Simplex Integration

By Domain Subdivision

Inhaltsverzeichnis

Teil I.
Theory

1. Problem

Total Energy in the System:

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

Degradation Function

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

mit

k . . . being a small but finite scalar such as 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

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

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

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)

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

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

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

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

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

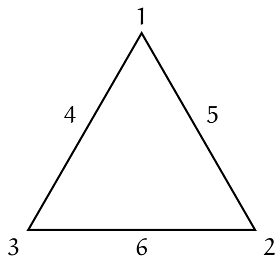
$$\Delta_{U_i}\, \delta_{U_i}\Pi = U_i \cdot \int_\Omega g(\phi)\frac{\partial\varepsilon}{\partial U_i} \cdot \mathbb{C} \cdot \frac{\partial\varepsilon}{\partial U_i}\, d\Omega \cdot \delta U_i \quad [1.12]$$

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

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

2. Element Description

Shape Functions in barycentric coordinates



$$N_1(\xi_1, \xi_2, \xi_3) = \xi_1 \quad [2.1]$$

$$N_2(\xi_1, \xi_2, \xi_3) = \xi_2 \quad [2.2]$$

$$N_3(\xi_1, \xi_2, \xi_3) = \xi_3 \quad [2.3]$$

$$N_4(\xi_1, \xi_2, \xi_3) = 4\xi_1\xi_3 \quad [2.4]$$

$$N_5(\xi_1, \xi_2, \xi_3) = 4\xi_1\xi_2 \quad [2.5]$$

$$N_6(\xi_1, \xi_2, \xi_3) = 4\xi_2\xi_3 \quad [2.6]$$

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

$$P(\xi_1, \xi_2, \xi_3) = p_1\xi_1 + p_2\xi_2 + p_3\xi_3 \quad [2.7]$$

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

ξ-η-Transformation

$$\xi_1 := 1 - \xi - \eta \quad [2.8]$$

$$\xi_2 := \xi \quad [2.9]$$

$$\xi_3 := \eta \quad [2.10]$$

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

Es gilt:

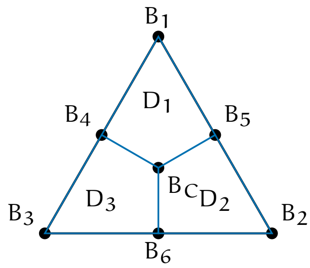
$$T(\xi, \eta) = \begin{bmatrix} 1 - \xi - \eta \\ \xi \\ \eta \end{bmatrix} \quad [2.11]$$

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

3. Simplex Integration in $n = 2$

3.1. Simplex Integration

Characteristic points in barycentric coordinates



$$B_C = \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{bmatrix} \quad [3.1]$$

$$B_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad B_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \qquad B_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad [3.2]$$

$$B_4 = \begin{bmatrix} 0.5 \\ 0 \\ 0.5 \end{bmatrix} \qquad B_5 = \begin{bmatrix} 0.5 \\ 0.5 \\ 0 \end{bmatrix} \qquad B_6 = \begin{bmatrix} 0 \\ 0.5 \\ 0.5 \end{bmatrix} \quad [3.3]$$

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

$$\boldsymbol{\Delta} = D_1 \cup D_2 \cup D_3 \quad [3.4]$$

Therefore the double-Integral

$$\iint_{\boldsymbol{\Delta}} F \, d\boldsymbol{\Delta} = \iint_{D_1} F \, dD_1 + \iint_{D_2} F \, dD_2 + \iint_{D_3} F \, dD_3 \quad [3.5]$$

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

$$g_1(X) = \frac{X}{2} + \frac{1}{2} \qquad g_2(X) = -\frac{X}{2} + \frac{1}{2} \quad [3.6]$$

$$\frac{\partial g_1}{\partial X} = \frac{1}{2} \qquad \frac{\partial g_2}{\partial X} = -\frac{1}{2} \quad [3.7]$$

$$g_1(Y) = \frac{Y}{2} + \frac{1}{2} \qquad g_2(Y) = -\frac{Y}{2} + \frac{1}{2} \quad [3.8]$$

$$\frac{\partial g_1}{\partial Y} = \frac{1}{2} \qquad \frac{\partial g_2}{\partial Y} = -\frac{1}{2} \quad [3.9]$$

$$G_1(X, Y) = g_1(X)g_1(Y) \qquad G_2(X, Y) = g_1(X)g_2(Y) \quad [3.10]$$

$$G_3(X, Y) = g_2(X)g_1(Y) \qquad G_4(X, Y) = g_2(X)g_2(Y) \quad [3.11]$$

to barycentric coordinates of the D_1, D_2, D_3 Quadrilaterials

$$B_{D_1}(X, Y) = B_1 \cdot G_1(X, Y) + B_5 \cdot G_2(X, Y) + B_4 \cdot G_3(X, Y) + B_C \cdot G_4(X, Y) \quad [3.12]$$

