Simplex Integration

By Domain Subdivision

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Teil I.
Theory

1. Problem

Total Energy in the System:

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

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

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

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

1.1. Ansatz functions

$$u = \sum_i N_i u_i + \sum_i N_i F a_i \qquad [1.5]$$

mit

   N_i ...are quadratic lagrange (standard) shape functions for tetrahedrons
   $U_i = u_i, a_i$...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

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

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

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

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

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

$$\tag{1.14}$$

2. Element Description

Shape Functions in barycentric coordinates

$$N_1(\xi_1,\xi_2,\xi_3) = \xi_1 \tag{2.1}$$
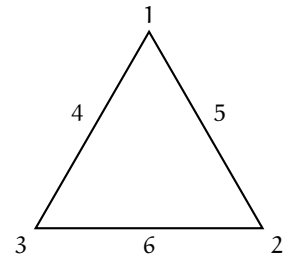$$N_2(\xi_1,\xi_2,\xi_3) = \xi_2 \tag{2.2}$$
$$N_3(\xi_1,\xi_2,\xi_3) = \xi_3 \tag{2.3}$$
$$N_4(\xi_1,\xi_2,\xi_3) = 4\xi_1\xi_3 \tag{2.4}$$
$$N_5(\xi_1,\xi_2,\xi_3) = 4\xi_1\xi_2 \tag{2.5}$$
$$N_6(\xi_1,\xi_2,\xi_3) = 4\xi_2\xi_3 \tag{2.6}$$

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

$$P(\xi_1,\xi_2,\xi_3) = p_1\xi_1 + p_2\xi_2 + p_3\xi_3 \tag{2.7}$$

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

ξ-η-Transformation

$$\xi_1 := 1 - \xi - \eta \tag{2.8}$$
$$\xi_2 := \xi \tag{2.9}$$
$$\xi_3 := \eta \tag{2.10}$$

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

Es gilt:

$$T(\xi,\eta) = \begin{bmatrix} 1 - \xi - \eta \\ \xi \\ \eta \end{bmatrix} \tag{2.11}$$

$$T^{-1}(\xi_1,\xi_2,\xi_3) = \xi_1\begin{bmatrix}0\\0\end{bmatrix} + \xi_2\begin{bmatrix}1\\0\end{bmatrix} + \xi_3\begin{bmatrix}0\\1\end{bmatrix} \tag{2.12}$$

3. Simplex Integration in $n = 2$

First start with definitions:

Pure Integrator   is any quadrature formula of the simplex:

$$I = \iint_\Delta f(\xi_1, \xi_2, \xi_3) \, d\Delta \approx \sum_i w_i f(\xi_{1,i}, \xi_{2,i}, \xi_{3,i}) \tag{3.1}$$

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

Subdivision Integrators   are Integrators of the form:

$$I = \iint_\Delta f(\xi_1, \xi_2, \xi_3) \, d\Delta = \sum_i \iint_{\Delta_i} f(\xi_1, \xi_2, \xi_3) \, d\Delta_i \tag{3.2}$$

which then will be evaluated by pure Integrators.
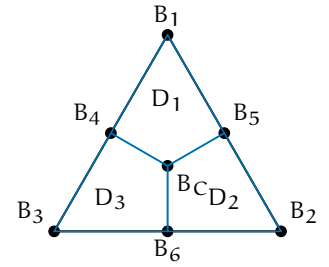
3.1. Pure Integrators

3.1.1. Quadrilaterial Integrator

Characteristic points in barycentric coordinates

$$B_C = \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{bmatrix} \tag{3.3}$$

$$B_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad B_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \qquad B_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \tag{3.4}$$

$$B_4 = \begin{bmatrix} 0.5 \\ 0 \\ 0.5 \end{bmatrix} \qquad B_5 = \begin{bmatrix} 0.5 \\ 0.5 \\ 0 \end{bmatrix} \qquad B_6 = \begin{bmatrix} 0 \\ 0.5 \\ 0.5 \end{bmatrix} \tag{3.5}$$

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

$$\Delta = D_1 \cup D_2 \cup D_3 \tag{3.6}$$

Therefore the double-Integral

$$\iint_\Delta F \, d\Delta = \iint_{D_1} F \, dD_1 + \iint_{D_2} F \, dD_2 + \iint_{D_3} F \, dD_3 \tag{3.7}$$

