PROPERTIES OF NATURAL ELEMENT COORDINATES ON ANY POLYHEDRON

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ABSTRACT

Traditional finite elements are based on simple geometrical elements such as edges in the one-dimensional space, triangles and quadrangles in the plane as well as tetra- and hexahedrons in the three-dimensional space. The extension of the geometrical basis to any polyhedron is enabled by the definition of a local coordinate system called the natural element coordinates. The formulation of interpolation and test functions in natural element coordinates enables the formulation of generalized finite elements. The differentiation and integration of these interpolation and test functions are essential for finite element approximations. In the paper convex and special non convex polyhedron are considered as geometrical basis for generalized finite elements as well as for the formulation of interpolation and test functions on natural element coordinates. Furthermore, methods for the numerical differentiation and integration of functions on these generalized finite elements are introduced. The paper closed with two applications in the range of fluid mechanic and structural mechanics.

KEY WORDS

natural element coordinates, convex and non-convex polyhedron, finite element method, numerical integration and differentiation

INTRODUCTION

Physical processes in natural science and engineering are the deformation behavior of solids, the flow behavior of fluids or the temperature behavior of materials. These physical processes are describable by differential equations. The analytical solution of these equations is not or only with extensive complexity computable.

The finite element method is a numerical method for the interpolation of given basic values as well as for the numeric approximation of partial differential equations. The basic idea of the finite element method is to decompose the investigation area in subareas. The subareas are called finite elements. A finite element can be understood as a triple consisting of a geometrical basis, a set of degrees of freedom and a set of interpolation functions. Usually, the geometrical basis of classical finite elements are edges in the one dimensional space, triangles and quadrangles in the plane as well as tetra- and hexahedrons in the three dimensional Euclidian space.

The extension of the geometrical basis to any polyhedron is enabled by the definition of a local coordinate system called natural element coordinates. The natural element coordinates are computable for any convex and special non convex polyhedron. The formulation of generalized finite elements is enabled by the formulation of interpolation and test functions which base only on natural element coordinates. The differentiation and the integration of the natural element coordinates are essential for finite element approximations.

NATURAL ELEMENT COORDINATES

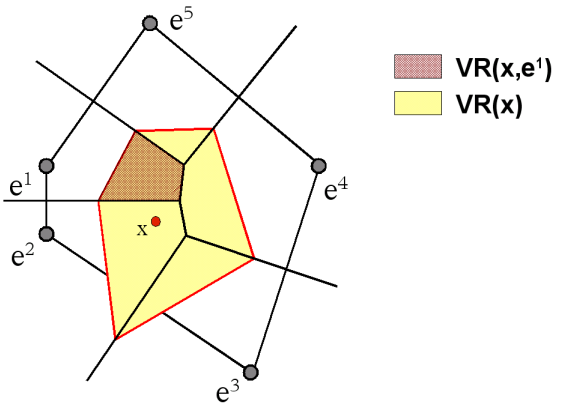
For a generalized consideration of any polyhedron as basis for finite elements a uniform description of all points of the finite element is necessary. This is achieved with the definition of the natural element coordinates [Milbradt 2001].

CONVEX POLYHEDRON

There are several approaches to describe convex polyhedron. The description of the convex polyhedron Z by the Minkowsky product of its vertices E suggests using the factors λ_i of the linear combination as element coordinates.

$$Z := \{ p : p = \lambda_1 e^1 + \lambda_2 e^2 + ... + \lambda_N e^N, \lambda_i \geq 0 \wedge \sum_i \lambda_i = 1 \}$$

If a *m*-dimensional convex polyhedron has *m+1* linear independent vertices, the factors are unique and called barycentric coordinates. If a convex polyhedron consists of more than *m+1* vertices, the factors are not unique. If the natural neighborhood coordinates introduced by Sibson [Sibson 1980] are restricted to the convex polyhedron, one receives unique natural element coordinates, which are related to the vertices of the convex polyhedron. These natural element coordinates are consistent with the barycentric coordinates on simplexes. The determination of the natural element coordinates of a point x concerning the convex polyhedron Z is based on the computation of the Voronoi diagram of second order concerning the vertices and the point x.



The computation of natural element coordinates is formulated as follows:

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

Figure 1: Voronoi diagram of second order

The contour lines of natural element coordinates are shown in figure 2 for the regarded points e^1 , e^3 and e^4 .

