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**Symmetric Hierarchical Polynomials
for the h - p -Version of Finite
Elements**

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ABSTRACT

Adaptive numerical methods using the h - p -version of finite elements require special kinds of shape functions. Desirable properties of them are symmetry, hierarchy and simple coupling. In a first step it is demonstrated that for standard polynomial vector spaces not all of these features can be obtained simultaneously. However, this is possible if these spaces are extended. Thus a new class of polynomial shape functions is derived, which is well-suited for the p - and h - p -version of finite elements on unstructured simplices. The construction is completed by minimizing the condition numbers of the arising finite element matrices. The new shape functions are compared with standard functions widely used in the literature.

KEY WORDS

FEM, shape functions, p -version, h - p -version, multivariate interpolation

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INTRODUCTION

This paper deals with shape functions for the finite element method. If the solution area of a partial differential equation is discretized into finite-size elements, one has to represent functions on these elements. We choose the simplex as element, which is a triangle in 2-D and a tetrahedron in 3-D, and try to approximate a scalar solution (or each single component of a non-scalar solution) by a polynomial. For numerical calculations one has to choose a basis for the desired space of polynomials. This basis yields the so-called shape functions.

Many operations in the finite element method deal with functions in the finite element space and therefore with the shape function. In the context of conforming linear shape functions one usually uses node-based functions. There is no need for other linear shape functions and in this sense they are optimal. Working with higher polynomial degrees the choice should depend on the version of finite elements. Interpolatory and orthogonal polynomials are commonly used in this case. In spite of different suggestions [MP72, Nic72, Pea76, SB91, ZT89, BGP89, DORH89], there is no canonical set of polynomials concerning optimal condition number and simplicity of usage. There is no systematic analysis about shape functions on any simplex either (except for the interval).

On the interval, 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 of finite elements for the Laplace equation. A pure higher-order h -version may also use interpolatory Lagrange polynomials. For the p - and h - p -version on tensor product structures like rectangles and bricks one could generalize these integrated Legendre polynomials [SB91], loosing some of their good transformation properties and investing more degrees of freedom than necessary in the approximation sense. But for the simplex one has to give up some other nice characteristics of the Legendre polynomials and a more complicated approach [Pea76, SB91, ZT89] has to be used. For a pure h -version one can keep Lagrange interpolation [MP72, Nic72].

In the following we analyze the operations for solving a problem by an adaptive (multilevel) finite element code with respect to the operations on the shape functions. This leads to useful properties of 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. Keeping in mind the bad condition numbers of some polynomial bases, we construct optimal and quasi-optimal shape functions within these spaces. The comparison to other popular shape functions with respect to the mentioned properties covers the last part of the paper.

1 PROPERTIES OF SHAPE FUNCTIONS

1.1 THE PROBLEM

We consider a linear second order elliptic symmetrical boundary value problem of the type

$$\sum_{i,k=1}^d \partial_i \left(a_{ik}(x) \partial_k u(x) \right) + a_0(x) u(x) = f(x), \quad \forall x \in \Omega \quad (1.1)$$

on the Lipschitz domain $\Omega \subset \mathbb{R}^d$ with suitable boundary conditions on $\partial\Omega$, a_0 being non-negative. We want to calculate the solution $u(x) \in \mathbb{R}$ on Ω with the finite element method. Using the bilinear form

$$a(u, v) = \int_{\Omega} \left(a_0(x) u(x) v(x) + \sum_{i,k=1}^d a_{ik}(x) \partial_i u(x) \partial_k v(x) \right) dx \quad (1.2)$$

and the scalar product

$$\langle v, f \rangle = \int_{\Omega} v(x) f(x) dx \quad (1.3)$$

in the variational formulation, one has to set up and solve the discrete linear system of equations

$$Au = b \quad (1.4)$$

defined by $A_{ik} = \left(a(\phi_i, \phi_k) \right)$ and $b_k = \langle \phi_k, f \rangle$. A suitable set of conforming shape functions $\phi_i \in H^1(\Omega)$ has to be chosen. These shape functions are formed by local shape functions ψ_i on each finite element. If the solution is not accurate enough, one has to choose a better discretization ϕ_i and redo the calculation. One has to distinguish some versions of finite element methods:

- The h -version is based on element subdivision, using identical shape functions on all elements.
- The p -version keeps the elements, but creates enhanced shape functions on each element [BSK81].
- The h - p -version uses both procedures – subdivision and shape function enhancement [BS90].
- The s -version uses an overlay of a domain of smaller elements on the original elements with the same type of shape functions. In most cases the overlaid elements are generated by element subdivision (c.f. [Ran93]).
- The more traditional r -version creates smaller elements which are not correlated with the old ones.

Each version of finite elements methods can be applied adaptively (affecting only some parts of the domain) or globally (also called uniform refinement). The system of linear equations can be solved directly (e.g. by Cholesky decomposition) or iteratively. Iterative solvers need a solution to start with which can be supplied by the solution on the previous discretization level. Types of iterative solution techniques are the family of multigrid and multi-level solvers which exploit the history of coarser discretizations. Here information about the solution process is transferred between different discretization levels.

1.2 FINITE ELEMENT CODES

A general finite element method consists of the following modules and operations which can merge into one another:

- *Constructing or managing a tessellation of the domain Ω .* In this paper we consider conforming tessellations of d -dimensional simplices. This means that two connected simplices have one and only one complete face of their boundary (a lower dimensional simplex) in common. This prevents us from dealing with slave nodes which are local but not global degrees of freedom and have to be removed from the global system of

equations by static condensation. Another point to mention is that we are working with only one element type, thus not mixing bricks, wedges, pyramids and tetrahedrons e.g.

- *Assembling the local element-wise matrices A^{loc} and right hand sides b^{loc} .* The numerical calculation of the integrals in $A_{ik}^{\text{loc}} = (a(\psi_i, \psi_k))$ and $b_k^{\text{loc}} = \langle \psi_k, f \rangle$ requires cubature formulas. The evaluation of the shape functions ψ_i is necessary only at the points of cubature and can be done via tabulated function values. Using different sets of shape functions like in the p -version, one may have different cubature formulas. Hence for all formulas one needs such a table. The number is limited by the maximal polynomial degree which is usually lower than ten. In the case of constant or simple a_{ik} 's and a_0 's the integrals may be calculated in advance using a transformation formula and, if necessary, a linear combination of such integrals. Thus it is not necessary to evaluate the shape functions in the assembling procedures if one can do some work in advance and does not use more sophisticated methods of integration. We do not necessarily have to supply a numerical procedure for evaluation of shape functions which can be difficult or sometimes ill conditioned numerically in case of higher order polynomials.
- *Assembling the local terms into the global matrix A and right hand side b (coupling of the shape functions).* The simplest way of assembling is summing up the local matrices and vectors, having in mind the position of the local matrix elements in the global matrix. A more complicated situation arises in the assembly of slave nodes which leads to condensing them by solving local linear equations, a procedure which we excluded previously. General shape functions may cause the same trouble if they are not symmetrical in the sense of simple inter-element coupling. This means that for two connected elements each shape function ψ_i of one simplex E that is not vanishing on the common boundary $\overline{E} \cap \overline{E^*}$ there is a corresponding shape function ψ_k^* on the other simplex E^* which is identical on the border $\psi_k^*(x) = \psi_i(x) \quad \forall x \in \overline{E} \cap \overline{E^*}$. In adaptive p -versions there is the additional problem of coupling different sets and degrees of polynomials. In the simplest case, one set $\Psi = \{\psi_i\}$ of non-vanishing polynomials is a subset of the other one $\Psi^* = \{\psi_i^*\}$ on

the common boundary. There are two parts: coupling of the common functions $\Psi \cap \Psi^*$ as usual and coupling the hierarchic surplus $\Psi^* \setminus \Psi$ by restricting it to zero. In more generality one has to remove some degrees of freedom by static condensation.

- *Solving the linear system of equations.* Using fast iterative multigrid or multilevel solvers, one has to transfer functions and updates of solutions between discretization levels. This requires a fast local transfer from one set of shape functions to another one (p -version) and from one element to the subdivided elements or vice versa (h -version). Hierarchic shape functions (p - or h -hierarchical) allow a relatively convenient transfer by setting some coefficients to zero or by ignoring them. All solvers appreciate a well-conditioned and sparse global matrix A .
- *Estimating the error of the solution or determining whether the solution is acceptable.* Error estimation often leads to the comparison of different approximations which are sometimes only local. Hence it reduces work if one can expand or restrict (project) a calculated solution easily to another discretization. Following this line it is convenient to use p - or h -hierarchical shape functions or to allow a simple transfer in another way.
- *Constructing a new tessellation of the domain by considering the estimated local errors.* Apart from the algorithmical problem of constructing a new conforming tessellation which fulfills the necessary element angle conditions one may want to save the calculated solution. This can be achieved easily if the transfer operations between discretization levels are simple.
- *Postprocessing the solution.* After calculating the solution, we may want to determine some properties of the solution or simply visualize it. We may have to manipulate the solution using the shape functions.

1.3 NOTATION

DEFINITION 1. We introduce the barycentric co-ordinates (b_0, b_1, \dots, b_d) in a d dimensional space, sometimes called area or volume co-ordinates (=

the linear Lagrange polynomials on the d -simplex) with

$$\sum_{i=0}^d b_i(x) = 1, \quad \forall x \in \mathbb{R}^d$$

The d -simplex has the corners $(1, 0, \dots, 0), (0, 1, 0, \dots, 0), \dots, (0, \dots, 0, 1)$.

DEFINITION 2. We introduce the multi index notation $\alpha = (\alpha_0, \alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^{d+1}$ by

- $|\alpha| = \sum_{i=0}^d \alpha_i$ and
- $b^\alpha = \prod_{i=0}^d b_i^{\alpha_i}$.

DEFINITION 3. We define the vector space P_p^d of polynomials of degree p in d variables by the linear span of

$$P_p^d = \langle \bigcup_{|\alpha| \leq p} b^\alpha \rangle, \quad \alpha \in \mathbb{N}_0^{d+1}$$

REMARK 1. The usual vector space of polynomials for a d -dimensional cube is the tensor product vector space $P_p^{d,\otimes} = \bigotimes_{i=1}^d P_p^1$ with $\dim P_p^{d,\otimes} > \dim P_p^d$ for $d > 1$.

1.4 CONDITION NUMBERS AND HIERARCHY

DEFINITION 4. We call $\kappa(A)$ condition number and $\kappa_j(A)$ reduced condition number of a symmetrical positive semi-definite matrix A . If the eigenvalues of A are $\lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_n$ with $0 \leq \lambda_0$, then $\kappa(A)$ and $\kappa_j(A)$ are given by

$$\kappa(A) = \frac{\lambda_n}{\lambda_0} \in [1, \infty] \quad \text{and} \quad \kappa_j(A) = \frac{\lambda_n}{\lambda_j} \quad \text{for the lowest } j \text{ with } \lambda_j \neq 0$$

By definition condition numbers are greater or equal to one: $\kappa(A) \geq 1$, $\kappa_j(A) \geq 1$. The condition number of a symmetrical positive definite matrix A is $\kappa(A) = \|A\|_2 \|A^{-1}\|_2$. If the so-called Helmholtz term a_0 in equation (1.1) does vanish, the local matrix A^{loc} has one eigenvalue zero and the reduced

condition number $\kappa_1(A^{\text{loc}})$ has to be used. If the term a_0 is strictly greater than zero on the element, we use the condition number $\kappa(A^{\text{loc}}) = \kappa_0(A^{\text{loc}})$. In general we write $\kappa_j(A^{\text{loc}})$.

REMARK 2. *The Helmholtz term a_0 plays an important role in the solution of parabolic equations and in eigenvalue computations via inverse vector iterations.*

The local condition numbers strongly depend on the functions a_{ik} , a_0 and on the geometry of the element.

EXAMPLE 1. *We recall the definition of the orthogonal Legendre polynomials on the interval $[-1, 1]$*

$$f_j(x) = \frac{1}{2^j j!} \frac{d^j}{dx^j} \left((x^2 - 1)^j \right).$$

These polynomials are orthogonal with respect to the scalar product $\langle \cdot, \cdot \rangle$ of equation (1.3). They are hierarchical in their polynomial degree p and symmetrical to the origin. The symmetry behaviour is alternately odd and even. To exploit the orthogonality in the case of a 1-D problem for the Laplace operator (i.e. $a_0 \equiv 0$ and $a_{11} \equiv 1$) one has to use integrated polynomials as shape functions: $\int_{-1}^x f_j(t) dt$ [SB91]. Then the bilinear form $a(u, v) = \langle u', v' \rangle$ operates on the same terms as the scalar product in the previous case. The integrated polynomials are orthogonal with respect to the new bilinear form.

DEFINITION 5. *Here we associate the term ‘orthogonal’ polynomials with a sequence of nested sets of polynomials $P_1 \subset P_2 \subset \dots$ for a specific bilinear form. The polynomials are linearly independent. A polynomial $f \in P_i$ is orthogonal with respect to this bilinear form on the vector space generated by the basis P_{i-1} (no condition for P_1). The vector spaces generated by P_i usually are the vector spaces of polynomials P_{i+1}^d . The polynomials in $P_i \setminus P_{i-1}$ need not be orthogonal.*

Orthogonal polynomials are hierarchical in p by definition. Orthogonal polynomials do not necessarily lead to local matrices with condition numbers

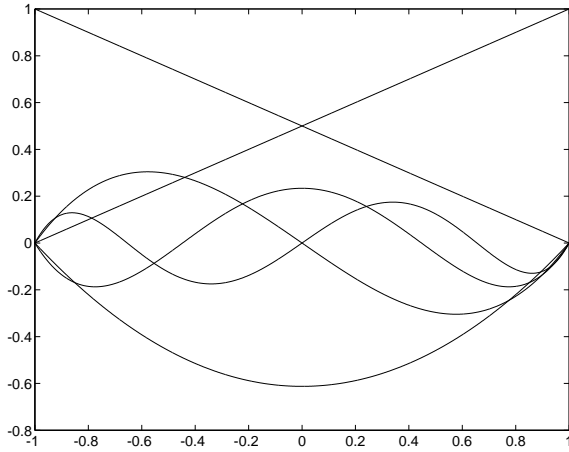


FIG. 1. The integrated Legendre polynomials

equal to one, $\kappa_j(A^{\text{loc}}) = 1$. However, a basis with this desirable property can be constructed:

LEMMA 1. *For every set of functions a_{ik} and a_0 of equation (1.1) there exists a set of shape functions yielding a local condition number equal to one.*

Proof. Consider the symmetric bilinear form $a(.,.)$ of equation (1.2) for a Gram-Schmidt orthogonalization of a vector space of polynomials. In the case of an eigenvalue zero take the corresponding eigenvector as additional shape function. In this case $a(.,.)$ is a semi-definite form. \square

These polynomials are orthogonal and therefore hierarchical in p .

RESULT 1. *We conclude that there are shape functions generating local matrices with condition number one. Some are hierarchical in p , too.*

A remark concerning hierarchy in h . Besides the so-called hierarchical basis algorithms [Ban88, DLY89, Yse86, CZZ84, ZGK83], shape functions being hierarchal in h are not very convenient. Some of these shape functions have a global support. They generate dense global matrices A which are expensive to compute with. Another problem is the number of hierarchical

levels in an h - p -version. We usually can restrict the order of p by a constant, say 10, but we cannot restrict the number of (adaptive) h refinements in that way. We can construct a family of ten p -hierarchical sets of shape functions, but we cannot precompute such an h -hierarchical set of shape functions for a number of unknown levels. If one uses h -hierarchy extensively, then only by an implicit transformation between a local and a hierarchical basis.

