Simplex Integration

Trials and Errors for transcendental Integrals

Inhaltsverzeichnis

Teil I.
Theory

1. Problem

Total Energy in the System:

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

Degradation Function

$$g(\phi) = \left(1-\phi^2\right) + k \qquad [1.2]$$

mit

k . . . being a small but finite scalar such as $10 \cdot 10^{-6}$
G_c . . . 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
$\nabla\phi$ . . . gradient of phase field parameter

$$\delta_u\Pi = \int_{\Omega} g(\phi)\sigma(\mathbf{u})\frac{\partial\varepsilon}{\partial\mathbf{u}}\,\delta\mathbf{u} = 0 \qquad [1.3]$$

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

1.1. Ansatz functions

$$\mathbf{u} = \sum_i N_i\mathbf{u}_i + \sum_i N_i F\mathbf{a}_i \qquad [1.5]$$

mit

N_i . . . are quadratic lagrange (standard) shape functions for tetrahedrons
$\mathbf{U}_i = \mathbf{u}_i, \mathbf{a}_i$ . . . are nodal degrees of freedom for displacement function
F . . . is an enrichment function (sigmoid like, depends on ϕ, later)

$$f_{base} = \sum_i N_i\phi_i \qquad [1.6]$$

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

mit

k_{reg} ... small but finite parameter

$$\phi = \exp(-\varsigma) \quad [1.8]$$
$$\phi = \exp(-\frac{\varsigma}{l}) \quad [1.9]$$

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

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

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

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

$$\Delta_{\phi_j}\, \delta_{\phi_i}\Pi = \phi_j \int_\Omega 2\left(\frac{\partial \phi}{\partial \phi_i}\right)^2 \psi(u)\, d\Omega\, \delta\phi_i + \phi_j \int_\Omega 2(\phi-1)\frac{\partial^2 \phi}{\partial \phi_i^2}\psi(u)\, d\Omega\, \delta\phi_i \quad [1.13]$$

$$+ \phi_j \frac{G_c}{l}\int_\Omega \frac{\partial \phi}{\partial \phi_i} + \frac{\partial^2 \phi}{\partial \phi_i^2} + l^2\frac{\partial \nabla\phi}{\partial \phi_j} \cdot \frac{\partial \nabla\phi}{\partial \phi_i} + l^2\nabla\phi \cdot \frac{\partial^2 \nabla\phi}{\partial \phi_i^2}\, d\Omega\, \delta\phi_i \quad [1.14]$$

1.2. Numerical Work

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

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

$$\frac{\partial^3 \varsigma}{\partial f_{base}^3} = \frac{3\left(-4k_{res}^2 + 12k_{res}f_{base}^2 + f_{base}^4\right)}{2\left(f_{base}^2 + k_{res}\right)^2} \cdot \frac{1}{4\sqrt[4]{f_{base}^2 + k_{res}}^5} \quad [1.17]$$

1.3. Setting up the Integrals in Question

The Vectors in Question are:

$$\mathbf{N} = \quad [1.18]$$
$$\mathbf{B} = \quad [1.19]$$

$$\frac{\partial \phi}{\partial \phi_i} = \frac{\partial \phi}{\partial \varsigma} \cdot \frac{\partial \varsigma}{\partial f_{base}} \cdot \frac{f_{base}}{\phi_i} \tag{1.20}$$

$$= -\frac{1}{l} \cdot \phi \cdot \frac{\partial \varsigma}{\partial f_{base}} \cdot N_i \tag{1.21}$$

$$\frac{\partial^2 \phi}{\partial \phi_i^2} = \frac{\partial}{\partial \phi_i}\left(-\frac{1}{l} \cdot \phi \cdot \frac{\partial \varsigma}{\partial f_{base}} \cdot N_i\right) \tag{1.22}$$

$$= -\frac{1}{l}\frac{\partial}{\partial \phi_i}\left(\phi \cdot \frac{\partial \varsigma}{\partial f_{base}}\right) \cdot N_i \tag{1.23}$$

$$= -\frac{1}{l}\left(\frac{\partial \phi}{\partial \phi_i} \cdot \frac{\partial \varsigma}{\partial f_{base}} + \phi \cdot \frac{\partial \varsigma}{\partial f_{base} \partial \phi}\right) \cdot N_i \tag{1.24}$$

$$= -\frac{1}{l}\left(\frac{\partial \phi}{\partial \phi_i} \cdot \frac{\partial \varsigma}{\partial f_{base}} + \phi \cdot \frac{\partial \varsigma}{\partial f_{base} \partial \phi}\right) \cdot N_i \tag{1.25}$$

$$= -\frac{1}{l}\left(\frac{\partial \phi}{\partial \phi_i} \cdot \frac{\partial \varsigma}{\partial f_{base}} + \phi \cdot \frac{\partial^2 \varsigma}{\partial f_{base}^2}\frac{\partial f_{base}}{\partial \phi}\right) \cdot N_i \tag{1.26}$$

$$= -\frac{1}{l}\left(-\frac{1}{l} \cdot \phi \cdot \left(\frac{\partial \varsigma}{\partial f_{base}}\right)^2 \cdot N_i + \phi \cdot \frac{\partial^2 \varsigma}{\partial f_{base}^2} N_i\right) \cdot N_i \tag{1.27}$$