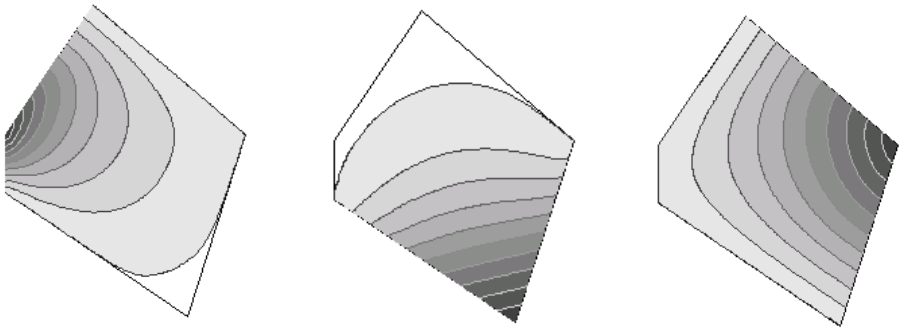


Figure 2: Natural element coordianates on a convex polhedron

An extension of the geometrical basis can be achieved through special non convex polyhedron.

NON CONVEX POLYHEDRON

The natural element coordinates of a convex polyhedron depends on the Voronoi decomposition of the vertices. The computation of natural element coordinates of a non convex polyhedron compared to a convex polyhedron is not transferable directly. An adjustment of the construction of the Voronoi decomposition is necessary.

The Voronoi decomposition of the first order concerning the vertices is shown in figure 3. The vertices e^9 , e^{10} and e^{11} form a region which is a part of the convex hull but not a part of the non convex polyhedron. These vertices are represented by the Voronoi vertex v^{11} . A description for the Voronoi vertices v^5 , v^6 and v^{12} can occur analogous.

The middle picture of figure 3 shows the Voronoi decomposition concerning the point x. The modified Voronoi decomposition without a consideration of the Voronoi vertices v^{11} and v^{12} are shown in the right picture.

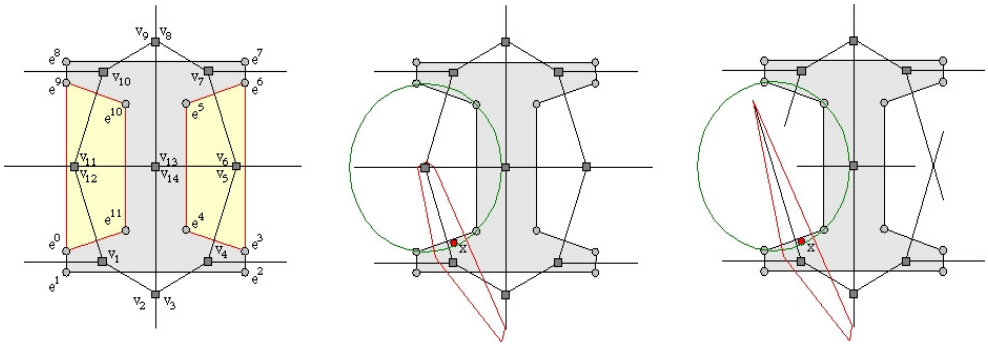


Figure 3: Voronoi decomposition of a non convex polyhedron

A computation of natural element coordinates with consideration of Voronoi vertex v^{11} leads to an influence of the needless vertices e^9 and e^{10} . Therefore, the corresponding Voronoi vertices have to be removed.

The left picture of figure 4 shows the contour lines of the wrong natural element coordinates which are computed with consideration of the Voronoi vertex v^{11} and v^{12} . The right picture shows the correct contour lines.

Figure 4: Contour lines of the natural element coordinates

A description of special non convex polyhedron can be achieved via regularized set operators. The regularized set operators are used on the convex hull of the non convex polyhedron and specific convex subareas. The convex subareas describe all points which are not part of the non convex polyhedron.

