QUADRATURE POINTS ON POLYHEDRAL ELEMENTS

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ABSTRACT

The method of the finite elements is a flexible numeric procedure both for interpolation and approximation of the solutions of partial differential equations. The generalized polyhedral finite elements (Milbradt 2004) lead to a greater flexibility in domain decomposition.

A general simple local coordinate system, the natural element coordinates, was developed, which makes a formulation of interpolation functions on polyhedral elements possible that are independent of the dimension of the space, of the localization and vertex number.

With these natural element coordinates, which can be understood as generalized barycentric coordinates, it is very easy to define interpolation functions for the use of the finite element method. This paper presents hierarchical edge based functions, which are formulated in natural element coordinates.

The unknown solution of the partial differential equation will be approximated by finite element interpolation. The resulting integral equations induce a system of linear equations, which needs to be solved with appropriate methods. The evaluation of the resulting integrals is the key ingredient in the proposed methodology. In this paper we present numerical approximations of such integrals over any polyhedrons. A fast and less computation intensive solution is the use of quadrature rules. This paper will show all steps needed to find quadrature points on any strict regular polyhedrons in any dimension. The existence of more then one set of quadrature points on higher polyhedrons is of interest.

KEY WORDS

quadrature, natural element coordinates, finite elements, barycentric decomposition, hierachical formfunction.

INTRODUCTION

Finite elements on the base of arbitrary polyhedrons (Milbradt 2001) offer a higher flexibility for the mesh generation and allow for a better mapping of natural and technical structures as they appear for example in biomechanics and crystallogics. To achieve this natural element coordinates were successfully introduced. The formulation of interpolation functions on the base of natural element coordinates leads to a generalized construction. The unknown

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solution of the numerical approximation of partial differential equations will be approximated by finite element interpolation. During this process integral equations arise, which are solved with suitable methods (Pick 2004). An analytical determination of these integrals over polyhedrons is normally not possible. They need to be realized by numerical approximation. An elaboration of those numerical approximations is the main focus of this article.

FINITE ELEMENT APPROXIMATION ON POLYHEDRONS

We focus on the numerical approximation of the solution $u(x)$ of a partial differential equation in a bounded domain Ω in $\mathbb{R}^n$ with the finite element method. The unknown solution *u* is approximated through a Galerkin procedure, which uses a linear combination of interpolation functions and the still unknown parameters u_i:

$$u(x) \simeq \tilde{u}(x) := \sum_{i=1}^{n} u_i \Phi_i(x)$$

Interpolation functions on classical finite elements are defined on triangles, quadrangles, tetrahedrons and quads. Hence, the domain Ω must be decomposed with such elements accordingly. The interpolation functions for each of these elements are well known. If necessary, a transformation on standard elements is done. The application of arbitrary polyhedrons as a base of finite elements needs a generalized formulation of these interpolation functions.

NATURAL ELEMENT COORDINATES

A general formulation of interpolation functions is possible with the introduction of natural element coordinates because they are usable for all convex polyhedrons in all positions, forms and dimensions. The natural element coordinates can be understood as the restriction of the natural neighbourhood interpolation introduced by Sibson (1980) to the convex polyhedron. They are computed using the Voronoi decomposition of the polyhedron.

The Voronoi decomposition of first order for a convex polyhedron is determined by its vertices e^i. Each vertex of the convex polyhedron has its own Voronoi region. The Voronoi region of a vertex e^i is the set of all points *p*, which have a smaller or equal distance to the vertex e^i as their distance to the remaining vertices e^j:

$$VR(e^i) := \left\{ p \in \mathbb{R}^n : d(p, e^i) \leq d(p, e^j) \, \forall j \neq i \right\}.$$