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

$$\frac{\partial^2 \phi}{\partial \phi_i^2} = \frac{1}{l^2}\left(\left(\frac{\partial \varsigma}{\partial f_{base}}\right)^2 - \frac{\partial^2 \varsigma}{\partial f_{base}^2}\right) N_i \cdot N_j \tag{1.29}$$

$$\tag{1.30}$$

2. Simplex Integration in $n = 2$

First start with definitions:

Pure Integration Strategy is any quadrature formula of the simplex:

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

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

Subdivision Integration Strategy are Integrators of the form:

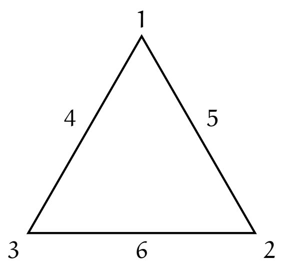
$$I = \iint_{\boldsymbol{\Delta}} f(\xi_1, \xi_2, \xi_3)\, d\boldsymbol{\Delta} = \sum_i \iint_{\boldsymbol{\Delta}_i} f(\xi_1, \xi_2, \xi_3)\, d\boldsymbol{\Delta}_i \qquad [2.2]$$

which then will be evaluated by pure Integrators.

2.1. Element Description

Shape Functions in barycentric coordinates

$$N_1(\xi_1, \xi_2, \xi_3) = \xi_1 \qquad [2.3]$$
$$N_2(\xi_1, \xi_2, \xi_3) = \xi_2 \qquad [2.4]$$
$$N_3(\xi_1, \xi_2, \xi_3) = \xi_3 \qquad [2.5]$$
$$N_4(\xi_1, \xi_2, \xi_3) = 4\xi_1\xi_3 \qquad [2.6]$$
$$N_5(\xi_1, \xi_2, \xi_3) = 4\xi_1\xi_2 \qquad [2.7]$$
$$N_6(\xi_1, \xi_2, \xi_3) = 4\xi_2\xi_3 \qquad [2.8]$$



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

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

mit $p_i \in \mathbb{R}^2$, $\xi_i \in [0, 1]$
ξ-η-Transformation

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

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

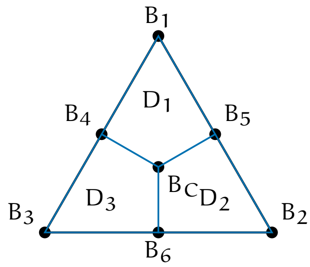
$$T(\xi, \eta) = \begin{bmatrix} 1 - \xi - \eta \\ \xi \\ \eta \end{bmatrix} \qquad [2.13]$$

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

2.2. Pure Integration Strategies

2.2.1. Quadrilaterial Integrator

Characteristic points in barycentric coordinates



$$B_C = \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{bmatrix} \quad [2.15]$$

$$B_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad B_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \qquad B_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad [2.16]$$

$$B_4 = \begin{bmatrix} 0.5 \\ 0 \\ 0.5 \end{bmatrix} \qquad B_5 = \begin{bmatrix} 0.5 \\ 0.5 \\ 0 \end{bmatrix} \qquad B_6 = \begin{bmatrix} 0 \\ 0.5 \\ 0.5 \end{bmatrix} \quad [2.17]$$

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

$$\boldsymbol{\Delta} = D_1 \cup D_2 \cup D_3 \quad [2.18]$$

Therefore the double-Integral

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

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

$$g_1(X) = \frac{X}{2} + \frac{1}{2} \qquad g_2(X) = -\frac{X}{2} + \frac{1}{2} \quad [2.20]$$

$$\frac{\partial g_1}{\partial X} = \frac{1}{2} \qquad \frac{\partial g_2}{\partial X} = -\frac{1}{2} \quad [2.21]$$

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

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

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

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

to barycentric coordinates of the D_1, D_2, D_3 Quadrilaterials

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

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

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

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

$$\iint_{[-1,1]\times[-1,1]} F(X,Y)\, d(X,Y) \approx \sum_i \sum_j F(X_i, X_j) w_i w_j \quad [2.29]$$

