Simplex Integration

Trials and Errors for transcendental Integrals

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Teil I.
Theory

1. Problem

Total Energy in the System:

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

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_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

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

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

1.1. Ansatz functions

$$\mathbf{u} = \sum_i N_i\mathbf{u}_i + \sum_i N_i F\mathbf{a}_i \tag{1.5}$$

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)

$$f_{base} = \sum_i N_i\phi_i \tag{1.6}$$

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

mit

k_{reg} ... small but finite parameter

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

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

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

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

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

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

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

1.2. Numerical Work

$$\frac{\partial\phi}{\partial\phi_i} = -\frac{1}{l}\phi\frac{\partial\varsigma}{\partial f_{base}}N_i \qquad [1.15]$$

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

$$\frac{\partial^2\varsigma}{\partial f_{base}^2} = \left(\frac{5f_{base}^3}{\left(f_{base}^2 + k_{res}\right)} - 6f_{base}\right)\cdot\frac{1}{4\sqrt[4]{f_{base}^2 + k_{res}}^{\,5}} \qquad [1.17]$$

$$\frac{\partial^3\varsigma}{\partial f_{base}^3} = \frac{3\left(-4k_{res}^2 + 12k_{res}f_{base}^2 + f_{base}^4\right)}{2\left(f_{base}^2 + k_{res}\right)^2}\cdot\frac{1}{4\sqrt[4]{f_{base}^2 + k_{res}}^{\,5}} \qquad [1.18]$$

$$\frac{\partial^2\phi}{\partial\phi_i^2} = \frac{1}{l^2}\left(\left(\frac{\partial\varsigma}{\partial f_{base}}\right)^2 - \frac{\partial^2\varsigma}{\partial f_{base}^2}\right)N_i\cdot N_i \qquad [1.19]$$

2. Simplex Integration in $n = 2$

First start with definitions:

Pure Integration Strategy is any quadrature formula of the simplex:

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

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

Subdivision Integration Strategy are Integrators of the form:

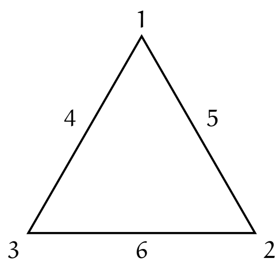
$$I = \iint_{\Delta} f(\xi_1, \xi_2, \xi_3)\, d\Delta = \sum_i \iint_{\Delta_i} f(\xi_1, \xi_2, \xi_3)\, d\Delta_i \tag{2.2}$$

which then will be evaluated by pure Integrators.

2.1. Element Description

Shape Functions in barycentric coordinates

$$N_1(\xi_1, \xi_2, \xi_3) = \xi_1 \tag{2.3}$$
$$N_2(\xi_1, \xi_2, \xi_3) = \xi_2 \tag{2.4}$$
$$N_3(\xi_1, \xi_2, \xi_3) = \xi_3 \tag{2.5}$$
$$N_4(\xi_1, \xi_2, \xi_3) = 4\xi_1\xi_3 \tag{2.6}$$
$$N_5(\xi_1, \xi_2, \xi_3) = 4\xi_1\xi_2 \tag{2.7}$$
$$N_6(\xi_1, \xi_2, \xi_3) = 4\xi_2\xi_3 \tag{2.8}$$



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

$$P(\xi_1, \xi_2, \xi_3) = p_1\xi_1 + p_2\xi_2 + p_3\xi_3 \tag{2.9}$$

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

$$\xi_1 := 1 - \xi - \eta \tag{2.10}$$
$$\xi_2 := \xi \tag{2.11}$$
$$\xi_3 := \eta \tag{2.12}$$

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

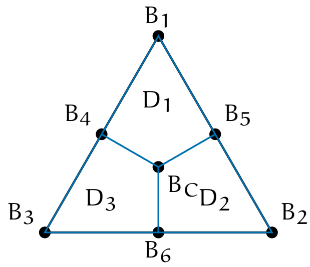
$$T(\xi, \eta) = \begin{bmatrix} 1 - \xi - \eta \\ \xi \\ \eta \end{bmatrix} \tag{2.13}$$