The Voronoi region of second order of a convex polyhedron is determined concerning its vertices e^i and a point *x* of the convex polyhedron. A Voronoi region of second order is the set of points *p*, whose distance to the point *x* is smaller or equal to the distance to a vertex e^i. If its distance to this vertex is smaller or equal their distance to the remaining vertices e^j is:

$$VR(x, e^i) := \left\{ p \in \mathbb{R}^n : d(p, x) \leq d(p, e^i) \leq d(p, e^j) \, \forall j \neq i \right\}.$$

The natural element coordinates of the point *x* concerning the vertex e^i are determined over the Voronoi regions of second order (see Figure 1). Each Voronoi region of first or second order assigns itself a Lebesgue measure $\mu\left(VR\left(e^i\right)\right)$. This measure is dimensional independent and corresponds to the length in 1d, to common surface area in 2d and volume in 3d Euclidean space. The ratio of the Lebesgue measure $\mu\left(VR\left(x,e^i\right)\right)$ from the Voronoi region of second order of the point *x* and a vertex e^i to the Lebesgue measure $\mu\left(VR\left(x\right)\right)$ of the Voronoi regions of first order of the point *x* is called the unique natural element coordinates. If the considered point *x* lies outside of the convex polyhedron, then no representation in natural element coordinates will exist.

$$\lambda_i(x)=\frac{\mu\left(VR\left(x,e^i\right)\right)}{\mu\left(VR\left(x\right)\right)}=\frac{\mu\left(VR\left(x,e^i\right)\right)}{\sum\mu\left(VR\left(x,e^i\right)\right)}$$

The natural element coordinates are not negative ($0\le\lambda_i\le1$) and take a value of one at the assigned point of reference and zero at all other points of reference:

$$\lambda_i\left(e^j\right)=\begin{cases}1 & i=j\\ 0 & i\neq j\end{cases}.$$

The natural coordinates satisfy the partition of unity:

$$\sum_{i=1}^{n}\lambda_i=1$$

and they are completely linear

$$\sum_{i=1}^{n}\lambda_i e^i=x\,.$$

As a result of this natural element coordinates construction for convex polyhedron, it is not necessary, that all local element coordinates of a point x depend on all vertices of the polyhedron. If the second order Voronoi region $VR\left(x,e^i\right)$ of the point x and the vertex e^i is empty the coordinate λ_i for this point regarding that vertex will have a zero value.

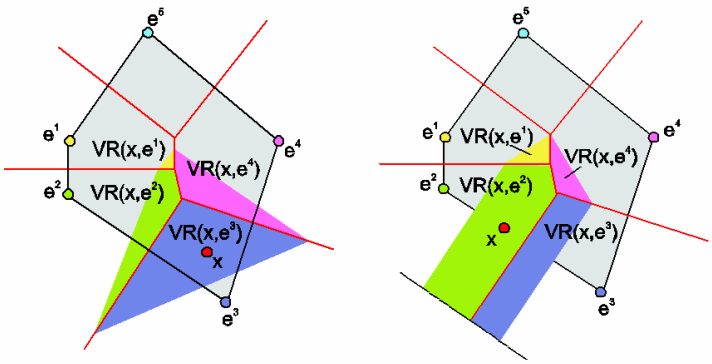

Figure 1: Voronoi decomposition

If the point *x* lies on a facet of the polyhedron the resulting Voronoi regions of second order will have infinite measures. It can be shown by limit value calculation (Milbradt 2001), that the calculation of the natural element coordinates depends only on vertices of the facet. Thus the calculation is limited to the convex polyhedron of the facet.

INTERPOLATION FUNCTIONS

The introduced natural element coordinates can directly be used as interpolation functions (Milbradt 2004).

$$\Phi_i\left(\vec{\lambda}(x)\right) := \lambda_i$$

It stands for an interpolation function, which has the value of one at vertex *i* of the polyhedron and is linear on the edges. It is also possible to define interpolation functions of higher order in lambda. Usually hierarchical interpolation functions are used for the p-version of the finite element method. The definition of hierarchical interpolation functions on polyhedrons is equivalent to classical hierarchical interpolation function. But it has the advantage that of geometry independence.