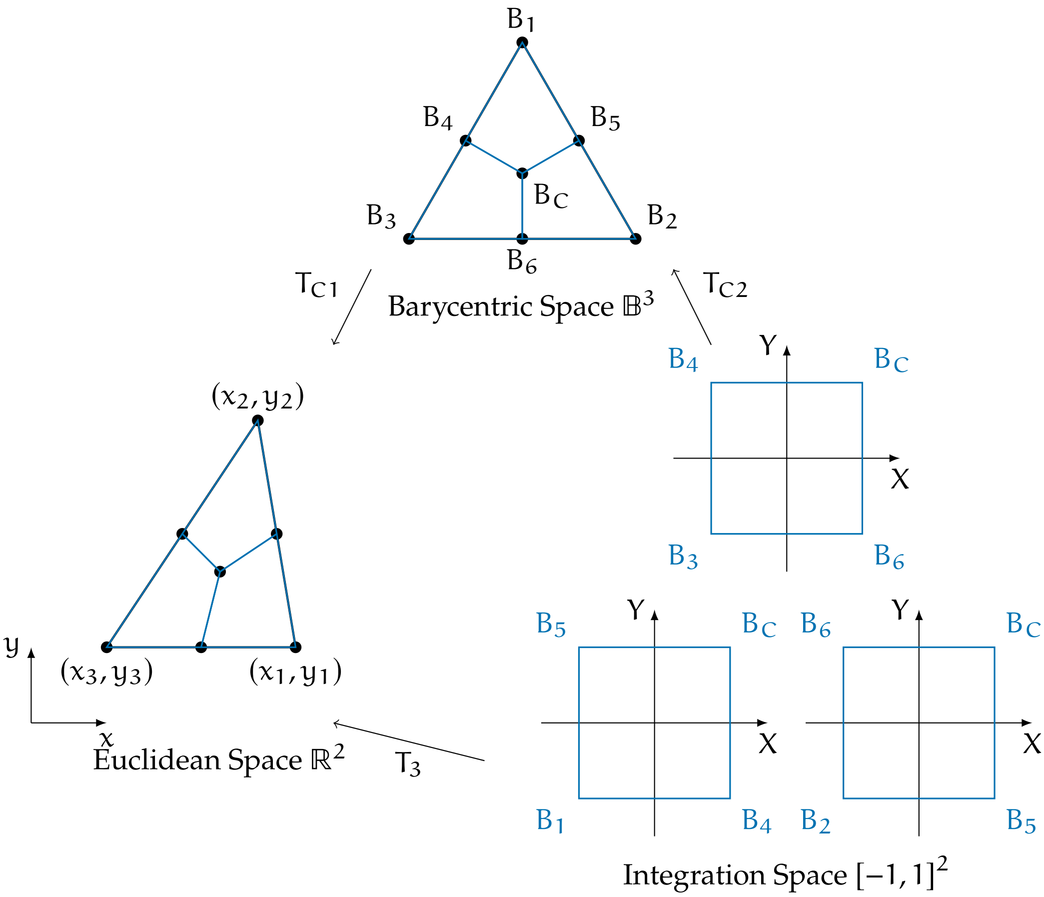
The Gauss-Points (X_i, X_j) and their weights w_i, w_j on the Square can be deduced from the one dimensional Gaussian Integration

$$\int_{-1}^{1} H(X)\,dX \approx \sum_i H(X_i) w_i \qquad [2.30]$$

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

$n = 1$	$X = 0$	$w = 2$
$n = 2$	$X = \sqrt{\frac{1}{3}}$	$w = 1$
	$X = -\sqrt{\frac{1}{3}}$	$w = 1$
$n = 3$	$X = \sqrt{\frac{3}{5}}$	$w = \frac{5}{9}$
	$X = 0$	$w = \frac{8}{9}$
	$X = -\sqrt{\frac{3}{5}}$	$w = \frac{5}{9}$

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

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

The Coordinates C_i of all characteristic points in Equations [2.15],[2.16] and [2.17] inside the simplex can be expressed in the following form

$$C_C = S \cdot B_C \quad [2.32]$$

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

.

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

$$B_{D_1}(X,Y) = \begin{bmatrix} B_1 & B_5 & B_4 & B_C \end{bmatrix} \begin{bmatrix} G_1(X,Y) \\ G_2(X,Y) \\ G_3(X,Y) \\ G_4(X,Y) \end{bmatrix} \quad [2.34]$$

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

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

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

$$C_{D_1}(X,Y) = S \begin{bmatrix} B_1 & B_5 & B_4 & B_C \end{bmatrix} \begin{bmatrix} G_1(X,Y) \\ G_2(X,Y) \\ G_3(X,Y) \\ G_4(X,Y) \end{bmatrix} \quad [2.37]$$

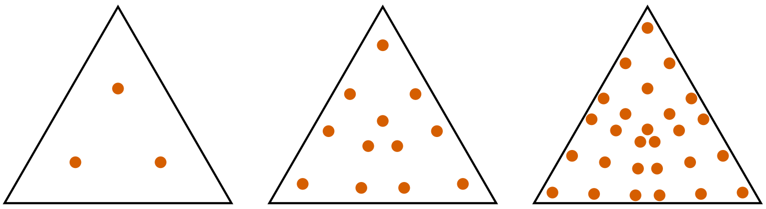
$$C_{D_2}(X,Y) = S \begin{bmatrix} B_2 & B_6 & B_5 & B_C \end{bmatrix} \begin{bmatrix} G_1(X,Y) \\ G_2(X,Y) \\ G_3(X,Y) \\ G_4(X,Y) \end{bmatrix} \quad [2.38]$$

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

With the Jacobi Matrix of any particular Domain being

$$J(C_{D_i}) = \begin{bmatrix} \frac{\partial C_{D_i}}{\partial X} & \frac{\partial C_{D_i}}{\partial Y} \end{bmatrix} = \begin{bmatrix} C_i & C_j & C_k & C_C \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial G_1}{\partial X} & \frac{\partial G_1}{\partial Y} \\ \frac{\partial G_2}{\partial X} & \frac{\partial G_2}{\partial Y} \\ \frac{\partial G_3}{\partial X} & \frac{\partial G_3}{\partial Y} \\ \frac{\partial G_4}{\partial X} & \frac{\partial G_4}{\partial Y} \end{bmatrix} \quad [2.40]$$

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]

The Integration Rules in [1] which satisfy the PI and $\nu = \bar{\nu}$ constraint. This only allows rules, which only allow positive weight where all points lie inside the triangle.

In combination with the edge subdivision scheme, integration points which lie on the boundary might be preferable.

Some Values were hard to read in my print of the paper.

