Whitepaper:
Elements based on the Lagrange shape-functions

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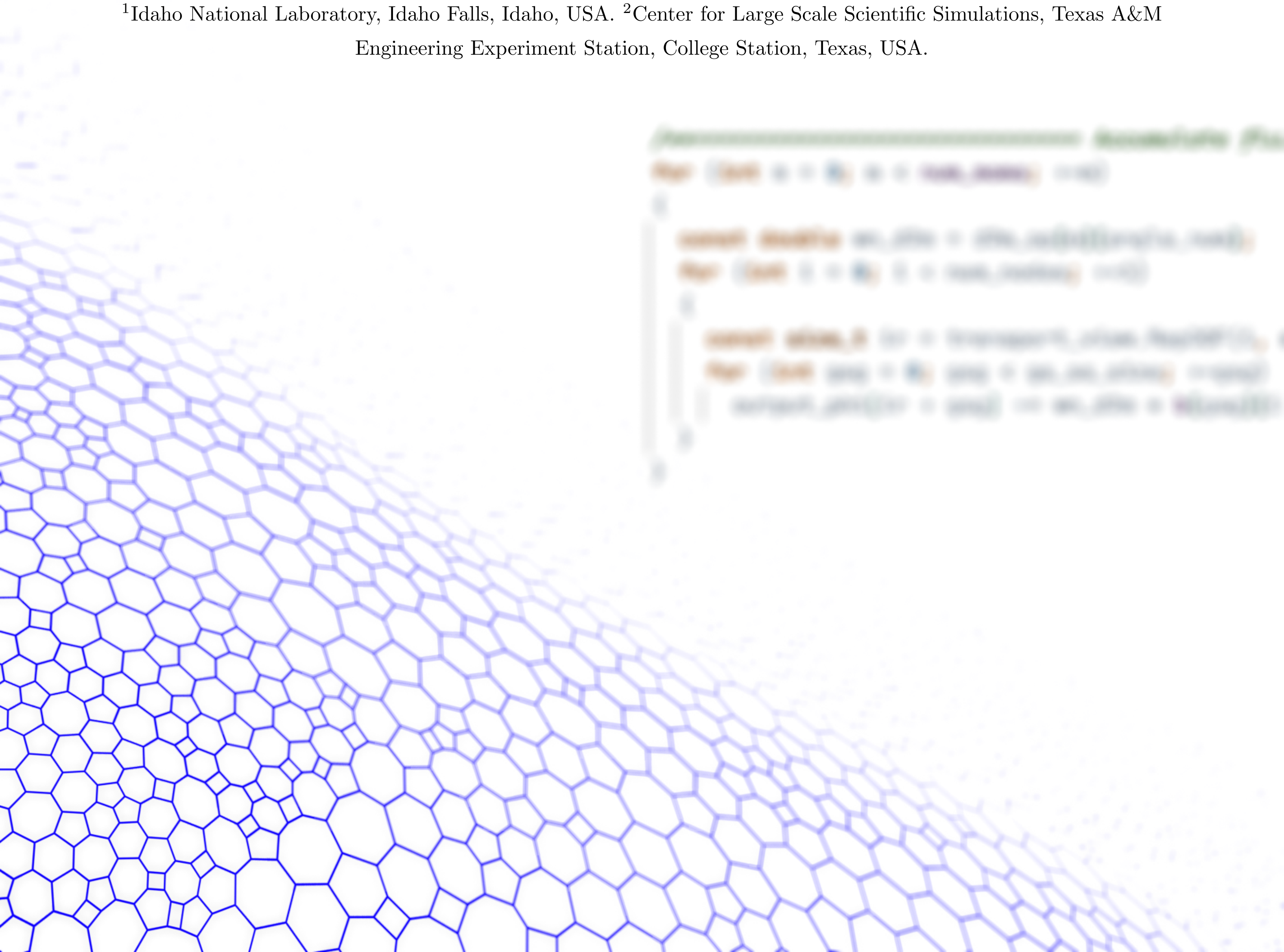

Abstract

The family of Lagrange finite elements shape functions are applied to the elements in ChiTech. This document details the mathematical formulations used in the code.