1.5 SYMMETRY

DEFINITION 6. *We denote the group of permutations of d elements with S_d and the subset of the alternating group with S_d^+ .*

DEFINITION 7. *We define the action of a group $S \subset S_{d+1}$ on a set of polynomials P 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.*

$$SP = \bigcup_{f \in P, s \in S} f(s^{-1}(b_0, b_1, \dots, b_d))$$

DEFINITION 8. *We call a polynomial f , a set of polynomials P and a vector space V of polynomials S -symmetrical, if it is invariant with respect to the action of S*

$$f = Sf, \quad P = SP \quad \text{and} \quad V = SV.$$

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 9. We define a set of polynomials P to be S^\pm -symmetrical in d variables by

$$\forall s \in S_{d+1} \text{ and } \forall f \in P \text{ holds } sf \in P \text{ or } -(sf) \in P.$$

S^\pm -symmetrical polynomials are zero. The definition of S^\pm -symmetrical

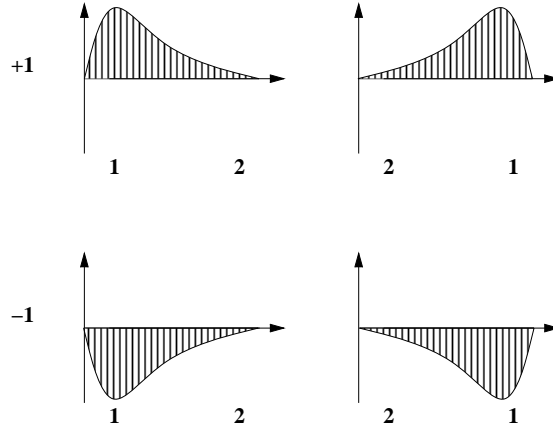


FIG. 2. $\pm S_2$ reflections of a 1-D function

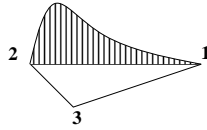


FIG. 3. A 2-D function f on the triangle

vector spaces does not make sense, because they are already S_{d+1} -symmetrical.

REMARK 3. Defining symmetry by $\forall s \forall f \in P \exists \lambda \in \mathbb{R} \setminus \{0\}$ with $\lambda(sf) \in P$ leads to $\lambda = \pm 1$, too.

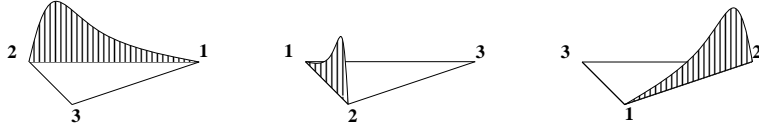


FIG. 4. S_3^+ reflections of a 2-D function f

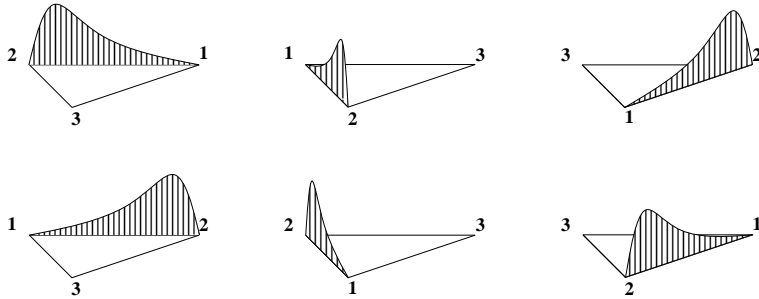


FIG. 5. S_3 reflections of a 2-D function f

LEMMA 2. *An S^\pm -symmetrical set P of polynomials is S^+ -symmetrical.*

Proof. Consider functions $\varphi : S^\pm \rightarrow \{+1, -1\}$, show that $\varphi^{-1}(+1) \subset S^+$ holds. \square

RESULT 2. *We conclude that there are S_d^\pm - and S_d -symmetrical shape functions.*

1.6 COUPLING

We call the assembly of local finite-element-matrices into a global one coupling. We have to guarantee that 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.

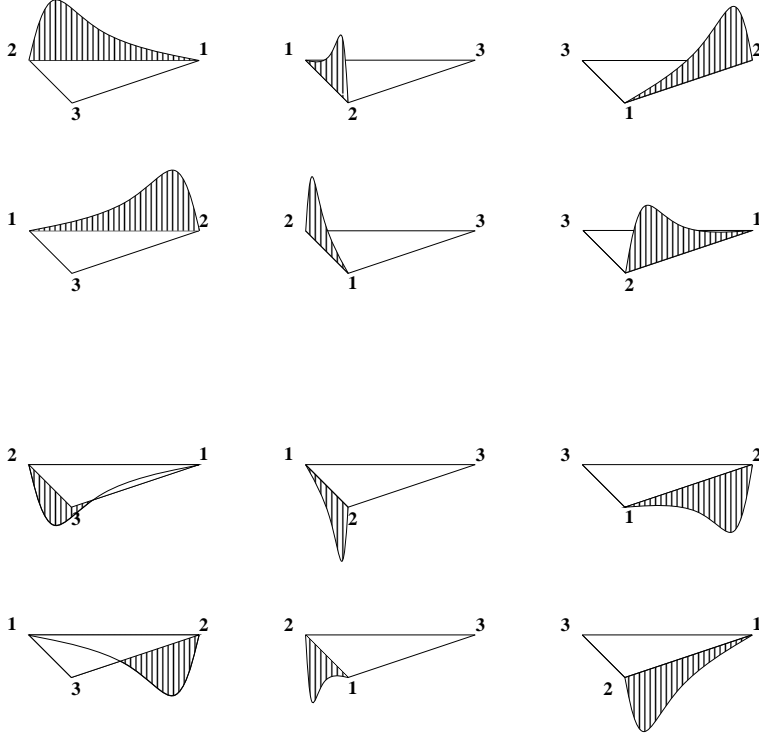


FIG. 6. $\pm S_3^\pm$ reflections of a 2-D function f , correlated with S_3^\pm

DEFINITION 10. *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 underdetermined 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

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

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

We introduce a stronger term of coupling by a special kind of minimal coupling which we call *simple*. The underdetermined 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 11. *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 2×1 non-zero blocks.*

The reduced matrix looks like this:

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

EXAMPLE 2. *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 $\tilde{C} = \tilde{C}_1 = \begin{pmatrix} 1 & -1 \end{pmatrix}$ and to*

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

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

EXAMPLE 3. *We recall the definition of the Bernstein polynomials on the simplex in the notation of chapter (1.3) [Far90]:*

$$f_\alpha = \binom{|\alpha|}{\alpha} b^\alpha, \quad \alpha \in \mathbb{N}_0^{d+1}$$

The Bernstein polynomials of degree $|\alpha| = p$ generate the vector space P_p^d .

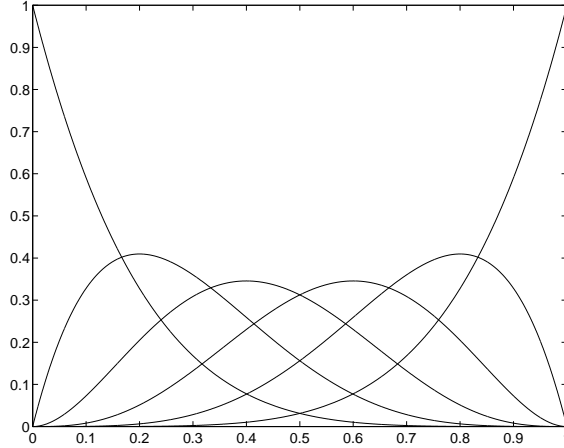


FIG. 7. The Bernstein polynomials of degree 5 in 1-D

This set of polynomials is S_{d+1} -symmetrical. They facilitate a *minimal* and *simple* coupling of blocks $\tilde{C}_i = (1 \quad -1)$ by identifying the proper functions being identical on the common boundary. The same holds for the standard Lagrange polynomials. On the other hand, it is harder to apply Dirichlet-boundary conditions. One has to interpolate the prescribed values using the polynomials non-vanishing on the boundary.

In general, only Lagrange interpolation polynomials permit a simple implementation of Dirichlet boundary conditions. The situation changes in the case of other boundary conditions like Neumann conditions. However $\partial\Omega$ is of lower complexity compared to Ω . Hence one may invest some more computational effort in calculating interpolatory conditions on the boundary for gaining some nicer properties in the inner domain Ω .

RESULT 3. *We conclude that there are shape functions with minimal and simple coupling. Some are S_{d+1} -symmetrical, too.*

1.7 CONDITION NUMBERS AND COUPLING

It is well known that the condition number of the global stiffness matrix for a fixed set of shape functions depends on the extension of the elements h . For elements of uniform size h , we get a sharp estimate (c.f. references in [Xu89])

$$\kappa(A) \leq C(a, p, \gamma)h^{-2}.$$

The constant C depends on the interior angles γ of the elements, on the differential operator a , on the set of shape functions and the associated polynomial degree p . In the case of non-uniform h and simplices we get a lower estimate [Xu89] with n denoting the number of simplices

$$\kappa(A) \leq C(a, p, \gamma) \cdot \begin{cases} n(1 + \log \frac{\max h}{\min h}) & \text{for } d = 2 \\ n^{2/d} & \text{for } d \geq 3 \end{cases}$$

Let us consider the p -dependence of the constants C . In the one-dimensional case there are shape functions with C independent from p , namely the integrated Legendre polynomials (chapter 3.3). Next we can conclude from sharp estimates in [BCMP91], that there are shape functions in two dimensions with global condition number

$$\kappa(A) \leq C(a, \gamma)h^{-2}(1 + \log^2 p)$$

for uniform h . The required functions are split into point-, edge- and internal shape functions in the usual way and the edge-functions have to be discrete harmonic with respect to the operator a . For dimensions higher than two ($d > 2$) an analogous construction delivers rapidly growing condition numbers in p [BCMP91].

If we now split the local condition numbers $\kappa_0(A_{\text{loc}})$ and $\kappa_1(A_{\text{loc}})$ into maximal and minimal eigenvalue $\lambda_{\max}(A_{\text{loc}})$ and $\lambda_{\min}(A_{\text{loc}})$ and look for the maximal λ_{\max} and the minimal λ_{\min} on all elements of a tessellation, we get a connection of local and global condition numbers. We conjecture an estimate for uniform h of the kind

$$\kappa(A) \leq C(\text{coupling})h^{-2} \frac{\max \lambda_{\max}(A_{\text{loc}})}{\min \lambda_{\min}(A_{\text{loc}})}$$

The constant C may also be written as a function of the minimal interior angle γ_{\min} and the family of shape functions. The conjecture is supported by numerical experiments and the estimates in this chapter.

1.8 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 a linear transformation . There are different possibilities to realize 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.

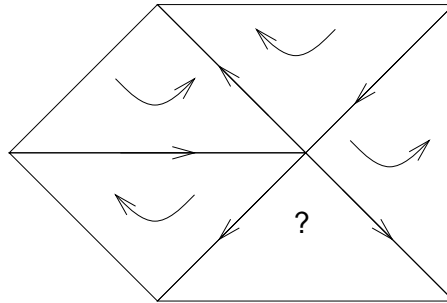


FIG. 8. Problems in orientating a tessellation

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 (figure 1.8).

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

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

Proof. We assign a permutation subgroup $G \subset S_{j+1}$ to each j -dimensional face of the reference simplex in a way that the non-vanishing shape functions are (S_{j+1}/G) -symmetrical. Dealing with a distinct set of shape functions, we are able to assign a subgroup G_{tot} of S_{d+1} to each simplex incorporating the

permutation groups of its faces. We now choose a tessellation in a way G_{tot} equals the identity leading to S_{j+1} -symmetry on the faces. The other way round is simple. \square

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

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

Proof. Analogously to the previous theorem. \square

RESULT 4. *S_{d+1} -symmetry is correlated with simple coupling of $(1 \ -1)$ and S_{d+1}^\pm -symmetry is correlated with simple coupling of $(1 \ \pm 1)$.*

1.9 SYMMETRY AND HIERARCHY

We now want to derive the correlation of symmetry and p -hierachy. The Legendre polynomials are p -hierachic and S_2^\pm -symmetrical, which simply means point or axial symmetry in 1-D. For d dimensions we get the following general statement:

THEOREM 2. *There is no p -hierarchical S_{d+1}^+ -symmetrical polynomial basis on the d -simplex for $d > 1$.*

Before we prove this, we recall the term irreducible:

DEFINITION 12. *We call a G -symmetric vector space V irreducible concerning a group G , if \emptyset and V are its only G -symmetric subspaces.*

Proof of theorem (2). We look at the p -hierarchical step from polynomial degree $j(d+1)$ to $j(d+1)+1$ with $j \in \mathbb{N}_0$. The set $\{b_0 - b_1, b_1 - b_2, \dots, b_{d-1} - b_d\}(b_0 \cdot b_1 \cdots b_d)^j$ is a basis of a subspace V of the vector space $P_{j(d+1)+1}^d$ not contained in the previous vector space $P_{j(d+1)}^d \cap V = \{0\}$. The vector space V is S_{d+1}^+ -symmetrical and is S_{d+1}^+ -irreducible with dimension $|V| = d$.

V is generated by the action of S_{d+1}^+ onto each of its elements, $f \in V \setminus \{0\} \Rightarrow \langle S_{d+1}^+ f \rangle = V$. Any S_{d+1}^+ -symmetrical set B of polynomials generating

V with $f \in B$ contains the complete space $S_{d+1}^+ f$. Hence it contains at least $d + 1$ elements, $|B| \geq d + 1$ and it is no linearly independent basis of V . \square

COROLLARY 2. *There is no p -hierarchical S_{d+1}^\pm -symmetrical polynomial basis on the d -simplex for $d > 1$.*

Proof. A direct conclusion of theorem (2). \square

THEOREM 3. *There is no p -hierarchical S_{d+1} -symmetrical polynomial basis on the d -simplex for $d \geq 1$.*

Proof. Analogously to the previous theorem (2). \square

COROLLARY 3. *There are no S_{d+1}^+ -symmetrical orthogonal polynomials on the d -simplex for $d > 1$.*

Proof. Orthogonal polynomials are p -hierarchical. Theorem (3). \square

RESULT 5. *Symmetry and simple coupling on the one hand and p -hierarchy for P_p^d on the other hand exclude each other.*

2 CONSTRUCTION OF SHAPE FUNCTIONS

2.1 SYMMETRY

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 1.8). It should be suitable for a p - and h - p -version of finite elements which means p -hierarchy in some sense. Both properties are not possible at the same time (chapter 1.9). We want to get low global condition numbers, too. This feature is correlated with local condition numbers (chapter 1.7) and often associated with orthogonal polynomials and therefore with p -hierarchy (chapter 1.4).

We have to cope with the limitations of theorem (2). We shall enlarge the polynomial vector spaces P_p^d slightly and construct new S_{d+1} -symmetrical vector spaces which avoid the irreducible subspaces of the proof of theorem (2).