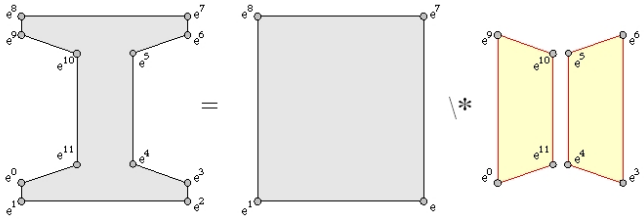
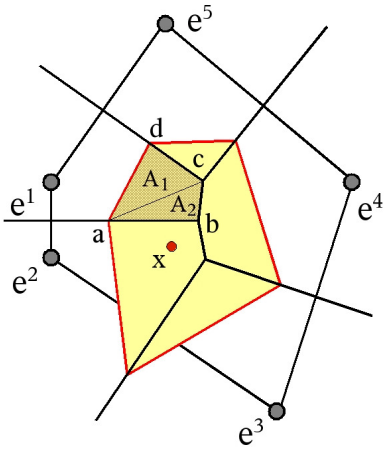


Figure 5: Convex hull and convex subareas

By adjusting the construction of the Voronoi decomposition the computation of the natural element coordinates of convex polyhedron is transferable to special non convex polyhedron. The local coordinate systems have the same characteristics. The introduced geometrical basis is used for a generalization of the finite elements.

DIFFERENTIATION OF NATURAL ELEMENT COORDINATES

The differentiation of natural element coordinates proceeds in an algorithmic-analytic manner. Retrospective, the computation of natural element coordinates depends on the Voronoi decompostions of first and second order. Using the quotient rule the differentiation of natural element coordinates can be formulated as:



$$\frac{\partial \lambda_k(x,e^k)}{\partial x_i} = \frac{\mu(VR(x))\frac{\partial \mu(VR(x,e^k))}{\partial x_i} - \mu(VR(x,e^k))\frac{\partial \mu(VR(x))}{\partial x_i}}{\mu(VR(x))^2}$$

The Voronoi regions of first and second order dependent on the point x are finite-bounded polygons which can be triangulated. The derivation of the measure of the Voronoi region can be considered as the sum of the derivation of the measure of all their triangles.

$$\frac{\partial \mu(VR)}{\partial x_i} = \sum \frac{\partial A_\Delta}{\partial x_i}$$

A generalized consideration of a triangle with the vertices a , b and c leads to:

$$\begin{aligned}\frac{\partial A_\Delta}{\partial x_i} = \frac{1}{2}(&a_1\frac{\partial b_2}{\partial x_i} + b_2\frac{\partial a_1}{\partial x_i} - a_2\frac{\partial b_1}{\partial x_i} - b_1\frac{\partial a_2}{\partial x_i} + a_2\frac{\partial c_1}{\partial x_i} + c_1\frac{\partial a_2}{\partial x_i} \\ &- a_1\frac{\partial c_2}{\partial x_i} - c_2\frac{\partial a_1}{\partial x_i} + b_1\frac{\partial c_2}{\partial x_i} + c_2\frac{\partial b_1}{\partial x_i} - b_2\frac{\partial c_1}{\partial x_i} - c_1\frac{\partial b_2}{\partial x_i})\end{aligned}$$

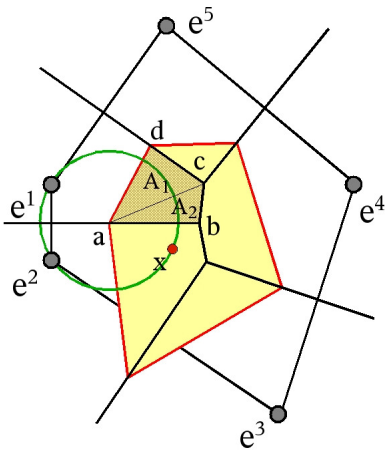
The vertices a , b and c of the triangle are either vertices of the Voronoi decomposition of first order or vertices of the Voronoi decomposition of second order.

In the figure above the Voronoi region $VR(x,e^1)$ is triangulated in the triangles A_1 and A_2 . The triangle A_2 is based on the vertices a , b and c . The vertex a is arose by the Voronoi decomposition of second order and depends on the point x . Instead of the vertices b and c are arose by the Voronoi decomposition of first order and independent of the point x . Therefore, the derivation of these vertices gets the value zero. The differentiation of the measure of triangle A_2 is shown below.

$$\frac{\partial A_2}{\partial x_i} = \frac{1}{2}\left(b_2\frac{\partial a_1}{\partial x_i} - b_1\frac{\partial a_2}{\partial x_i} + c_1\frac{\partial a_2}{\partial x_i} - c_2\frac{\partial a_1}{\partial x_i}\right)$$

The derivation of the Voronoi vertices of second order can be computed via the corresponding center of the Voronoi circle.