Edge quadratic hierarchical interpolation function:

$$\Phi_{1,2}(x) = \Phi_{1,2}\left(\vec{\lambda}(x)\right) := \lambda_1(x) \cdot \lambda_2(x)$$

Hereby, $\Phi_{1,2}$ is the interpolation function on the edge between vertex 1 and 2. Once found the advantage is that these functions can be used on any polyhedron in any position and space. This is because the natural element coordinates are defined there and have the proper attributes.

Hierarchical interpolation functions are used for p-adaptive methods. The local increasing of the polynomial degree leads to further columns and rows in the system matrix. Already calculated integrals can still be used.

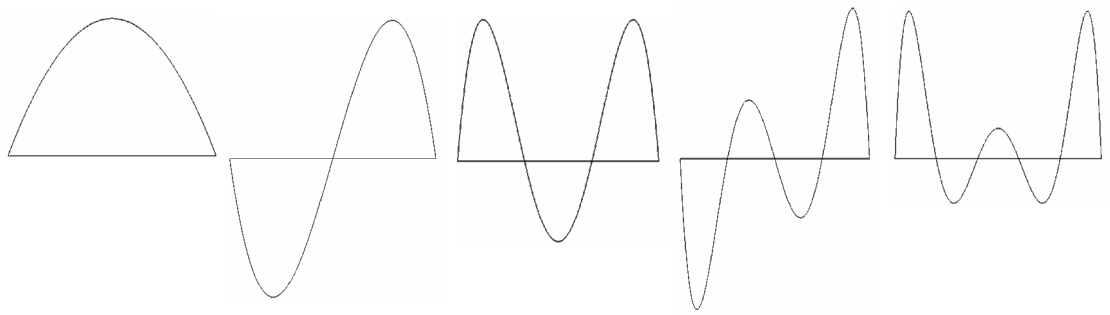

Figure 2: Normalized hierarchical interpolation functions in 1d

Edge oriented hierarchical interpolation functions on arbitrary polyhedrons can be build with the following rule:

$$\phi\left(\vec{\lambda}\right) := \prod_{k=1}^{n}\left(\lambda_i - \frac{k-1}{n-1}\left(\lambda_i + \lambda_j\right)\right)$$

Hereby is n the degree of the interpolation function, in relation to the natural element coordinates. These formulas can directly be used for 2d elements and results in the following functions.

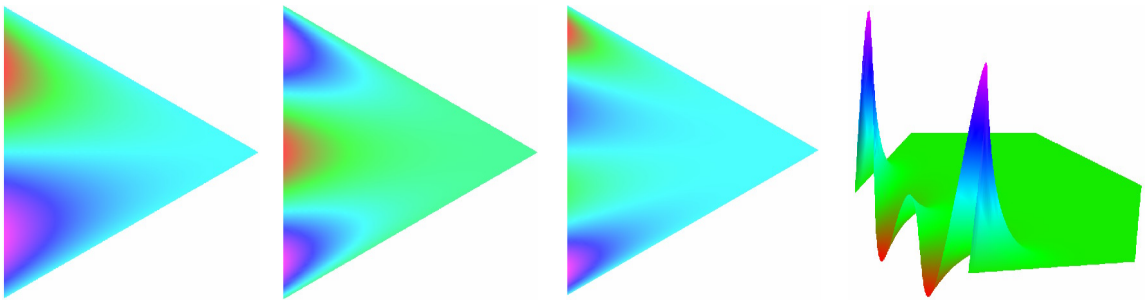

Figure 3: Hierarchical interpolation functions 2d

Figure 3 shows normalized interpolation functions of degree 3, 4 and 5 on a triangle and of degree 6 on a hexahedron.