We recursively construct a basis for the new vector space $P_p^{d,\text{sym}}$ by the span of the vector space $P_{p-1}^{d,\text{sym}}$ 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 $(B_{p-i-1}^i \cdot \prod_{j=0}^i b_j)$, $i < d$. The only difference to the standard polynomial spaces P_p^d is the beginning of the recursion. We start with $\{b_0\}$ for B_0^0 which actually has degree 1. If we want to get the standard polynomial spaces 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 13. *We recursively construct a basis for the new vector space in barycentric co-ordinates based on lower dimensions and lower degrees using the group of permutations S_d :*

- $B_0^0 = \{b_0\}$
- $B_p^0 = \emptyset$, $p > 0$
- $B_p^d = \bigcup_{i=0}^d S_{d+1}(B_{p-i-1}^i \cdot b_0 \cdot b_1 \cdots b_i)$, $d \geq 1$.

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

REMARK 4. *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 $\{b_0, b_1, \dots, b_d\}$.*

DEFINITION 14. *We now define the new polynomial vector spaces as the span of the basis functions in d dimensions: $P_p^{d,\text{sym}} = \langle \bigcup_{i=0}^p B_i^d \rangle$*

EXAMPLE 4. *In zero dimension we get the following sequence of polynomials, which are only useful for the construction of higher dimensional ones:*

$$\begin{aligned}
 P_0^{0,\text{sym}} &= \langle \{b_0\} \rangle \\
 P_1^{0,\text{sym}} &= P_0^{0,\text{sym}} \\
 P_2^{0,\text{sym}} &= P_0^{0,\text{sym}} \\
 &\vdots
 \end{aligned}$$

In one dimension we get the following S_2 -symmetrical sequence of polynomials:

$$\begin{aligned}
P_0^{1,\text{sym}} &= P_1^{1,\text{sym}} = \langle \{b_0, b_1\} \rangle \\
P_2^{1,\text{sym}} &= P_1^{3,\text{sym}} = \langle P_1^{1,\text{sym}} \cup \{b_0(b_0b_1), b_1(b_0b_1)\} \rangle \\
P_4^{1,\text{sym}} &= P_1^{5,\text{sym}} = \langle P_3^{1,\text{sym}} \cup \{b_0(b_0b_1)^2, b_1(b_0b_1)^2\} \rangle \\
P_6^{1,\text{sym}} &= P_1^{7,\text{sym}} = \langle P_5^{1,\text{sym}} \cup \{b_0(b_0b_1)^3, b_1(b_0b_1)^3\} \rangle \\
&\vdots
\end{aligned}$$

The polynomial spaces of odd degree contain one polynomial more than the former spaces P_p^2 . The polynomial spaces of even degree are equal. The basis leads to the two dimensional S_3 -symmetrical polynomials defined on the triangle by

$$\begin{aligned}
P_0^{2,\text{sym}} &= \langle \{b_0, b_1, b_2\} \rangle \\
P_1^{2,\text{sym}} &= P_0^{2,\text{sym}} \\
P_2^{2,\text{sym}} &= \langle P_1^{2,\text{sym}} \cup \{b_0(b_0b_1), b_1(b_0b_1), b_1(b_1b_2), \\
&\quad b_2(b_1b_2), b_2(b_2b_0), b_0(b_2b_0)\} \rangle \\
P_3^{2,\text{sym}} &= \langle P_2^{2,\text{sym}} \cup \{b_0(b_0b_1b_2), b_1(b_0b_1b_2), b_2(b_0b_1b_2)\} \rangle \\
P_4^{2,\text{sym}} &= \langle P_3^{2,\text{sym}} \cup \{b_0(b_0b_1)^2, b_1(b_0b_1)^2, b_1(b_1b_2)^2, \\
&\quad b_2(b_1b_2)^2, b_2(b_2b_0)^2, b_0(b_2b_0)^2\} \rangle \\
P_5^{2,\text{sym}} &= \langle P_4^{2,\text{sym}} \cup \{b_0(b_0b_1)(b_0b_1b_2), b_1(b_0b_1)(b_0b_1b_2), \\
&\quad b_1(b_1b_2)(b_0b_1b_2), b_2(b_1b_2)(b_0b_1b_2), \\
&\quad b_2(b_2b_0)(b_0b_1b_2), b_0(b_2b_0)(b_0b_1b_2)\} \rangle \\
&\vdots
\end{aligned}$$

The basis of these polynomial spaces contains much more polynomials than of the former spaces P_p^3 .

RESULT 6. The vector spaces $P_p^{d,\text{sym}}$ are S_{d+1} -symmetrical. Their bases $B_p^{d,\text{sym}}$ are p -hierarchical, facilitate minimal and simple coupling with blocks (1 ± 1) and are enlarged $P_p^d \subseteq P_p^{d,\text{sym}} \subseteq P_{p+1}^d$.

Proof. By induction. \square

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 ± 1) , we can reduce this high dimension, but we have to consider the group S_{d+1}^\pm (chapter 1.8).

DEFINITION 15. 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:

- $B_0^{0,\pm} = \{b_0\}$, $B_p^{0,\pm} = \emptyset$, $p > 0$
- $B_0^{0,\pm} = \{b_0, b_1\}$, $B_1^{0,\pm} = \emptyset$, $B_p^{1,\pm} = \{(b_1 - b_0)^p\}$, $p > 1$
- $B_p^{d,\pm} = \bigcup_{i=0}^d S_{d+1}^+(B_{p-i-1}^{i,\pm} \cdot b_0 \cdot b_1 \cdots b_i)$, $d > 1$.

REMARK 5. 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 $\{b_0, b_1, \dots, b_d\}$. Watch out for a systematical interpretation of “even”!

DEFINITION 16. We now define the new polynomial vector spaces as the span of the basis functions in d dimensions: $P_p^{d,\pm} = \langle \bigcup_{i=0}^p B_i^{d,\pm} \rangle$

EXAMPLE 5. In zero dimension we get the following sequence of polynomials, which are only useful for the construction of higher dimensional ones:

$$\begin{aligned} P_0^{0,\pm} &= \langle \{b_0\} \rangle \\ P_1^{0,\pm} &= P_0^{0,\pm} \\ P_2^{0,\pm} &= P_0^{0,\pm} \\ &\vdots \end{aligned}$$

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

$$\begin{aligned} P_0^{1,\pm} &= \langle \{b_0, b_1\} \rangle \\ P_1^{1,\pm} &= P_0^{1,\pm} \\ P_2^{1,\pm} &= \langle P_1^{1,\pm} \cup \{(b_1 - b_0)^2\} \rangle \\ P_3^{1,\pm} &= \langle P_2^{1,\pm} \cup \{(b_1 - b_0)^3\} \rangle \\ P_4^{1,\pm} &= \langle P_3^{1,\pm} \cup \{(b_1 - b_0)^4\} \rangle \\ &\vdots \end{aligned}$$

The spaces $P_p^{1,\pm}$ are equal to the former spaces P_p^1 . Thus they are smaller than the spaces $P_p^{1,\text{sym}}$. 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:

$$\begin{aligned}
P_0^{2,\pm} &= \langle \{b_0, b_1, b_2\} \rangle \\
P_1^{2,\pm} &= P_0^{2,\pm} \\
P_2^{2,\pm} &= \langle P_1^{2,\pm} \cup \{(b_1 - b_0)^2, (b_2 - b_1)^2, (b_0 - b_2)^2\} \rangle \\
P_3^{2,\pm} &= \langle P_2^{2,\pm} \cup \{(b_1 - b_0)^3, (b_2 - b_1)^3, (b_0 - b_2)^3\} \cup \\
&\quad \{b_0(b_0b_1b_2), b_1(b_0b_1b_2), b_2(b_0b_1b_2)\} \rangle \\
P_4^{2,\pm} &= \langle P_3^{2,\pm} \cup \{(b_1 - b_0)^4, (b_2 - b_1)^4, (b_0 - b_2)^4\} \rangle \\
P_5^{2,\pm} &= \langle P_4^{2,\pm} \cup \{(b_1 - b_0)^5, (b_2 - b_1)^5, (b_0 - b_2)^5\} \cup \\
&\quad \{(b_1 - b_0)^2(b_0b_1b_2), (b_2 - b_1)^2(b_0b_1b_2), \\
&\quad (b_0 - b_2)^2(b_0b_1b_2)\} \rangle \\
P_6^{2,\pm} &= \langle P_5^{2,\pm} \cup \{(b_1 - b_0)^6, (b_2 - b_1)^6, (b_0 - b_2)^6\} \cup \\
&\quad \{(b_1 - b_0)^3(b_0b_1b_2), (b_2 - b_1)^3(b_0b_1b_2), \\
&\quad (b_0 - b_2)^3(b_0b_1b_2)\} \cup \\
&\quad \{b_0(b_0b_1b_2)^2, b_1(b_0b_1b_2)^2, b_2(b_0b_1b_2)^2\} \rangle \\
&\vdots
\end{aligned}$$

On the triangle the polynomial sets for a degree p which is not divisible by 3 are identical to P_p^2 , all other vector spaces are generated by P_p^2 and 2 additional polynomials.

REMARK 6. The usual linear Lagrange polynomials are contained in both $P_1^{d,\text{sym}}$ and $P_1^{d,\pm}$. The associated hierarchical quadratic polynomials are contained in $P_2^{d,\pm}$, too.

REMARK 7. The linear Lagrange polynomials can be interpreted as symmetrization of the canonical basis of $P_1^d: \{1\} \cup \{b_1, b_2, \dots, b_d\}$.

RESULT 7. The vector spaces $P_p^{d,\pm}$ are S_{d+1}^\pm -symmetrical. Their bases $B_p^{d,\pm}$ are p -hierarchical, facilitate minimal and simple coupling with blocks (1 ± 1) , are only slightly enlarged ($P_p^d \subseteq P_p^{d,\pm} \subseteq P_p^{d,\text{sym}} \subseteq P_{p+1}^d$) and have got an even lower dimension than $P_p^{d,\text{sym}}$.

Proof. By induction. \square

2.2 CONDITION NUMBERS

We want to construct the final version of our shape functions by using the polynomial vector spaces $P_p^{d,\text{sym}}$ and $P_p^{d,\pm}$ of chapter (1.8). The set of func-

tions should maintain the symmetry and coupling properties of the original basis $B_p^{d,\text{sym}}$ and $B_p^{d,\pm}$. P -hierarchy is guaranteed by the nesting of the vector spaces. The only missing property is a low condition number.

There are several ways towards low local condition numbers. A straightforward one is Gram-Schmidt orthogonalization, which leads to orthogonal polynomials. In the case of polynomial vector spaces P_p^d we saw that these orthogonal polynomials are not S_{d+1}^\pm -symmetrical (chapter 1.9) and hence do not allow *simple* coupling of shape functions (chapter 1.8). We now have got slightly modified vector spaces and we cannot apply these arguments. But we have to be careful not to lose the symmetry of the original basis $B_p^{d,\text{sym}}$ and $B_p^{d,\pm}$.

DEFINITION 17. *We recall the definition of the Gram-Schmidt orthogonalization procedure for a basis $\{\phi_i\}$ of a vector space V :*

$$\begin{aligned} v_1 &:= \phi_1 \\ v_k &:= \phi_k - \sum_{i=1}^{k-1} \frac{\langle \phi_k, v_i \rangle}{\langle v_i, v_i \rangle} v_i, \quad k = 2, \dots \end{aligned} \tag{2.1}$$

The $\{v_i/\sqrt{\langle v_i, v_i \rangle}\}$ form an orthogonal basis of V .

We call the elements v_i in the sum competition elements which means that the elements ϕ_k are orthogonalized with respect to them.

We cannot expect symmetry after orthogonalization if the bilinear form $a(.,.)$ is not symmetric on the element E which is invariant under the permutations of the corners of E with S_{d+1} . In this case the coefficients a_{ik} and a_0 have to be constant on E or invariant under permutations. The latter condition is rather unlikely for non-constant materials. In general there are two alternatives:

- For an adaptive refinement procedure the coefficients a_{ik} and a_0 are constant on each element of the coarsest tessellation. All new elements are just subdivisions of these elements.
- We optimize the shape functions for an S_{d+1} -symmetrical $\tilde{a}(.,.)$ which only approximates the true $a(.,.)$ on the domain Ω .

If we now orthogonalize an S -symmetrical polynomial f to a vector space V with S -symmetrical $a(.,.)$, we have to be sure that V is at least S -

symmetrical. Hence we do not orthogonalize the polynomials step by step by the original Gram-Schmidt procedure but we will orthogonalize for some symmetrical subsets of the original basis. We will at most get orthogonality in the sense of space-wise orthogonality (like orthogonal polynomials are orthogonal only on spaces of some previous polynomials).

Next we have to maintain the coupling properties of the original basis functions. We want to use the same coupling matrix \tilde{C} on each face of an element. This means that the number of non-vanishing polynomials on each face must remain the same. Standard orthogonalization of *internal* functions f (functions vanishing on the element boundary) generates additional coupling on the boundary, because the scalar products $\langle f, \phi \rangle \neq 0$ with the boundary functions ϕ (functions that do not vanish on the element boundary) used previously in the orthogonalization procedure (definition 2.1) do not vanish in general.

A way out of this trouble is the restriction of the *competition* functions (of the Gram-Schmidt procedure) for *internal* functions to *internal* functions and for *boundary* functions to *internal* functions together with *boundary* functions non-vanishing on a higher-dimensional face.

RESULT 8. *When we optimize the basis functions we have to restrict the set of competition functions and we have to keep the sets of functions optimized simultaneously sufficiently large.*

We make a more general approach to optimization. The optimal polynomials are in a linear vector space $V = \langle \psi_1, \psi_2, \dots \rangle$. Every optimized polynomial v_k has a representation of

$$v_k := \sum_{i=1}^k \alpha_{ki} \psi_i, \quad k = 1, \dots$$

We have to determine the coefficients α_{ki} that v_k has got the desired properties. There are several ways to implement this approach:

- We can use a restricted Gram-Schmidt procedure, hoping for low condition numbers. That means that we just omit a number of scalar products.
- Instead of trying to force off-diagonal elements of a matrix to vanish, we can minimize the square sum of the non-diagonal elements in a least-

squares sense. We have to keep the corresponding diagonal element large enough, say 1, thus arriving at a non-linear process. We can iterate some steps of normalization (diagonal elements set to 1) and least squares minimization. In the experiments we iterate just one step.

- The attempt to solve the optimization problem directly may lead to a (Quasi-)Newton procedure minimizing the condition number of the matrix. We tried this approach, too.

All 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 basis functions are in some cases (optimized) shape functions of previous optimization steps and in some cases symmetrizations of them.

3 COMPARISON

3.1 PROPERTIES

Here we show some properties of different families of shape functions:

| polynomials | reference | <i>simple</i> coupling | symm. on the faces | symm. in the element | hierarch. in p |
|-----------------------------|--------------------------------|---------------------------|--------------------------|----------------------------|---------------------|
| monomials | $\prod_{i=1}^d x_i^{\alpha_i}$ | – | – | – | × |
| orthogonal | [AF26, GM78] | – | – | – | × |
| mod. Legendre | [SB91] | × | 2-D only | – | × |
| mod. monomials | [Pea76] | × | 2-D only | – | × |
| p -hierarch. original* | mod. [ZT89] [ZT89] | × | 2-D only* | –* | × |
| Lagrange | [MP72, Nic72] | × | × | × | – |
| Bernstein | [Far90] | × | × | × | – |
| symm. hierarch. | chapter (2) | × | × | × | × |

The reader should not be surprised that we can separate two classes of shape functions: The p -hierarchical and the symmetrical ones. The only

exception are the new symmetric hierarchical polynomials. The asterisk * denotes our modification of the polynomials originally proposed by [ZT89]. The original shape functions on the triangle are not p -hierarchical for the step from degree 3 to 4. We modified the basis to be hierarchical, loosing symmetry.