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

$$g_1(X) = \frac{X}{2} + \frac{1}{2} \qquad\qquad g_2(X) = -\frac{X}{2} + \frac{1}{2} \tag{3.8}$$

$$\frac{\partial g_1}{\partial X} = \frac{1}{2} \qquad\qquad \frac{\partial g_2}{\partial X} = -\frac{1}{2} \tag{3.9}$$

$$g_1(Y) = \frac{Y}{2} + \frac{1}{2} \qquad\qquad g_2(Y) = -\frac{Y}{2} + \frac{1}{2} \tag{3.10}$$

$$\frac{\partial g_1}{\partial Y} = \frac{1}{2} \qquad\qquad \frac{\partial g_2}{\partial Y} = -\frac{1}{2} \tag{3.11}$$

$$G_1(X, Y) = g_1(X)g_1(Y) \qquad\qquad G_2(X, Y) = g_1(X)g_2(Y) \tag{3.12}$$

$$G_3(X, Y) = g_2(X)g_1(Y) \qquad\qquad G_4(X, Y) = g_2(X)g_2(Y) \tag{3.13}$$

to barycentric coordinates of the D_1, D_2, D_3 Quadrilaterials

$$B_{D_1}(X, Y) = B_1 \cdot G_1(X, Y) + B_5 \cdot G_2(X, Y) + B_4 \cdot G_3(X, Y) + B_C \cdot G_4(X, Y) \qquad [3.14]$$
$$B_{D_2}(X, Y) = B_2 \cdot G_1(X, Y) + B_6 \cdot G_2(X, Y) + B_5 \cdot G_3(X, Y) + B_C \cdot G_4(X, Y) \qquad [3.15]$$
$$B_{D_3}(X, Y) = B_3 \cdot G_1(X, Y) + B_4 \cdot G_2(X, Y) + B_6 \cdot G_3(X, Y) + B_C \cdot G_4(X, Y) \qquad [3.16]$$

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

$$\iint_{[-1,1] \times [-1,1]} F(X, Y) \, d(X, Y) \approx \sum_i \sum_j F(X_i, X_j) w_i w_j \qquad [3.17]$$
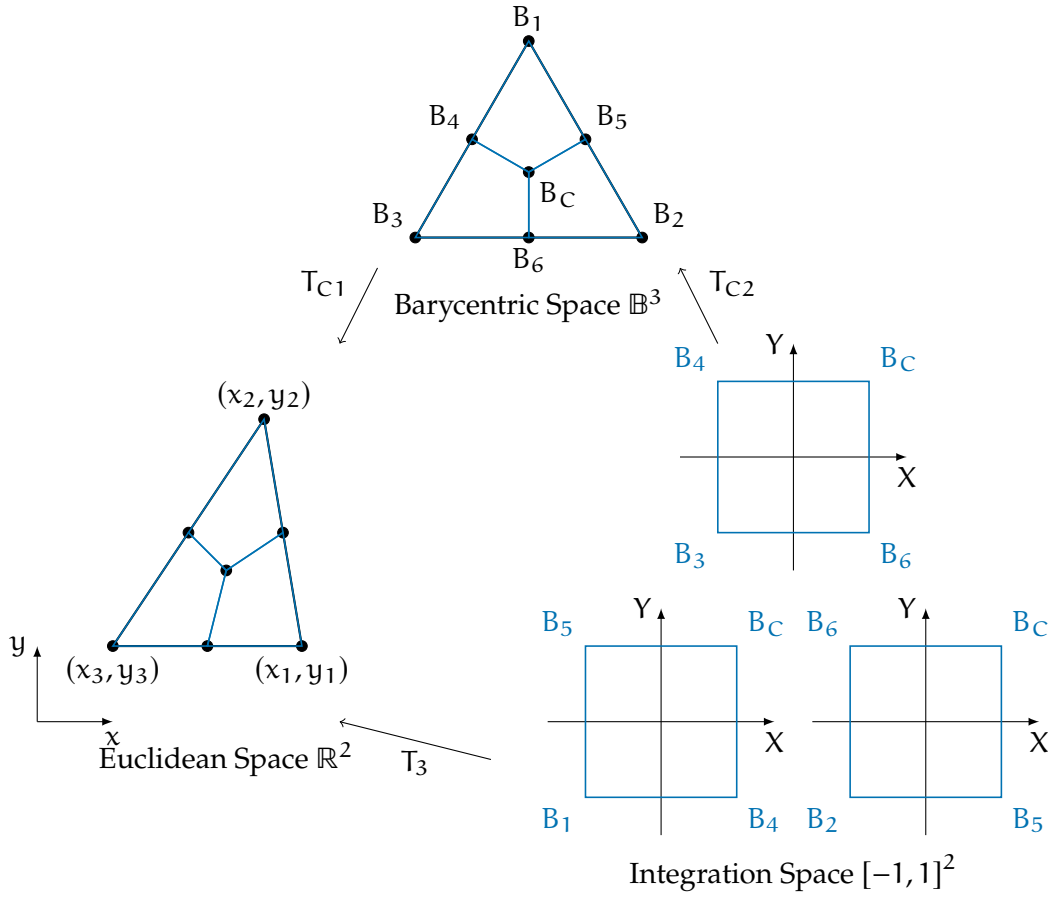
The Gauss-Points (X_i, X_j) and their weights w_i, w_j on the Square can be deduced from the one dimensional Gaussian Integration

