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

$$\phi = \exp(-\varsigma) \tag{1.8}$$
$$\phi = \exp(-\frac{\varsigma}{l}) \tag{1.9}$$

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

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

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

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

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

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

1.2. Numerical Work

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

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

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

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

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

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.

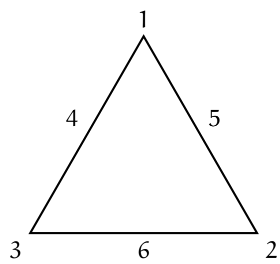
Subdivision Integration Strategy are Integrators of the form:

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

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

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

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:

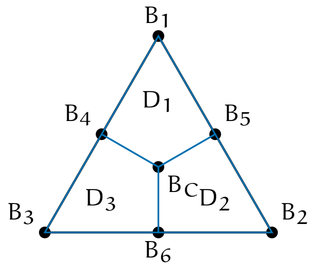
$$T(\xi, \eta) = \begin{bmatrix} 1 - \xi - \eta \\ \xi \\ \eta \end{bmatrix} \quad [2.13]$$

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

2.2. Pure Integration Strategies

2.2.1. Quadrilaterial Integrator

Characteristic points in barycentric coordinates



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

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

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

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

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

Therefore the double-Integral

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

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

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

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

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

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

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

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

to barycentric coordinates of the D_1, D_2, D_3 Quadrilaterials

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

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

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

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

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

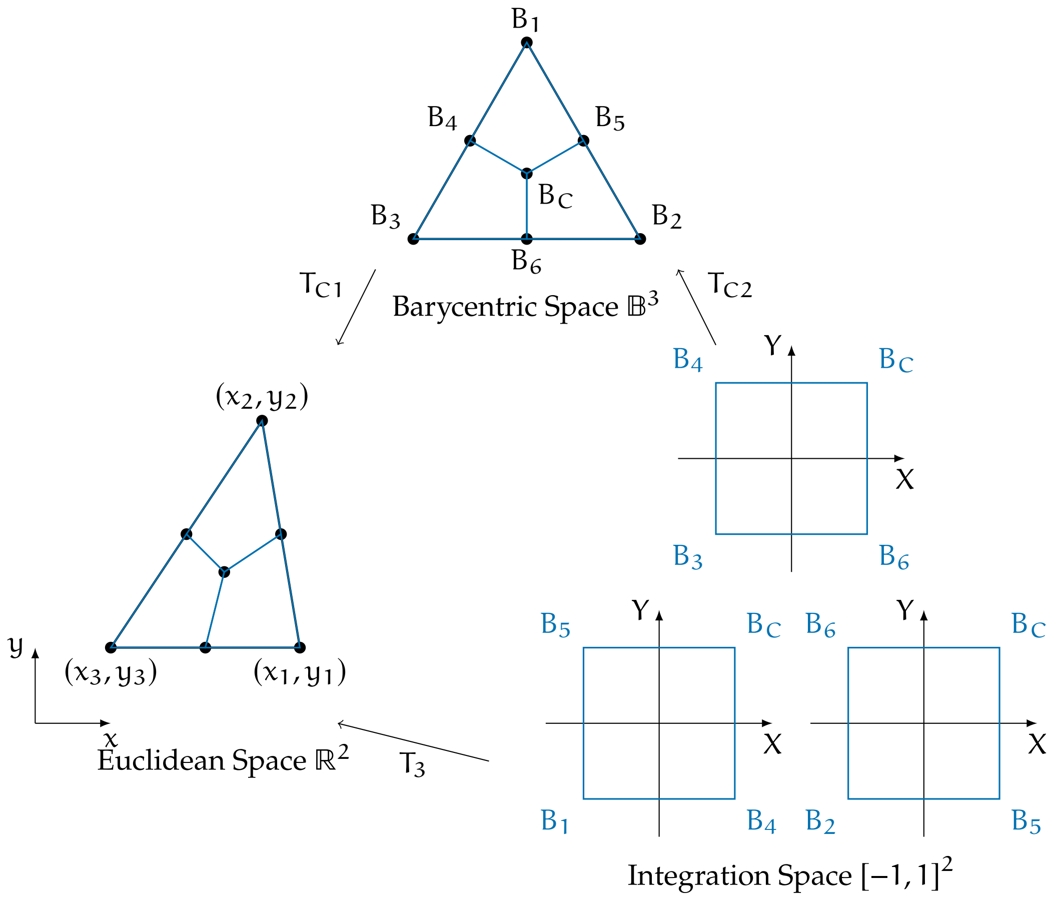
The Gauss-Points (X_i, X_j) and their weights w_i, w_j on the Square can be deduced from the one dimensional Gaussian Integration