Deg	Weight w_i	ξ_1	ξ_2	ξ_3	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	0.152 534 719 110 616 4	0.873 821 971 016 996 5	0.063 089 014 491 501 77	$1 - \xi_1 - \xi_2$	3
6	0.497 106 453 710 337 5	0.636 502 499 121 393 9	0.053 145 049 844 832 16	$1 - \xi_1 - \xi_2$	6

2.2.3. Integration Rules in [2]

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

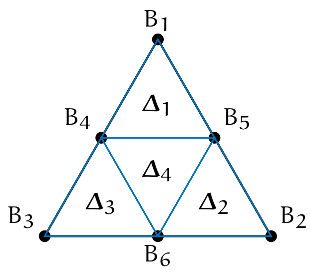
Deg	Weight w_i	ξ_1	ξ_2	ξ_3	Mult
1	1.0	0.333 333 333 333 333	0.333 333 333 333 333	$1 - \xi_1 - \xi_2$	1
2	0.333 333 333 333 333	0.666 666 666 666 667	0.166 666 666 666 667	$1 - \xi_1 - \xi_2$	3
3	−0.562 500 000 000 000	0.333 333 333 333 333	0.333 333 333 333 333	$1 - \xi_1 - \xi_2$	1
3	0.520 833 333 333 333	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 $\boldsymbol{\Delta}_p$, can be expressed as an Integral over 4 Child Simpleces $\boldsymbol{\Delta}_i$:

$$\iint_{\boldsymbol{\Delta}_p} F\,d\boldsymbol{\Delta}_p = \iint_{\boldsymbol{\Delta}_1} F\,d\boldsymbol{\Delta}_1 + \iint_{\boldsymbol{\Delta}_2} F\,d\boldsymbol{\Delta}_2 + \iint_{\boldsymbol{\Delta}_3} F\,d\boldsymbol{\Delta}_3 + \iint_{\boldsymbol{\Delta}_4} F\,d\boldsymbol{\Delta}_4 \quad [2.41]$$



The Coordinates of a Child Simplex $\boldsymbol{\Delta}_i$ can be expressed in local-barycentric coordinates $\xi'_{i,1}$, $\xi'_{i,2}$, $\xi'_{i,3}$

The corresponding Transformation from the local coordinate System into the global is given by

$$T_{lg}(\xi'_{i,1}, \xi'_{i,2}, \xi'_{i,3}) = B_{i,1}\xi'_{i,1} + B_{i,2}\xi'_{i,2} + B_{i,3}\xi'_{i,3} \quad [2.42]$$

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

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

2.4. Hierarchic Simplex Subdivision

A Criterion for adaptive integration from [3]

$$Q = \iint_{\boldsymbol{\Delta}} F\,d\boldsymbol{\Delta} \quad [2.43]$$

$$\varepsilon = \left| Q - \iint_{\boldsymbol{\Delta}_p} F\,d\boldsymbol{\Delta}_p \right| \quad [2.44]$$

The Coordinates of the Verteces of the 4 Child Simplizes $\boldsymbol{\Delta}_i$ can be calculated with S by

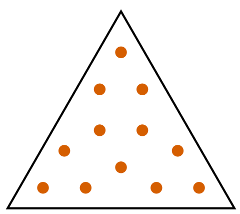
$$S_{\boldsymbol{\Delta},1} = S \cdot B_{\boldsymbol{\Delta},1} = S \cdot \begin{bmatrix} B_1 & B_5 & B_4 \end{bmatrix} = S \cdot \begin{bmatrix} 1 & 0.5 & 0.5 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \quad [2.45]$$

$$S_{\boldsymbol{\Delta},2} = S \cdot B_{\boldsymbol{\Delta},2} = S \cdot \begin{bmatrix} B_2 & B_6 & B_5 \end{bmatrix} = S \cdot \begin{bmatrix} 0 & 0 & 0.5 \\ 1 & 0.5 & 0.5 \\ 0 & 0.5 & 0 \end{bmatrix} \quad [2.46]$$

$$S_{\boldsymbol{\Delta},3} = S \cdot B_{\boldsymbol{\Delta},3} = S \cdot \begin{bmatrix} B_3 & B_4 & B_6 \end{bmatrix} = S \cdot \begin{bmatrix} 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \\ 1 & 0.5 & 0.5 \end{bmatrix} \quad [2.47]$$

$$S_{\boldsymbol{\Delta},4} = S \cdot B_{\boldsymbol{\Delta},4} = S \cdot \begin{bmatrix} B_4 & B_5 & B_6 \end{bmatrix} = S \cdot \begin{bmatrix} 0.5 & 0.5 & 0 \\ 0 & 0.5 & 0.5 \\ 0.5 & 0 & 0.5 \end{bmatrix} \quad [2.48]$$

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



2.5. 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

$$i_1 + i_2 + i_3 = r \qquad [2.49]$$

The barycentric coordinates of any points can be calculated by

$$B = \begin{bmatrix} \frac{i_1}{r} \\ \frac{i_2}{r} \\ \frac{i_3}{r} \end{bmatrix} \qquad [2.50]$$

An example edgewise subdivision is given in figure 1.