Keywords: Lagrange finite element shape functions

Contents

List of Figures

1 Need-to-know information

In the section that follows we define each element mapping we support. We refer to **world coordinates** with the vector $\mathbf{x}$ where $\mathbf{x} = [x, y, z]$, and subsequently **node coordinates** with $\mathbf{x}_i$ for the respective i-th node on an element where $\mathbf{x}_i = [x_i, y_i, z_i]$. We refer to **natural coordinates** with the $\bar{x}, \bar{y}, \bar{z}$ and element shape functions $N_i(\bar{x})$, $N_i(\bar{x}, \bar{y})$ or $N_i(\bar{x}, \bar{y}, \bar{z})$ depending on the element dimension. Shape function derivatives, $\dfrac{\partial N_i}{\partial \bar{x}}$ etc. are denoted with $\partial N_{i,\bar{x}}$.

1.1 The recipe for each element

For element definitions we follow the same recipe on each element, i.e.,

- Define the coordinate system in both natural- and world coordinates
- Define the spatial interpolation function
- Define the shape functions in natural coordinates
- Define the shape function derivatives in natural coordinates
- Define Jacobian entries
- Define the Jacobian (not explicitly)

1.2 Transformation of shape function gradients

Finite Element weak forms often require the shape function gradients, i.e.,

$$\int_V \boldsymbol{\nabla} N_i \boldsymbol{\cdot} \boldsymbol{\nabla} N_j dV \quad \text{or} \quad \int_V N_i \boldsymbol{\nabla} N_j dV, \tag{1.1}$$

however these gradients are needed in world coordinates. For the components of the gradient we use the chain rule to write

$$\begin{aligned}
\frac{\partial N_i}{\partial \bar{x}} &= \frac{\partial x}{\partial \bar{x}}\frac{\partial N_i}{\partial x} + \frac{\partial y}{\partial \bar{x}}\frac{\partial N_i}{\partial y} + \frac{\partial z}{\partial \bar{x}}\frac{\partial N_i}{\partial z} \\
\frac{\partial N_i}{\partial \bar{y}} &= \frac{\partial x}{\partial \bar{y}}\frac{\partial N_i}{\partial x} + \frac{\partial y}{\partial \bar{y}}\frac{\partial N_i}{\partial y} + \frac{\partial z}{\partial \bar{y}}\frac{\partial N_i}{\partial z} \\
\frac{\partial N_i}{\partial \bar{z}} &= \frac{\partial x}{\partial \bar{z}}\frac{\partial N_i}{\partial x} + \frac{\partial y}{\partial \bar{z}}\frac{\partial N_i}{\partial y} + \frac{\partial z}{\partial \bar{z}}\frac{\partial N_i}{\partial z}
\end{aligned} \tag{1.2}$$

which can be written in vector and matrix format as

$$\begin{bmatrix} \dfrac{\partial N_i}{\partial \bar{x}} \\ \dfrac{\partial N_i}{\partial \bar{y}} \\ \dfrac{\partial N_i}{\partial \bar{z}} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial x}{\partial \bar{x}} & \dfrac{\partial y}{\partial \bar{x}} & \dfrac{\partial z}{\partial \bar{x}} \\ \dfrac{\partial x}{\partial \bar{y}} & \dfrac{\partial y}{\partial \bar{y}} & \dfrac{\partial z}{\partial \bar{y}} \\ \dfrac{\partial x}{\partial \bar{z}} & \dfrac{\partial y}{\partial \bar{z}} & \dfrac{\partial z}{\partial \bar{z}} \end{bmatrix} \begin{bmatrix} \dfrac{\partial N_i}{\partial x} \\ \dfrac{\partial N_i}{\partial y} \\ \dfrac{\partial N_i}{\partial z} \end{bmatrix} \tag{1.3}$$

Moreover, the Jacobian matrix is fundamentally defined as

$$J = \begin{bmatrix} \dfrac{\partial x}{\partial \bar{x}} & \dfrac{\partial x}{\partial \bar{y}} & \dfrac{\partial x}{\partial \bar{z}} \\ \dfrac{\partial y}{\partial \bar{x}} & \dfrac{\partial y}{\partial \bar{y}} & \dfrac{\partial y}{\partial \bar{z}} \\ \dfrac{\partial z}{\partial \bar{x}} & \dfrac{\partial z}{\partial \bar{y}} & \dfrac{\partial z}{\partial \bar{z}} \end{bmatrix} \tag{1.4}$$

and therefore we can see that the following identity holds

$$\boldsymbol{\nabla} N_i = \begin{bmatrix} \partial N_{i,x} \\ \partial N_{i,y} \\ \partial N_{i,z} \end{bmatrix} = (J^T)^{-1} \begin{bmatrix} \partial N_{i,\bar{x}} \\ \partial N_{i,\bar{y}} \\ \partial N_{i,\bar{z}} \end{bmatrix}. \tag{1.5}$$