$$\int_{-1}^{1} H(X) \, dX \approx \sum_i H(X_i) w_i \qquad [3.18]$$

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

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

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

$$S = \begin{bmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{bmatrix}$$ [3.19]

The Coordinates C_i of all characteristic points in Equations [3.3],[3.4] and [3.5] inside the simplex can be expressed in the following form

$$C_C = S \cdot B_C$$ [3.20]
$$C_i = S \cdot B_i \quad \forall i \in 1, 2, \ldots, 6$$ [3.21]

.

The transformation from points in the Integration Domain to the points in the bary-

centric given in [3.14],[3.15] and [3.16] can be expressed as

$$B_{D_1}(X, Y) = \begin{bmatrix} B_1 & B_5 & B_4 & B_C \end{bmatrix} \begin{bmatrix} G_1(X, Y) \\ G_2(X, Y) \\ G_3(X, Y) \\ G_4(X, Y) \end{bmatrix} \qquad [3.22]$$

$$B_{D_2}(X, Y) = \begin{bmatrix} B_2 & B_6 & B_5 & B_C \end{bmatrix} \begin{bmatrix} G_1(X, Y) \\ G_2(X, Y) \\ G_3(X, Y) \\ G_4(X, Y) \end{bmatrix} \qquad [3.23]$$

$$B_{D_3}(X, Y) = \begin{bmatrix} B_3 & B_4 & B_6 & B_C \end{bmatrix} \begin{bmatrix} G_1(X, Y) \\ G_2(X, Y) \\ G_3(X, Y) \\ G_4(X, Y) \end{bmatrix} \qquad [3.24]$$

With the Relationship given in [3.20] and [3.21] one can rewrite this as

$$C_{D_1}(X, Y) = S \begin{bmatrix} B_1 & B_5 & B_4 & B_C \end{bmatrix} \begin{bmatrix} G_1(X, Y) \\ G_2(X, Y) \\ G_3(X, Y) \\ G_4(X, Y) \end{bmatrix} \qquad [3.25]$$

$$C_{D_2}(X, Y) = S \begin{bmatrix} B_2 & B_6 & B_5 & B_C \end{bmatrix} \begin{bmatrix} G_1(X, Y) \\ G_2(X, Y) \\ G_3(X, Y) \\ G_4(X, Y) \end{bmatrix} \qquad [3.26]$$

$$C_{D_3}(X, Y) = S \begin{bmatrix} B_3 & B_4 & B_6 & B_C \end{bmatrix} \begin{bmatrix} G_1(X, Y) \\ G_2(X, Y) \\ G_3(X, Y) \\ G_4(X, Y) \end{bmatrix} \qquad [3.27]$$

With the Jacobi Matrix of any particular Domain being

$$J(C_{D_i}) = \begin{bmatrix} \frac{\partial C_{D_i}}{\partial X} & \frac{\partial C_{D_i}}{\partial Y} \end{bmatrix} = \begin{bmatrix} C_i & C_j & C_k & C_C \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial G_1}{\partial X} & \frac{\partial G_1}{\partial Y} \\ \frac{\partial G_2}{\partial X} & \frac{\partial G_2}{\partial Y} \\ \frac{\partial G_3}{\partial X} & \frac{\partial G_3}{\partial Y} \\ \frac{\partial G_4}{\partial X} & \frac{\partial G_4}{\partial Y} \end{bmatrix} \qquad [3.28]$$