3.2 CONDITION NUMBERS

We now compare the resulting local condition numbers like in [BGP89]. We choose the Laplace operator Δu (i.e. $a_0 \equiv 0$ and $a_{ik} \equiv I$) and vary the geometry of the elements. Equivalently we could have changed the differential operator keeping the element fixed. The absolute scaling of the elements is not relevant, hence we only change angles and aspect ratios. The condition numbers are evaluated numerically.

3.3 1-D

We compare the condition numbers of the local matrices for the Laplace operator on the interval $[0, 1]$. We may draw conclusions from this 1-D case for edge based shape functions in higher dimensions.

The polynomials compared are:

- the monomials x^p for $p \in \mathbb{N}_0$
- p -hierarchical polynomials proposed by [ZT89], which are of Hermitean type till degree two

$$f_p(x) = \begin{cases} \frac{1}{p!}(x^p - 1) & p \text{ even} \\ \frac{1}{p!}(x^p - x) & p \text{ odd} \end{cases}$$

- normalized polynomials ϕ_i . ϕ_i is substituted by $\frac{\phi_i}{\sqrt{\langle \phi_i, \phi_i \rangle}}$, if the (semi-) norm of the polynomial is not zero ($\sqrt{\langle \phi_i, \phi_i \rangle} \neq 0$).
- Lagrange polynomials which are interpolation polynomials for the equidistributed interpolation points $x_i = i/p$, $i \in \{0, 1, \dots, p\}$ on the interval $[0, 1]$.

$$f_{ip}(x_i) = \begin{cases} 1 & \text{for } i = p \\ 0 & \text{for } i \neq p \end{cases}$$

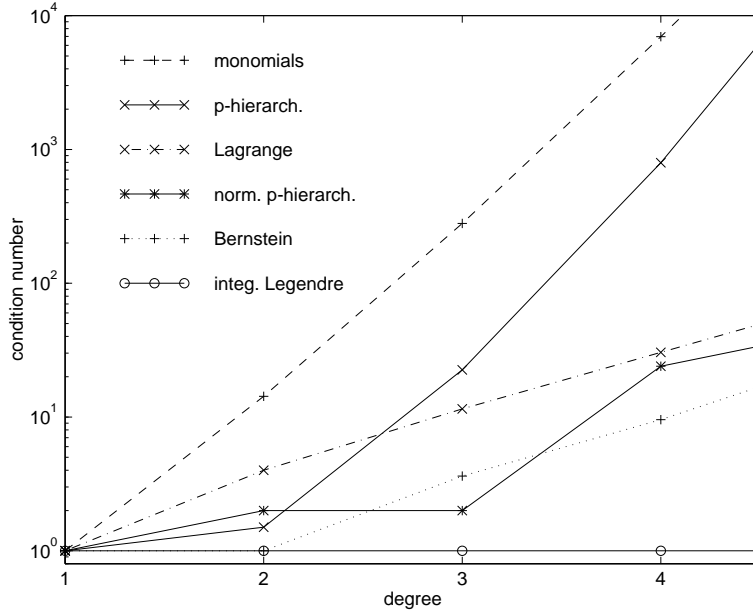


FIG. 9. Local condition numbers for the Laplace operator on the interval for different polynomials of degree 1 to 4 (detail)

- Bernstein polynomials of degree p [Far90]

$$f_{ip}(x) = \frac{p!}{i!(p-i)!} (1-x)^i x^{p-i}$$

- the integrated Legendre polynomials on $[-1, 1]$ [SB91]

$$f_p(x) = \begin{cases} \frac{1+x}{2} & \text{for } p < 2 \\ \frac{1}{2(2p-1)} (f_p(x) - f_{p-2}(x)) & \text{for } p \geq 2 \end{cases}$$

with Legendre polynomials f_p defined in example (1).

We observe the following: For degree one all condition numbers start with a low number. For degree two, the quadratic case, the condition numbers

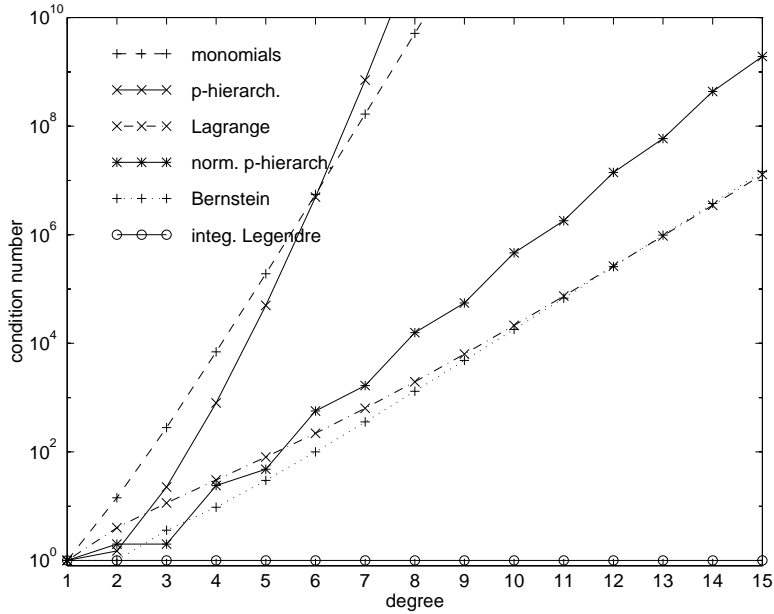


FIG. 10. Local condition numbers for the Laplace operator on the interval for different polynomials of degree 1 to 15

diverge, but not with the same pattern as in the asymptotic case. The Bernstein polynomials keep optimal for degree two. The p -hierarchical polynomials are slightly better than the normalized ones in the quadratic case, but are outperformed for higher degrees. The integrated Legendre polynomials keep the optimal constant condition number due to their construction.

The numbers of the monomials and the p -hierarchic polynomials increase drastically. At first the monomials are worse, but are caught at degree 6, getting unacceptable for higher degrees. The normalized p -hierarchic polynomials perform better. One can obtain a “staircase effect” for odd and even degrees. The non-hierarchical Bernstein and the Lagrange polynomials asymptotically show the same behavior.

3.4 2-D

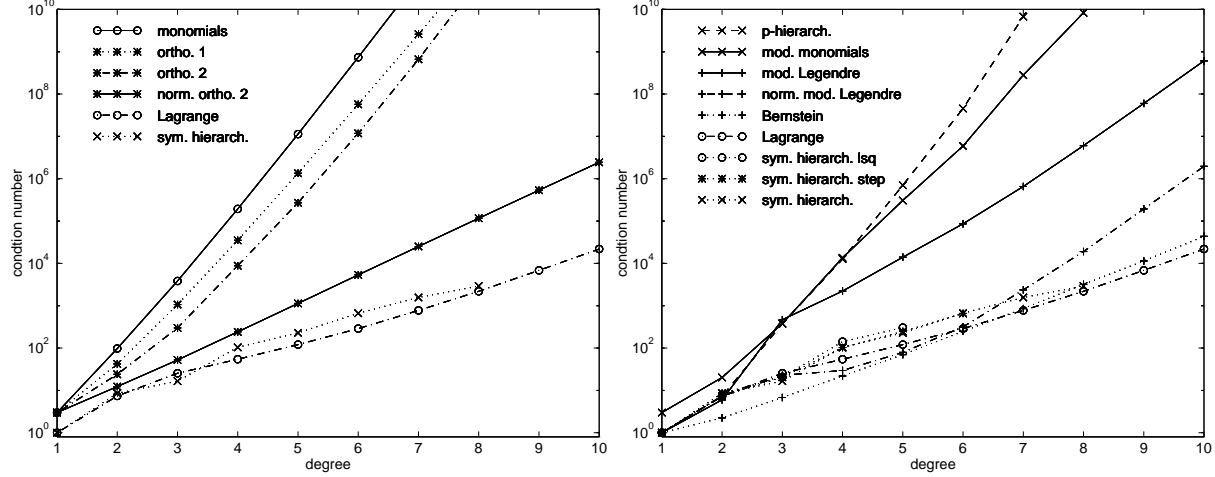


FIG. 11. Local condition numbers for the Laplace operator on the *equilateral triangle* for different polynomials of degree 1 to 10

We compare the condition numbers of the local matrices for the Laplace operator on the triangle. The results only depend on the angles of the triangle.

The polynomials compared are:

- the *monomials* $x^i y^j$ with $i + j = p \in \mathbb{N}_0$
- the orthogonal (*ortho. 1*) polynomials proposed by [GM78] for the d -simplex:

$$f_\alpha = \sum_{\beta \leq \alpha} (-1)^{|\alpha|+|\beta|} \frac{(d-1+|\alpha|+|\beta|)!}{(d-1+2|\alpha|)!} (\alpha-\beta)! \left(\frac{\alpha!}{(\alpha-\beta)! \beta!} \right)^2 b^\beta, \alpha, \beta \in \mathbb{N}_0^d$$

- the orthogonal (*ortho. 2*) polynomials proposed by [AF26] for the d -simplex

$$f_\alpha = \partial^\alpha \left(1 - \sum_{j=1}^d b_j \right)^{|\alpha|} b^\alpha, \alpha \in \mathbb{N}_0^d$$

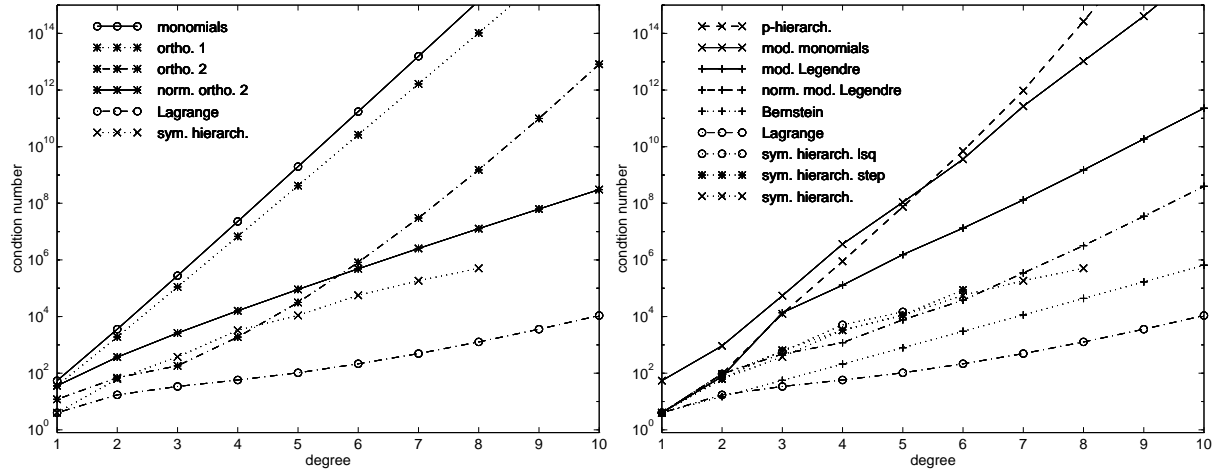


FIG. 12. Local condition numbers for the mass-matrix on the *equilateral triangle* for different polynomials of degree 1 to 10

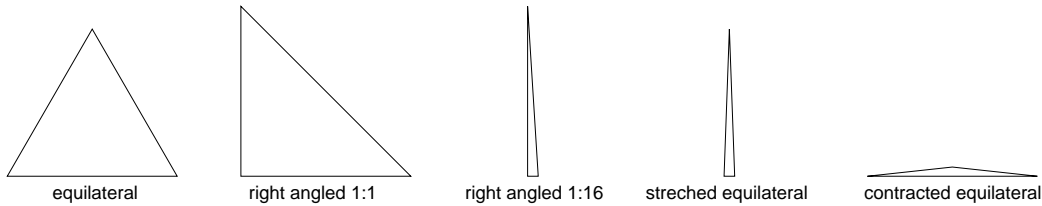


FIG. 13. The different triangle shapes

with derivatives ∂^i with respect to b_i .

- *normalized* polynomials ϕ_i . ϕ_i is substituted by $\frac{\phi_i}{\sqrt{\langle \phi_i, \phi_i \rangle}}$, if the (semi-) norm of the polynomial is not zero ($\sqrt{\langle \phi_i, \phi_i \rangle} \neq 0$).
- a modified version of the *p-hierarchical* polynomials proposed by [ZT89], which are a generalization of the one-dimensional polynomi-

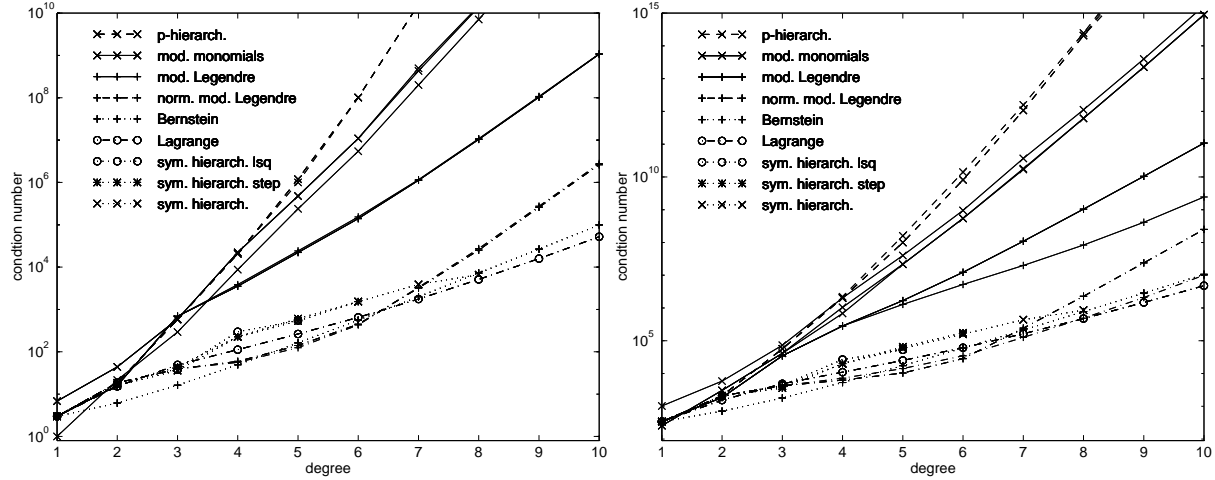


FIG. 14. Local condition numbers for the Laplace operator on the *right-angled triangle* with short edges of length 1 : 1 and 1 : 16 for different polynomials of degree 1 to 10

als. We have the linear functions $\{b_0, b_1, b_2\}$ and the edge-functions generated by rotations (cyclic permutations) of:

$$f_p(x) = \begin{cases} \frac{1}{p!} ((b_2 - b_1)^p - (b_2 + b_1)^p) & p \text{ even} \\ \frac{1}{p!} ((b_2 - b_1)^p - (b_2 - b_1)(b_2 + b_1)^{p-1}) & p \text{ odd} \end{cases}$$

Additionally, the internal function $b_0 b_1 b_2$ is proposed for degree 3 and the functions $\{b_0(b_0 b_1 b_2), b_1(b_0 b_1 b_2), b_2(b_0 b_1 b_2)\}$ for degree 4 as a substitution for it. Hence the functions are not p -hierarchical any longer. We modify this step using the the usual monomials multiplied by the “bubble”-function $b_1^i b_2^j (b_0 b_1 b_2)$ with $i + j + 3 = p$. Hence we enforce p -hierarchy and violate symmetry on the triangle. Thus the polynomials are defined for all degrees p , not only till degree 4.