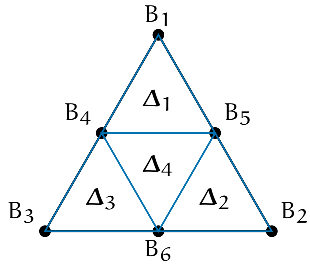
$$B_{D_2}(X, Y) = B_2 \cdot G_1(X, Y) + B_6 \cdot G_2(X, Y) + B_5 \cdot G_3(X, Y) + B_C \cdot G_4(X, Y) \quad [3.13]$$

$$B_{D_3}(X, Y) = B_3 \cdot G_1(X, Y) + B_4 \cdot G_2(X, Y) + B_6 \cdot G_3(X, Y) + B_C \cdot G_4(X, Y) \quad [3.14]$$

3.2. Simplex Subdivision

The Integral over a parent Simplex $\boldsymbol{\Delta}_p$, can be expressed as an Integral over 4 Child Simpleces $\boldsymbol{\Delta}_i$:

$$\iint_{\Delta_p} F \, d\boldsymbol{\Delta}_p = \iint_{\Delta_1} F \, d\boldsymbol{\Delta}_1 + \iint_{\Delta_2} F \, d\boldsymbol{\Delta}_2 + \iint_{\Delta_3} F \, d\boldsymbol{\Delta}_3 + \iint_{\Delta_4} F \, d\boldsymbol{\Delta}_4 \qquad [3.15]$$



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

$$T_{lg}(\xi'_{i,1}, \xi'_{i,2}, \xi'_{i,3}) = B_{i,1}\xi'_{i,1} + B_{i,2}\xi'_{i,2} + B_{i,3}\xi'_{i,3} \qquad [3.16]$$

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.

3.3. Numerical Integration Scheme

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

$$\iint_{[-1,1]\times[-1,1]} F(X,Y) \, d(X,Y) \approx \sum_i \sum_j F(X_i, X_j) w_i w_j \qquad [3.17]$$

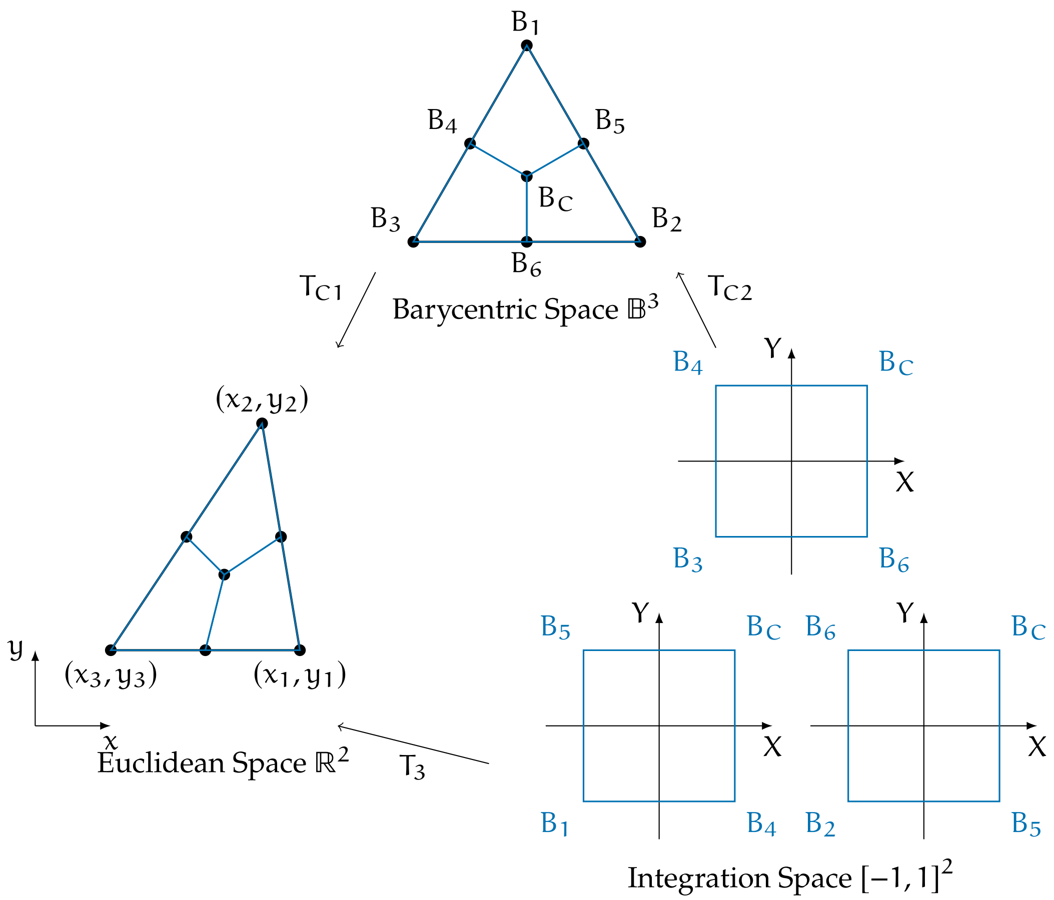
The Gauss-Points (X_i, X_j) and their weights w_i, w_j on the Square can be deduced from the one dimensional Gaussian Integration

