# **Simplex Integration**

Trials and Errors for transcendental Integrals

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I Theory

1 Problem

## Teil I.

# **Theory**

#### 1. Problem

Total Energy in the System:

$$\Pi = \int_{\Omega} g(\phi)\psi(\mathfrak{u}) d\Omega + \frac{G_c}{2l} \int_{\Omega} \phi^2 + l^2 \nabla \phi \cdot \nabla \phi d\Omega \to \min$$
 [1.1]

**Degradation Function** 

$$g(\phi) = \left(1 - \phi^2\right) + k \tag{1.2}$$

mit

k ... being a small but finite scalar such as  $10 \cdot 10^{-6}$ 

G<sub>c</sub> ... critical energy release rate, material parameter

l ... width of phase field

 $\psi(u)$ ...strain energy density function

u ... displacement function

φ ... phase field parameter, ansatz function discussed below

 $\nabla \varphi$  ...gradient of phase field parameter

$$\delta_{\mathbf{u}}\Pi = \int_{\Omega} g(\phi)\sigma(\mathbf{u})\frac{\partial \varepsilon}{\partial \mathbf{u}} \,\delta\mathbf{u} = 0 \tag{1.3}$$

$$\delta_{\phi}\Pi = \int_{\Omega} 2(\phi - 1) \,\delta\phi\psi(\mathbf{u}) \,d\Omega + \frac{G_c}{l} \int_{\Omega} \phi \,\delta\phi + l^2 \nabla\phi \cdot \nabla \,\delta\phi \,d\Omega = 0 \qquad [1.4]$$

#### 1.1. Ansatz functions

$$\mathbf{u} = \sum_{i} N_{i} \mathbf{u}_{i} + \sum_{i} N_{i} \mathbf{F} \mathbf{a}_{i}$$
 [1.5]

mit

N<sub>i</sub> ... are quadratic lagrange (standard) shape functions for tetrahedrons

 $U_i = u_i, a_i \dots$  are nodal degrees of freedom for displacement function

F ... is an enrichment function (sigmoid like, depends on  $\phi$ , later)

$$f_{\text{base}} = \sum_{i} N_{i} \phi_{i}$$
 [1.6]

$$\varsigma = \frac{f_{\text{base}}}{\sqrt[4]{f_{\text{base}}^2 + k_{\text{res}}}}$$
[1.7]

mit

I Theory

1 Problem

 $k_{reg}$  . . . small but finite parameter

$$\phi = \exp(-\varsigma) \tag{1.8}$$

$$\Phi = \exp(-\frac{\zeta}{l}) \tag{1.9}$$

we need to be able to integrate the residual vectors and the stiffness matrices efficiently and accurately

$$\delta_{\mathbf{U}_{i}}\Pi = \int_{\Omega} g(\phi)\sigma(\mathbf{u})\frac{\partial \varepsilon}{\partial \mathbf{u}} \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{U}} d\Omega \cdot \delta \mathbf{U}_{i}$$
 [1.10]

$$\delta_{\varphi_i}\Pi = \int_{\Omega} 2(\varphi - 1) \frac{\partial \varphi}{\partial \varphi_i} \psi(u) \, d\Omega \, \delta \varphi_i + \frac{G_c}{l} \int_{\Omega} \varphi \frac{\partial \varphi}{\partial \varphi_i} + l^2 \nabla \varphi \cdot \frac{\partial \nabla \varphi}{\partial \varphi_i} \, d\Omega \, \delta \varphi_i = 0 \ \ [1.11]$$

$$\Delta_{\mathbf{U}_{i}} \, \delta_{\mathbf{U}_{i}} \Pi = \mathbf{U}_{i} \cdot \int_{\Omega} g(\phi) \frac{\partial \varepsilon}{\partial \mathbf{U}_{i}} \cdot \mathbb{C} \cdot \frac{\partial \varepsilon}{\partial \mathbf{U}_{i}} \, d\Omega \cdot \delta \mathbf{U}_{i}$$
 [1.12]

$$\begin{split} \Delta_{\varphi_{i}}\,\delta_{\varphi_{i}}\Pi &= \varphi_{j} \int_{\Omega} 2\left(\frac{\partial\varphi}{\partial\varphi_{i}}\right)^{2}\psi(u)\,d\Omega\,\delta\varphi_{i} + \varphi_{j} \int_{\Omega} 2(\varphi-1)\frac{\partial^{2}\varphi}{\partial\varphi_{i}^{2}}\psi(u)\,d\Omega\,\delta\varphi_{i} \\ &+ \varphi_{j}\frac{G_{c}}{l} \int_{\Omega} \frac{\partial\varphi}{\partial\varphi_{i}} + \frac{\partial^{2}\varphi}{\partial\varphi_{i}^{2}} + l^{2}\frac{\partial\nabla\varphi}{\partial\varphi_{j}} \cdot \frac{\partial\nabla\varphi}{\partial\varphi_{i}} + l^{2}\nabla\varphi \cdot \frac{\partial^{2}\nabla\varphi}{\partial\varphi_{i}^{2}}\,d\Omega\,\delta\varphi_{i} \end{split}$$
 [1.13]

[1.14]

#### 1.2. Numerical Work

$$\frac{\partial \varsigma}{\partial f_{\text{base}}} = \left(1 - \frac{f_{\text{base}}^2}{2(f_{\text{base}}^2 + k_{\text{res}})}\right) \cdot \frac{1}{\sqrt[4]{f_{\text{base}}^2 + k_{\text{res}}}}$$
[1.15]

$$\frac{\partial^2 \zeta}{\partial f_{\text{base}}^2} = \left(\frac{5f_{\text{base}}^3}{\left(f_{\text{base}}^2 + k_{\text{res}}\right)} - 6f_{\text{base}}\right) \cdot \frac{1}{4\sqrt[4]{f_{\text{base}}^2 + k_{\text{res}}}}$$
[1.16]

$$\frac{\partial^{3} \zeta}{\partial f_{\text{base}}^{3}} = \frac{3 \left( -4k_{\text{res}}^{2} + 12k_{\text{res}}f_{\text{base}}^{2} + f_{\text{base}}^{4} \right)}{2 \left( f_{\text{base}}^{2} + k_{\text{res}} \right)^{2}} \cdot \frac{1}{4 \sqrt[4]{f_{\text{base}}^{2} + k_{\text{res}}}}$$
[1.17]