- the modified monomials for the triangle proposed by [Pea76]:

$$\begin{aligned} f_1^0 &= 1 \\ f_{1,2}^1 &= b_1, b_2 \quad \text{point functions} \end{aligned}$$

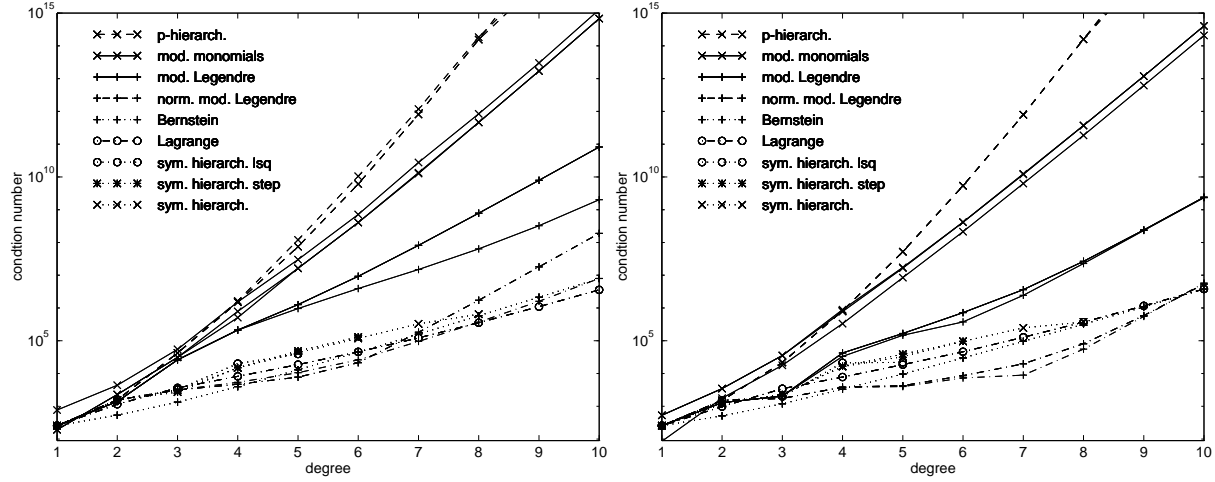


FIG. 15. Local condition numbers for the Laplace operator on the *distorted equilateral triangle* stretched and contracted by a factor of 16 for different polynomials of degree 1 to 10

$$\begin{aligned}
 f_{1,2,3}^p &= b_0^{p-1} b_1, b_1^{p-1} b_2, b_2^{p-1} b_0 \quad \text{edge functions, } p > 1 \\
 f_{i+3}^p &= f_i^{p-3} b_0 b_1 b_2 \quad \text{internal functions, } i \geq 0
 \end{aligned}$$

After construction of the polynomials we substitute the usual linear polynomial b_0 for f_1^0 .

- Lagrange polynomials which are interpolation polynomials for the equidistributed interpolation points $x_i = i/p$ and $y_j = j/p$, $i, j \in \{0, 1, \dots, p\}$ on the reference triangle $(x + y) \leq 1$, $(i + j) \leq p$ (for details see [MP72, Nic72]).

$$f_{ij}(x_k, y_l) = \begin{cases} 1 & \text{for } i = k \text{ and } j = l \\ 0 & \text{else} \end{cases}$$

- Bernstein polynomials of degree p [Far90]

$$f_{ijp}(x, y) = \frac{p!}{i!j!(p-i-j)!} x^i y^j (1-x-y)^{p-i-j}$$

- a construction using Legendre polynomials on the triangle [SB91]: point functions $\{b_0, b_1, b_2\}$ as usual,

$$F_p = \sqrt{8(2p-1)} \frac{b_0 b_1}{1 - (b_0 - b_1)^2} \int_{-1}^{b_0 - b_1} f_{p-1}(x) dx$$

the edge function for the edge $(0, 1)$ together with its cyclic permutations, and internal functions

$$F_{p,q} = b_0 b_1 b_2 f_p(b_1 - b_0) f_q(2b_2 - 1)$$

with Legendre polynomials f_p defined in example (1).

- the *symmetric hierarchical least squares* polynomials of the polynomial vector space $P_p^{2,\pm}$, optimized consecutively by a least squares method.
- the *symmetric hierarchical step-wise/* consecutively (by a Gauß-Seidel method) optimized polynomials of the polynomial vector space $P_p^{2,\pm}$. Each polynomial generating a symmetrical subset is optimized with respect to the previous optimized polynomials.
- the *symmetric hierarchical* polynomials of the polynomial vector space $P_p^{2,\pm}$, optimized by a Gauß-Seidel method for each space $P_p^{2,\pm}$, $p = 1, 2, \dots$

We observe the following: For degree one all condition numbers start with a low number. For degree two, the quadratic case, the condition numbers diverge, but not in the same pattern as in the asymptotic case. For non-symmetric triangles we could get up to six different condition numbers depending on the orientation of the triangle, but actually we do get only three different numbers. We see that a suitable orientation pays off in this case. The symmetric polynomials have got only one unique condition number independent of orientation.

We can separate the polynomials into three different groups (figure 11). The highest condition numbers are produced by the monomials, the modified monomials, the orthogonal polynomials and the p -hierarchical polynomials. The condition numbers are not acceptable for higher p and grow dramatically. The second group contains the normalized orthogonal polynomials number 2, the modified Legendre polynomials and, asymptotically, the normalized

modified Legendre polynomials. The slowest growth of condition numbers show the Bernstein and Lagrange polynomials and the symmetric hierarchical polynomials. The different versions of optimization procedures do not differ much from each other. We have chosen the best optimization as a reference for the following tests. Looking at the details for low degrees we see a cluster until $p = 3$ or 4 . An optimal choice in these sections may differ from a choice for higher p . In this range the condition numbers are generally not very high, hence other properties than condition numbers may become a criterion of higher priority.

The comparison of the condition numbers for the Laplace-operator and the pure mass-matrix (i.e. $a_0 \equiv 1$ and $a_{ik} \equiv 0$) on the equilateral triangle shows that the numbers are approximately of the same size but are not equally clustered (figure 12). Some polynomials perform significantly better for the mass-matrix and some perform in a similar way. The orthogonal polynomials number 2 do benefit from this operator, whereas the normalized ones (normalized for the Laplace-operator) are slightly better in the beginning until $p = 5$, but are asymptotically worse. The Lagrange polynomials have got smaller condition numbers, too. In this case they generally differ from the numbers of the Bernstein-polynomials. The symmetric hierarchical polynomials perform similarly to the modified Legendre-polynomials. Besides the similarity of condition numbers for the different differential-operators for the equilateral triangle one has to mention the fact that the eigenvalues for the mass-matrix scale in a different way in h than they do for the Laplace-operator.

Let us look at some other triangles. A “canonical” one is the right-angled triangle with short edges of length 1 and the hypotenuse of length $\sqrt{2}$ (figure 14). The triangle is no longer symmetric which means that non-symmetric polynomials are sensitive for orientation. We can see this effect for the modified monomials which split into two different paths of condition numbers. We can see that the Bernstein-polynomials perform slightly worse for small p , but in general there is not much difference to the equilateral triangle.

Things change for a distorted right-angled triangle with short edges of length 1 and 16 (figure 14). The condition numbers are approximately a factor of 16^2 higher than for the undistorted case. We obtain a splitting of condition number histories not only for the modified monomials (up to 3 branches) but also for the p -hierarchical polynomials and the modified Legendre-polynomials.

The difference between different orientations diverges for the Legendre-polynomials starting with $p = 5$, which means that a proper orientation of the polynomials depending on the geometry does pay off. Both for the normalized and the original modified Legendre-polynomials the best condition numbers (lowest branch) do not suffer as much from the distortion as the other polynomials do.

Going further into details we look at two other triangles distorted by a factor of 16 which gives a stretched and a contracted equilateral triangle (figure 15). The condition numbers for the stretched triangle do not differ much from the long right-angled triangle. In the contracted case the splitting of the condition numbers for the modified Legendre-polynomials converges for high p , which was not the case for the previous triangles. The normalized Legendre-polynomials perform better than before in a medium range of p .

We can summarize this by saying that the lowest condition numbers are gained with the Lagrange and Bernstein polynomials. They are not far away from the numbers for the new symmetric hierarchical polynomials and the modified Legendre polynomials, which depend on orientation. The exact ranking depends on the triangle and the differential operator itself.

3.5 3-D

We compare the condition numbers of the local matrices for the Laplace operator on the tetrahedron. The results only depend on the angles of the tetrahedron.

The polynomials compared are:

- the *monomials* $x^i y^j z^k$ with $i + j + k = p \in \mathbb{N}_0$
- the orthogonal (*ortho. 1*) polynomials proposed by [GM78] for the d -simplex defined in chapter (3.4).
- the orthogonal (*ortho. 2*) polynomials proposed by [AF26] for the d -simplex defined in chapter (3.4).
- a modified version of the *p-hierarchical* polynomials proposed by [ZT89], which are a generalization of the one- and two-dimensional polynomials. We take the usual linear functions $\{b_0, b_1, b_2, b_3\}$ and

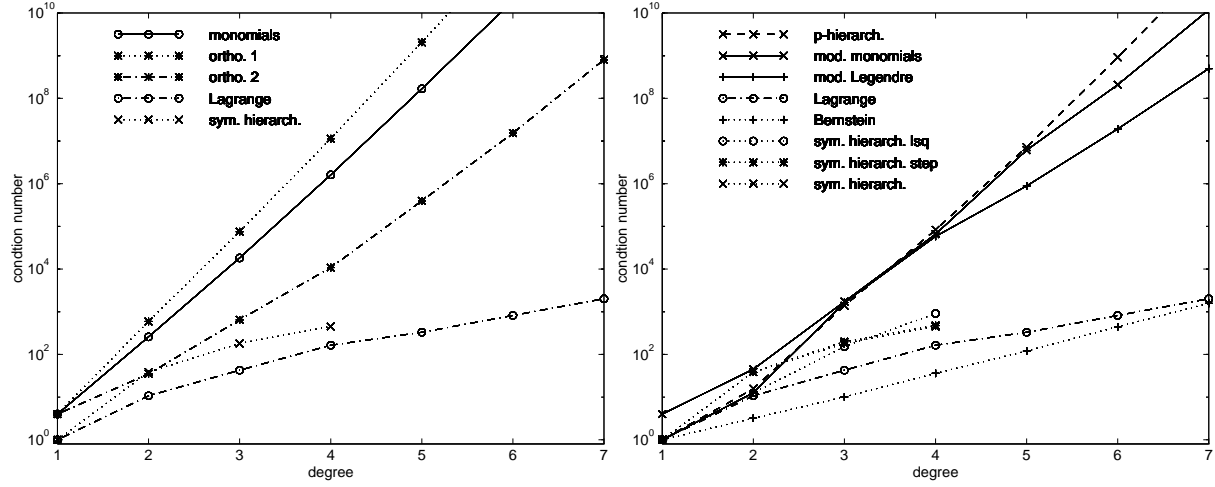


FIG. 16. Local condition numbers for the Laplace operator on the *equilateral tetrahedron* for different polynomials of degree 1 to 7

the edge-functions generated by permutations of:

$$f_p = \begin{cases} \frac{1}{p!} ((b_2 - b_1)^p - (b_2 + b_1)^p) & p \text{ even} \\ \frac{1}{p!} ((b_2 - b_1)^p - (b_2 - b_1)(b_2 + b_1)^{p-1}) & p \text{ odd} \end{cases}$$

Analogously to the two dimensional case we enforce p -hierarchy and violate symmetry by constructing internal functions and functions on the triangular faces with standard monomials and “bubble” functions $b_0 \cdot b_1 \cdots b_d$.

- the *modified monomials* originally proposed by [Pea76] for the triangle, generalized for the d -simplex:

$$\begin{aligned} F_0^d &= \{1\} \\ F_1^d &= \{b_1, b_2, \dots, b_d\} \\ F_p^1 &= \{b_0^p\} \\ F_p^d &= \bigcup_k \text{permutations of } F_{p-k-1}^k \cdot b_0 \cdot b_1 \cdots b_k \end{aligned}$$

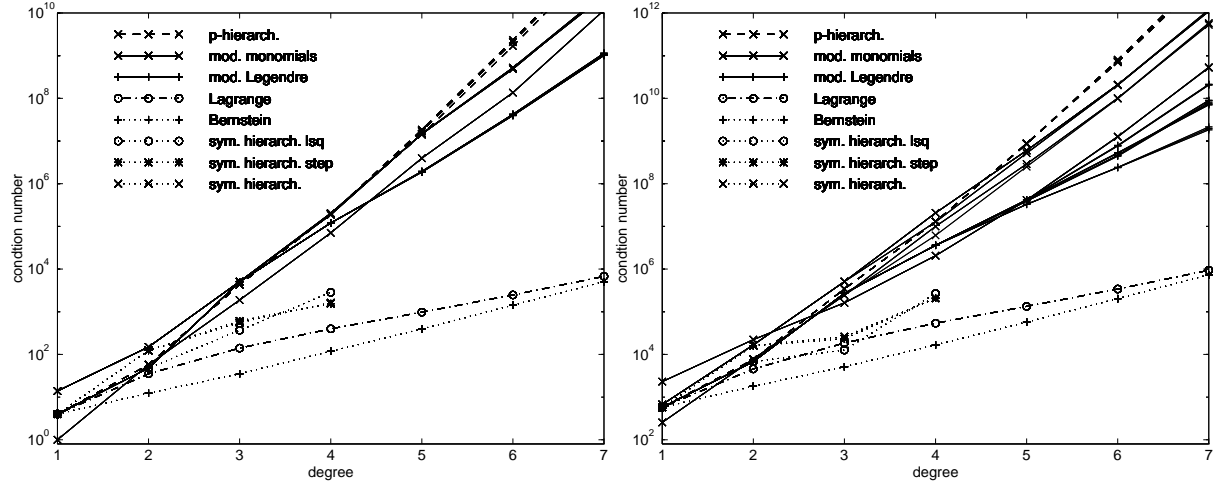


FIG. 17. Local condition numbers for the Laplace operator on the *right-angled tetrahedron* with short edges of length 1 : 1 : 1 and 1 : 1 : 16 for different polynomials of degree 1 to 7

After the construction of the polynomials we substitute the usual linear polynomial $\{b_0\}$ for F_0^d .