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

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

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

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

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

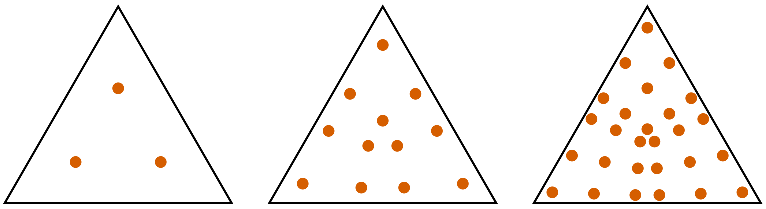
$$C_{D_2}(X, Y) = S \begin{bmatrix} B_2 & B_6 & B_5 & B_C \end{bmatrix} \begin{bmatrix} G_1(X, Y) \\ G_2(X, Y) \\ G_3(X, Y) \\ G_4(X, Y) \end{bmatrix} \tag{2.38}$$

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

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

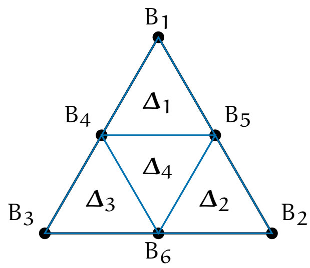
2.2.3. Other Quadrature Formulas

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 $\boldsymbol{\Delta}_i$:

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



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. Simplex Subdivision

A Criterion for adaptive integration from [1]

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

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

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

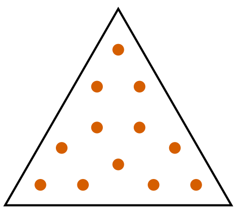
$$S_{\boldsymbol{\Delta},1} = S \cdot B_{\boldsymbol{\Delta},1} = S \cdot \begin{bmatrix} B_1 & B_5 & B_4 \end{bmatrix} = S \cdot \begin{bmatrix} 1 & 0.5 & 0.5 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \quad [2.45]$$

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

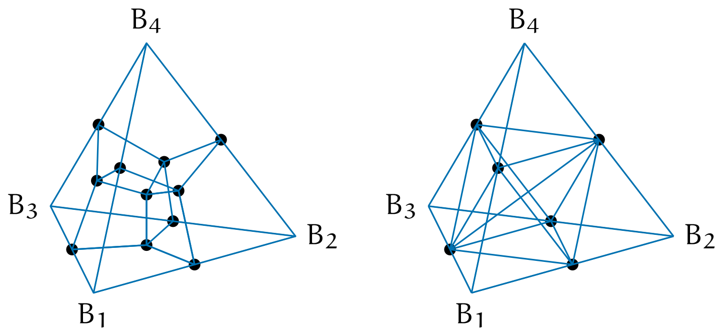
$$S_{\boldsymbol{\Delta},3} = S \cdot B_{\boldsymbol{\Delta},3} = S \cdot \begin{bmatrix} B_3 & B_4 & B_6 \end{bmatrix} = S \cdot \begin{bmatrix} 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \\ 1 & 0.5 & 0.5 \end{bmatrix} \quad [2.47]$$

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

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



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 $\mathbb{R}^3$

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

The points C_i can be written in Matrix Form

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

A mapping $M_B : \mathbb{B}^4 \longrightarrow \mathbb{R}^3$ 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** $\mathbb{R}^3_r$ can be mapped via $M_R : \mathbb{R}^3_r \longrightarrow \mathbb{B}^4$ to barycentric coordinates