INTEGRATION WITH RIEMANN SUM

For the solution of partial differential equations with Galerkin approximation it is necessary to integrate the interpolation functions over the polyhedrons. Usually, there is no analytical solution to these interpolation functions. Hence, a numerical method is used. Experience shows that Gaussian quadrature formulas deliver good solutions. Usually, they use special chosen sampling points and weights for these points (Bronstein 2001). However, such points do not exist for arbitrary polyhedrons. In order to find such points, it is initially necessary to calculate the integrals with another method once.

If a function is bounded, a Riemann integral can be build:

$$\int_a^b f(x)dx = \lim_{\substack{\Delta x_i \to 0 \\ n \to \infty}} \sum_{i=1}^{n} \left[f(\xi_i) \cdot \Delta x_i \right]$$

Here, the integral is decomposed in *n* arbitrary parts Δx_i. The sum of all volumes of these parts multiplied with a function value within the parts, approximate the integral.

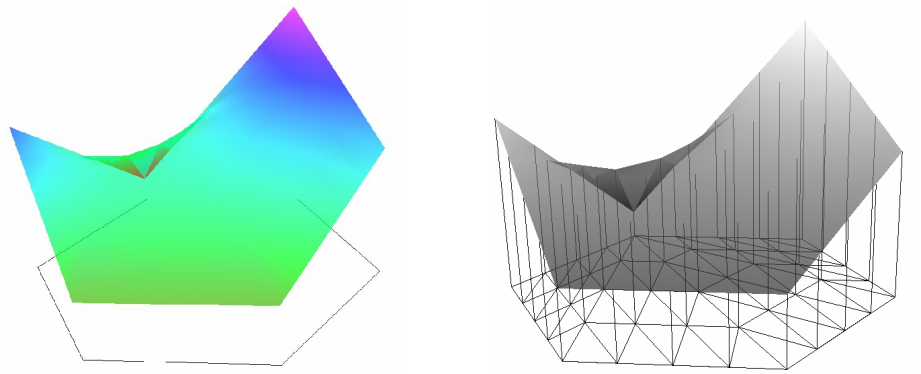

Figure 4: Simplex decomposition of a polyhedron

Figure 4 shows an edge linear interpolation over a hexahedron. This function is the sum of six interpolation functions of degree 1 with different weights. The weights correspond to the values on the vertices, because they have the corresponding interpolation functions values equal to one. The right figure shows a decomposition of the hexahedron in triangles for the purpose of integration. The integral of the function is equivalent to the volume under the surface and can be approximated by the 64 prisms underneath.

BARYCENTRIC DECOMPOSITION

The design of the Riemann integral is based on the decomposition of the integration area in well known sub domains, such as triangles und quads. Due to this, a minimal barycentric simplecial decomposition will be introduced. A minimal barycentric simplecial decomposition is the barycentric decomposition of highest order that consists only of simplexes.

The barycentric decomposition of order *n* can be constructed by the following recursive algorithm.

I. Determine the order *m* of the polyhedron.

II. If *m*>*n*, then

  a) calculate the barycenter of polyhedron

  b) barycentric decomposition of order *n* of all facets of the polyhedron I.)

  c) build polyhedrons out of the polyhedrons of b) and the barycenter of a)

  ⇒ new polyhedron of order *m*

III. Else:

  Stop

Algortihm 1: Minimal barycentic simplicial decomposition algorithm

It is essential for all convex polyhedrons that the barycenter lies inside. A facet is the border of the element. In 3d case are this surfaces, in 2d the border lines and in 1d the points.