- Lagrange polynomials which are interpolation polynomials for the regular equidistant interpolation points x_α on the reference simplex:

$$f_\beta(x_\alpha) = \begin{cases} 1 & \text{for } \alpha = \beta \\ 0 & \text{for } \alpha \neq \beta \end{cases}$$

- Bernstein polynomials of degree p for the d -simplex [Far90]

$$f_\alpha = \binom{|\alpha|}{\alpha} b^\alpha$$

- a construction using Legendre polynomials on the tetrahedron [SB91]: point functions $\{b_0, b_1, b_2, b_3\}$ defined as usual,

$$F_p = \sqrt{8(2p-1)} \frac{b_0 b_1}{1 - (b_0 - b_1)^2} \int_{-1}^{b_0 - b_1} f_{p-1}(x) dx$$

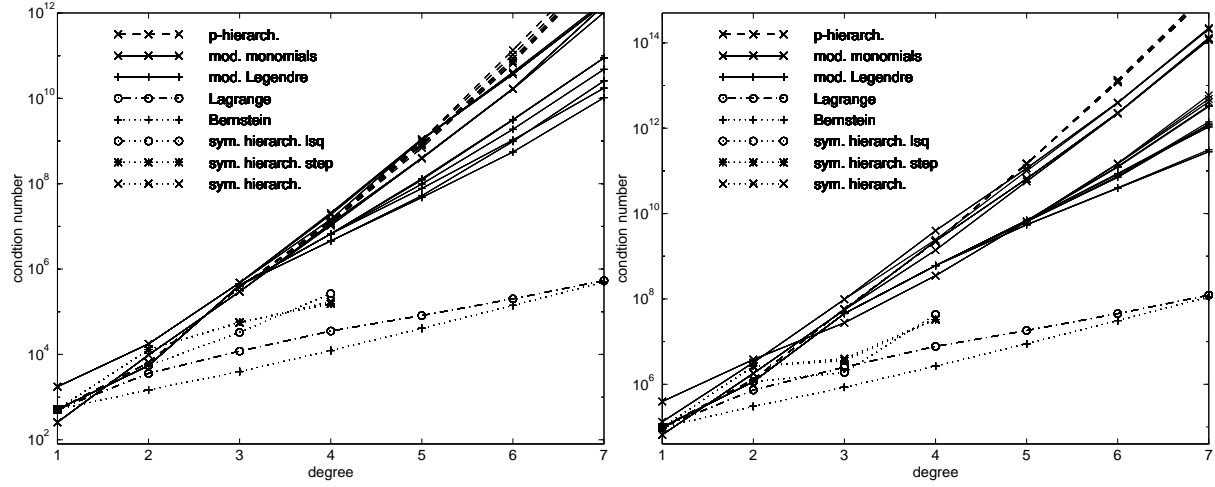


FIG. 18. Local condition numbers for the Laplace operator on the *right-angled tetrahedron* with short edges of length $1 : 16 : 16$ and $1 : 16 : 16^2$ for different polynomials of degree 1 to 7

as edge function for the edge $(0, 1)$ together with permutations for the other edges,

$$F_{p,q} = b_0 b_1 b_2 f_p(b_1 - b_0) f_q(2b_2 - 1)$$

as triangle function for the triangular face $(0, 1, 2)$ together with permutations for the other faces,

$$F_\alpha = b_0 \cdot b_1 \cdots b_d f_{\alpha_1}(b_1 - b_0) f_{\alpha_2}(2b_2 - 1) \cdot f_{\alpha_3}(2b_3 - 1) \cdots$$

as general internal functions for a d -simplex with $|\alpha| = d$ and with Legendre polynomials f_p defined in example (1).

- the *symmetric hierarchical least squares* polynomials of the polynomial vector space $P_p^{3,\pm}$, optimized by a step-wise least squares method.
- the *symmetric hierarchical step-wise/* consecutively (by a Gauß-Seidel method) optimized polynomials of the polynomial vector space $P_p^{3,\pm}$.

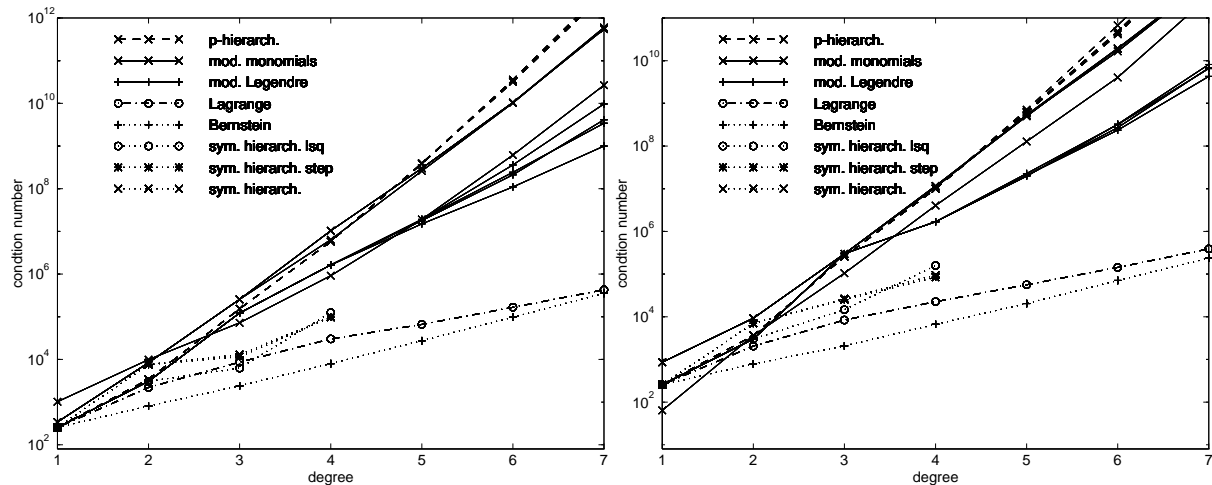


FIG. 19. Local condition numbers for the Laplace operator on the *distorted equilateral tetrahedron* stretched and contracted by a factor of 16 for different polynomials of degree 1 to 7

Each polynomial which generates a symmetrical subset is optimized with respect to the previous optimized polynomials.

- the *symmetric hierarchical* polynomials of the polynomial vector space $P_p^{3,\pm}$, optimized by a Gauß-Seidel method for each space $P_p^{3,\pm}$, $p = 1, 2, \dots$

We observe the following: For degree one all condition numbers start with a low number. For degree two, the quadratic case, the condition numbers diverge, but not with the same pattern as in the asymptotic case. For non-symmetric tetrahedrons we could get up to 24 different condition numbers depending on the orientation of the tetrahedron, but actually we get up to six different condition numbers. We see that a suitable orientation pays off in this case. The symmetric polynomials have got only one unique condition number independent from orientation.

In more detail we can see in figure (16) an analogous pattern of condition numbers for the equilateral tetrahedron. We can split the polynomials

into groups of lower or higher growth of condition numbers. The monomials, the orthogonal polynomials, the p -hierarchical polynomials, the modified monomials and the modified Legendre-polynomials belong to the group with rapidly growing condition numbers. On the triangle the modified Legendre-polynomials were in the group with better condition numbers, but this is not the case for the tetrahedron. Now the Bernstein-polynomials perform best and the Lagrange-polynomials are slightly worse. In general the lowest condition numbers are of the same magnitude like on the triangle, but other ones may be much higher. We have to keep in mind that the number of polynomials involved for each p grows an order of p faster in 3D than in 2D.

Looking at right-angled tetrahedrons we have to consider different situations concerning a factor 16 of distortion (figures 17 and 18). The distortions are applied analogously to the 2-D case (figure 13). We take the edges $1 : 1 : 1$, $1 : 1 : 16$, $1 : 16 : 16$ and $1 : 16 : 16^2$ preserving the right-angle. The $1 : 1 : 1$ situation produces only slightly higher condition numbers than the equilateral tetrahedron. The other distorted tetrahedrons have a factor of 16^2 and the twice distorted ones ($1 : 16 : 16^2$) an even higher factor. The condition numbers for the $1 : 16 : 16$ case are slightly better than for the $1 : 1 : 16$ one. In each case the symmetric hierarchical polynomials have the lowest condition number of all hierarchical polynomials. Only Bernstein- and Lagrange-polynomials have lower ones, but are not far away. The different distortions lead to a splitting of the condition number histories, which diverge for modified monomials and modified Legendre-polynomials. For high p a proper orientation pays off for these polynomials.

Proceeding to distortions of an equilateral tetrahedron (figure 19), we can observe a similar pattern but with different scaling. We have contracted and stretched a tetrahedron by a factor 16. The contracted one leads to a smaller divergence of non-symmetric polynomials and at some points to a slightly lower condition number. The general behavior and the division into groups remains the same. At degree $p = 3$ we can see small deviations for some polynomials.

We can summarize the results saying that the lowest condition numbers arise in the case of Bernstein and Lagrange polynomials. They are not far away from the numbers for the new symmetric hierarchical polynomials. The modified Legendre polynomials have got higher condition numbers, which additionally depend on orientation. The exact ranking depends on the tetra-

hedron shape and the differential operator itself.

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We have done the symbolic computations including the management of polynomials and permutation groups with list-oriented features of REDUCE [Hea93], which triggered an optimization procedure written in C++. The final results were computed and drawn by MATLAB [Mat92]. Some illustrations were drawn using UNIDRAW [Vli90].

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A APPENDIX

A.1 TRIANGLE

We have listed the *symmetric hierarchical* polynomials of the polynomial vector space $P_p^{2,\pm}$, optimized by a Gauß-Seidel method for each space $P_p^{2,\pm}$, $p = 1, 2, \dots, 8$. The optimization was done rather roughly, but the condition numbers in chapter (3.4) were calculated based on the polynomials given here.

We only print every third polynomial, the rest can be obtained rotating the triangle twice ($b_0 \rightarrow b_1 \rightarrow b_2 \rightarrow b_0$).

The linear polynomials (point-functions) $p = 1$:

$$f_0 = b_0$$

The quadratic polynomials (edge-functions) $p = 2$:

$$f_3 = (-36837 b_0 b_1)/10000$$

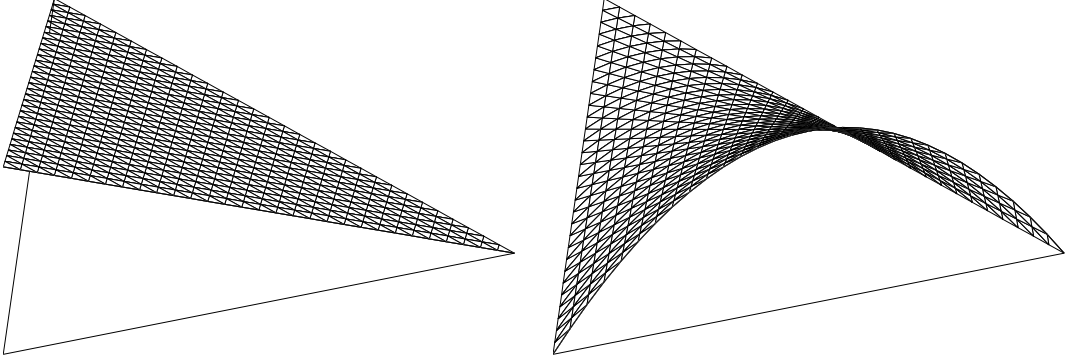


FIG. 20. *Symmetric hierarchical* polynomials f_0 and $-f_3$ in $P_1^{2,\pm}$ and $P_2^{2,\pm}$

Polynomials for $P_3^{2,\pm}$ (internal functions) $p = 3$:

$$f_6 = (133659 b_0 b_1^2 b_2)/5000$$

Polynomials for $P_3^{2,\pm}$ (edge-functions) $p = 3$:

$$f_9 = (b_0 b_1 (-16635193 b_0 b_2 + 7277900 b_0 + 16635193 b_1 b_2 - 7277900 b_1))/1000000$$

Polynomials for $P_4^{2,\pm}$ (edge-functions) $p = 4$:

$$f_{12} = (b_0 b_1 (45850375 b_0^2 - 91700750 b_0 b_1 - 36167375 b_0 b_2 + 45850375 b_1^2 - 36167375 b_1 b_2 - 159096 b_2^2 - 45850375))/12500000$$

Polynomials for $P_5^{2,\pm}$ (internal functions) $p = 5$:

$$f_{15} = (b_0 b_1 b_2 (11754500 b_0 b_1 - 1627056 b_0 - 1627056 b_1 + 250071 b_2))/50000$$

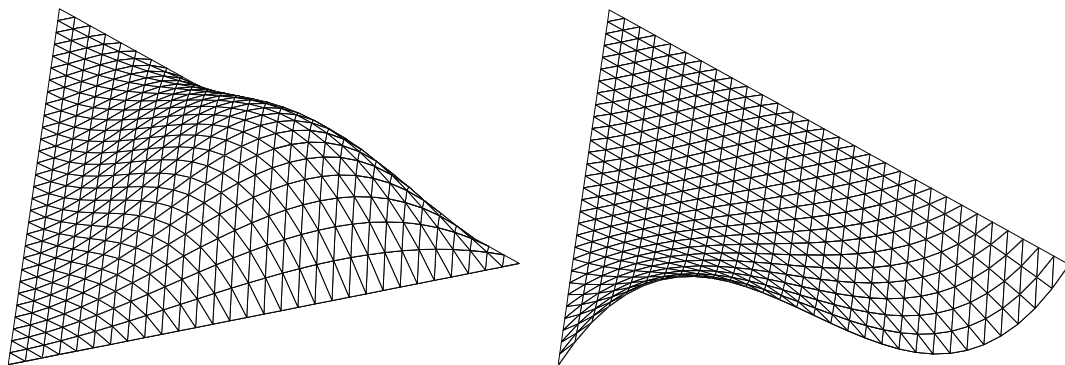


FIG. 21. *Symmetric hierarchical polynomials f_6 and f_9 in $P_3^{2,\pm}$*

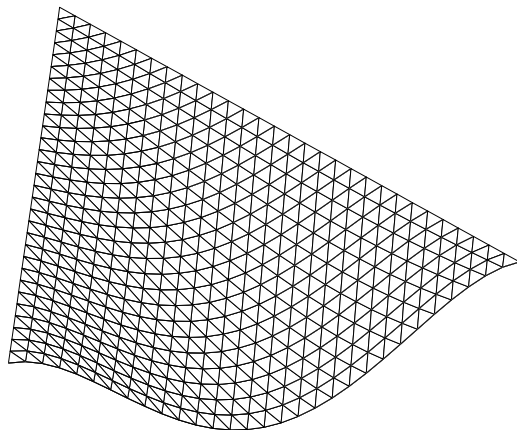


FIG. 22. *Symmetric hierarchical polynomial f_{12} in $P_4^{2,\pm}$*

Polynomials for $P_5^{2,\pm}$ (edge-functions) $p = 5$:

$$f_{18} = \left(b_0 b_1 \right. \\ \left. (284147 b_0^3 - 852441 b_0^2 b_1 + 852441 b_0 b_1^2 + 89792 b_0 b_2^2 + 67950 b_0 b_2 - \right. \\ \left. 284147 b_0 - 284147 b_1^3 - 89792 b_1 b_2^2 - 67950 b_1 b_2 + 284147 b_1) \right) / 100000$$