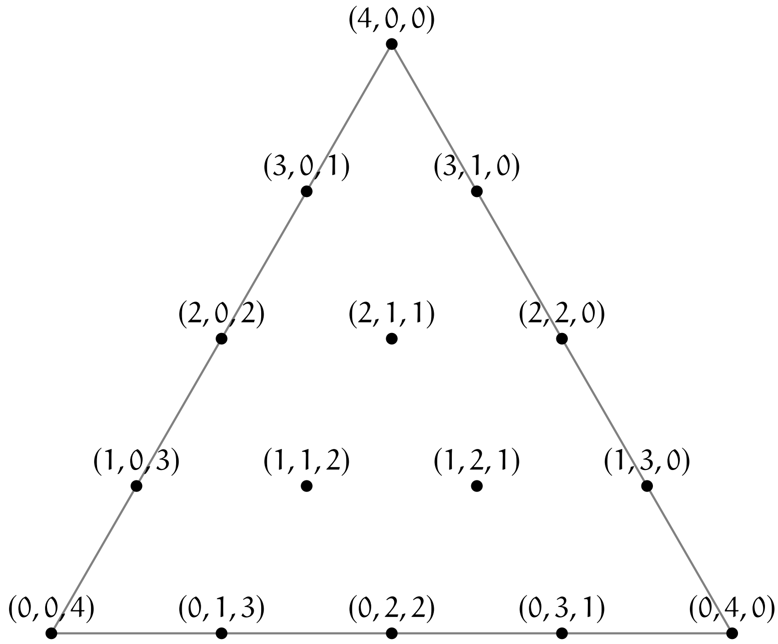


Abbildung 1: The points of the 4-th edge subdivision

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

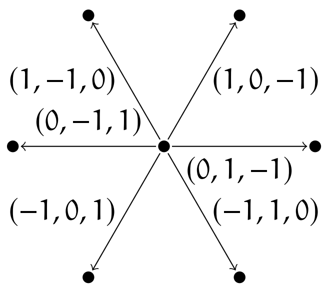


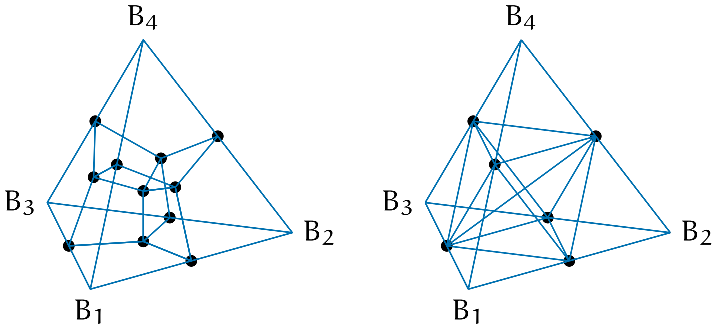
Abbildung 2: Traversal through the points

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:

$$I_1 = (i_1, i_2, i_3) + (0, -1, 1) \quad I_2 = (i_1, i_2, i_3) + (-1, 0, 1) \quad I_3 = (i_1, i_2, i_3) + (-1, 1, 0) \tag{2.51}$$

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:

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

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

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

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

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

3.2. Common Mappings

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

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

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

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

3.3. Pure Integration Strategy

3.3.1. Quadrilateral Integration

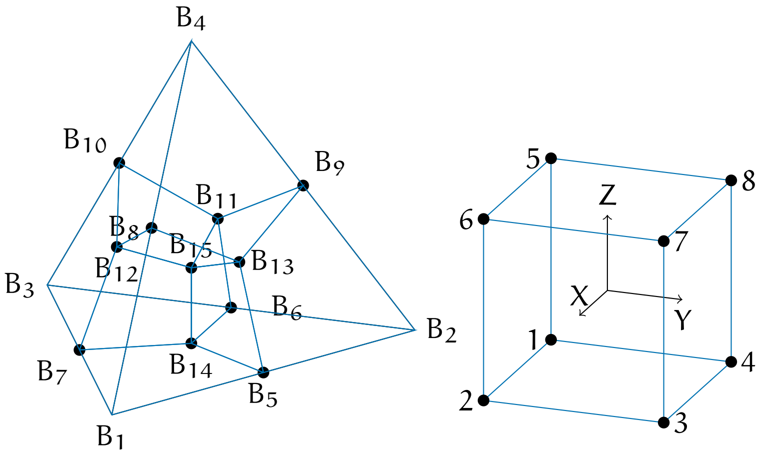
Similar to the 2D Case, Quadrilaterals can be identified inside the tetrahedron for which, normal gaussian quadrature rules can be applied. In this Integration Space $\mathbb{R}^3_I := [-1,1] \times [-1,1] \times [-1,1]$ a transformation must be formulated.

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

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

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

$$G_1(X,Y,Z) = g_2(X)g_2(Y)g_2(Z) \qquad G_2(X,Y,Z) = g_1(X)g_2(Y)g_2(Z) \qquad [3.8]$$
$$G_3(X,Y,Z) = g_1(X)g_1(Y)g_2(Z) \qquad G_4(X,Y,Z) = g_2(X)g_1(Y)g_2(Z) \qquad [3.9]$$
$$G_5(X,Y,Z) = g_2(X)g_2(Y)g_1(Z) \qquad G_6(X,Y,Z) = g_1(X)g_2(Y)g_1(Z) \qquad [3.10]$$
$$G_7(X,Y,Z) = g_1(X)g_1(Y)g_1(Z) \qquad G_8(X,Y,Z) = g_2(X)g_1(Y)g_1(Z) \qquad [3.11]$$