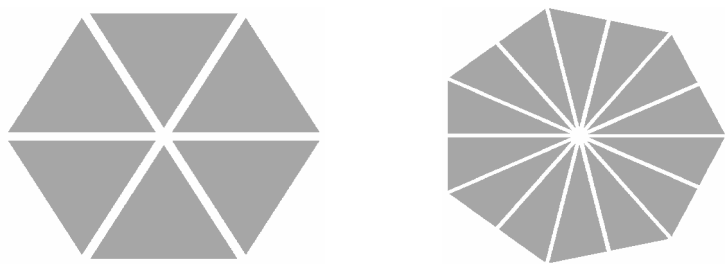

Figure 5: Barycentric decomposition in 2d

Figure 5 shows the barycentric decomposition of order 1 and 0. The smallest angle becomes smaller with decreasing order. For this reason, the left version is more suitable for the approximation of the integration.

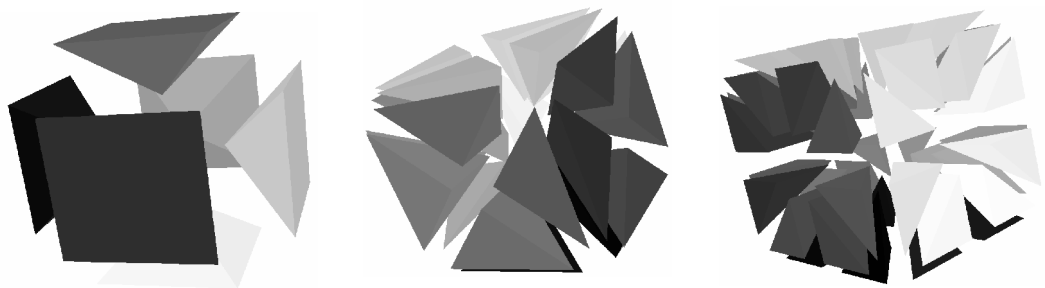

Figure 6: Barycentric decomposition in 3d

Figure 6 shows that not every barycentric decomposition leads to a simplecial complex. The minimal barycentric simplecial decomposition of the cube shown in the middle has the order 1.

Now, an explicit method is obtained, that uniquely decomposes every convex polyhedron into a small number of simplexes. For the Riemann sum it may be better to refine these simplexes into smaller simplexes, which are similar to the original simplexes. In the 2d case such decomposition is possible.

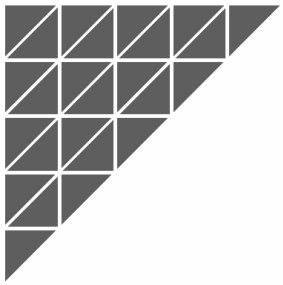

Figure 7: Regular triangle refinement

Such a refinement does not exist in 3d. However, for higher dimensions is the method of longest side refinement (Rivara 1996) suitable. The longest side of the simplex will be divided in this method. From a technical view, it looks as if the longest edge is split into two edges, each connected to all other points. In this process two simplexes are build from the one, which have the same order as the original with a smaller angle. It can be shown that the angle in this construction does not become too bad and stays within a certain interval.

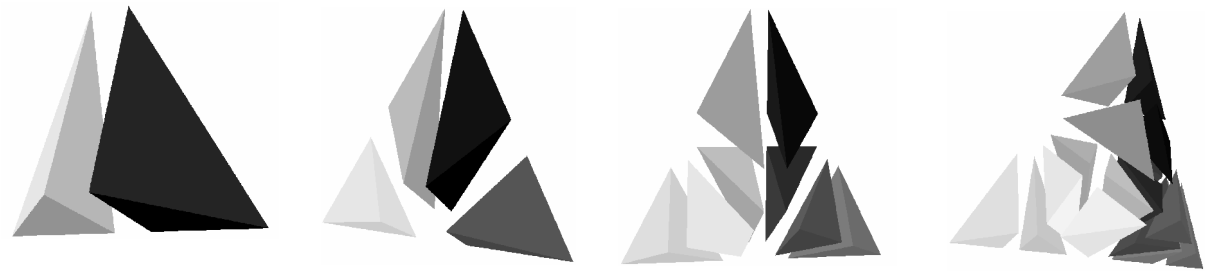

Figure 8: Longest Side Refinement

Figure 8 shows the refinements of order 1, 2, 3 and 4. Each convex polyhedron can be refined by a combination of minimal barycentric simplex decompositions and as many longest side refinement as wanted. Theoretically, an arbitrarily accurate approximation of the integral is possible with this procedure.