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

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

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

3.4. Integraltransformation



Let S denote a Matrix of the coordinates of the vertices of the simplex in the following form

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

The Coordinates C_i of all characteristic points in Equations [3.1],[3.2] and [3.3] inside the simplex can be expressed in the following form

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

.

The transformation from points in the Integration Domain to the points in the barycentric given in [3.12],[3.13] and [3.14] can be expressed as

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

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

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

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

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

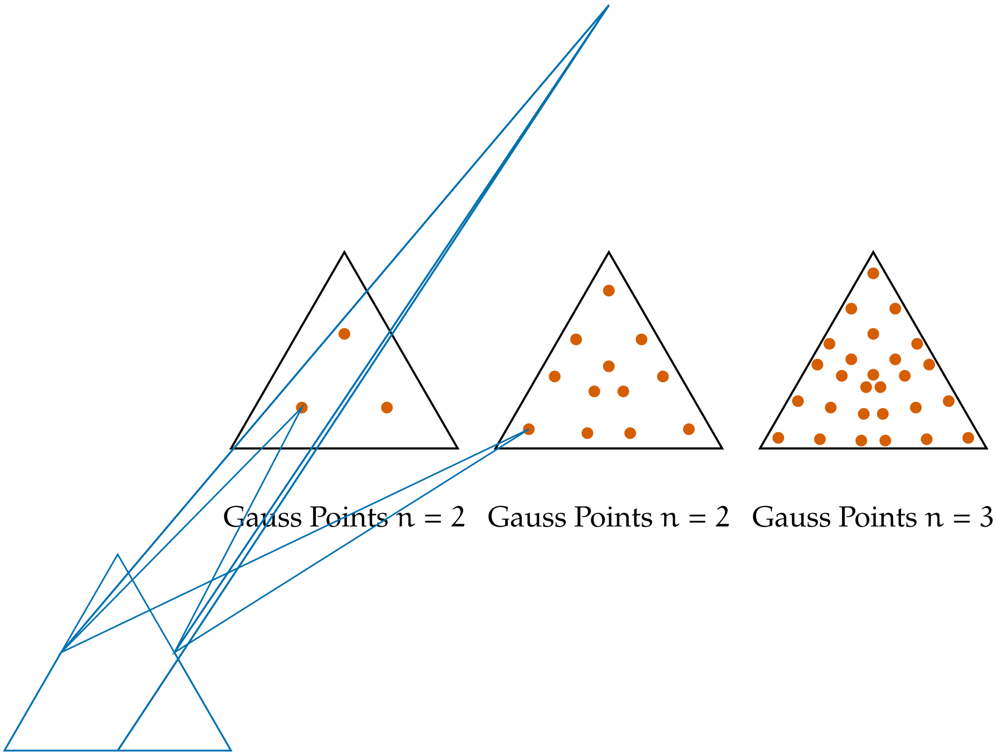
$$C_{D_2}(X,Y) = S \begin{bmatrix} B_2 & B_6 & B_5 & B_C \end{bmatrix} \begin{bmatrix} G_1(X,Y) \\ G_2(X,Y) \\ G_3(X,Y) \\ G_4(X,Y) \end{bmatrix} \quad [3.26]$$

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

With the Jacobi Matrix of any particular Domain being

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

3.4.1. Gauss Point Distribution



Gauss Points $n = 2$ Gauss Points $n = 2$ Gauss Points $n = 3$

4. Simplex Integration in $n = 3$