1.3 Volume integrations

When computing volume integrals on an element we follow the quadrature-rule integration paradigm:

$$\int_V g_i(\mathbf{x}) f(\mathbf{x}) dV = \int_V g_i(\bar{\mathbf{x}}_q) f(\mathbf{x}_q)\ |J(\bar{\mathbf{x}}_q)| d\bar{x} d\bar{y} d\bar{z} = \sum_q \bar{w}_q |J(\bar{\mathbf{x}}_q)| g_i(\bar{\mathbf{x}}_q) f(\mathbf{x}_q), \tag{1.6}$$

where $\bar{w}_q$ is the quadrature weight, $|J(\bar{\mathbf{x}}_q)|$ is the determinant of the Jacobian at the quadrature point, $\bar{\mathbf{x}}_q$ is the quadrature point in natural coordinates, $\mathbf{x}_q$ is the quadrature point in world coordinates, and g_i is either the shape function N_i or its gradient $\boldsymbol{\nabla} N_i$. We can precompute the following values at each quadrature point:

- The effective quadrature weight, w_q, which is the product of the quadrature weight and the Jacobian's determinant, $w_q = \bar{w}_q |J(\bar{\mathbf{x}}_q)|$
- The shape function values, N_i
- The shape function gradient values, $\boldsymbol{\nabla} N_i$
- The quadrature point world coordinates, $\mathbf{x}_q$

In order to compute the necessary values at the quadrature points we apply the following procedure:

```
for qp in qp_indices:
  qpoint = volume_quadrature.qpoints[qp]
  J = element.GetJacobian(qpoint)
  JT = Transpose(J)
  JTinv = Inverse(JT)
  detJ = Determinant(J)


  weight = quadrature.weight * detJ

  qpoint_world = [0,0,0]
  for i in node_indices:
    shape_i = element.Shape(i, qpoint)
    grad_shape_i = MatMult(JTinv, element.GradShape(i, qpoint))

    qpoint_world += shape_i * x_i
```

1.4 Surface integrations

Dealing with surface integrals on elements can be a confusing endeavour. Firstly, the surface integrals are performed per face of an element. On such faces the quadrature-rule is very much different from the volumetric quadrature-rule because it has one less dimension, consequently the transformation involves a different Jacobian-determinant, i.e., from the surface Jacobian, J_s. The paradigm is as follows:

$$\int_S \mathbf{n}\ g_i(\mathbf{x}) f(\mathbf{x}) dA = \int_S \mathbf{n}\ g_i(\bar{\mathbf{x}}) f(\mathbf{x})\ |J_s(\bar{\mathbf{x}})| d\bar{x} d\bar{y} = \sum_q \mathbf{n}_q \bar{w}_q |J_s(\bar{\mathbf{x}}_q)| g_i(\bar{\mathbf{x}}) f(\mathbf{x}_q). \tag{1.7}$$

Here we need the same quantities that we needed for the volume integration (N_i are now the surface shape functions), however, in addition we need, $\mathbf{n}_q$, the normal at the quadrature point, and $|J_s(\bar{\mathbf{x}}_q)|$, the determinant of the **surface** Jacobian at the quadrature point.

1.4.1 1D elements

For 1D elements the faces are points and therefore no transformation is required, i.e., $|J_s| = 1$ and the face normal is constant.

1.4.2 2D elements

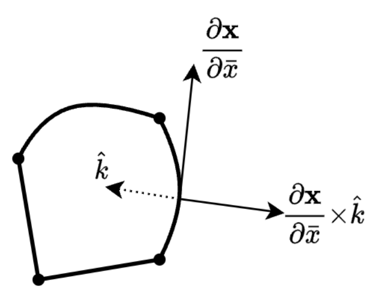

Figure 1.1: Orientations for 2D surface integrals. $\hat{k}$ is pointing out of the page.