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

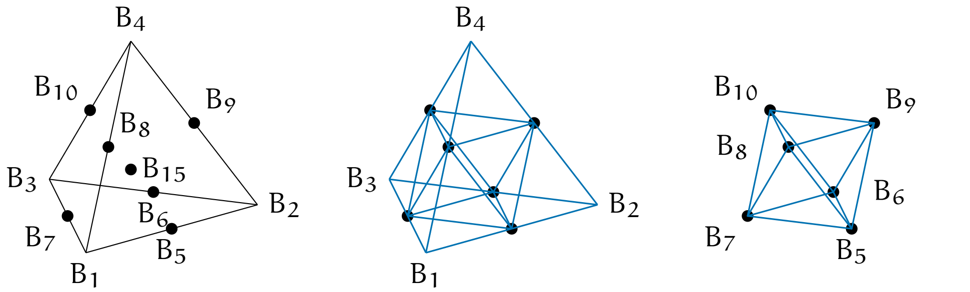
A Transformation of the subspace $\mathbb{B}^4_S$-Space with its supspace barycentric coordinates $\xi_{S,i}$ into its greater space $\mathbb{B}^4$ can be denoted by

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

3.3. Pure Integration Strategy

3.4. Subdivision Integration Strategy

3.4.1. Edge Subdivision



Simplex with characteristic points Child Simplices Child Octahedron

The smooth subdivision scheme proposed in [2] can be adapted to serve a uniform decomposition of a unit tetrahedron. This Approach circumvents numerical errors due to a directional bias in the subdivision scheme.

The points being

$$B_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad B_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad B_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad B_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \qquad [3.7]$$

$$B_5 = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \\ 0 \end{bmatrix} \quad B_6 = \begin{bmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{bmatrix} \quad B_7 = \begin{bmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \\ 0 \end{bmatrix} \quad B_8 = \begin{bmatrix} \frac{1}{2} \\ 0 \\ 0 \\ \frac{1}{2} \end{bmatrix} \quad B_9 = \begin{bmatrix} 0 \\ \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{bmatrix} \quad B_{10} = \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} \qquad [3.8]$$

$$B_{11} = \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ 0 \\ \frac{1}{3} \end{bmatrix} \quad B_{12} = \begin{bmatrix} \frac{1}{3} \\ 0 \\ \frac{1}{3} \\ \frac{1}{3} \end{bmatrix} \quad B_{13} = \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ 0 \\ \frac{1}{3} \end{bmatrix} \quad B_{14} = \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \\ 0 \end{bmatrix} \quad B_{15} = \begin{bmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{bmatrix} \qquad [3.9]$$

The tetrahedral integration Domains can be expressed as

$$\mathbf{\Delta}_1 = \begin{bmatrix} B_1 & B_5 & B_7 & B_8 \end{bmatrix} \qquad \mathbf{\Delta}_2 = \begin{bmatrix} B_5 & B_2 & B_6 & B_9 \end{bmatrix} \qquad [3.10]$$

$$\mathbf{\Delta}_3 = \begin{bmatrix} B_7 & B_8 & B_3 & B_{10} \end{bmatrix} \qquad \mathbf{\Delta}_4 = \begin{bmatrix} B_8 & B_9 & B_{10} & B_4 \end{bmatrix} \qquad [3.11]$$

Whereas the vertices of the octahedral domain are expressable as

$$\mathbf{O}_5 = \begin{bmatrix} B_5 & B_6 & B_7 & B_8 & B_9 & B_{10} \end{bmatrix} \qquad [3.12]$$

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

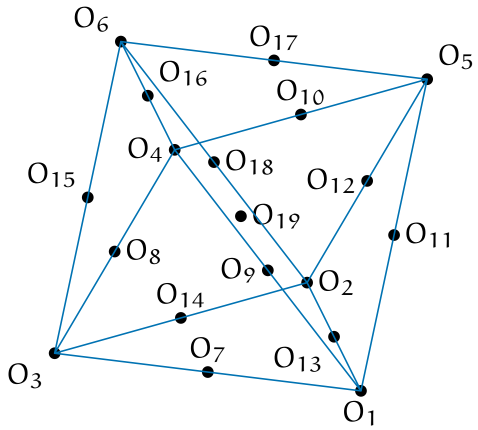
octahedron integration The standard integration will subdivide the octahedron along its diagonal creating 4 deformed tetrahedrons. These deformed tetrahedrons are defined by following points: TODO Update Numbering to coincide with numbering of the mapping

$$\boldsymbol{\Delta}_{O,1} = \begin{bmatrix} B_5 & B_7 & B_9 & B_8 \end{bmatrix} \qquad \boldsymbol{\Delta}_{O,2} = \begin{bmatrix} B_8 & B_7 & B_9 & B_{10} \end{bmatrix} \tag{3.13}$$