QUADRATURE POINTS

The Gaussian point integration is an efficient method for the calculation of integrals and is well known for triangles and quadrangles. The integration is achieved by a multiplication of function values on a few well selected points and their related weights. The selection of these

Gaussian points and weights ensures an exact integration for the designed functions. In this chapter the quadrature is enhanced by a special class of polyhedrons. Usually, quadrature is based on functions of a linear space with basis functions f_i. Because of properties of sum and integral it is sufficient for the integration of any function of that space that the basis functions f_i are calculated exactly. To achieve this, m points p_i and weights w_i are selected, so that the following identities are true:

$$\int f_1 \partial\Omega = \left(\sum_{i=1}^{n} f_1(p_i) \cdot w_i \right) \cdot \Delta$$

$$\int f_2 \partial\Omega = \left(\sum_{i=1}^{n} f_2(p_i) \cdot w_i \right) \cdot \Delta$$

$$\vdots$$

$$\int f_m \partial\Omega = \left(\sum_{i=1}^{n} f_m(p_i) \cdot w_i \right) \cdot \Delta .$$

Herein, Δ is the volume of the polyhedron. The normalization with the volume Δ leads to a nonlinear system of equations of the form $b = A(x)$ with m rows and the unknowns p_i and w_i. Since the basis functions are the known interpolation functions and a Riemann integrations is possible, the left side is known. An approach to find the solution of the nonlinear system of equations will be shown in the following.

NEWTON METHOD

To find a solution for the nonlinear system of equations the Newton method is used. It is an iteration method that converges with a suitable starting condition. The considered system of equation can be written in the following way.

$$T(x) = 0$$

whereas:

$$T(x) = A(x) - b$$

The iteration method is:

$$x_{n+1} = x_n - \left[T'(x_n) \right]^{-1} \cdot T(x_n) .$$

Herein, $T'(x)$ is a componentwise derivative of $T(x)$ with respect to the unknowns, such that the following $m \times (n \cdot 3)$ matrix arises.

$$T'(x)=\begin{bmatrix} \frac{\partial f_1(p_1)}{\partial p_1.x}w_1 & \frac{\partial f_1(p_1)}{\partial p_1.y}w_1 & f_1(p_1) & \cdots & \frac{\partial f_1(p_n)}{\partial p_n.y}w_1 & f_1(p_n) \\ \frac{\partial f_2(p_1)}{\partial p_1.x}w_1 & \frac{\partial f_2(p_1)}{\partial p_1.y}w_1 & f_2(p_1) & \cdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial f_m(p_1)}{\partial p_1.x}w_1 & \frac{\partial f_m(p_1)}{\partial p_1.y}w_1 & f_m(p_1) & \cdots & \frac{\partial f_m(p_n)}{\partial p_n.y}w_1 & f_m(p_n) \end{bmatrix}$$

The derivation of the natural element coordinates with respect to the cartesian coordinates (Milbradt 2005) is computationally expensive.

In order to avoid the determination of the inverse matrix, the linear system of equations $T'(x_n)\cdot\bar{x}=T(x_n)$ is solved instead. It has exactly one solution, if $m=(n\cdot 3)$ and the matrix is not singular. It has more solutions, if $m>(n\cdot 3)$ or rows are linear dependent.

TRIANGLE

The scenario, shown below, is the easiest 2d possibility and is used to illustrate the method. The task is to find one quadrature point. The polyhedron used is a triangle with linear interpolation functions, hence $n=1$ and $m=3$. Three vertices deliver three linear interpolation functions. The resulting system of equation has exactly one solution. The used triangle Ω has the vertices $vertex_1=(0,0)$, $vertex_2=(1,0)$, $vertex_3=(0,1)$ and the volume

of $\Delta=0.5$.