Quadrilateral Domains Reference Quadrilateral

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

with

$$B_{D_1}(X,Y,Z) = \begin{bmatrix} B_1 & B_5 & B_{14} & B_7 & B_8 & B_{13} & B_{15} & B_{12} \end{bmatrix} \cdot G \qquad [3.13]$$
$$B_{D_2}(X,Y,Z) = \begin{bmatrix} B_2 & B_6 & B_{14} & B_5 & B_9 & B_{11} & B_{15} & B_{13} \end{bmatrix} \cdot G \qquad [3.14]$$
$$B_{D_3}(X,Y,Z) = \begin{bmatrix} B_3 & B_7 & B_{14} & B_6 & B_{10} & B_{12} & B_{15} & B_{11} \end{bmatrix} \cdot G \qquad [3.15]$$
$$B_{D_4}(X,Y,Z) = \begin{bmatrix} B_4 & B_8 & B_{12} & B_{10} & B_9 & B_{13} & B_{15} & B_{11} \end{bmatrix} \cdot G \qquad [3.16]$$

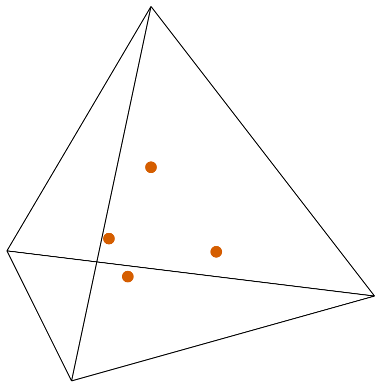
and

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

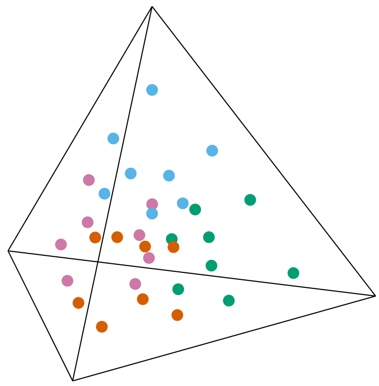
The Jacobi-Determinant of any particular Domain being

$$J(B_{D_i}) = B_i \begin{bmatrix} \frac{\partial G_1}{\partial X} & \frac{\partial G_2}{\partial X} & \frac{\partial G_3}{\partial X} & \frac{\partial G_4}{\partial X} & \frac{\partial G_5}{\partial X} & \frac{\partial G_6}{\partial X} & \frac{\partial G_7}{\partial X} & \frac{\partial G_8}{\partial X} \\ \frac{\partial G_1}{\partial Y} & \frac{\partial G_2}{\partial Y} & \frac{\partial G_3}{\partial Y} & \frac{\partial G_4}{\partial Y} & \frac{\partial G_5}{\partial Y} & \frac{\partial G_6}{\partial Y} & \frac{\partial G_7}{\partial Y} & \frac{\partial G_8}{\partial Y} \\ \frac{\partial G_1}{\partial Z} & \frac{\partial G_2}{\partial Z} & \frac{\partial G_3}{\partial Z} & \frac{\partial G_4}{\partial Z} & \frac{\partial G_5}{\partial Z} & \frac{\partial G_6}{\partial Z} & \frac{\partial G_7}{\partial Z} & \frac{\partial G_8}{\partial Z} \end{bmatrix}^T \qquad [3.18]$$

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



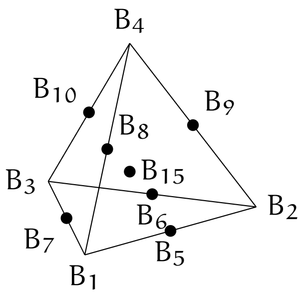
Gauss Points $n = 1$



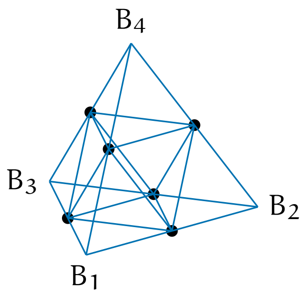
Gauss Points $n = 2$

3.4. Subdivision Integration Strategy

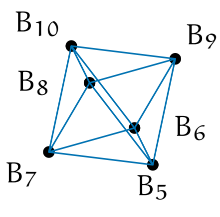
3.4.1. Edge Subdivision



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.

The points being

$$B_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad B_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad B_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad B_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{3.19}$$

$$B_5 = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \\ 0 \end{bmatrix} \quad B_6 = \begin{bmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{bmatrix} \quad B_7 = \begin{bmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \\ 0 \end{bmatrix} \quad B_8 = \begin{bmatrix} \frac{1}{2} \\ 0 \\ 0 \\ \frac{1}{2} \end{bmatrix} \quad B_9 = \begin{bmatrix} 0 \\ \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{bmatrix} \quad B_{10} = \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} \tag{3.20}$$

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

The tetrahedral integration Domains can be expressed as

$$\boldsymbol{\Delta}_1 = \begin{bmatrix} B_1 & B_5 & B_7 & B_8 \end{bmatrix} \qquad \boldsymbol{\Delta}_2 = \begin{bmatrix} B_5 & B_2 & B_6 & B_9 \end{bmatrix} \tag{3.22}$$

$$\boldsymbol{\Delta}_3 = \begin{bmatrix} B_7 & B_6 & B_3 & B_{10} \end{bmatrix} \qquad \boldsymbol{\Delta}_4 = \begin{bmatrix} B_8 & B_9 & B_{10} & B_4 \end{bmatrix} \tag{3.23}$$