In the figure below the Voronoi vertex a is the center of the Voronoi circle pass through the vertices e^1 , e^2 and point x . The corresponding circle equations are:



$$\left(e_1^1-a_1\right)^2+\left(e_2^1-a_2\right)^2=r^2$$

$$\left(e_1^2-a_1\right)^2+\left(e_2^2-a_2\right)^2=r^2$$

$$\left(x_1-a_1\right)^2+\left(x_2-a_2\right)^2=r^2$$

and leads to

$$\underbrace{\begin{bmatrix} e_1^1-x_1 & e_2^1-x_2 \\ e_1^2-x_1 & e_2^2-x_2 \end{bmatrix}}_{\underline{\underline{E}}} \underbrace{\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}}_{\underline{a}} = \underbrace{\begin{bmatrix} 0.5\left((e_1^1)^2+(e_2^1)^2-(x_1)^2-(x_2)^2\right) \\ 0.5\left((e_1^2)^2+(e_2^2)^2-(x_1)^2-(x_2)^2\right) \end{bmatrix}}_{\underline{y}}$$

The coordinate vector of the center $\underline{a}$ can be formulated as: $\underline{a}=\underline{y}\,\underline{\underline{E}}^{-1}$ with

$$\underline{\underline{E}}^{-1}=\frac{1}{det\,\underline{\underline{E}}}\begin{bmatrix} e_2^2-x_2 & -e_2^1-x_2 \\ -e_1^2+x_1 & e_1^1-x_1 \end{bmatrix}$$

The components of $\underline{a}$ are quotients, therefore the quotient rule is used:

$$\frac{\partial a_i}{\partial x_i}=\frac{\partial u*v-u*\partial v}{v^2}$$

For example, the operands u and v for the coordinate a_1 are shown below:

$$\begin{aligned} u= \;& (e_1^1)^2 e_2^2+(e_2^1)^2 e_2^2-x_1^2 e_2^2-x_2^2 e_2^2-(e_1^1)^2 x_2-(e_2^1)^2 x_2 \\ & -(e_1^2)^2 e_2^1-(e_2^2)^2 e_2^1+x_1^2 e_2^1+x_2^2 e_2^1+(e_1^2)^2 x_2+(e_2^2)^2 x_2 \\ v= \;& 2e_1^1 e_2^2-2e_1^1 x_2-2e_2^1 e_1^2+2e_2^1 x_1-2e_2^2 x_1+2e_1^2 x_2 \end{aligned}$$

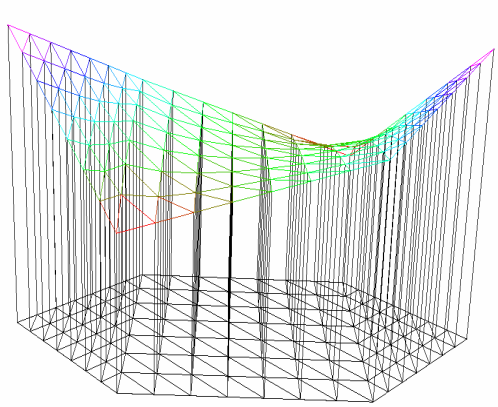
The derivation of the operands u and v with respect to x_1 is mentioned below:

$$\begin{aligned} \partial u &= -2x_1 e_2^2+2x_1 e_2^1 \\ \partial v &= -2e_2^2+2e_2^1 \end{aligned}$$

NUMERICAL INTEGRATION

The approximation of partial differential equations with the finite element method leads to integral equations whose integrals generally are not analytic computable. The main problem is the computation of the integral over the geometrical basis Ω_E of the finite elements.

$$\int_{\Omega_E} f(\lambda) d\Omega_E$$



Special methods for a numerical integration [Fröbel 2004] also known as quadrature are essential for the use of the finite element method. The complexity of the computation depends of the chosen method. The definition of the Riemann integral shows a possible numerical approximation. With a gradually refinement of the sub-regions the accuracy level of the approximation can be increased.

The numerical integration of the polyhedron E can be formulated as a sum of an integration of all sub-regions E_i . The numerical integration of the sub-regions can be achieved via quadrature formulas.

$$\int_{\Omega_E} f(\lambda) d\Omega_E = \sum_{E_i} \int_{\Omega_{E_i}} f(\lambda) d\Omega_{E_i} = \sum_{E_i} \sum_{j=0}^{N} w_j^{(N)} f(\lambda_j^{(N)})$$

The values of the coefficients $w_j^{(N)}$ and $\lambda_j^{(N)}$ depends on the selected quadrature formula. One kind of a quadrature formula is the Gaussian quadrature formula.

