

Simplex Integration

Trials and Errors for transcendental Integrals

Inhaltsverzeichnis

I. Theory	3
1. Problem	3
1.1. Ansatz functions	3
1.2. Numerical Work	4
2. Simplex Integration in $n = 2$	5
2.1. Element Description	5
2.2. Pure Integration Strategies	6
2.2.1. Quadrilateral Integrator	6
2.2.2. Sphere Integrator	9
2.2.3. Other Quadrature Formulas	9
2.3. Subdivision Integration Strategy	10
2.4. Simplex Subdivision	10
3. Simplex Integration in $n = 3$	11
3.1. Space Definition	11
3.2. Common Mappings	11
3.3. Pure Integration Strategy	12
3.4. Subdivision Integration Strategy	12
3.4.1. Edge Subdivision	12

Teil I.

Theory

1. Problem

Total Energy in the System:

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

Degradation Function

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

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

$\psi(\mathbf{u})$... strain energy density function

\mathbf{u} ... displacement function

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

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

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

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

1.1. Ansatz functions

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

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)

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

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

mit

$k_{\text{reg}} \dots$ small but finite parameter

$$\phi = \exp(-\varsigma) \quad [1.8]$$

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

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

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

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

$$\Delta_{\mathbf{u}_i} \delta \mathbf{u}_i \Pi = \mathbf{u}_i \cdot \int_{\Omega} g(\phi) \frac{\partial \varepsilon}{\partial \mathbf{u}_i} \cdot \mathbb{C} \cdot \frac{\partial \varepsilon}{\partial \mathbf{u}_i} d\Omega \cdot \delta \mathbf{U}_i \quad [1.12]$$

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

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

1.2. Numerical Work

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

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

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

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

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

2. Simplex Integration in $n = 2$

First start with definitions:

Pure Integration Strategy is any quadrature formula of the simplex:

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

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

Subdivision Integration Strategy are Integrators of the form:

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

which then will be evaluated by pure Integrators.

2.1. Element Description

Shape Functions in barycentric coordinates

$$N_1(\xi_1, \xi_2, \xi_3) = \xi_1 \quad [2.3]$$

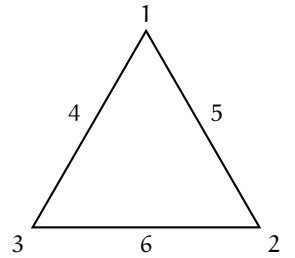
$$N_2(\xi_1, \xi_2, \xi_3) = \xi_2 \quad [2.4]$$

$$N_3(\xi_1, \xi_2, \xi_3) = \xi_3 \quad [2.5]$$

$$N_4(\xi_1, \xi_2, \xi_3) = 4\xi_1\xi_3 \quad [2.6]$$

$$N_5(\xi_1, \xi_2, \xi_3) = 4\xi_1\xi_2 \quad [2.7]$$

$$N_6(\xi_1, \xi_2, \xi_3) = 4\xi_2\xi_3 \quad [2.8]$$



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

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

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

ξ - η -Transformation

$$\xi_1 := 1 - \xi - \eta \quad [2.10]$$

$$\xi_2 := \xi \quad [2.11]$$

$$\xi_3 := \eta \quad [2.12]$$

mit $\xi \in [0, 1]$, $\eta \in [0, 1]$

Es gilt:

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

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

2.2. Pure Integration Strategies

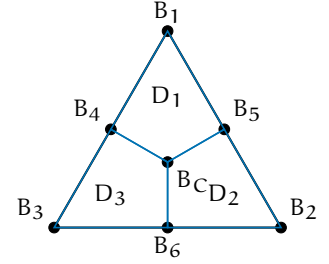
2.2.1. Quadrilateral Integrator

Characteristic points in barycentric coordinates

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

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

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



Domain of a Simplex Δ can be decomposed into three disjunct subdomains:

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

Therefore the double-Integral

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

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

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

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

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

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

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

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

to barycentric coordinates of the D_1, D_2, D_3 Quadrilaterals

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

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

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

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

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

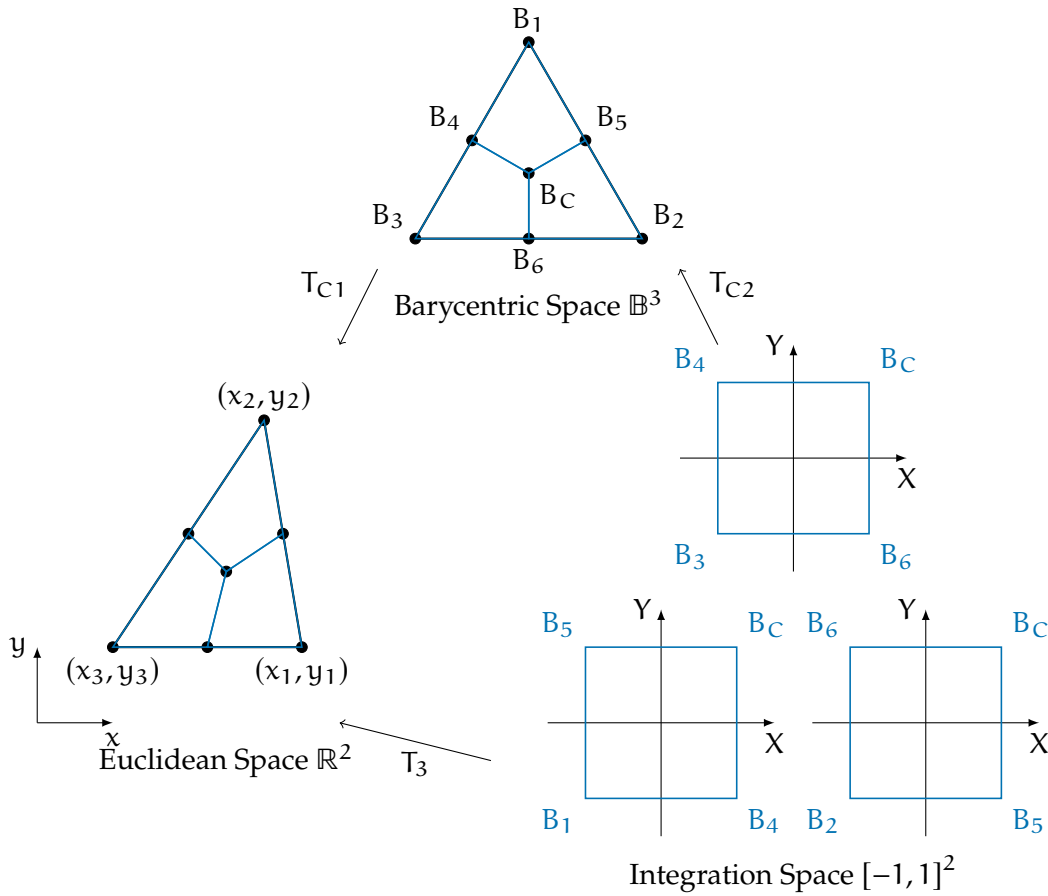
The Gauss-Points (X_i, X_j) and their weights w_i, w_j on the Square can be deduced from the one dimensional Gaussian Integration

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

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

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

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

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

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

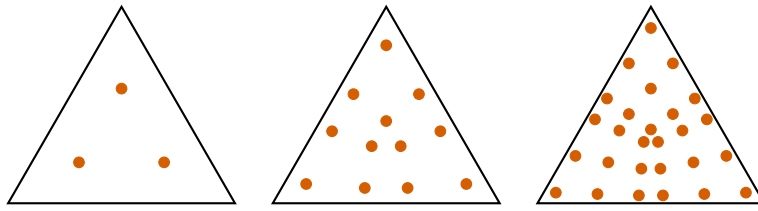
$$C_{D_2}(X, Y) = S \begin{bmatrix} B_2 & B_6 & B_5 & B_C \end{bmatrix} \begin{bmatrix} G_1(X, Y) \\ G_2(X, Y) \\ G_3(X, Y) \\ G_4(X, Y) \end{bmatrix} \quad [2.38]$$