For 2D elements the faces are 1D and we need

$$\frac{\partial \mathbf{x}}{\partial \bar{x}} = \sum_i \frac{\partial N_i}{\partial \bar{x}} \mathbf{x}_i, \tag{1.8}$$

as shown in Figure 1.1, from which $|J_s|$ is the magnitude of this vector at the quadrature point,

$$|J_s| = ||\frac{\partial \mathbf{x}}{\partial \bar{x}}||. \tag{1.9}$$

As a byproduct the normal can be computed using the upward (out of the page) point $\hat{k}$ as

$$\mathbf{n}_q = \frac{\frac{\partial \mathbf{x}}{\partial \bar{x}} \times \hat{k}}{||\frac{\partial \mathbf{x}}{\partial \bar{x}} \times \hat{k}||} \tag{1.10}$$

1.4.3 3D elements

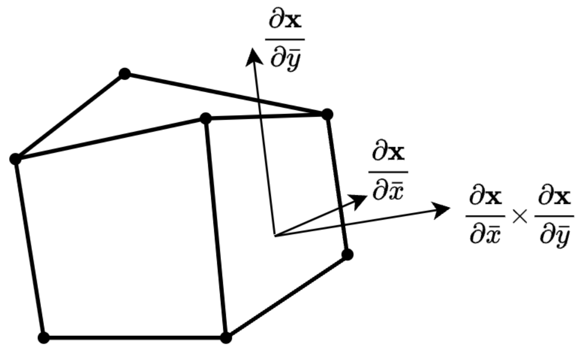

Figure 1.2: Orientations for 3D surface integrals.

For 3D elements the faces are 2D and we need the two vectors

$$\begin{aligned} \frac{\partial \mathbf{x}}{\partial \bar{x}} &= \sum_i \frac{\partial N_i}{\partial \bar{x}} \mathbf{x}_i \\ \frac{\partial \mathbf{x}}{\partial \bar{y}} &= \sum_i \frac{\partial N_i}{\partial \bar{y}} \mathbf{x}_i \end{aligned} \tag{1.11}$$

after which the surface jacobian is the magnitude of the cross product of these two vectors

$$|J_s| = ||\frac{\partial \mathbf{x}}{\partial \bar{x}} \times \frac{\partial \mathbf{x}}{\partial \bar{y}}||. \tag{1.12}$$

As a byproduct this cross-product can also be used to compute the normal at that point,

$$\mathbf{n}_q = \frac{\frac{\partial \mathbf{x}}{\partial \bar{x}} \times \frac{\partial \mathbf{x}}{\partial \bar{y}}}{||\frac{\partial \mathbf{x}}{\partial \bar{x}} \times \frac{\partial \mathbf{x}}{\partial \bar{y}}||} = \frac{1}{|J_s|} \frac{\partial \mathbf{x}}{\partial \bar{x}} \times \frac{\partial \mathbf{x}}{\partial \bar{y}} \tag{1.13}$$

1.4.4 Computing the surface quadrature point data

In order to compute the necessary values at the surface quadrature points we apply the following procedure:

```
f = face_index
for qp in qp_indices:
  qpoint_face = surface_quadrature.qpoints[qp]
  qpoint = element.ConvertFaceQPToElement(qpoint_face)
  J = element.GetJacobian(qpoint)
  JT = Transpose(J)
  JTinv = Inverse(JT)

  detJ, normal_q = element.GetFaceDetJandNormal(f, qpoint_face)

  weight = quadrature.weight * detJ

  qpoint_world = [0,0,0]
```

```
for i in node_indices:
shape_i = element.Shape(i, qpoint)
grad_shape_i = MatMult(JTinv, element.GradShape(i, qpoint))

qpoint_world += shape_i * x_i
```

2 Element definitions

2.1 One dimensional Slab elements

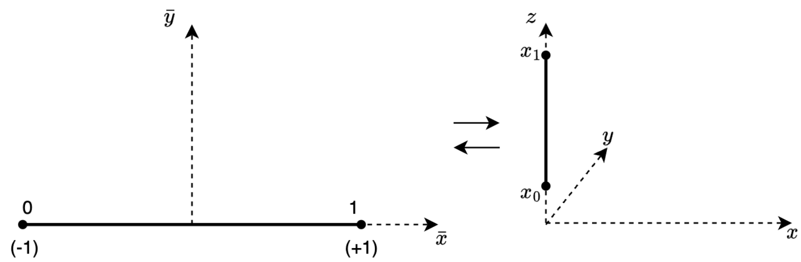

Figure 2.1: Reference coordinates for a slab.