#### 1.3. Setting up the Integrals in Question

The Vectors in Question are:

$$N = [1.18]$$

$$\mathbf{B} = [1.19]$$

$$= -\frac{1}{l} \cdot \phi \cdot \frac{\partial \zeta}{\partial f_{\text{base}}} \cdot N_{i}$$
 [1.21]

$$\frac{\partial^2 \Phi}{\partial \Phi_i^2} = \frac{\partial}{\partial \Phi_i} \left( -\frac{1}{l} \cdot \Phi \cdot \frac{\partial \zeta}{\partial f_{\text{base}}} \cdot N_i \right)$$
 [1.22]

$$= -\frac{1}{l} \frac{\partial}{\partial \phi_{i}} \left( \phi \cdot \frac{\partial \zeta}{\partial f_{\text{base}}} \right) \cdot N_{i}$$
 [1.23]

$$= -\frac{1}{l} \left( \frac{\partial \phi}{\partial \phi_{i}} \cdot \frac{\partial \zeta}{\partial f_{\text{base}}} + \phi \cdot \frac{\partial \zeta}{\partial f_{\text{base}} \partial \phi} \right) \cdot N_{i}$$
 [1.24]

$$= -\frac{1}{l} \left( \frac{\partial \phi}{\partial \phi_{i}} \cdot \frac{\partial \zeta}{\partial f_{\text{base}}} + \phi \cdot \frac{\partial \zeta}{\partial f_{\text{base}} \partial \phi} \right) \cdot N_{i}$$

$$= -\frac{1}{l} \left( \frac{\partial \phi}{\partial \phi_{i}} \cdot \frac{\partial \zeta}{\partial f_{\text{base}}} + \phi \cdot \frac{\partial \zeta}{\partial f_{\text{base}} \partial \phi} \right) \cdot N_{i}$$
[1.24]

$$= -\frac{1}{l} \left( \frac{\partial \phi}{\partial \phi_{i}} \cdot \frac{\partial \zeta}{\partial f_{\text{base}}} + \phi \cdot \frac{\partial^{2} \zeta}{\partial f_{\text{base}}^{2}} \frac{\partial f_{\text{base}}}{\partial \phi} \right) \cdot N_{i}$$
 [1.26]

$$= -\frac{1}{l} \left( -\frac{1}{l} \cdot \phi \cdot \left( \frac{\partial \zeta}{\partial f_{\text{base}}} \right)^{2} \cdot N_{i} + \phi \cdot \frac{\partial^{2} \zeta}{\partial f_{\text{base}}^{2}} N_{i} \right) \cdot N_{i}$$
 [1.27]

$$= \frac{1}{l^2} \phi \left( \left( \frac{\partial \zeta}{\partial f_{base}} \right)^2 - l \cdot \frac{\partial^2 \zeta}{\partial f_{base}^2} \right) \cdot N_i^2$$
 [1.28]

$$\frac{\partial^2 \Phi}{\partial \Phi_i^2} = \frac{1}{l^2} \left( \left( \frac{\partial \zeta}{\partial f_{base}} \right)^2 - \frac{\partial^2 \zeta}{\partial f_{base}^2} \right) N_i \cdot N_j$$
 [1.29]

[1.30]

I Theory

2 Simplex Integration in n = 2

### 2. Simplex Integration in n = 2

First start with definitions:

**Pure Integration Strategy** is any quadrature formula of the simplex:

$$I = \iint_{\Delta} f(\xi_1, \xi_2, \xi_3) d\Delta \approx \sum_{i} w_i f(\xi_{1,i}, \xi_{2,i}, \xi_{3,i})$$
 [2.1]

The Term *pure* is used for telling them apart from subdivision integrators.

**Subdivision Integration Strategy** are Integrators of the form:

$$I = \iint_{\Delta} f(\xi_1, \xi_2, \xi_3) d\Delta = \sum_{i} \iint_{\Delta_i} f(\xi_1, \xi_2, \xi_3) d\Delta_i$$
 [2.2]

which then will be evaluated by pure Integrators.

#### 2.1. Element Description

Shape Functions in barycentric coordinates

$$N_{1}(\xi_{1}, \xi_{2}, \xi_{3}) = \xi_{1} 
N_{2}(\xi_{1}, \xi_{2}, \xi_{3}) = \xi_{2} 
N_{3}(\xi_{1}, \xi_{2}, \xi_{3}) = \xi_{3} 
N_{4}(\xi_{1}, \xi_{2}, \xi_{3}) = 4\xi_{1}\xi_{3} 
N_{5}(\xi_{1}, \xi_{2}, \xi_{3}) = 4\xi_{1}\xi_{2} 
N_{6}(\xi_{1}, \xi_{2}, \xi_{3}) = 4\xi_{2}\xi_{3}$$
[2.3]
$$[2.4] \\
5 \\
[2.5] \\
[2.6] \\
[2.7] \\
3$$

$$[2.7] \\
3$$

$$[2.8]$$

Barycentric Interpolation Formula  $P: \mathbb{B}^3 \to \mathbb{R}^2$ 

$$P(\xi_1, \xi_2, \xi_3) = p_1 \xi_1 + p_2 \xi_2 + p_3 \xi_3$$
 [2.9]

 $\min p_i \in \mathbb{R}^2, \, \xi_i \in [0,1]$ 

 $\xi$ -η-Transformation

$$\xi_1 := 1 - \xi - \eta$$
 [2.10]  
 $\xi_2 := \xi$  [2.11]  
 $\xi_3 := \eta$  [2.12]

mit  $\xi \in [0, 1]$ ,  $\eta \in [0, 1]$ Es gilt:

$$T(\xi, \eta) = \begin{bmatrix} 1 - \xi - \eta \\ \xi \\ \eta \end{bmatrix}$$
 [2.13]

$$T^{-1}(\xi_1, \xi_2, \xi_3) = \xi_1 \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \xi_2 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \xi_3 \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$
 [2.14]

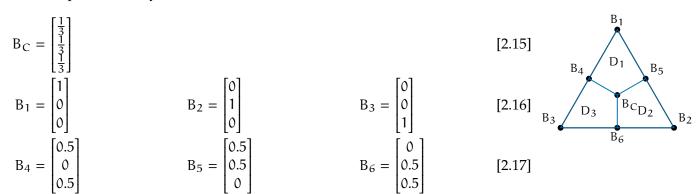
Theory

Simplex Integration in n = 2

#### 2.2. Pure Integration Strategies

#### 2.2.1. Quadrilaterial Integrator

Characteristic points in barycentric coordinates



Domain of a Simplex  $\Delta$  can be decomposed into three disjunct subdomains:

$$\Delta = D_1 \cup D_2 \cup D_3 \tag{2.18}$$

Therefore the double-Integral

$$\iint_{\Delta} F d\Delta = \iint_{D_1} F dD_1 + \iint_{D_2} F dD_2 + \iint_{D_3} F dD_3$$
 [2.19]