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

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:

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

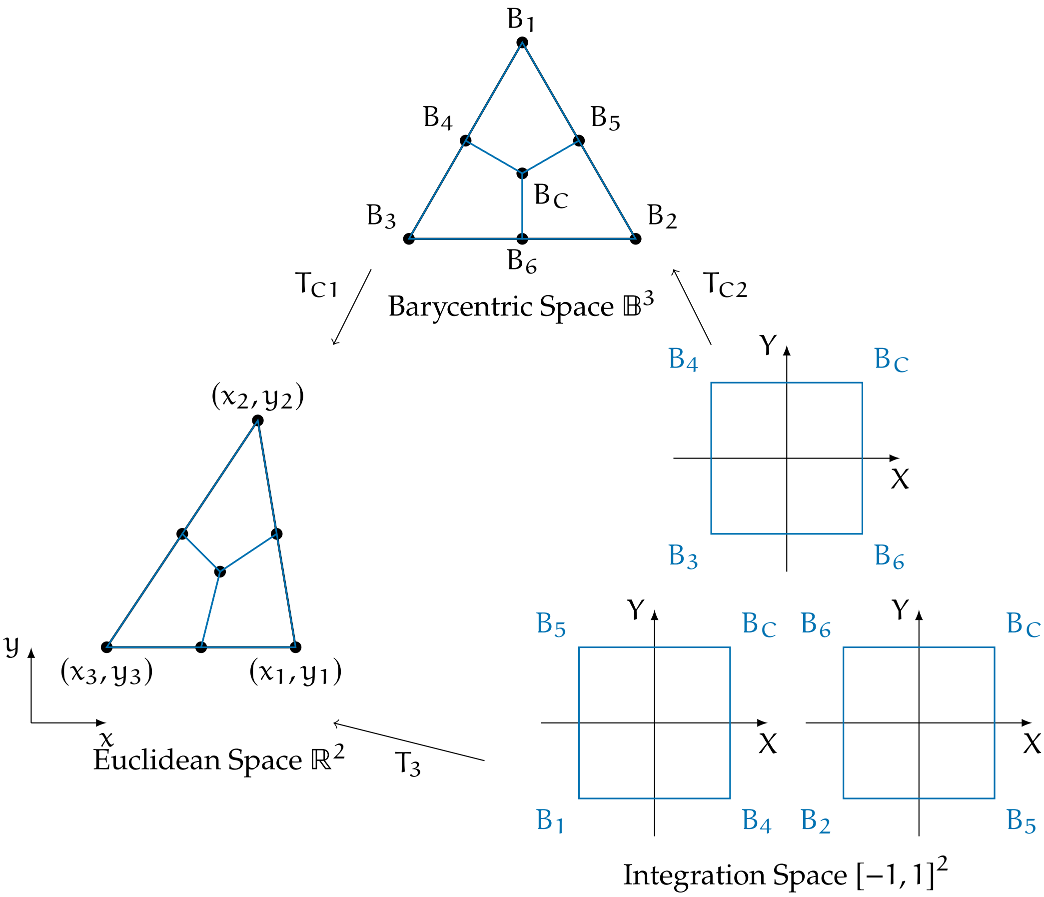
The Gauss-Points (X_i, X_j) and their weights w_i, w_j on the Square can be deduced from the one dimensional Gaussian Integration

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

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

$$
\begin{array}{lll}
n = 1 & X = 0 & w = 2 \\
n = 2 & X = \sqrt{\frac{1}{3}} & w = 1 \\
 & X = -\sqrt{\frac{1}{3}} & w = 1 \\
n = 3 & X = \sqrt{\frac{3}{5}} & w = \frac{5}{9} \\
 & X = 0 & w = \frac{8}{9} \\
 & X = -\sqrt{\frac{3}{5}} & w = \frac{5}{9}
\end{array}
$$

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

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

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

$$C_C = S \cdot B_C \tag{2.32}$$

$$C_i = S \cdot B_i \quad \forall i \in 1, 2, \dots, 6 \tag{2.33}$$

.