Fundamental interpolation function:

$$\mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ y \\ \sum_i N_i(\bar{x}) z_i \end{bmatrix} \tag{2.1}$$

Shape function definitions:

$$N_0(\bar{x}) = \frac{1-\bar{x}}{2}, \quad N_1(\bar{x}) = \frac{1+\bar{x}}{2} \tag{2.2}$$

Derivatives:

$$\partial N_{0,\bar{x}} = -\frac{1}{2}, \quad \partial N_{1,\bar{x}} = \frac{1}{2} \tag{2.3}$$

Jacobian entries:

$$\frac{\partial z}{\partial \bar{x}} = \sum_i \partial N_{i,\bar{x}} z_i = -\frac{1}{2} z_0 + \frac{1}{2} z_1 \tag{2.4}$$

Jacobian:

$$J = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{\partial z}{\partial \bar{x}} \end{bmatrix} \tag{2.5}$$

2.2 Two dimensional Triangle elements

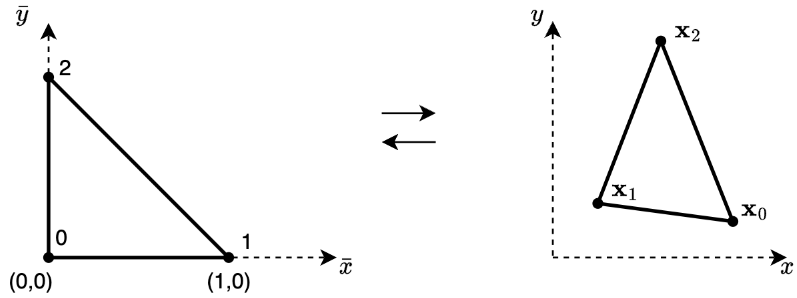

Figure 2.2: Reference coordinates for a triangle

Fundamental interpolation function:

$$\mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \sum_i N_i(\bar{x},\bar{y})x_i \\ \sum_i N_i(\bar{x},\bar{y})y_i \\ z \end{bmatrix} \tag{2.6}$$

Shape function definitions:

$$\begin{aligned} N_0(\bar{x},\bar{y}) &= 1-\bar{x}-\bar{y} \\ N_1(\bar{x},\bar{y}) &= \bar{x} \\ N_2(\bar{x},\bar{y}) &= \bar{y} \end{aligned} \tag{2.7}$$

Derivatives:

$$\begin{aligned} \partial N_{0,\bar{x}} &= -1, \quad \partial N_{0,\bar{y}} = -1 \\ \partial N_{1,\bar{x}} &= 1, \quad \partial N_{1,\bar{y}} = 0 \\ \partial N_{2,\bar{x}} &= 0, \quad \partial N_{2,\bar{y}} = 1 \end{aligned} \tag{2.8}$$

Jacobian entries, $d = [x,y]$, $\bar{d} = [\bar{x},\bar{y}]$:

$$\frac{\partial d}{\partial \bar{d}} = \sum_i \partial N_{i,\bar{d}}\, d_i \tag{2.9}$$

$$\begin{aligned} \frac{\partial x}{\partial \bar{x}} &= x_1-x_0, \quad \frac{\partial x}{\partial \bar{y}} = x_2-x_0 \\ \frac{\partial y}{\partial \bar{x}} &= y_1-y_0, \quad \frac{\partial y}{\partial \bar{y}} = y_2-y_0 \end{aligned} \tag{2.10}$$

Jacobian:

$$J = \begin{bmatrix} \frac{\partial x}{\partial \bar{x}} & \frac{\partial x}{\partial \bar{y}} & 0 \\ \frac{\partial y}{\partial \bar{x}} & \frac{\partial y}{\partial \bar{y}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{2.11}$$