Two triples of polynomials for $P_6^{2,\pm}$ (internal functions) $p = 6$:

$$f_{21} = (b_0 b_1 b_2$$

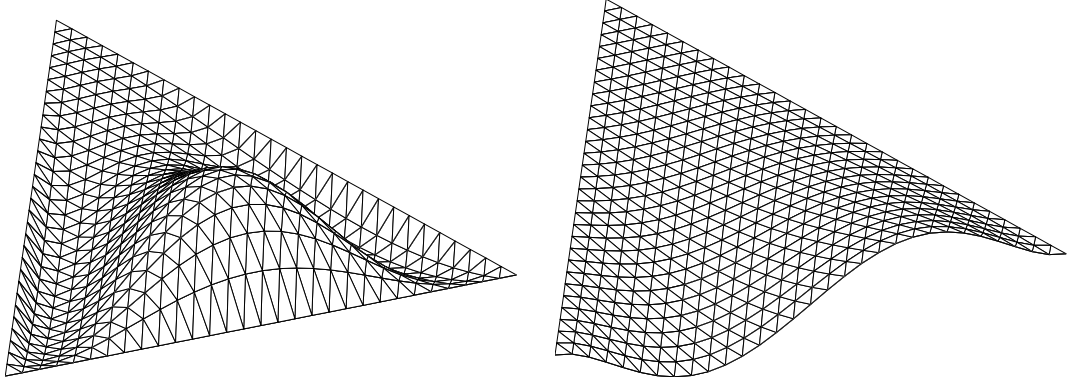


FIG. 23. *Symmetric hierarchical polynomials* f_{15} and f_{18} in $P_5^{2,\pm}$

$$(10371440000 b_0 b_1^2 b_2 - 81393100 b_0 b_1 - 474864000 b_0 b_2 + 26585293 b_0 - 81393100 b_1 b_2 + 37947000 b_1 + 26585293 b_2) / 10000000$$

and

$$f_{24} = (b_0 b_1 b_2 (-107151020 b_0^2 b_1 b_2 + 76672000 b_0^2 b_1 + 107151020 b_0 b_1^2 b_2 - 76672000 b_0 b_1^2 + 16173954 b_0 b_2 - 6890163 b_0 - 16173954 b_1 b_2 + 6890163 b_1)) / 100000$$

Polynomials for $P_6^{2,\pm}$ (edge-functions) $p = 6$:

$$f_{27} = (b_0 b_1 (20291425 b_0^4 - 81165700 b_0^3 b_1 + 121748550 b_0^2 b_1^2 - 304084000 b_0^2 b_1 b_2^2 + 16279800 b_0^2 b_2^2 - 24349710 b_0^2 - 81165700 b_0 b_1^3 - 304084000 b_0 b_1^2 b_2^2 + 213762000 b_0 b_1 b_2^3 + 16688400 b_0 b_1 b_2 + 48699420 b_0 b_1 - 16279800 b_0 b_2^3 - 3943304 b_0 b_2^2 - 58480 b_0 b_2 + 20291425 b_1^4 + 16279800 b_1^2 b_2^2 - 24349710 b_1^2 - 16279800 b_1 b_2^3 - 3943304 b_1 b_2^2 - 58480 b_1 b_2 + 9680800 b_2^2 + 4058285)) / 2000000$$

Polynomials for $P_7^{2,\pm}$ (internal functions) $p = 7$:

$$f_{30} = (b_0 b_1 b_2 (204343000 b_0^3 b_1 - 408686000 b_0^2 b_1^2 - 81061000 b_0^2 b_1 b_2 + 20704700 b_0^2 b_2 + 204343000 b_0 b_1^3 - 81061000 b_0 b_1^2 b_2 - 28501800 b_0 b_1 b_2^2 + 38345000 b_0 b_1 -$$

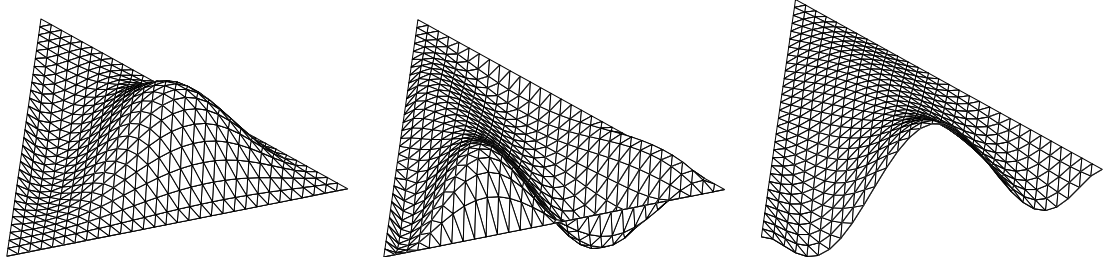


FIG. 24. *Symmetric hierarchical polynomials* f_{21} , f_{24} and f_{27} in $P_6^{2,\pm}$

$$\begin{aligned} & 20704700 b_0 b_2^2 + 20004200 b_0 b_2 - 12352751 b_0 + 20704700 b_1^2 b_2 - \\ & 20704700 b_1 b_2^2 + \\ & 20004200 b_1 b_2 - 12352751 b_1 + 4315040 b_2) / 1000000 \end{aligned}$$

Polynomials for $P_7^{2,\pm}$ (edge-functions) $p = 7$:

$$\begin{aligned} f_{33} = & (b_0 b_1 \\ & (200550000 b_0^5 - 1002750000 b_0^4 b_1 + 2005500000 b_0^3 b_1^2 + 801302870 b_0^3 b_2^2 - \\ & 286500000 b_0^3 - 2005500000 b_0^2 b_1^3 - 2030145900 b_0^2 b_1 b_2^2 + \\ & 398956000 b_0^2 b_1 b_2 + \\ & 859500000 b_0^2 b_1 - 1602605740 b_0^2 b_2^2 + 183375700 b_0^2 b_2 + 1002750000 b_0 b_1^4 + \\ & 2030145900 b_0 b_1^2 b_2^2 - 398956000 b_0 b_1^2 b_2 - 859500000 b_0 b_1^2 + \\ & 801302870 b_0 b_2^4 - \\ & 183375700 b_0 b_2^3 + 297443130 b_0 b_2^2 + 25007201 b_0 b_2 + 85950000 b_0 - \\ & 200550000 b_1^5 - \\ & 801302870 b_1^3 b_2^2 + 286500000 b_1^3 + 1602605740 b_1^2 b_2^3 - 183375700 b_1^2 b_2^2 - \\ & 801302870 b_1 b_2^4 + 183375700 b_1 b_2^3 - 297443130 b_1 b_2^2 - 25007201 b_1 b_2 - \\ & 85950000 b_1) / 10000000 \end{aligned}$$

Two triples of polynomials for $P_8^{2,\pm}$ (internal functions) $p = 8$:

$$\begin{aligned} f_{36} = & (b_0 b_1 b_2 \\ & (31373400 b_0^3 b_1 + 3540224 b_0^3 b_2 + 936696000 b_0^2 b_1^2 b_2 - 62746800 b_0^2 b_1^2 - \\ & 168326200 b_0^2 b_1 b_2 - 7080448 b_0^2 b_2^2 - 11059300 b_0^2 b_2 + 31373400 b_0 b_1^3 - \\ & 168326200 b_0 b_1^2 b_2 - 20606560 b_0 b_1 b_2^2 + 13286600 b_0 b_1 + 3540224 b_0 b_2^3 + \\ & 11059300 b_0 b_2^2 + 483951 b_0 b_2 - 2316856 b_0 + 3540224 b_1^3 b_2 - \\ & 7080448 b_1^2 b_2^2 - \\ & 11059300 b_1^2 b_2 + 3540224 b_1 b_2^3 + 11059300 b_1 b_2^2 + 483951 b_1 b_2 - \end{aligned}$$

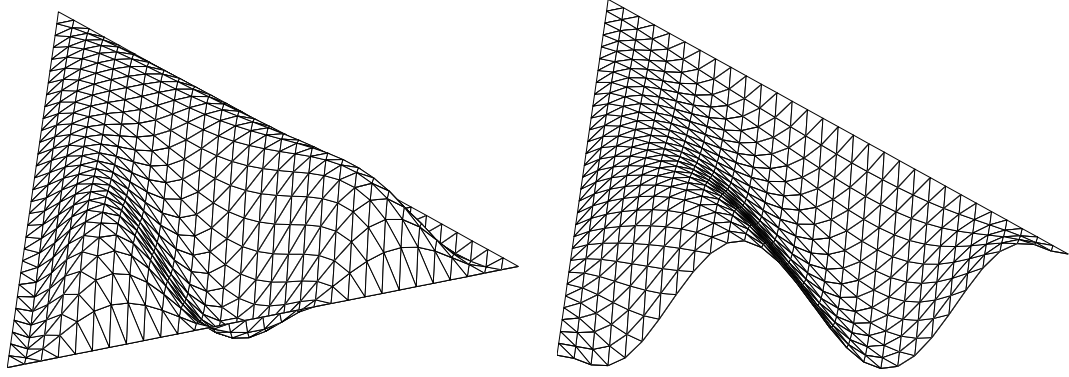


FIG. 25. *Symmetric hierarchical* polynomials f_{30} and f_{33} in $P_7^{2,\pm}$

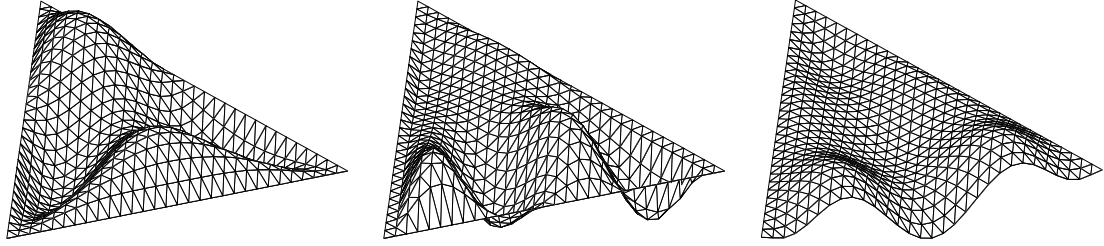


FIG. 26. *Symmetric hierarchical* polynomials f_{36} , f_{39} and f_{42} in $P_8^{2,\pm}$

$$2316856 b_1 + 1885820 b_2) / 200000$$

and

$$f_{39} = \left(b_0 b_1 b_2 (14571400 b_0^4 b_1 - 43714200 b_0^3 b_1^2 + 14265 b_0^3 b_2 + 43714200 b_0^2 b_1^3 + 26008348 b_0^2 b_1 b_2^2 - 11352642 b_0^2 b_1 b_2 + 46920 b_0^2 b_1 - 28530 b_0^2 b_2^2 + 1050552 b_0^2 b_2 - 14571400 b_0 b_1^4 - 26008348 b_0 b_1^2 b_2^2 + 11352642 b_0 b_1^2 b_2 - 46920 b_0 b_1^2 + 14265 b_0 b_2^3 - 1050552 b_0 b_2^2 + 553029 b_0 b_2 - 387563 b_0 - 14265 b_1^3 b_2 + 28530 b_1^2 b_2^2 - 1050552 b_1^2 b_2 - 14265 b_1 b_2^3 + 1050552 b_1 b_2^2 - 553029 b_1 b_2 + 387563 b_1) \right) / 20000$$

Polynomials for $P_8^{2,\pm}$ (edge-functions) $p = 8$:

$$\begin{aligned}
f_{42} = & \left(b_0 b_1 \right. \\
& (3708747 b_0^6 - 22252482 b_0^5 b_1 + 55631205 b_0^4 b_1^2 + 57088550 b_0^4 b_2^2 - \\
& 6181245 b_0^4 - \\
& 74174940 b_0^3 b_1^3 + 16168880 b_0^3 b_1 b_2 + 24724980 b_0^3 b_1 - 171265650 b_0^3 b_2^3 - \\
& 8817189 b_0^3 b_2^2 + 55631205 b_0^2 b_1^4 + 346212400 b_0^2 b_1^2 b_2^2 - 32337760 b_0^2 b_1^2 b_2 - \\
& 37087470 b_0^2 b_1^2 - 140255200 b_0^2 b_1 b_2^3 - 68062060 b_0^2 b_1 b_2^2 + 171265650 b_0^2 b_2^4 + \\
& 17634378 b_0^2 b_2^3 + 224190 b_0^2 b_2^2 + 2649105 b_0^2 - 22252482 b_0 b_1^5 + \\
& 16168880 b_0 b_1^3 b_2 + 24724980 b_0 b_1^3 - 140255200 b_0 b_1^2 b_2^3 - \\
& 68062060 b_0 b_1^2 b_2^2 + \\
& 40048800 b_0 b_1 b_2^3 + 3865040 b_0 b_1 b_2 - 5298210 b_0 b_1 - 57088550 b_0 b_2^5 - \\
& 8817189 b_0 b_2^4 - 224190 b_0 b_2^3 - 1360531 b_0 b_2^2 - 340880 b_0 b_2 + 3708747 b_1^6 + \\
& 57088550 b_1^4 b_2^2 - 6181245 b_1^4 - 171265650 b_1^3 b_2^3 - 8817189 b_1^3 b_2^2 + \\
& 171265650 b_1^2 b_2^4 + 17634378 b_1^2 b_2^3 + 224190 b_1^2 b_2^2 + 2649105 b_1^2 - \\
& 57088550 b_1 b_2^5 - 8817189 b_1 b_2^4 - 224190 b_1 b_2^3 - 1360531 b_1 b_2^2 - \\
& 340880 b_1 b_2 + \\
& \left. 2994332 b_2^2 - 176607 \right) / 200000
\end{aligned}$$

A.2 TETRAHEDRON

Now we consider the *symmetric hierarchical* polynomials in $P_p^{3,\pm}$, $p = 1, 2, 3, 4$. The polynomials have been used in chapter (3.5).

We only print the first polynomial of each symmetrical set, the rest can be obtained by even permutations of the variables b_0, b_1, b_2, b_3 .

The 4 linear polynomials (point-functions) $p = 1$:

$$f_0 = b_0$$

The 6 quadratic polynomials (edge-functions) $p = 2$:

$$f_4 = \left(-460461897 b_1 b_2 \right) / 62500000$$

The 12 polynomials for $P_3^{3,\pm}$ (triangle-functions) $p = 3$:

$$f_{10} = \left(2520584851 b_0 b_1 b_2^2 \right) / 50000000$$

The 6 polynomials for $P_3^{3,\pm}$ (edge-functions) $p = 3$:

$$\begin{aligned}
f_{22} = & \left(b_1 b_2 \right. \\
& \left. - 35669479477 b_0 b_1 + 35669479477 b_0 b_2 - 35669479477 b_1 b_3 + \right.
\end{aligned}$$

$$17822747392 b_1 + 35669479477 b_2 b_3 - 17822747392 b_2) / 1000000000$$

The 4 polynomials for $P_4^{3,\pm}$ (internal functions) $p = 4$:

$$f_{28} = (4117143117 b_0 b_1 b_2^2 b_3) / 100000000$$

The 6 polynomials for $P_4^{3,\pm}$ (edge-functions) $p = 4$:

$$f_{32} = (b_1 b_2 (-58436191856 b_0^2 b_3 + 31087963700 b_0^2 + 48601598362 b_0 b_1 b_3 - 13736554971 b_0 b_1 + 48601598362 b_0 b_2 b_3 - 13736554971 b_0 b_2 - 58436191856 b_0 b_3^2 + 6507381544 b_1^2 - 13014763088 b_1 b_2 - 13736554971 b_1 b_3 + 6507381544 b_2^2 - 13736554971 b_2 b_3 + 31087963700 b_3^2 - 6507381544)) / 1000000000$$

The 12 polynomials for $P_5^{3,\pm}$ (triangle-functions) $p = 5$:

$$f(38) := (b_0 b_1 b_2 (-8769504191 b_0 b_3 - 8328968708 b_0 + 166728839300 b_1 b_2 + 36572623855 b_1 b_3 - 22058761161 b_1 + 36572623855 b_2 b_3 - 22058761161 b_2 + 3702426378 b_3^2)) / 500000000$$

The 6 polynomials for $P_5^{3,\pm}$ (edge-functions) $p = 5$:

$$f(50) := (b_1 b_2 (18758276598 b_0^2 b_1 - 18758276598 b_0^2 b_2 - 32865620574 b_0 b_1 b_3 + 25529946079 b_0 b_1 + 32865620574 b_0 b_2 b_3 - 25529946079 b_0 b_2 + 5682941970 b_1^3 - 17048825910 b_1^2 b_2 + 17048825910 b_1 b_2^2 + 18758276598 b_1 b_3^2 + 25529946079 b_1 b_3 - 5682941970 b_1 - 5682941970 b_3^2 - 18758276598 b_2 b_3^2 - 25529946079 b_2 b_3 + 5682941970 b_2)) / 1000000000$$

A.3 4-SIMPLEX

Now we consider the *symmetric hierarchical* polynomials in $P_p^{4,\pm}$, $p = 1, 2, 3, 4$.