NUMERICAL INTEGRATION VIA GAUSSIAN QUADRATURE FORMULA

The computation of the coefficients $w_j^{(N)}$ and $\lambda_j^{(N)}$ on the interval [-1, 1] can be achieved with Legendre polynomials. In the literature well known Gaussian points are given for edges in the 1-dimensional space, for triangles and quadrangles in the 2-dimensional space as well as for tetra- or hexahedrons in the 3-dimensional space.

A transformation of the well known Gaussian points on the sub-regions of the polyhedron is necessary. The transformation is accomplished via the Jacobian matrix. The Jacobian matrix allows establishing a relationship between both local coordinate systems.

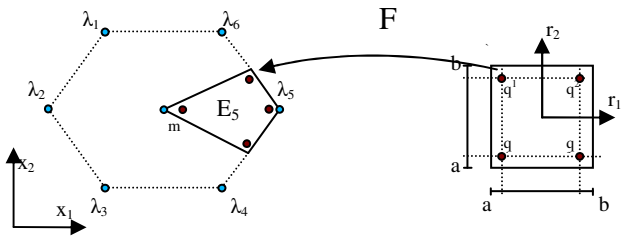


Figure 6: Transformation of the unit polyhedron to the convex polyhedron

FINITE ELEMENT APPROXIMATION

The finite element approximation is a numerical method to approximate a solution of the unknown function $u(x)$ which satisfy the equation

$$F(u)=0 \ .$$

Now, we consider the equation above to be a boundary value problem. Generally, the equation is a system of partial differential equations with associated boundary conditions. The idea of this method is to find the unknown solution $u(x)$ not in the infinite-dimensional space but to find an optimal approximation $u_h(x)$ of the solution in a finite-dimensional sub-space. The finite-dimensional sub-space is spanned by a finite set of interpolation functions ϕ_i formulated in natural element coordinates and called basic functions. The approximation of the unknown solution has the form:

$$u(x) \approx u_h(x) = \sum_{i=1}^{n} \phi_i \cdot u^i$$

If we insert the approximation $u_h(x)$ of the solution $u(x)$ into the equation which we like to solve, this equation is not fulfilled accurately in all cases. The occurring difference is called defect or residual:

$$\epsilon = F(\hat{u})$$

In order to receive an optimal approximation the defect must be minimized. The standard Galerkin method assumes that the defect may not lie in the finite-dimensional sub-space of the approximation. The defect should be orthogonal to all basic functions ϕ_i of the interpolation space:

$$\int_{\Omega} \phi_i \epsilon = 0$$

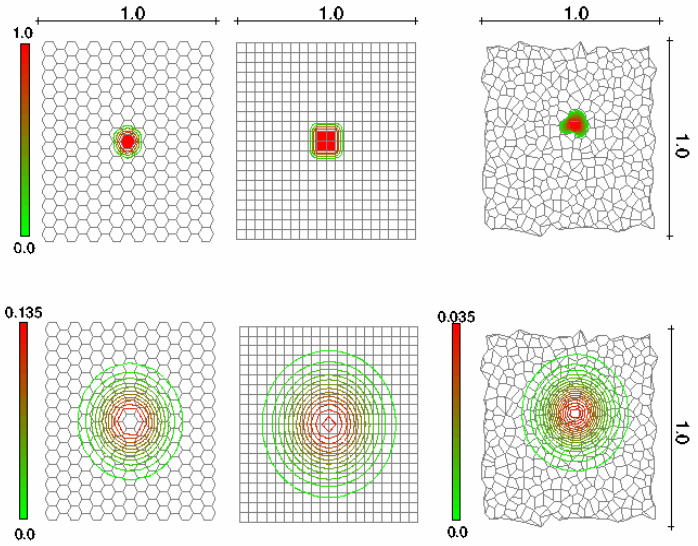
APPLICATIONS

The first application from the range of a flow behavior computes the propagation of a material concentration. The corresponding two-dimensional diffusion equation can be formulated as follows:

$$\frac{\partial c(x,y,t)}{\partial t} - k \nabla^2 c(x,y) = 0$$

The standard Galerkin method and the implicit Euler method lead to the system of equations below. M is the mass matrix and D the corresponding diffusion matrix.

$$(\boldsymbol{M} - \boldsymbol{D})\, \hat{u}^{t+dt} = \boldsymbol{M}\, \hat{u}^{t}$$



As initial condition a material concentration in the middle of the investigation area is injected. Figure 7 shows the used decompositions and the corresponding initial conditions. The used decompositions based on quadrangles and hexagons as well as on Voronoi cells.