Mapping functions from the  $[-1,1] \times [-1,1] \times [-1]$  X-Y-Unit Square

$$g_{1}(X) = \frac{X}{2} + \frac{1}{2}$$

$$g_{2}(X) = -\frac{X}{2} + \frac{1}{2}$$

$$\frac{\partial g_{1}}{\partial X} = \frac{1}{2}$$

$$g_{1}(Y) = \frac{Y}{2} + \frac{1}{2}$$

$$g_{2}(Y) = -\frac{Y}{2} + \frac{1}{2}$$

$$g_{2}(Y) = -\frac{Y}{2} + \frac{1}{2}$$

$$[2.20]$$

$$g_1(Y) = \frac{Y}{2} + \frac{1}{2}$$
  $g_2(Y) = -\frac{Y}{2} + \frac{1}{2}$  [2.22]

$$\frac{\partial g_1}{\partial Y} = \frac{1}{2} \qquad \qquad \frac{\partial g_2}{\partial Y} = -\frac{1}{2} \qquad [2.23]$$

$$G_1(X,Y) = g_1(X)g_1(Y)$$
  $G_2(X,Y) = g_1(X)g_2(Y)$  [2.24]

$$G_3(X,Y) = g_2(X)g_1(Y)$$
  $G_4(X,Y) = g_2(X)g_2(Y)$  [2.25]

to barycentric coordinates of the D<sub>1</sub>, D<sub>2</sub>, D<sub>3</sub> Quadrilaterials

$$B_{D_1}(X,Y) = B_1 \cdot G_1(X,Y) + B_5 \cdot G_2(X,Y) + B_4 \cdot G_3(X,Y) + B_C \cdot G_4(X,Y)$$
 [2.26]

$$B_{D_2}(X,Y) = B_2 \cdot G_1(X,Y) + B_6 \cdot G_2(X,Y) + B_5 \cdot G_3(X,Y) + B_C \cdot G_4(X,Y)$$
 [2.27]

$$B_{D_3}(X,Y) = B_3 \cdot G_1(X,Y) + B_4 \cdot G_2(X,Y) + B_6 \cdot G_3(X,Y) + B_C \cdot G_4(X,Y)$$
 [2.28]

**Numerical Integration Scheme** The Integration is done on the Square  $[-1,1] \times [-1,1]$ , which allows for Gaussian Integration to be used:

$$\iint_{[-1,1]\times[-1,1]} F(X,Y) d(X,Y) \approx \sum_{i} \sum_{j} F(X_{i},X_{j}) w_{i} w_{j}$$
 [2.29]

The Gauss-Points  $(X_i, X_j)$  and their weights  $w_i, w_j$  on the Square can be deduced from the one dimensional Gaussian Integration

$$\int_{-1}^{1} H(X) dX \approx \sum_{i} H(X_{i}) w_{i}$$
 [2.30]

The Weights and Points of the 1D Gauss-Legendre Integration are given as:

$$n = 1$$

$$X = 0$$

$$w = 2$$

$$X = \sqrt{\frac{1}{3}}$$

$$w = 1$$

$$X = -\sqrt{\frac{1}{3}}$$

$$w = 1$$

$$X = \sqrt{\frac{3}{5}}$$

$$X = 0$$

$$W = \frac{5}{9}$$

$$X = -\sqrt{\frac{3}{5}}$$

$$W = \frac{5}{9}$$

$$W = \frac{5}{9}$$

**Integral transformation** from the 3 Domains into any simplex.



Let S denote a Matrix of the coordinates of the vertices of the simplex in the following form

$$S = \begin{bmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{bmatrix}$$
 [2.31]

The Coordinates C<sub>i</sub> of all characteristic points in Equations [2.15],[2.16] and [2.17] inside the simplex can be expressed in the following form

$$C_{C} = S \cdot B_{C}$$
 [2.32]

$$C_i = S \cdot B_i \quad \forall i \in 1, 2, ..., 6$$
 [2.33]

The transformation from points in the Integration Domain to the points in the barycentric given in [2.26],[2.27] and [2.28] can be expressed as

$$B_{D_{1}}(X,Y) = \begin{bmatrix} B_{1} & B_{5} & B_{4} & B_{C} \end{bmatrix} \begin{bmatrix} G_{1}(X,Y) \\ G_{2}(X,Y) \\ G_{3}(X,Y) \\ G_{4}(X,Y) \end{bmatrix}$$

$$B_{D_{2}}(X,Y) = \begin{bmatrix} B_{2} & B_{6} & B_{5} & B_{C} \end{bmatrix} \begin{bmatrix} G_{1}(X,Y) \\ G_{2}(X,Y) \\ G_{2}(X,Y) \\ G_{3}(X,Y) \\ G_{4}(X,Y) \end{bmatrix}$$
[2.34]

$$B_{D_2}(X,Y) = \begin{bmatrix} B_2 & B_6 & B_5 & B_C \end{bmatrix} \begin{bmatrix} G_1(X,Y) \\ G_2(X,Y) \\ G_3(X,Y) \\ G_4(X,Y) \end{bmatrix}$$
 [2.35]

$$B_{D_3}(X,Y) = \begin{bmatrix} B_3 & B_4 & B_6 & B_C \end{bmatrix} \begin{bmatrix} G_1(X,Y) \\ G_2(X,Y) \\ G_3(X,Y) \\ G_4(X,Y) \end{bmatrix}$$
[2.36]

With the Relationship given in [2.32] and [2.33] one can rewrite this as

$$C_{D_{1}}(X,Y) = S \begin{bmatrix} B_{1} & B_{5} & B_{4} & B_{C} \end{bmatrix} \begin{bmatrix} G_{1}(X,Y) \\ G_{2}(X,Y) \\ G_{3}(X,Y) \\ G_{4}(X,Y) \end{bmatrix}$$

$$C_{D_{2}}(X,Y) = S \begin{bmatrix} B_{2} & B_{6} & B_{5} & B_{C} \end{bmatrix} \begin{bmatrix} G_{1}(X,Y) \\ G_{2}(X,Y) \\ G_{3}(X,Y) \\ G_{4}(X,Y) \end{bmatrix}$$

$$C_{D_{3}}(X,Y) = S \begin{bmatrix} B_{3} & B_{4} & B_{6} & B_{C} \end{bmatrix} \begin{bmatrix} G_{1}(X,Y) \\ G_{2}(X,Y) \\ G_{2}(X,Y) \\ G_{3}(X,Y) \\ G_{3}(X,Y) \\ G_{3}(X,Y) \end{bmatrix}$$

$$[2.39]$$

$$C_{D_{2}}(X,Y) = S \begin{bmatrix} B_{2} & B_{6} & B_{5} & B_{C} \end{bmatrix} \begin{bmatrix} G_{1}(X,Y) \\ G_{2}(X,Y) \\ G_{3}(X,Y) \\ G_{4}(X,Y) \end{bmatrix}$$
[2.38]