Gauss Point Distribution   for the three Orders of Integration used.
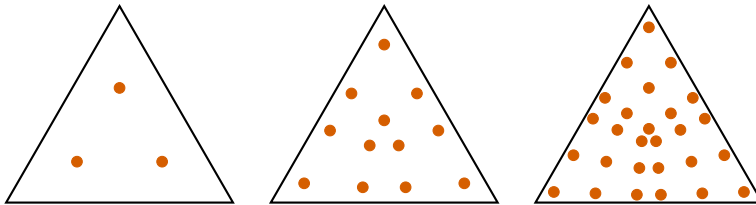
Gauss Points $n = 1$ Gauss Points $n = 2$ Gauss Points $n = 3$

3.1.2. Sphere Integrator

3.1.3. Other Quadrature Formulas

3.2. Subdivision Integrator

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 Simpleces Δ_i:

$$\iint_{\Delta_p} F\,d\Delta_p = \iint_{\Delta_1} F\,d\Delta_1 + \iint_{\Delta_2} F\,d\Delta_2 + \iint_{\Delta_3} F\,d\Delta_3 + \iint_{\Delta_4} F\,d\Delta_4 \qquad [3.29]$$
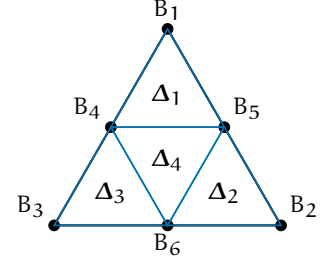
The Coordinates of a Child Simplex Δ_i can be expressed in local-barycentric coordinates $\xi'_{i,1}, \xi'_{i,2}, \xi'_{i,3}$

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

$$T_{lg}(\xi'_{i,1}, \xi'_{i,2}, \xi'_{i,3}) = B_{i,1}\xi'_{i,1} + B_{i,2}\xi'_{i,2} + B_{i,3}\xi'_{i,3} \qquad [3.30]$$

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.

3.3. Simplex Subdivision

A Criterion for adaptive integration

$$Q = \iint_{\Delta} F\,d\Delta \qquad [3.31]$$

$$\varepsilon = \left| Q - \iint_{\Delta_p} F\,d\Delta_p \right| \qquad [3.32]$$

The Coordinates of the Verteces of the 4 Child Simplizes Δ_i can be calculated with S by
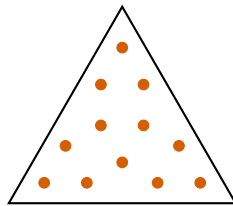
$$S_{\Delta,1} = S \cdot B_{\Delta,1} = S \cdot \begin{bmatrix} B_1 & B_5 & B_4 \end{bmatrix} = S \cdot \begin{bmatrix} 1 & 0.5 & 0.5 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \qquad [3.33]$$

$$S_{\Delta,2} = S \cdot B_{\Delta,2} = S \cdot \begin{bmatrix} B_2 & B_6 & B_5 \end{bmatrix} = S \cdot \begin{bmatrix} 0 & 0 & 0.5 \\ 1 & 0.5 & 0.5 \\ 0 & 0.5 & 0 \end{bmatrix} \qquad [3.34]$$

$$S_{\Delta,3} = S \cdot B_{\Delta,3} = S \cdot \begin{bmatrix} B_3 & B_4 & B_6 \end{bmatrix} = S \cdot \begin{bmatrix} 0 & 0.5 & 0 \\ 0 & 0 & 0.5 \\ 1 & 0.5 & 0.5 \end{bmatrix} \qquad [3.35]$$

$$S_{\Delta,4} = S \cdot B_{\Delta,4} = S \cdot \begin{bmatrix} B_4 & B_5 & B_6 \end{bmatrix} = S \cdot \begin{bmatrix} 0.5 & 0.5 & 0 \\ 0 & 0.5 & 0.5 \\ 0.5 & 0 & 0.5 \end{bmatrix} \qquad [3.36]$$

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

4. **Simplex Integration in** $n = 3$