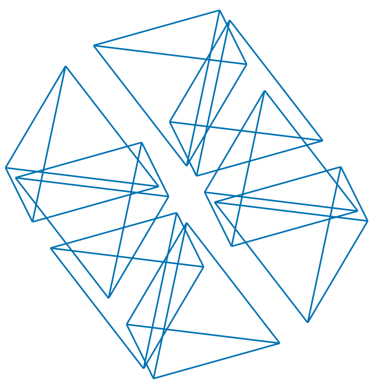
$$\boldsymbol{\Delta}_{O,3} = \begin{bmatrix} B_{10} & B_7 & B_9 & B_6 \end{bmatrix} \qquad \boldsymbol{\Delta}_{O,4} = \begin{bmatrix} B_6 & B_7 & B_9 & B_5 \end{bmatrix} \tag{3.14}$$

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

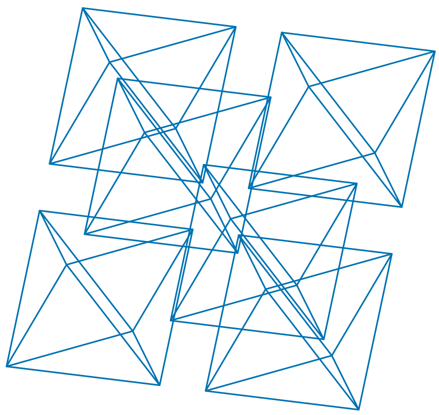
octahedron subdivision The subdivision will subdivide the octahedron into 6 octahedrons and 8 tetrahedrons, where the 6 octahedrons will be again subdivided into 4 deformed tetrahedrons. This results in 32 tetrahedrons of equal volume. For ease of implementation and reduced complexicity, the subregions 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 $\boldsymbol{\Delta}_{O,i}$



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

The Child simplizes are

$$\boldsymbol{\Delta}_{O,1} = \begin{bmatrix} O_7 & O_{13} & O_{14} & O_{19} \end{bmatrix} \qquad \boldsymbol{\Delta}_{O,2} = \begin{bmatrix} O_7 & O_8 & O_9 & O_{19} \end{bmatrix} \tag{3.15}$$

$$\boldsymbol{\Delta}_{O,3} = \begin{bmatrix} O_9 & O_{10} & O_{11} & O_{19} \end{bmatrix} \qquad \boldsymbol{\Delta}_{O,4} = \begin{bmatrix} O_{10} & O_{16} & O_{17} & O_{19} \end{bmatrix} \tag{3.16}$$

$$\boldsymbol{\Delta}_{O,5} = \begin{bmatrix} O_{15} & O_{16} & O_8 & O_{19} \end{bmatrix} \qquad \boldsymbol{\Delta}_{O,6} = \begin{bmatrix} O_{14} & O_{15} & O_{18} & O_{19} \end{bmatrix} \tag{3.17}$$

$$\boldsymbol{\Delta}_{O,7} = \begin{bmatrix} O_{11} & O_{13} & O_{12} & O_{19} \end{bmatrix} \qquad \boldsymbol{\Delta}_{O,8} = \begin{bmatrix} O_{12} & O_{17} & O_{18} & O_{19} \end{bmatrix} \tag{3.18}$$

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).

[2] S. Schaefer, J. Hakenberg und J. Warren. “Smooth subdivision of tetrahedral meshes”. In: *Proceedings of the 2004 Eurographics/ACM SIGGRAPH symposium on Geometry processing*. SGP04: Symposium on Geometry Processing. Nice France: ACM, 8. Juli 2004, S. 147–154. ISBN: 978-3-905673-13-5. DOI: 10.1145/1057432.1057452. URL: https://dl.acm.org/doi/10.1145/1057432.1057452 (besucht am 12. 05. 2023).