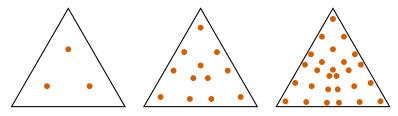
$$C_{D_3}(X,Y) = S \begin{bmatrix} B_3 & B_4 & B_6 & B_C \end{bmatrix} \begin{bmatrix} G_1(X,Y) \\ G_2(X,Y) \\ G_3(X,Y) \\ G_4(X,Y) \end{bmatrix}$$
[2.39]

With the Jacobi Matrix of any particular Domain being

$$J(C_{D_i}) = \begin{bmatrix} \frac{\partial C_{D_i}}{\partial X} & \frac{\partial C_{D_i}}{\partial Y} \end{bmatrix} = \begin{bmatrix} C_i & C_j & C_k & C_C \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial G_1}{\partial X} & \frac{\partial G_1}{\partial Y} \\ \frac{\partial G_2}{\partial X} & \frac{\partial G_2}{\partial Y} \\ \frac{\partial G_3}{\partial X} & \frac{\partial G_3}{\partial Y} \\ \frac{\partial G_3}{\partial X} & \frac{\partial G_3}{\partial Y} \end{bmatrix}$$
[2.40]

10

**Gauss Point Distribution** for the three Orders of Integration used.



Gauss Points n = 1 Gauss Points n = 2 Gauss Points n = 3

#### 2.2.2. Integration Rules in [1]

boundary might be preferable.

0.497 106 453 710 337 5

The Integration Rules in [1] which satisfy the PI and  $v = \overline{v}$  constraint. This only allows rules, which only allow positive weight where all points lie inside the triangle. Some Values were hard to In combination with the edge subdivision scheme, integration points which lie on the read in my print of the paper.

 $0.053\,145\,049\,844\,832\,16$   $1-\xi_1-\xi_2$  6

Deg	Weight w <sub>i</sub>	ξ <sub>1</sub>	ξ <sub>2</sub>	ξ3	Mult
4	0.329 855 230 965 965 5	0.816 847 572 980 458 5	0.091 576 213 509 770 73	$1 - \xi_1 - \xi_2$	3
4	0.670 144 769 034 034 5	0.108 103 018 168 070 2	0.445 948 490 915 964 90	$1 - \xi_1 - \xi_2$	3
6	0.350 358 827 179 022 2	0.501 426 509 658 134 2	0.249 286 745 170 932 9	$1 - \xi_1 - \xi_2$	3
6	0.1525347191106164	0.873 821 971 016 996 5	0.063 089 014 491 501 77	$1 - \xi_1 - \xi_2$	3

The jacobi determinant will be calculated by expressing  $\xi_3$  as

0.636 502 499 121 393 9

$$\xi_3 = 1 - \xi_1 - \xi_2 \tag{2.41}$$

Therefore the integral will be transformed into the  $\xi_1^*$ ,  $\xi_2^*$  space, using the interpolation functions  $N_1, N_2, N_3$ , with the jacobi determinant being:

$$J = \begin{bmatrix} C_1 & C_2 & C_3 \end{bmatrix} \begin{bmatrix} \frac{\partial N_1}{\partial \xi_1^+} & \frac{\partial N_1}{\partial \xi_2^+} \\ \frac{\partial N_2}{\partial \xi_1^+} & \frac{\partial N_2}{\partial \xi_2^+} \\ \frac{\partial N_3}{\partial \xi_1^+} & \frac{\partial N_3}{\partial \xi_2^+} \end{bmatrix}$$
 [2.42]

and

$$\frac{\partial N_{\alpha}}{\partial \xi_{j}^{*}} = \frac{N_{\alpha}}{\xi_{j}} - \frac{N_{\alpha}}{\xi_{3}} \quad \forall j = 1, 2$$
 [2.43]

Therefore

$$J = \begin{bmatrix} C_1 & C_2 & C_3 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{bmatrix}$$
 [2.44]

#### 2.2.3. Integration Rules in [2]

The Integration Rules in [2] up to order 5 are implemented.

# 

Deg	Weight w <sub>i</sub>	ξ <sub>1</sub>	ξ <sub>2</sub>	ξ3	Mult
1	1.0	0.333 333 333 333 333	0.333 333 333 333 333	$1 - \xi_1 - \xi_2$	1
2	0.333 333 333 333 333	0.666 666 666 666 667	0.166 666 666 666 667	$1 - \xi_1 - \xi_2$	3
3	-0.562 500 000 000 000	0.333 333 333 333 333	0.333 333 333 333 333	$1 - \xi_1 - \xi_2$	1
3	0.520 833 333 333 333	0.6	0.2	$1 - \xi_1 - \xi_2$	3
4	0.223 381 589 678 011	0.108 103 018 168 070	0.445 948 490 915 965	$1 - \xi_1 - \xi_2$	3
4	0.109 951 743 655 322	0.816 847 572 980 459	0.091 576 213 509 771	$1 - \xi_1 - \xi_2$	3
5	0.225 000 000 000 000	0.333 333 333 333 333	0.333 333 333 333 333	$1 - \xi_1 - \xi_2$	1
5	0.132 394 152 788 506	0.059 715 871 789 770	0.470 142 064 105 115	$1 - \xi_1 - \xi_2$	3
5	0.125 939 180 544 827	0.797 426 985 353 087	0.101 286 507 323 456	$1 - \xi_1 - \xi_2$	3







#### 2.3. Subdivision Integration Strategy

Because any triangle can be decomposed into 4 similar triangles, the subdivision algorithm turns out to be quite practical in implementation.