Figure 9: Interpolation functions f_1, f_2 and f_3

In contrast to all other polyhedrons simplexes are advantageous, since the derivation of the interpolation functions of order 1 are constant in one direction all over the simplex. This simplifies the Newton method. The starting point of the iteration is the point $p_1=(0.2,0.2)$ with the weight $w=1$. The solution of this problem is well known in literature with the point $p=(\frac{1}{3},\frac{1}{3})$ and weight $w=1$.

The following calculation steps lead to this solution:

$$T(x) = A(x) - b = \begin{bmatrix} f_1(p_1)\cdot w_1 - \int f_1 \partial\Omega : \Delta \\ f_2(p_1)\cdot w_1 - \int f_2 \partial\Omega : \Delta \\ f_3(p_1)\cdot w_1 - \int f_3 \partial\Omega : \Delta \end{bmatrix} = \begin{bmatrix} 0.6 - 1/6 : 1/2 \\ 0.2 - 1/6 : 1/2 \\ 0.2 - 1/6 : 1/2 \end{bmatrix} = \begin{bmatrix} 0.2666 \\ -0.1333 \\ -0.1333 \end{bmatrix}.$$

Two edges of the triangle are parallel to the cartesian coordinate axes. This and the fact that these edges have the length of one lead to derivations of -1/1 and the following derivation matrix:

$$T'(x) = \begin{bmatrix} -1 & -1 & 0.6 \\ 1 & 0 & 0.2 \\ 0 & 1 & 0.2 \end{bmatrix} \quad \Rightarrow \bar{x} = \begin{bmatrix} -0.133 \\ -0.133 \\ 0 \end{bmatrix} \qquad x_1 = x_0 - \bar{x} = \begin{bmatrix} 0.2 \\ 0.2 \\ 1 \end{bmatrix} - \begin{bmatrix} -0.133 \\ -0.133 \\ 0 \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1 \end{bmatrix}.$$

The Newton method converged for this trivial test case in one step.

STRICT REGULAR POLYHEDRON

The objective is to find quadrature points for arbitrary polyhedrons. A first step is done, when points are found for strict regular polyhedrons. These are polyhedrons where each edge has the same length and each facet consists of the same number of points. One of the questions is how many quadrature points are necessary to integrate the used functions exactly.

The edge oriented hierarchical interpolation functions of order 3 may not be completely cubical; however they are suitable for the p-version. With regard to Newton method they are advantageous, because the resulting system of equation has always exactly one solution.

Example hexahedron:

6 vertices	$\Rightarrow$	6 interpolation functions of order 1
6 edges	$\Rightarrow$	6 hierarchical functions of order 2
		6 hierarchical functions of order 3

$\Rightarrow$ 18 equations

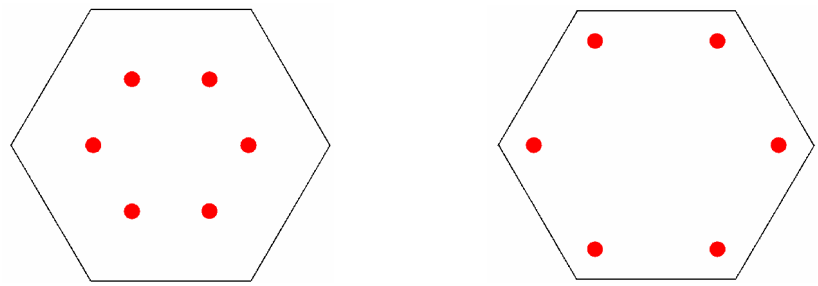

Figure 10: Quadrature points on hexahedron

Hence, six points are necessary to compute one solution. When the number of points is determined, it is most important to choose a good starting position for them, because only suitable starting positions will deliver a solution. Naturally, the rotation symmetry of the polyhedron is used. It has been shown that a position on the virtual line between the vertices and the barycenter is a suitable starting point and all points have the same weight of $w = 1/6$. Interestingly, the result showed that two sets of points are possible for the quadrature points.