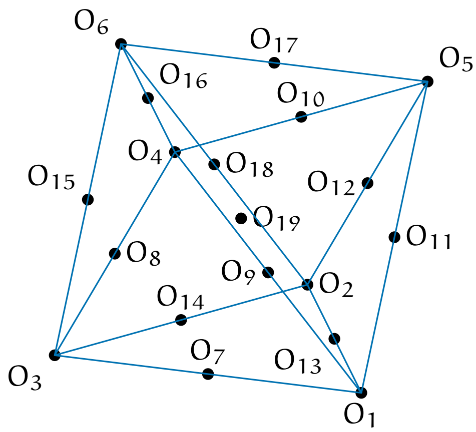
Whereas the vertices of the octahedral domain are expressable as

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

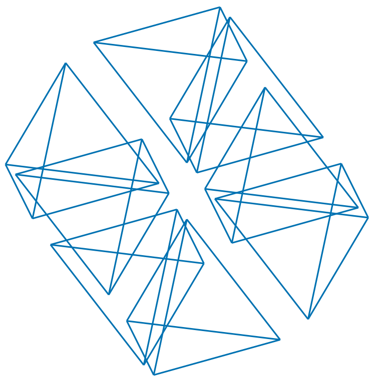
This map implies a order of the octahedrons vertices, which is now necessarily a condition to uphold.

This order is necessary to uphold. Every even permutation of the order is also okay. The first and last coordinates must be opposing.

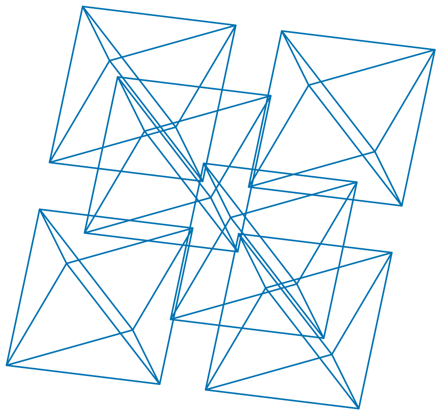
octahedron subdivision The subdivision will subdivide the octahedron into 6 octahedrons and 8 tetrahedrons, where the 6 octahedrons will be again subdivided into 4 deformed tetrahedrons. This results in 32 tetrahedrons of equal volume. For ease of implementation and reduced complexicity, the subregions 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.



Octahedron $\mathbf{O}$



Child tetrahedrons $\mathbf{\Delta}_{O,i}$



Child octahedrons $\mathbf{O}_{O,i}$

$$O_1 = \begin{bmatrix}1\\0\\0\\0\\0\\0\end{bmatrix} \quad O_2 = \begin{bmatrix}0\\1\\0\\0\\0\\0\end{bmatrix} \quad O_3 = \begin{bmatrix}0\\0\\1\\0\\0\\0\end{bmatrix} \quad O_4 = \begin{bmatrix}0\\0\\0\\1\\0\\0\end{bmatrix} \quad O_5 = \begin{bmatrix}0\\0\\0\\0\\1\\0\end{bmatrix} \quad O_6 = \begin{bmatrix}0\\0\\0\\0\\0\\1\end{bmatrix} \tag{3.25}$$

$$O_7 = \begin{bmatrix}0.5\\0\\0.5\\0\\0\\0\end{bmatrix} \quad O_8 = \begin{bmatrix}0\\0\\0.5\\0.5\\0\\0\end{bmatrix} \quad O_9 = \begin{bmatrix}0.5\\0\\0\\0.5\\0\\0\end{bmatrix} \quad O_{10} = \begin{bmatrix}0\\0\\0\\0.5\\0.5\\0\end{bmatrix} \quad O_{11} = \begin{bmatrix}0.5\\0\\0\\0\\0.5\\0\end{bmatrix} \quad O_{12} = \begin{bmatrix}0\\0.5\\0\\0\\0.5\\0\end{bmatrix} \tag{3.26}$$

$$O_{13} = \begin{bmatrix}0.5\\0.5\\0\\0\\0\\0\end{bmatrix} \quad O_{14} = \begin{bmatrix}0\\0.5\\0.5\\0\\0\\0\end{bmatrix} \quad O_{15} = \begin{bmatrix}0\\0\\0.5\\0\\0\\0.5\end{bmatrix} \quad O_{16} = \begin{bmatrix}0\\0\\0\\0.5\\0\\0.5\end{bmatrix} \quad O_{17} = \begin{bmatrix}0\\0\\0\\0\\0.5\\0.5\end{bmatrix} \quad O_{18} = \begin{bmatrix}0\\0.5\\0\\0\\0\\0.5\end{bmatrix} \tag{3.27}$$

$$O_{19} = \begin{bmatrix}0.5\\0\\0\\0\\0\\0.5\end{bmatrix} \tag{3.28}$$

The child octahedrons are

$$\mathbf{O}_{O,1} = \begin{bmatrix}O_1 & O_7 & O_9 & O_{11} & O_{13} & O_{19}\end{bmatrix} \tag{3.29}$$
$$\mathbf{O}_{O,2} = \begin{bmatrix}O_{13} & O_2 & O_{14} & O_{19} & O_{12} & O_{18}\end{bmatrix} \tag{3.30}$$
$$\mathbf{O}_{O,3} = \begin{bmatrix}O_7 & O_3 & O_8 & O_{19} & O_{14} & O_{15}\end{bmatrix} \tag{3.31}$$
$$\mathbf{O}_{O,4} = \begin{bmatrix}O_9 & O_4 & O_{10} & O_{19} & O_8 & O_{16}\end{bmatrix} \tag{3.32}$$
$$\mathbf{O}_{O,5} = \begin{bmatrix}O_{11} & O_5 & O_{12} & O_{19} & O_{10} & O_{17}\end{bmatrix} \tag{3.33}$$
$$\mathbf{O}_{O,6} = \begin{bmatrix}O_{19} & O_{15} & O_{16} & O_{17} & O_{18} & O_6\end{bmatrix} \tag{3.34}$$