The Integral over a parent Simplex  $\Delta_p$ , can be expressed as an Integral over 4 Child Simpleces  $\Delta_i$ :

$$\iint_{\Delta_{p}} F d\Delta_{p} = \iint_{\Delta_{1}} F d\Delta_{1} + \iint_{\Delta_{2}} F d\Delta_{2} + \iint_{\Delta_{3}} F d\Delta_{3} + \iint_{\Delta_{4}} F d\Delta_{4}$$
 [2.45]

The Coordinates of a Child Simplex  $\Delta_i$  can be expressed in local-barycentric coordi-

nates  $\xi'_{i,1}$ ,  $\xi'_{i,2}$ ,  $\xi'_{i,3}$  The corresponding Transformation from the local coordinate System into the global is given by

$$B_4$$
 $\Delta_1$ 
 $B_5$ 
 $\Delta_3$ 
 $\Delta_4$ 
 $\Delta_2$ 
 $\Delta_2$ 
 $\Delta_3$ 
 $\Delta_4$ 
 $\Delta_2$ 
 $\Delta_3$ 
 $\Delta_4$ 
 $\Delta_2$ 
 $\Delta_3$ 

$$T_{lg}(\xi'_{i,1}, \xi'_{i,2}, \xi'_{i,3}) = B_{i,1}\xi'_{i,1} + B_{i,2}\xi'_{i,2} + B_{i,3}\xi'_{i,3}$$
[2.46]

where  $B_{i,j}$  are the coordinates of the Verteces of the Child Simplex  $\Delta_i$ .

This can be done recursively, to get a desired accuracy.

#### 2.3.1. Hierarchic Simplex Subdivision

A Criterion for adaptive integration from [3]

$$Q = \iint_{\Delta} F d\Delta$$
 [2.47]

$$\varepsilon = \left| Q - \iint_{\Delta_{p}} F \, d\Delta_{p} \right| \tag{2.48}$$

The Coordinates of the Verteces of the 4 Child Simplizes  $\Delta_i$  can be calculated with S by

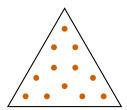
$$S_{\Delta,1} = S \cdot B_{\Delta,1} = S \cdot \begin{bmatrix} B_1 & B_5 & B_4 \end{bmatrix} = S \cdot \begin{bmatrix} 1 & 0.5 & 0.5 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \end{bmatrix}$$
 [2.49]

$$S_{\Delta,2} = S \cdot B_{\Delta,2} = S \cdot \begin{bmatrix} B_2 & B_6 & B_5 \end{bmatrix} = S \cdot \begin{bmatrix} 0 & 0 & 0.5 \\ 1 & 0.5 & 0.5 \\ 0 & 0.5 & 0 \end{bmatrix}$$
 [2.50]

$$S_{\Delta,3} = S \cdot B_{\Delta,3} = S \cdot \begin{bmatrix} B_3 & B_4 & B_6 \end{bmatrix} = S \cdot \begin{bmatrix} 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \\ 1 & 0.5 & 0.5 \end{bmatrix}$$
 [2.51]

$$S_{\Delta,4} = S \cdot B_{\Delta,4} = S \cdot \begin{bmatrix} B_4 & B_5 & B_6 \end{bmatrix} = S \cdot \begin{bmatrix} 0.5 & 0.5 & 0 \\ 0 & 0.5 & 0.5 \\ 0.5 & 0 & 0.5 \end{bmatrix}$$
 [2.52]

Coordinates of any Grandchild-Simplizes can be calculated by chaining  $B_{\Delta,i}$  Transformations



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#### 2.3.2. Edgewise Simplex Subdivision

The edgewise simplex subdivision can also be applied to uniformly subdivide any simplex. The points inside the r-th edgewise subdivision are indexed by 3 integers  $i_1$ ,  $i_2$ ,  $i_3$ , which satisfy following relation

$$i_1 + i_2 + i_3 = r$$
 [2.53]

The barycentric coordinates of any points can be calculated by

$$B = \begin{bmatrix} \frac{i_1}{r} \\ \frac{i_2}{r} \\ \frac{i_3}{r} \end{bmatrix}$$
 [2.54]

An example edgewise subdivision is given in figure 1.

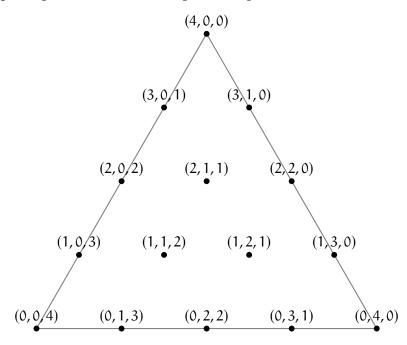


Abbildung 1: The points of the 4-th edge subdivision

In the r-th edge subdivision, traversal of the points can be done with the vectors indicated in

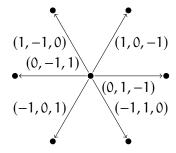
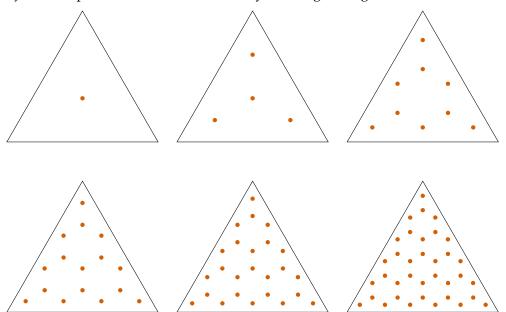


Abbildung 2: Traversal through the points

The integration domains will be identified by their *first-most* point  $I_0 = (i_1, i_2, i_3)$ . In order to calculate the neighboring points the following formulas will be used:

$$I_1 = (i_1, i_2, i_3) + (0, -1, 1) \quad I_2 = (i_1, i_2, i_3) + (-1, 0, 1) \quad I_3 = (i_1, i_2, i_3) + (-1, 1, 0)$$
[2.55]

The *first-most* points will be enumerated by iterating through the 2 first most indeces.



## 3. Simplex Integration in n = 3



#### 3.1. Space Definition

In a  $\mathbb{R}^3$  Simplex, the barycentric coordinates  $\mathbb{B}^4$  need to be used:

$$\mathbb{B}^4 = \{\xi_1, \, \xi_2, \, \xi_3, \, \xi_4 \in [0, 1] | \xi_1 + \xi_2 + \xi_3 + \xi_4 = 1\}$$
 [3.1]

where each set of coordinates corresponds to a point inside the simplex, spanned by the Coordinates in  $\mathbb{R}^3$ 

$$C_1 = \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} \qquad C_2 = \begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} \qquad C_3 = \begin{bmatrix} x_3 \\ y_3 \\ z_3 \end{bmatrix} \qquad C_4 = \begin{bmatrix} x_4 \\ y_4 \\ z_4 \end{bmatrix} \qquad [3.2]$$

The points  $C_i$  can be written in Matrix Form

$$\underline{\mathbf{C}} = \begin{bmatrix} C_1 & C_2 & C_3 & C_4 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \\ z_1 & z_2 & z_3 & z_4 \end{bmatrix}$$
[3.3]

A mapping  $M_B: \mathbb{B}^4 \to \mathbb{R}^3$  can be written as

$$C = \underline{C} \cdot \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \end{bmatrix}$$
 [3.4]