2.3 Two dimensional Quadrilateral elements

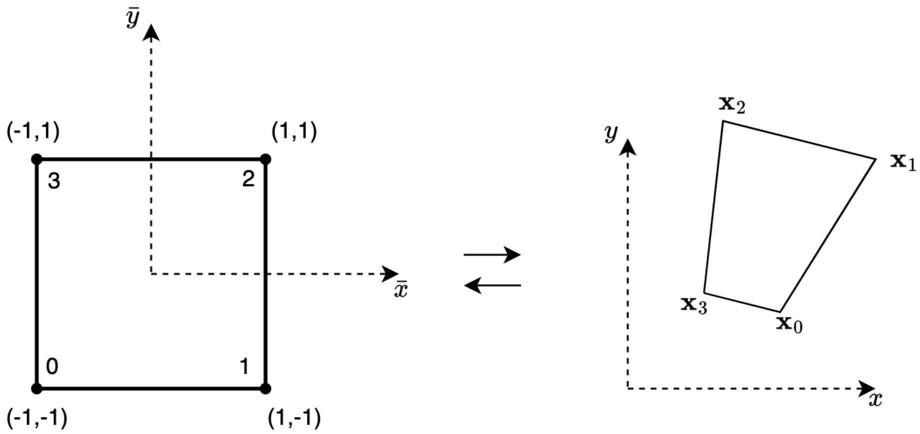

Figure 2.3: Reference coordinates for a quadrilateral

Fundamental interpolation function:

$$\mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \sum_i N_i(\bar{x},\bar{y})x_i \\ \sum_i N_i(\bar{x},\bar{y})y_i \\ z \end{bmatrix} \tag{2.12}$$

Shape function definitions:

$$\begin{aligned} a, b &= \bar{x}_i, \bar{y}_i \\ N_i(\bar{x},\bar{y}) &= \frac{1}{4}(1{+}a\bar{x})(1{+}b\bar{y}) \end{aligned} \tag{2.13}$$

Derivatives:

$$\begin{aligned} \partial N_{i,\bar{x}} &= \tfrac{1}{4}(a{+}ab\bar{y}) \\ \partial N_{i,\bar{y}} &= \tfrac{1}{4}(b{+}ab\bar{x}) \end{aligned} \tag{2.14}$$

Jacobian entries, $d = [x, y]$, $\bar{d} = [\bar{x}, \bar{y}]$:

$$\frac{\partial d}{\partial \bar{d}} = \sum_i \partial N_{i,\bar{d}}\; d_i \tag{2.15}$$

Jacobian:

$$J = \begin{bmatrix} \dfrac{\partial x}{\partial \bar{x}} & \dfrac{\partial x}{\partial \bar{y}} & 0 \\ \dfrac{\partial y}{\partial \bar{x}} & \dfrac{\partial y}{\partial \bar{y}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{2.16}$$

2.4 Three dimensional Tetrahedral elements

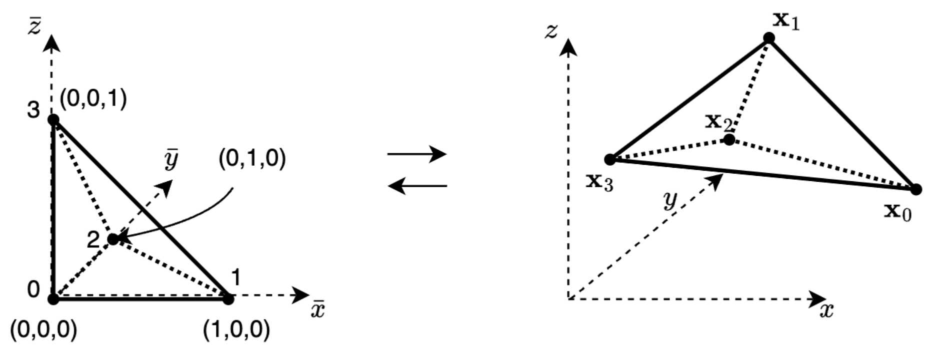

Figure 2.4: Reference coordinates for a tetrahedron

Fundamental interpolation function: Fundamental interpolation function:

$$\mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \sum_i N_i(\bar{x}, \bar{y}, \bar{z}) x_i \\ \sum_i N_i(\bar{x}, \bar{y}, \bar{z}) y_i \\ \sum_i N_i(\bar{x}, \bar{y}, \bar{z}) z_i \end{bmatrix} \tag{2.17}$$

Shape function definitions:

$$\begin{aligned} N_0(\bar{x}, \bar{y}, \bar{z}) &= 1 - \bar{x} - \bar{y} - \bar{z} \\ N_1(\bar{x}, \bar{y}, \bar{z}) &= \bar{x} \\ N_2(\bar{x}, \bar{y}, \bar{z}) &= \bar{y} \\ N_3(\bar{x}, \bar{y}, \bar{z}) &= \bar{z} \end{aligned} \tag{2.18}$$