We only print the first polynomial of each symmetrical set, the rest can be obtained by even permutations of the variables b_0, b_1, b_2, b_3, b_4 .

The 5 linear polynomials (point-functions) $p = 1$:

$$f_0 = b_0$$

The 10 quadratic polynomials (edge-functions) $p = 2$:

$$f_5 = 5527802379 b_0 b_3 / 2500000000$$

The 30 polynomials for $P_3^{4,\pm}$ (triangle-functions) $p = 3$:

$$f_{15} = 568294197 b_0 b_2 b_3^2 / 500000000$$

The 10 polynomials for $P_3^{4,\pm}$ (edge-functions) $p = 3$:

$$f_{45} = \left(3 b_0 b_3 \right. \\ \left. (3713723093 b_0 b_1 + 3713723093 b_0 b_2 + 3713723093 b_0 b_4 - 1016500455 b_0 - \right. \\ \left. 3713723093 b_1 b_3 - 3713723093 b_2 b_3 - 3713723093 b_3 b_4 + \right. \\ \left. 1016500455 b_3) \right) / 2500000000$$

The 20 polynomials for $P_4^{4,\pm}$ (tetrahedron-functions) $p = 4$:

$$f_{55} = 129844041 b_0 b_1 b_2 b_3^2 / 1250000$$

The 10 polynomials for $P_4^{4,\pm}$ (edge-functions) $p = 4$:

$$f_{75} = \left(b_0 b_3 \right. \\ \left. (27578210199 b_0^2 + 627173420137 b_0 b_1 b_2 + 627173420137 b_0 b_1 b_4 - \right. \\ \left. 7613815925 b_0 b_1 \right. \\ \left. + 627173420137 b_0 b_2 b_4 - 7613815925 b_0 b_2 - 55156420398 b_0 b_3 - \right. \\ \left. 7613815925 b_0 b_4 - \right. \\ \left. 448021375170 b_1^2 b_2 - 448021375170 b_1^2 b_4 + 180300619660 b_1^2 - \right. \\ \left. 448021375170 b_1 b_2^2 \right)$$

$$\begin{aligned}
& + 627173420137 b_1 b_2 b_3 + 627173420137 b_1 b_3 b_4 - 7613815925 b_1 b_3 - \\
& 448021375170 b_1 b_4^2 - 448021375170 b_2^2 b_4 + 180300619660 b_2^2 + \\
& 627173420137 b_2 b_3 b_4 - 7613815925 b_2 b_3 - 448021375170 b_2 b_4^2 + \\
& 27578210199 b_3^2 - \\
& 7613815925 b_3 b_4 + 180300619660 b_4^2 - 27578210199) / 5000000000
\end{aligned}$$

A.4 CODE

We repeat the listing of the polynomials in a more machine-readable fashion. The terms are written in a different bracketed form. We use a multivariate Horner-scheme for a better numeric performance.

The polynomials on the triangle of chapter (A.1) are:

```

f(0) =
b0;
f(3) =
(-36837.*b1*b0)/10000.;
f(6) =
(133659.*b2*b1**2*b0)/5000.;
f(9) =
((( -16635193.*b2+7277900.)*b1*b0+(16635193.*b2-7277900.)*b1**2)*b0)/
1000000.;
f(12) =
(((45850375.*b1*b0+(-91700750.*b1-36167375.*b2)*b1)*b0+((45850375.*
b1-36167375.*b2)*b1-159096.*b2**2-45850375.)*b1)*b0)/12500000.;
f(15) =
(((11754500.*b2*b1-1627056.*b2)*b1*b0+(-1627056.*b2*b1+250071.*
b2**2)*b1)*b0)/50000.;
f(18) =
((( (284147.*b1*b0-852441.*b1**2)*b0+(852441.*b1**2+(89792.*b2+
67950.)*b2-284147.)*b1)*b0+(-284147.*b1**2+(-89792.*b2-67950.)*b2+
284147.)*b1**2)*b0)/100000.;
f(21) =
((( (10371440000.*b2**2*b1-81393100.*b2)*b1+(-474864000.*b2+
26585293.)*b2)*b1*b0+((-81393100.*b2+37947000.)*b2*b1+26585293.*
b2**2)*b1)*b0)/10000000.;
f(24) =
((( (-107151020.*b2+76672000.)*b2*b1**2*b0+((107151020.*b2-

```

$76672000.) * b_2 * b_1^{**2} + (16173954. * b_2 - 6890163.) * b_2) * b_1) * b_0 + (-16173954. * b_2 + 6890163.) * b_2 * b_1^{**2} * b_0) / 100000.;$
 $f(27) =$
 $(((((20291425. * b_1 * b_0 - 81165700. * b_1^{**2}) * b_0 + ((121748550. * b_1 - 304084000. * b_2^{**2}) * b_1 + 16279800. * b_2^{**2} - 24349710.) * b_1) * b_0 + (((-81165700. * b_1 - 304084000. * b_2^{**2}) * b_1 + (213762000. * b_2^{**2} + 16688400.) * b_2 + 48699420.) * b_1 + ((-16279800. * b_2 - 3943304.) * b_2 - 58480.) * b_2) * b_1) * b_0 + ((20291425. * b_1^{**2} + 16279800. * b_2^{**2} - 24349710.) * b_1 + ((-16279800. * b_2 - 3943304.) * b_2 - 58480.) * b_2) * b_1 + 9680800. * b_2^{**2} + 4058285.) * b_1) * b_0) / 2000000.;$
 $f(30) =$
 $(((((204343000. * b_2 * b_1^{**2} * b_0 + ((-408686000. * b_2 * b_1 - 81061000. * b_2^{**2}) * b_1 + 20704700. * b_2^{**2}) * b_1) * b_0 + ((204343000. * b_2 * b_1 - 81061000. * b_2^{**2}) * b_1 + (-28501800. * b_2^{**2} + 38345000.) * b_2) * b_1 + ((-20704700. * b_2 + 20004200.) * b_2 - 12352751.) * b_2) * b_1) * b_0 + ((20704700. * b_2^{**2} * b_1 + ((-20704700. * b_2 + 20004200.) * b_2 - 12352751.) * b_2) * b_1 + 4315040. * b_2^{**2}) * b_1) * b_0) / 1000000.;$
 $f(33) =$
 $(((((200550000. * b_1 * b_0 - 1002750000. * b_1^{**2}) * b_0 + (2005500000. * b_1^{**2} + 801302870. * b_2^{**2} - 286500000.) * b_1) * b_0 + ((-2005500000. * b_1^{**2} + (-2030145900. * b_2 + 398956000.) * b_2 + 859500000.) * b_1 + (-1602605740. * b_2 + 183375700.) * b_2^{**2}) * b_1) * b_0 + ((1002750000. * b_1^{**2} + (2030145900. * b_2 - 398956000.) * b_2 - 859500000.) * b_1^{**2} + ((801302870. * b_2 - 183375700.) * b_2 + 297443130.) * b_2 + 25007201.) * b_2 + 859500000.) * b_1) * b_0 + (((-200550000. * b_1^{**2} - 801302870. * b_2^{**2} + 286500000.) * b_1 + (1602605740. * b_2 - 183375700.) * b_2^{**2}) * b_1 + (((-801302870. * b_2 + 183375700.) * b_2 - 297443130.) * b_2 - 25007201.) * b_2 - 859500000.) * b_1^{**2}) * b_0) / 10000000.;$
 $f(36) =$
 $(((((31373400. * b_2 * b_1 + 3540224. * b_2^{**2}) * b_1 * b_0 + ((936696000. * b_2 - 62746800.) * b_2 * b_1 - 168326200. * b_2^{**2}) * b_1 + (-7080448. * b_2 - 11059300.) * b_2^{**2}) * b_1) * b_0 + ((31373400. * b_2 * b_1 - 168326200. * b_2^{**2}) * b_1 + (-20606560. * b_2^{**2} + 13286600.) * b_2) * b_1 + ((3540224. * b_2 + 11059300.) * b_2 + 483951.) * b_2 - 2316856.) * b_2) * b_1) * b_0 + ((3540224. * b_2^{**2} * b_1 + (-7080448. * b_2 - 11059300.) * b_2^{**2}) * b_1 + ((3540224. * b_2 + 11059300.) * b_2 + 483951.) * b_2 - 2316856.) * b_2) * b_1 + 1885820. * b_2^{**2}) * b_1) * b_0) / 200000.;$
 $f(39) =$
 $(((((14571400. * b_2 * b_1^{**2} * b_0 + (-43714200. * b_2 * b_1^{**2} + 14265. * b_2^{**2}) * b_1) * b_0 + ((43714200. * b_2 * b_1^{**2} + (26008348. * b_2 - 11352642.) * b_2 + 46920.) * b_2) * b_1 + (-28530. * b_2 + 1050552.) * b_2^{**2}) * b_1) * b_0 + ((-14571400. * b_2 * b_1^{**2} + ((-26008348. * b_2 + 11352642.) * b_2 - 46920.) * b_2) * b_1^{**2} + ((14265. * b_2 - 1050552.) * b_2 + 553029.) * b_2 - 387563.) * b_2) * b_1) * b_0 + ((-14265. * b_2^{**2} * b_1 +$

$$(28530.*b2-1050552.)*b2**2)*b1+(((-14265.*b2+1050552.)*b2-553029.)*b2+387563.)*b2)*b1**2)*b0)/20000.;$$

$$f(42) =$$

$$(((((((3708747.*b1*b0-22252482.*b1**2)*b0+(55631205.*b1**2+57088550.*b2**2-6181245.)*b1)*b0+((-74174940.*b1**2+16168880.*b2+24724980.)*b1+(-171265650.*b2-8817189.)*b2**2)*b1)*b0+(((55631205.*b1**2+(346212400.*b2-32337760.)*b2-37087470.)*b1+(-140255200.*b2-68062060.)*b2**2)*b1+((171265650.*b2+17634378.)*b2+224190.)*b2**2+2649105.)*b1)*b0+(((-22252482.*b1**2+16168880.*b2+24724980.)*b1+(-140255200.*b2-68062060.)*b2**2)*b1+(40048800.*b2**2+3865040.)*b2-5298210.)*b1+(((-57088550.*b2-8817189.)*b2-224190.)*b2-1360531.)*b2-340880.)*b2)*b1)*b0+((((3708747.*b1**2+57088550.*b2**2-6181245.)*b1+(-171265650.*b2-8817189.)*b2**2)*b1+((171265650.*b2+17634378.)*b2+224190.)*b2**2+2649105.)*b1+(((-57088550.*b2-8817189.)*b2-224190.)*b2-1360531.)*b2-340880.)*b2)*b1+2994332.*b2**2-176607.)*b1)*b0)/200000.;$$

The polynomials on the tetrahedron of chapter (A.2) are:

$$f(0) =$$

$$b0;$$

$$f(4) =$$

$$(-460461897.*b2*b1)/62500000.;$$

$$f(10) =$$

$$(2520584851.*b2**2*b1*b0)/50000000.;$$

$$f(22) =$$

$$((-35669479477.*b2*b1+35669479477.*b2**2)*b1*b0+((-35669479477.*b3+17822747392.)*b2*b1+(35669479477.*b3-17822747392.)*b2**2)*b1)/100000000.;$$

$$f(28) =$$

$$(4117143117.*b3*b2**2*b1*b0)/100000000.;$$

$$f(32) =$$

$$(((((-58436191856.*b3+31087963700.)*b2*b1*b0+((48601598362.*b3-13736554971.)*b2*b1+((48601598362.*b3-13736554971.)*b2-58436191856.*b3**2)*b2)*b1)*b0+((6507381544.*b2*b1+(-13014763088.*b2-13736554971.*b3)*b2)*b1+((6507381544.*b2-13736554971.*b3)*b2+31087963700.*b3**2-6507381544.)*b2)*b1)/1000000000.;$$

$$f(38) =$$

$$(((-8769504191.*b3-8328968708.)*b2*b1*b0+((166728839300.*b2+36572623855.*b3-22058761161.)*b2*b1+((36572623855.*b3-$$

$$22058761161.) * b_2 + 3702426378. * b_3^{**2} * b_2) * b_1) * b_0) / 500000000. ;$$

$$f(50) =$$

$$(((18758276598. * b_2 * b_1 - 18758276598. * b_2^{**2}) * b_1 * b_0 + ((-32865620574. * b_3 + 25529946079.) * b_2 * b_1 + (32865620574. * b_3 - 25529946079.) * b_2^{**2}) * b_1) * b_0 + (((5682941970. * b_2 * b_1 - 17048825910. * b_2^{**2}) * b_1 + (17048825910. * b_2^{**2} + (18758276598. * b_3 + 25529946079.) * b_3 - 5682941970.) * b_2) * b_1 + (-5682941970. * b_2^{**2} + (-18758276598. * b_3 - 25529946079.) * b_3 + 5682941970.) * b_2^{**2}) * b_1) / 1000000000. ;$$

The polynomials on the 4-simplex of chapter (A.3) are:

$$f(0) =$$

$$b_0;$$

$$f(5) =$$

$$(5527802379. * b_3 * b_0) / 2500000000. ;$$

$$f(15) =$$

$$(568294197. * b_3^{**2} * b_2 * b_0) / 500000000. ;$$

$$f(45) =$$

$$(((11141169279. * b_3 * b_1 + 11141169279. * b_3 * b_2 + (11141169279. * b_4 - 3049501365.) * b_3) * b_0 - 11141169279. * b_3^{**2} * b_1 - 11141169279. * b_3^{**2} * b_2 + (-11141169279. * b_4 + 3049501365.) * b_3^{**2}) * b_0) / 2500000000. ;$$

$$f(55) =$$

$$(129844041. * b_3^{**2} * b_2 * b_1 * b_0) / 1250000. ;$$

$$f(75) =$$

$$(((27578210199. * b_3 * b_0 + (627173420137. * b_3 * b_2 + (627173420137. * b_4 - 7613815925.) * b_3) * b_1 + (627173420137. * b_4 - 7613815925.) * b_3 * b_2 + (-55156420398. * b_3 - 7613815925. * b_4) * b_3) * b_0 + ((-448021375170. * b_3 * b_2 + (-448021375170. * b_4 + 180300619660.) * b_3) * b_1 + (-448021375170. * b_3 * b_2 + 627173420137. * b_3^{**2}) * b_2 + ((627173420137. * b_4 - 7613815925.) * b_3 - 448021375170. * b_4^{**2}) * b_3) * b_1 + ((-448021375170. * b_4 + 180300619660.) * b_3 * b_2 + ((627173420137. * b_4 - 7613815925.) * b_3 - 448021375170. * b_4^{**2}) * b_3) * b_2 + ((27578210199. * b_3 - 7613815925. * b_4) * b_3 + 180300619660. * b_4^{**2} - 27578210199.) * b_3) * b_0) / 5000000000. ;$$