#### 3.2. Common Mappings

The Reference Element in Finite Element Analysis is often given in a  $\xi$ ,  $\eta$ ,  $\zeta$  Coordinates. The set of coordinates spanning this **Reference Space**  $\mathbb{R}^3_r$  can be mapped via  $M_R: \mathbb{R}^3_r \to \mathbb{B}^4$  to barycentric coordinates

$$B = \begin{bmatrix} -1 & -1 & -1 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \xi \\ \eta \\ \zeta \\ 1 \end{bmatrix} \qquad R = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \end{bmatrix}$$
[3.5]

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A Transformation of the subspace  $\mathbb{B}^4_S$ -Space with its supspace barycentric coordinates  $\xi_{S,i}$  into its greater space  $\mathbb{B}^4$  can be denoted by

$$B = \begin{bmatrix} B_1 & B_2 & B_3 & B_4 \end{bmatrix} \cdot \begin{bmatrix} \xi_{S,1} \\ \xi_{S,2} \\ \xi_{S,3} \\ \xi_{S,4} \end{bmatrix}$$
 [3.6]

#### 3.3. Pure Integration Strategy

#### 3.3.1. Quadrilateral Integration

Similar to the 2D Case, Quadrilaterals can be identified inside the tetrahedron for which, normal gaussian quadrature rules can be applied. In this Integration Space  $\mathbb{R}^3_{\mathrm{I}} := [-1,1] \times [-1,1] \times [-1,1]$  a transformation must be formulated.

For brevity, the interpolation functions  $g_1$ ,  $g_2$  will again be defined

$$g_1(a) = \frac{1}{2} + \frac{a}{2}$$
  $g_2(a) = \frac{1}{2} - \frac{a}{2}$  [3.7]

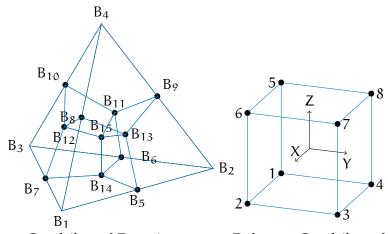
For which, the Interpolation functions for the points can be defined:

$$G_1(X, Y, Z) = g_2(X)g_2(Y)g_2(Z)$$
  $G_2(X, Y, Z) = g_1(X)g_2(Y)g_2(Z)$  [3.8]

$$G_3(X,Y,Z) = g_1(X)g_1(Y)g_2(Z)$$
  $G_4(X,Y,Z) = g_2(X)g_1(Y)g_2(Z)$  [3.9]

$$G_5(X,Y,Z) = g_2(X)g_2(Y)g_1(Z)$$
  $G_6(X,Y,Z) = g_1(X)g_2(Y)g_1(Z)$  [3.10]

$$G_7(X,Y,Z) = g_1(X)g_1(Y)g_1(Z)$$
  $G_8(X,Y,Z) = g_2(X)g_1(Y)g_1(Z)$  [3.11]



Quadrilateral Domains

Reference Quadrilateral

$$\iiint_{\Delta} F d\Delta = \iiint_{D_1} F dD_1 + \iiint_{D_2} F dD_2 + \iiint_{D_3} F dD_3 + \iiint_{D_4} F dD_4$$
 [3.12]

with

$$B_{D_1}(X, Y, Z) = \begin{bmatrix} B_1 & B_5 & B_{14} & B_7 & B_8 & B_{13} & B_{15} & B_{12} \end{bmatrix} \cdot G$$
 [3.13]

$$B_{D_2}(X, Y, Z) = \begin{bmatrix} B_2 & B_6 & B_{14} & B_5 & B_9 & B_{11} & B_{15} & B_{13} \end{bmatrix} \cdot G$$
 [3.14]

$$B_{D_3}(X,Y,Z) = \begin{bmatrix} B_3 & B_7 & B_{14} & B_6 & B_{10} & B_{12} & B_{15} & B_{11} \end{bmatrix} \cdot G$$
 [3.15]

$$B_{D_4}(X,Y,Z) = \begin{bmatrix} B_4 & B_8 & B_{12} & B_{10} & B_9 & B_{13} & B_{15} & B_{11} \end{bmatrix} \cdot G$$
 [3.16]

and

$$G(X,Y,Z) = \begin{bmatrix} G_1 & G_2 & G_3 & G_4 & G_5 & G_6 & G_7 & G_8 \end{bmatrix}^T$$
 [3.17]

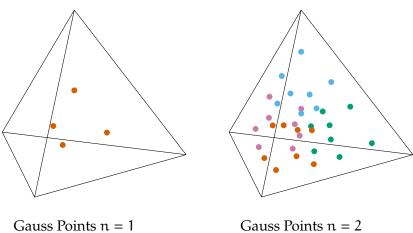
The Jacobi-Determinant of any particular Domain being

$$J(B_{D_{i}}) = B_{i} \begin{bmatrix} \frac{\partial G_{1}}{\partial X} & \frac{\partial G_{2}}{\partial X} & \frac{\partial G_{3}}{\partial X} & \frac{\partial G_{4}}{\partial X} & \frac{\partial G_{5}}{\partial X} & \frac{\partial G_{6}}{\partial X} & \frac{\partial G_{7}}{\partial X} & \frac{\partial G_{8}}{\partial X} \end{bmatrix}^{T}$$

$$\frac{\partial G_{1}}{\partial Y} & \frac{\partial G_{2}}{\partial Y} & \frac{\partial G_{3}}{\partial Y} & \frac{\partial G_{4}}{\partial Y} & \frac{\partial G_{5}}{\partial Y} & \frac{\partial G_{6}}{\partial Y} & \frac{\partial G_{7}}{\partial Y} & \frac{\partial G_{8}}{\partial Y} \\ \frac{\partial G_{1}}{\partial Z} & \frac{\partial G_{2}}{\partial Z} & \frac{\partial G_{3}}{\partial Z} & \frac{\partial G_{4}}{\partial Z} & \frac{\partial G_{5}}{\partial Z} & \frac{\partial G_{6}}{\partial Z} & \frac{\partial G_{7}}{\partial Z} & \frac{\partial G_{8}}{\partial Z} \end{bmatrix}^{T}$$

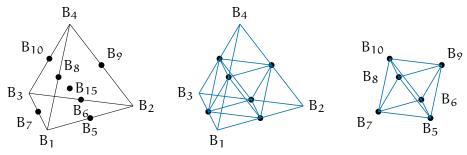
$$[3.18]$$

With the added benefit, that the integration points and their weights can be precomputed.



#### 3.4. Subdivision Integration Strategy

#### 3.4.1. Edge Subdivision



Simplex with characteristic points Child Simplices

Child Octahedron

The smooth subdivision scheme proposed in [4] can be adapted to serve a uniform decomposition of a unit tetrahedron. This approach circumvents a directional bias in the subdivision scheme.