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

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

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

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

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

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

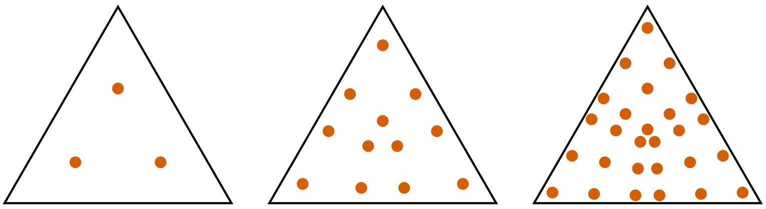
$$C_{D_2}(X, Y) = S \begin{bmatrix} B_2 & B_6 & B_5 & B_C \end{bmatrix} \begin{bmatrix} G_1(X, Y) \\ G_2(X, Y) \\ G_3(X, Y) \\ G_4(X, Y) \end{bmatrix} \tag{2.38}$$

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

With the Jacobi Matrix of any particular Domain being

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

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. Sphere Integrator

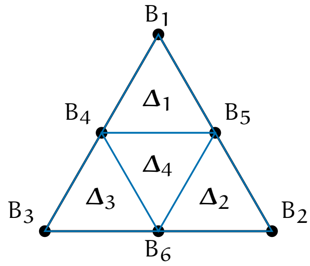
2.2.3. Other Quadrature Formulas

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 $\boldsymbol{\Delta}_i$:

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



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

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

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. Simplex Subdivision

A Criterion for adaptive integration from [1]

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

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

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

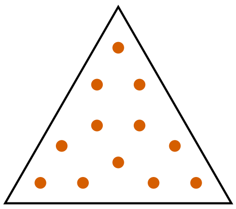
$$S_{\boldsymbol{\Delta},1} = S \cdot B_{\boldsymbol{\Delta},1} = S \cdot \begin{bmatrix} B_1 & B_5 & B_4 \end{bmatrix} = S \cdot \begin{bmatrix} 1 & 0.5 & 0.5 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \qquad [2.45]$$

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

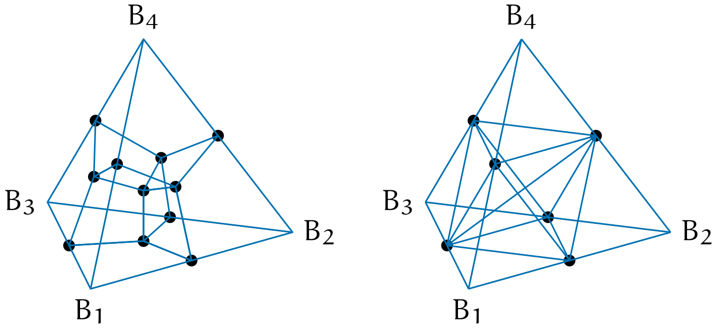
$$S_{\boldsymbol{\Delta},3} = S \cdot B_{\boldsymbol{\Delta},3} = S \cdot \begin{bmatrix} B_3 & B_4 & B_6 \end{bmatrix} = S \cdot \begin{bmatrix} 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \\ 1 & 0.5 & 0.5 \end{bmatrix} \qquad [2.47]$$

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

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



3. Simplex Integration in $n = 3$



Literatur

[1] Pedro Gonnet. “A Review of Error Estimation in Adaptive Quadrature”. In: *ACM Computing Surveys* 44.4 (Aug. 2012), S. 1–36. ISSN: 0360-0300, 1557-7341. DOI: 10.1145/2333112.2333117. URL: https://dl.acm.org/doi/10.1145/2333112.2333117 (besucht am 07. 05. 2023).