The finite element approximation on the three decompositions generates the expected distribution.

Figure 7: Initial conditions and concentration after 10 minutes

The second application is a standard benchmark problem [Stein 2003]. A stretched plate with a circular central hole under plane strain condition is considered. An elastic material behavior is assumed. Due to the symmetric geometry of the system only the consideration of a quarter plate is necessary.

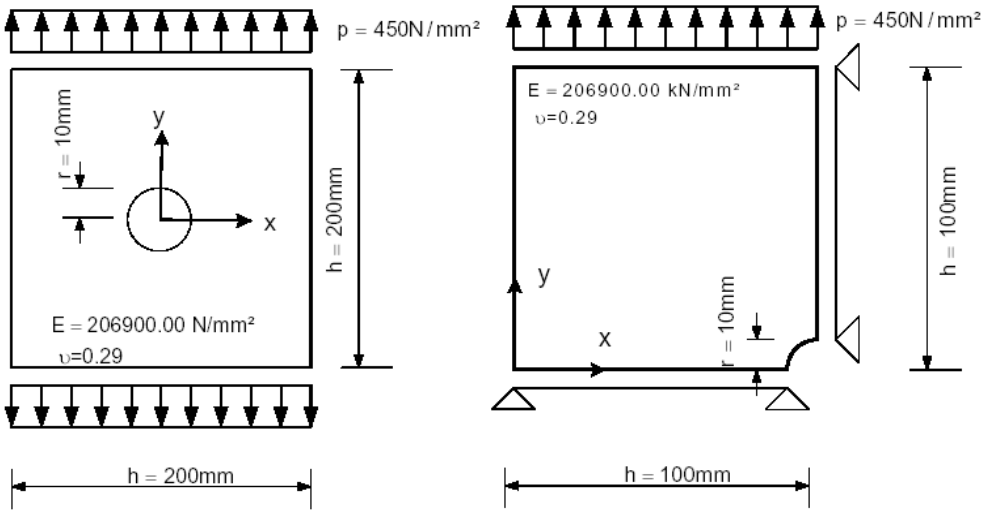


Figure 8: Structural system of the perforated pane

The weak form of the corresponding differential equation can be formulated as:

$$\int_{\Omega} [\boldsymbol{Lv}]^T \boldsymbol{C} [\boldsymbol{Lu}] \, d\Omega = \int_{\Omega} \boldsymbol{v}^T \boldsymbol{f} \, d\Omega + \int_{\Gamma_N} \boldsymbol{v}^T \bar{\boldsymbol{t}} \, d\Gamma$$

The computation was carried out with edge-quadratic test function of second order. The underlying decompositions are quadrangles with 1273 degrees of freedom and hexagons with 627 degrees of freedom. The results of the stress are shown in figure 9 below.

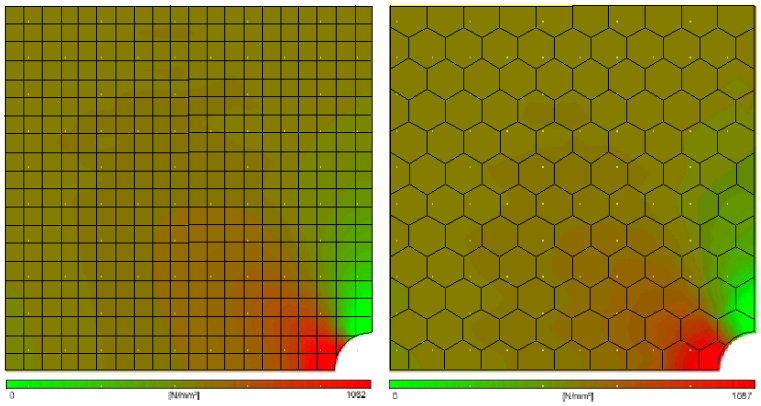


Figure 9: Plots of the computed stress

In spite of the small number of degrees of freedom the decomposition based on hexagons leads to a better approximation of the maximum displacement as well as a better displacement on the perforation.

CONCLUSIONS

Generalized finite elements on the basis of convex and non-convex polyhedron are presented. The new flexibility achieved by generalized finite elements leads to simplified mesh generation and adaptive decomposition. Methods for optimization of decompositions are the consequence of a transfer of well known criteria from triangles and quadrangles to polyhedron.

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