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The points being

$$B_{1} = \begin{bmatrix} 1\\0\\0\\0\\0 \end{bmatrix} \quad B_{2} = \begin{bmatrix} 0\\1\\0\\0\\0 \end{bmatrix} \quad B_{3} = \begin{bmatrix} 0\\0\\1\\0\\0 \end{bmatrix} \quad B_{4} = \begin{bmatrix} 0\\0\\0\\0\\1\\1 \end{bmatrix}$$

$$B_{5} = \begin{bmatrix} \frac{1}{2}\\\frac{1}{2}\\0\\0\\0 \end{bmatrix} \quad B_{6} = \begin{bmatrix} 0\\\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\\0 \end{bmatrix} \quad B_{7} = \begin{bmatrix} \frac{1}{2}\\0\\\frac{1}{2}\\0\\0\\\frac{1}{2} \end{bmatrix} \quad B_{8} = \begin{bmatrix} \frac{1}{2}\\0\\0\\0\\\frac{1}{2} \end{bmatrix} \quad B_{9} = \begin{bmatrix} 0\\\frac{1}{2}\\0\\0\\\frac{1}{2} \end{bmatrix} \quad B_{10} = \begin{bmatrix} 0\\0\\0\\\frac{1}{2}\\\frac{1}{2} \end{bmatrix} \quad [3.20]$$

$$B_{11} = \begin{bmatrix} 0\\\frac{1}{3}\\\frac{1}{3}\\\frac{1}{3}\\\frac{1}{3} \end{bmatrix} \quad B_{12} = \begin{bmatrix} \frac{1}{3}\\0\\\frac{1}{3}\\\frac{1}{3}\\\frac{1}{3} \end{bmatrix} \quad B_{13} = \begin{bmatrix} \frac{1}{3}\\\frac{1}{3}\\0\\\frac{1}{3}\\\frac{1}{3} \end{bmatrix} \quad B_{14} = \begin{bmatrix} \frac{1}{3}\\\frac{1}{3}\\\frac{1}{3}\\0\\0 \end{bmatrix} \quad B_{15} = \begin{bmatrix} \frac{1}{4}\\\frac{1}{4}\\\frac{1}{4}\\\frac{1}{4} \end{bmatrix} \quad [3.21]$$

The tetrahedral integration Domains can be expressed as

$$\Delta_{1} = \begin{bmatrix} B_{1} & B_{5} & B_{7} & B_{8} \end{bmatrix}$$
 $\Delta_{2} = \begin{bmatrix} B_{5} & B_{2} & B_{6} & B_{9} \end{bmatrix}$ 
 $\Delta_{3} = \begin{bmatrix} B_{7} & B_{6} & B_{3} & B_{10} \end{bmatrix}$ 
 $\Delta_{4} = \begin{bmatrix} B_{8} & B_{9} & B_{10} & B_{4} \end{bmatrix}$ 
[3.22]
 $\Delta_{3} = \begin{bmatrix} B_{7} & B_{6} & B_{3} & B_{10} \end{bmatrix}$ 

$$\Delta_3 = \begin{bmatrix} B_7 & B_6 & B_3 & B_{10} \end{bmatrix}$$
  $\Delta_4 = \begin{bmatrix} B_8 & B_9 & B_{10} & B_4 \end{bmatrix}$  [3.23]

Whereas the vertices of the octahedral domain are expressable as

$$\mathbf{O}_5 = \begin{bmatrix} B_5 & B_6 & B_7 & B_8 & B_9 & B_{10} \end{bmatrix}$$
 [3.24]

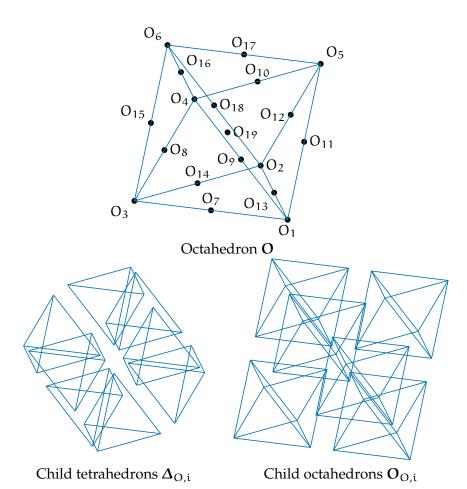
This map implies a order of the octahedrons vertices, which is now necessarily a This order is necessary to condition to uphold.

**octahedron subdivision** The subdivision will subdivide the octahedron into 6 octa- dinates must be opposing. hedrons and 8 tetrahedrons, where the 6 octahedrons will be again subdivided into 4 deformed tetrahedrons. This results in 32 tetrahedrons of equal volume. For ease of implementation and reduced complexicity, the subregions of the octahedron will be expressed in generalized barycentric coordinates. Unfortunately these barycentric coordinates are not unique for any given point inside the octahedron. Fortunately these coordinates only serve the purpose of interpolation of points inside any octahedron, where we can choose the coordinates of the octahedron in such a way, that the minimal number of points required is used.

uphold. Every even permutation of the order is also okay. The first and last coor-

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3 Simplex Integration in n = 3



$$O_{1} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad O_{2} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad O_{3} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad O_{4} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad O_{5} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad O_{6} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$[3.25]$$

$$O_{7} = \begin{bmatrix} 0.5 \\ 0 \\ 0.5 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad O_{8} = \begin{bmatrix} 0 \\ 0 \\ 0.5 \\ 0.5 \\ 0 \\ 0 \end{bmatrix} \qquad O_{9} = \begin{bmatrix} 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0 \\ 0 \end{bmatrix} \qquad O_{10} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \\ 0 \end{bmatrix} \qquad O_{11} = \begin{bmatrix} 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0 \end{bmatrix} \qquad O_{12} = \begin{bmatrix} 0 \\ 0.5 \\ 0 \\ 0.5 \\ 0 \end{bmatrix}$$

$$[3.26]$$

$$O_{13} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad O_{14} = \begin{bmatrix} 0 \\ 0.5 \\ 0.5 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad O_{15} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0.5 \\ 0 \\ 0.5 \end{bmatrix} \qquad O_{16} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0.5 \\ 0 \\ 0.5 \end{bmatrix} \qquad O_{17} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{18} = \begin{bmatrix} 0 \\ 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix}$$

$$O_{19} = \begin{bmatrix} 0.5 \\ 0 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{18} = \begin{bmatrix} 0 \\ 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{18} = \begin{bmatrix} 0 \\ 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0 \\ 0 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix} \qquad O_{19} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0$$