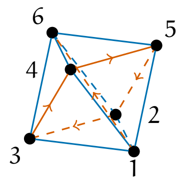


Abbildung 3: Orientation of Points

The child simplizes are

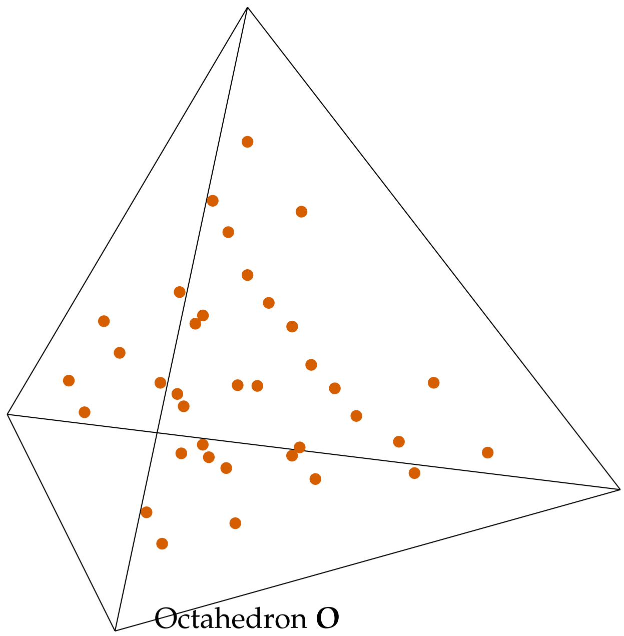
$$\mathbf{\Delta}_{O,1} = \begin{bmatrix}O_7 & O_{13} & O_{14} & O_{19}\end{bmatrix} \qquad \mathbf{\Delta}_{O,2} = \begin{bmatrix}O_7 & O_8 & O_9 & O_{19}\end{bmatrix} \tag{3.35}$$
$$\mathbf{\Delta}_{O,3} = \begin{bmatrix}O_9 & O_{10} & O_{11} & O_{19}\end{bmatrix} \qquad \mathbf{\Delta}_{O,4} = \begin{bmatrix}O_{10} & O_{16} & O_{17} & O_{19}\end{bmatrix} \tag{3.36}$$
$$\mathbf{\Delta}_{O,5} = \begin{bmatrix}O_{15} & O_{16} & O_8 & O_{19}\end{bmatrix} \qquad \mathbf{\Delta}_{O,6} = \begin{bmatrix}O_{14} & O_{18} & O_{15} & O_{19}\end{bmatrix} \tag{3.37}$$
$$\mathbf{\Delta}_{O,7} = \begin{bmatrix}O_{11} & O_{13} & O_{12} & O_{19}\end{bmatrix} \qquad \mathbf{\Delta}_{O,8} = \begin{bmatrix}O_{12} & O_{17} & O_{18} & O_{19}\end{bmatrix} \tag{3.38}$$

octahedron integration The standard integration will subdivide the octahedron along its diagonal creating 4 deformed tetrahedrons. These deformed tetrahedrons are defined by following points:

$$\boldsymbol{\Delta}_{O,1} = \begin{bmatrix} O_3 & O_4 & O_1 & O_5 \end{bmatrix} \qquad \boldsymbol{\Delta}_{O,2} = \begin{bmatrix} O_3 & O_1 & O_2 & O_5 \end{bmatrix} \tag{3.39}$$

$$\boldsymbol{\Delta}_{O,3} = \begin{bmatrix} O_3 & O_2 & O_6 & O_5 \end{bmatrix} \qquad \boldsymbol{\Delta}_{O,4} = \begin{bmatrix} O_3 & O_6 & O_4 & O_5 \end{bmatrix} \tag{3.40}$$

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



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
	$\boldsymbol{\Delta}_1$	$\boldsymbol{\Delta}_2$	$\boldsymbol{\Delta}_3$	$\boldsymbol{\Delta}_4$	$\boldsymbol{\Delta}_{O,1}$	$\boldsymbol{\Delta}_{O,2}$	$\boldsymbol{\Delta}_{O,3}$	$\boldsymbol{\Delta}_{O,4}$	$\boldsymbol{\Delta}_{O,5}$	$\boldsymbol{\Delta}_{O,6}$	$\boldsymbol{\Delta}_{O,7}$	$\boldsymbol{\Delta}_{O,8}$

13	14	15	16	17	18	19
$\mathbf{O}_5$	$\mathbf{O}_{O,1}$	$\mathbf{O}_{O,2}$	$\mathbf{O}_{O,3}$	$\mathbf{O}_{O,4}$	$\mathbf{O}_{O,5}$	$\mathbf{O}_{O,6}$

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