. *Internat. J. Numer. Methods Engrg.*, 36:3759–3779, 1993.

[7] L. Demkowicz, A. Karafiat, and J.T. Oden. Solution of elastic scattering problems in linear acoustics using h-p boundary element method. *Comput. Methods Appl. Mech. Engrg.*, 101:251–282, 1992.

[8] L. Demkowicz, J. T. Oden, W. Rachowicz, and O. Hardy. Toward a universal h-p adaptive finite element strategy. i: Constrained approximation and data structure. *Comput. Methods Appl. Mech. Engrg.*, 77:79–112, 1989.

[9] P. Deuflhard. Cascadic conjugate gradient methods for elliptic partial differential equations. Algorithm and numerical results. In D. Keyes and J. Xu, editors, *Proceedings of the 7th International Conference on Domain Decomposition Methods 1993.* AMS, Providence, 1994.

[10] P. Deuflhard, P. Leinen, and H. Yserentant. Concepts of an adaptive hierarchical finite element code. *IMPACT Comput. Sci. Engrg.*, 1:3–35, 1989.

[11] M. Dubiner. Spectral methods on triangles and other domains. *J. Sci. Comp.*, 6(4):345–390, 1991.

[12] W. Gui and I. Babuška. The h, p and h-p versions of the finite element method in 1 dimension. i., ii., iii. *Numer. Math.*, 49:577–612, 613–657, 659–683, 1986.

[13] J. Mandel. Two-level domain decomposition preconditioning for the p-version finite element method in three dimensions. *Internat. J. Numer. Methods Engrg.*, 29:1095–1108, 1990.

[14] J. T. Oden. Optimal h-p finite element methods. *Comput. Methods Appl. Mech. Engrg.*, 112, 1994.

[15] J. T. Oden, L. Demkowicz, W. Rachowicz, and T. A. Westermann. Toward a universal h-p adaptive finite element strategy. ii: A posteriori error estimation. *Comput. Methods Appl. Mech. Engrg.*, 77:113–180, 1989.

[16] L. F. Pavarino. Additive Schwarz methods for the p-version finite element method. *Numer. Math.*, 66(4):493–515, 1994.

[17] L. F. Pavarino. Schwarz methods with local refinement for the p-version finite element method. *Numer. Math.*, 69(2):185–211, 1994.

[18] A. G. Peano. Hierarchies of conforming finite elements for plane elasticity and plate bending. *Comput. Math. Appl.*, 2:211–224, 1976.

[19] W. Rachowicz, J. T. Oden, and L. Demkowicz. Toward a universal h-p adaptive finite element strategy. iii: Design of h-p meshes. *Comput. Methods Appl. Mech. Engrg.*, 77:181–212, 1989.

[20] S. J. Sherwin and G. E. Karniadakis. Triangular and tetrahedral spectral elements. In *ICOSAHOM'95*, 1995.

[21] B. A. Szabó and I. Babuška. *Finite Element Analysis.* J. Wiley & Sons, New York, 1991.

[22] G. W. Zumbusch. Symmetric hierarchical polynomials for the h-p-version of finite elements. Preprint SC 93-32 ZIB, 1993.