Derivatives:

$$\begin{array}{ccc} \partial N_{0,\bar{x}} = -1 & \partial N_{0,\bar{y}} = -1 & \partial N_{0,\bar{z}} = -1 \\ \partial N_{1,\bar{x}} = 1 & \partial N_{1,\bar{y}} = 0 & \partial N_{1,\bar{z}} = 0 \\ \partial N_{2,\bar{x}} = 0 & \partial N_{2,\bar{y}} = 1 & \partial N_{2,\bar{z}} = 0 \\ \partial N_{3,\bar{x}} = 0 & \partial N_{3,\bar{y}} = 0 & \partial N_{3,\bar{z}} = 1 \end{array} \tag{2.19}$$

Jacobian entries, $d = [x, y, z]$, $\bar{d} = [\bar{x}, \bar{y}, \bar{z}]$:

$$\frac{\partial d}{\partial \bar{d}} = \sum_i \partial N_{i,\bar{d}} \, d_i \tag{2.20}$$

Jacobian:

$$J = \begin{bmatrix} \frac{\partial x}{\partial \bar{x}} & \frac{\partial x}{\partial \bar{y}} & \frac{\partial x}{\partial \bar{z}} \\ \frac{\partial y}{\partial \bar{x}} & \frac{\partial y}{\partial \bar{y}} & \frac{\partial y}{\partial \bar{z}} \\ \frac{\partial z}{\partial \bar{x}} & \frac{\partial z}{\partial \bar{y}} & \frac{\partial z}{\partial \bar{z}} \end{bmatrix} \tag{2.21}$$

2.5 Three dimensional Hexahedral elements

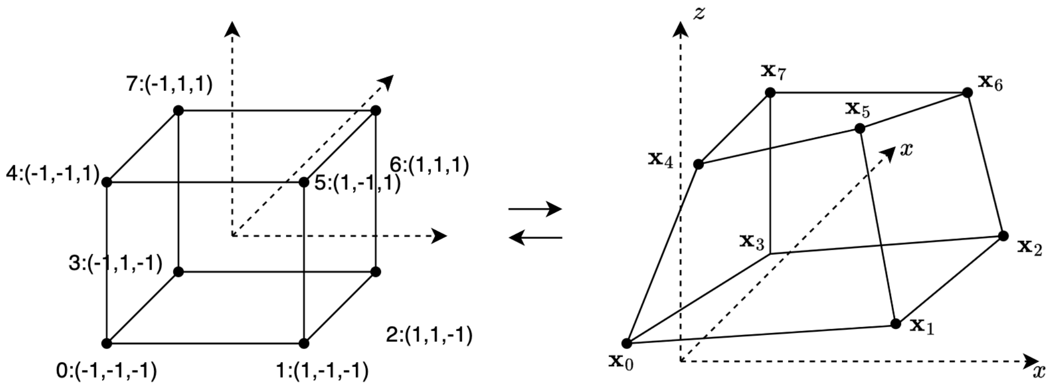

Figure 2.5: Reference coordinates of a hexahedron

Fundamental interpolation function:

$$\mathbf{x} = \sum_i N_i(\bar{x})\mathbf{x}_i \tag{2.22}$$

Shape function definitions:

$$\begin{aligned} a, b, c &= \bar{x}_i, \bar{y}_i, \bar{z}_i \\ N_i(\bar{x}, \bar{y}, \bar{z}) &= \frac{1}{8}(1+a\bar{x})(1+b\bar{y})(1+c\bar{z}) \\ &= \frac{1}{8}(1+a\bar{x}+b\bar{y}+c\bar{z}+ab\bar{x}\bar{y}+bc\bar{y}\bar{z}+ac\bar{x}\bar{z}+abc\bar{x}\bar{y}\bar{z}) \end{aligned} \tag{2.23}$$

Derivatives:

$$\begin{aligned} \partial N_{i,\bar{x}} &= \tfrac{1}{8}(a+ab\bar{y}+ac\bar{z}+abc\bar{y}\bar{z}) \\ \partial N_{i,\bar{y}} &= \tfrac{1}{8}(b+ab\bar{x}+bc\bar{z}+abc\bar{x}\bar{z}) \\ \partial N_{i,\bar{z}} &= \tfrac{1}{8}(c+bc\bar{y}+ac\bar{x}+abc\bar{x}\bar{y}) \end{aligned} \tag{2.24}$$