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

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. 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 Δ_p , can be expressed as an Integral over 4 Child Simplexes Δ_i :

$$\iint_{\Delta_p} F d\Delta_p = \iint_{\Delta_1} F d\Delta_1 + \iint_{\Delta_2} F d\Delta_2 + \iint_{\Delta_3} F d\Delta_3 + \iint_{\Delta_4} F d\Delta_4 \quad [2.41]$$

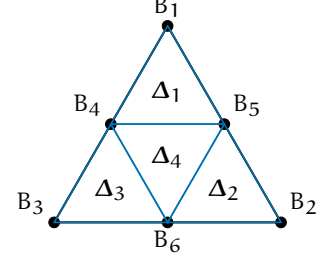
The Coordinates of a Child Simplex Δ_i can be expressed in local-barycentric coordinates $\xi'_{i,1}, \xi'_{i,2}, \xi'_{i,3}$

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 Δ_i .

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



2.4. Simplex Subdivision

A Criterion for adaptive integration from [1]

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

$$\varepsilon = \left| Q - \iint_{\Delta_p} F d\Delta_p \right| \quad [2.44]$$

The Coordinates of the Verteces of the 4 Child Simplizes Δ_i can be calculated with S by

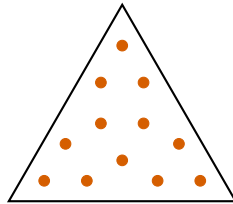
$$S_{\Delta,1} = S \cdot B_{\Delta,1} = S \cdot [B_1 \ B_5 \ B_4] = S \cdot \begin{bmatrix} 1 & 0.5 & 0.5 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \quad [2.45]$$

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

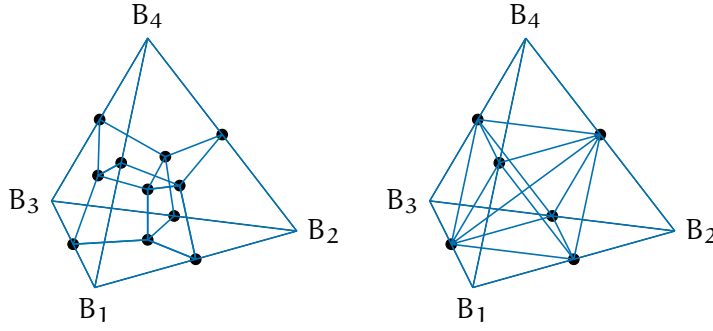
$$S_{\Delta,3} = S \cdot B_{\Delta,3} = S \cdot [B_3 \ B_4 \ B_6] = S \cdot \begin{bmatrix} 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \\ 1 & 0.5 & 0.5 \end{bmatrix} \quad [2.47]$$

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

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



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:

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

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

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

The points C_i can be written in Matrix Form

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

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

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

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}_r^3 can be mapped via $M_R : \mathbb{R}_r^3 \rightarrow \mathbb{B}^4$ to barycentric coordinates

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

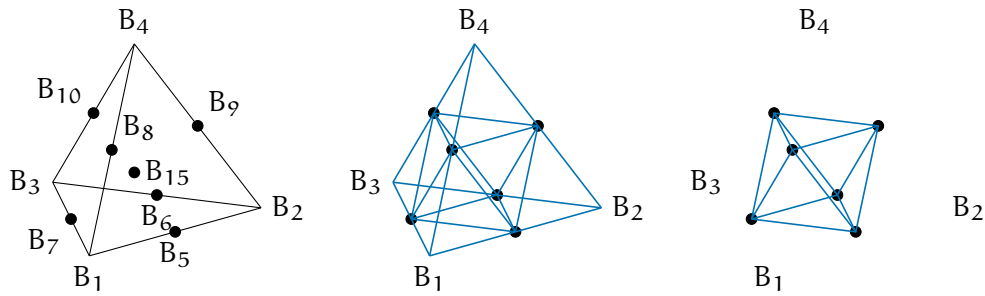
A Transformation of the subspace \mathbb{B}_S^4 -Space with its supspace barycentric coordinates $\xi_{S,i}$ into its greater space \mathbb{B}^4 can be denoted by

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

3.3. Pure Integration Strategy

3.4. Subdivision Integration Strategy

3.4.1. Edge Subdivision



Simplex with characteristic points Child Simplices

Child Octahedron

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).