The child octahedrons are

$$\mathbf{O}_{O,1} = \begin{bmatrix} O_1 & O_7 & O_9 & O_{11} & O_{13} & O_{19} \end{bmatrix}$$

$$\mathbf{O}_{O,2} = \begin{bmatrix} O_{13} & O_2 & O_{14} & O_{19} & O_{12} & O_{18} \end{bmatrix}$$

$$\mathbf{O}_{O,3} = \begin{bmatrix} O_7 & O_3 & O_8 & O_{19} & O_{14} & O_{15} \end{bmatrix}$$

$$\mathbf{O}_{O,4} = \begin{bmatrix} O_9 & O_4 & O_{10} & O_{19} & O_8 & O_{16} \end{bmatrix}$$

$$\mathbf{O}_{O,5} = \begin{bmatrix} O_{11} & O_5 & O_{12} & O_{19} & O_{10} & O_{17} \end{bmatrix}$$

$$\mathbf{O}_{O,6} = \begin{bmatrix} O_{19} & O_{15} & O_{16} & O_{17} & O_{18} & O_6 \end{bmatrix}$$

$$\mathbf{O}_{O,6} = \begin{bmatrix} O_{19} & O_{15} & O_{16} & O_{17} & O_{18} & O_6 \end{bmatrix}$$

$$\mathbf{O}_{O,6} = \begin{bmatrix} O_{19} & O_{15} & O_{16} & O_{17} & O_{18} & O_6 \end{bmatrix}$$

$$\mathbf{O}_{O,6} = \begin{bmatrix} O_{19} & O_{15} & O_{16} & O_{17} & O_{18} & O_6 \end{bmatrix}$$

$$\mathbf{O}_{O,6} = \begin{bmatrix} O_{19} & O_{15} & O_{16} & O_{17} & O_{18} & O_6 \end{bmatrix}$$

$$\mathbf{O}_{O,6} = \begin{bmatrix} O_{19} & O_{15} & O_{16} & O_{17} & O_{18} & O_6 \end{bmatrix}$$

$$\mathbf{O}_{O,6} = \begin{bmatrix} O_{19} & O_{15} & O_{16} & O_{17} & O_{18} & O_6 \end{bmatrix}$$

The child simplizes are

$$\Delta_{O,1} = \begin{bmatrix} O_7 & O_{13} & O_{14} & O_{19} \end{bmatrix} \qquad \Delta_{O,2} = \begin{bmatrix} O_7 & O_8 & O_9 & O_{19} \end{bmatrix} \qquad [3.35]$$

$$\Delta_{O,3} = \begin{bmatrix} O_9 & O_{10} & O_{11} & O_{19} \end{bmatrix} \qquad \Delta_{O,4} = \begin{bmatrix} O_{10} & O_{16} & O_{17} & O_{19} \end{bmatrix} \qquad [3.36]$$

$$\Delta_{O,5} = \begin{bmatrix} O_{15} & O_{16} & O_8 & O_{19} \end{bmatrix} \qquad \Delta_{O,6} = \begin{bmatrix} O_{14} & O_{18} & O_{15} & O_{19} \end{bmatrix} \qquad [3.37]$$

$$\Delta_{O,7} = \begin{bmatrix} O_{11} & O_{13} & O_{12} & O_{19} \end{bmatrix} \qquad \Delta_{O,8} = \begin{bmatrix} O_{12} & O_{17} & O_{18} & O_{19} \end{bmatrix} \qquad [3.38]$$

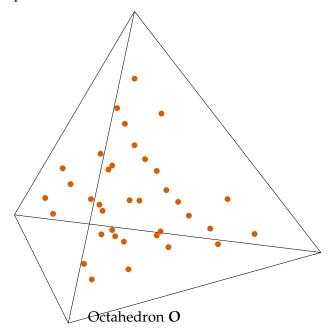
**octahedron integration** The standard integration will subdivide the octahedron along its diagonal creating 4 deformed tetrahedrons. These deformed tetrahedrons are defined

by following points:

$$\Delta_{O,1} = \begin{bmatrix} O_3 & O_4 & O_1 & O_5 \end{bmatrix} \qquad \Delta_{O,2} = \begin{bmatrix} O_3 & O_1 & O_2 & O_5 \end{bmatrix} \qquad [3.39]$$

$$\Delta_{O,3} = \begin{bmatrix} O_3 & O_2 & O_6 & O_5 \end{bmatrix} \qquad \Delta_{O,4} = \begin{bmatrix} O_3 & O_6 & O_4 & O_5 \end{bmatrix} \qquad [3.40]$$

The domains  $\Delta_{\rm O,i}$  can the be integrated with a pure simplex integrator. This results in 4 tetrahedrons of equal volume.



II Implementation 22

5 3D Case

# Teil II. Implementation

#### 4. 2D Case

Many formulas have been implemented 1-to-1 into code, shifting indizes as needed.

For the hierarchic subdivision algorithm a tree data structure has been utilized. The depth of the tree corresponds to the number of subdivisions, while the tree nodes visited contain a number. Every node also contains the information, whether a refinement has been tested. That way, repeated function evaluations are circumvented.

The tree nodes are visited via a depth-first traversal. This choice is arbitrary. Upon visiting a leaf node, it will be refined, if it hasn't been refined before. If the error of the unrefined leaf and the refined leaf is above the accepted threshold, the refined leaves will remain in the tree. This procedure will be done until, no leafs have been refined in an iteration.

Therefore any tree encodes a specific subdivision for a simplex.

#### 4.1. Magic Numbers and other arbitrary decisions

In the 2D Simplex, the subdomains are indexed as introduced in 2.3. With a list of indeces the subdomain transformation can be derived.

#### 5. 3D Case

#### 5.1. Magic Numbers and other arbitrary decisions

In the 3D Simplex, the subdivision scheme needs to index every domain. As there are two types of domains, a distiction must be made.

The Domains listed in 3.4.1 will be indexed in the following way:

0 1 2 3 4 5 6 7 8 9 10 11 12 
$$\Delta_1$$
  $\Delta_2$   $\Delta_3$   $\Delta_4$   $\Delta_{O,1}$   $\Delta_{O,2}$   $\Delta_{O,3}$   $\Delta_{O,4}$   $\Delta_{O,5}$   $\Delta_{O,6}$   $\Delta_{O,7}$   $\Delta_{O,8}$  13 14 15 16 17 18 19  $O_5$   $O_{O,1}$   $O_{O,2}$   $O_{O,3}$   $O_{O,4}$   $O_{O,5}$   $O_{O,6}$ 

5 Literatur

#### Literatur

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