The potential of the points on the virtual line can be calculated and are shown in the following picture for a triangle, quadrangle, hexahedron and a decahedron. Of special interest are the points of minimum.

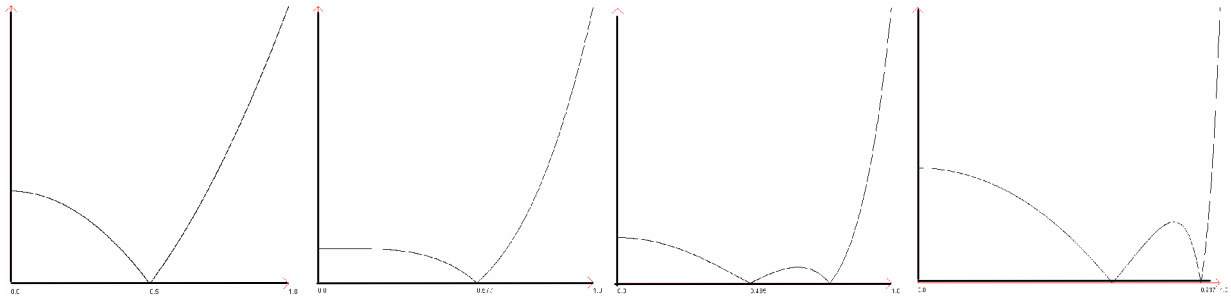

Figure 11: Potential of quadrature points

Two sets of points start with the five angle element and seem to be found afterwards in all elements. The quadrature points can be found in 3d as well. In that case, the derivate with respect to the z- coordinate has to be added with the Newton method.

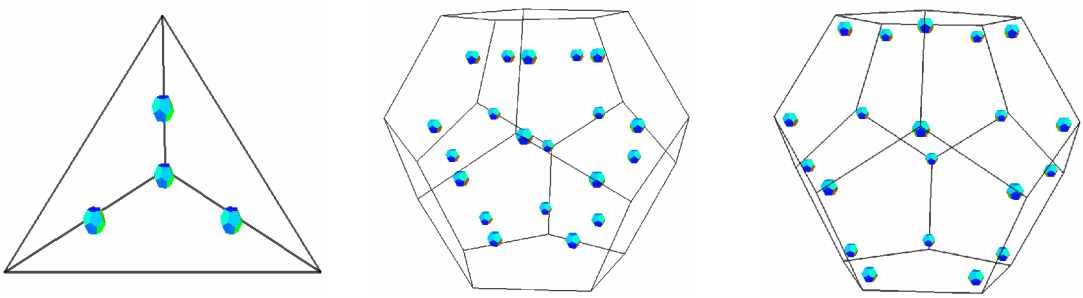

Figure 12: Quadrature points in 3d

Figure 12 shows quadrature points for a tetrahedron and a dodecahedron, where two sets of points are possible as well.

CONCLUSION AND OUTLOOK

Hierarchical edge oriented interpolation functions were introduced, which are suitable for the approximation of partial differential equations within the finite element method. The differentiation and integration of such interpolation functions is essential for the application of the FEM approximation. A numerical integration, the Riemann integral, was introduced on the base of a simplex decomposition. For this reason, a minimal barycentric simplecial decomposition was established, which could be arbitrarily refined by longest side refinement.

With this numerical integration, it was possible to find quadrature points on strict regular polyhedrons in 2d and 3d. It is expected that with the analysis of these results and further investigations, it may be possible to find quadrature points for all convex polyhedrons. First applications have shown that the quadrature points lead to a more efficient realisation of finite element approximation on polyhedral decompositions.

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