Jacobian entries, $d = [x, y, z]$, $\bar{d} = [\bar{x}, \bar{y}, \bar{z}]$:

$$\frac{\partial d}{\partial \bar{d}} = \sum_i \partial N_{i,\bar{d}}\; d_i \tag{2.25}$$

Jacobian:

$$J = \begin{bmatrix} \frac{\partial x}{\partial \bar{x}} & \frac{\partial x}{\partial \bar{y}} & \frac{\partial x}{\partial \bar{z}} \\ \frac{\partial y}{\partial \bar{x}} & \frac{\partial y}{\partial \bar{y}} & \frac{\partial y}{\partial \bar{z}} \\ \frac{\partial z}{\partial \bar{x}} & \frac{\partial z}{\partial \bar{y}} & \frac{\partial z}{\partial \bar{z}} \end{bmatrix} \tag{2.26}$$

2.6 Three dimensional Wedge elements

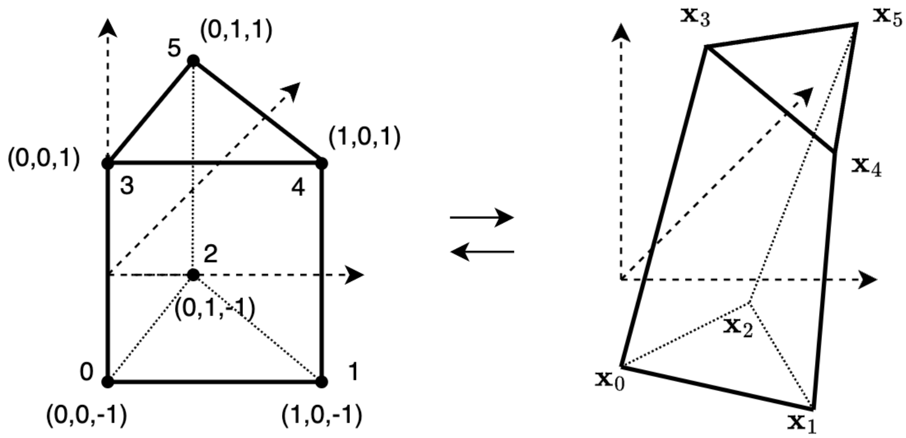

Figure 2.6: Reference coordinates for a wedge.

Shape function definitions:

$$
\begin{aligned}
N_0(\bar{x},\bar{y},\bar{z}) &= (1-\bar{x}-\bar{y})\left(\frac{1-\bar{z}}{2}\right)\\
N_1(\bar{x},\bar{y},\bar{z}) &= \bar{x}\left(\frac{1-\bar{z}}{2}\right)\\
N_2(\bar{x},\bar{y},\bar{z}) &= \bar{y}\left(\frac{1-\bar{z}}{2}\right)\\
N_3(\bar{x},\bar{y},\bar{z}) &= (1-\bar{x}-\bar{y})\left(\frac{1+\bar{z}}{2}\right)\\
N_4(\bar{x},\bar{y},\bar{z}) &= \bar{x}\left(\frac{1+\bar{z}}{2}\right)\\
N_5(\bar{x},\bar{y},\bar{z}) &= \bar{y}\left(\frac{1+\bar{z}}{2}\right)
\end{aligned}
\tag{2.27}
$$

Jacobian entries, $d = [x, y, z]$, $\bar{d} = [\bar{x}, \bar{y}, \bar{z}]$:

$$
\frac{\partial d}{\partial \bar{d}} = \sum_i \partial N_{i,\bar{d}}\; d_i \tag{2.28}
$$

Jacobian:

$$
J = \begin{bmatrix}
\frac{\partial x}{\partial \bar{x}} & \frac{\partial x}{\partial \bar{y}} & \frac{\partial x}{\partial \bar{z}}\\
\frac{\partial y}{\partial \bar{x}} & \frac{\partial y}{\partial \bar{y}} & \frac{\partial y}{\partial \bar{z}}\\
\frac{\partial z}{\partial \bar{x}} & \frac{\partial z}{\partial \bar{y}} & \frac{\partial z}{\partial \bar{z}}
\end{bmatrix} \tag{2.29}
$$

References

[1] Huebner K.H., Thornton E.A., Byrom T.G., *The Finite Element Method for Engineers*, third edition. 1995.