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# **Development of a FEM code for fluid-structure coupling**

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# 1 Introduction

Here comes the introduction. And before that the abstract (that needs to be put into LaTeX as special paragraph)

## 2 Framework Evaluation

Part of the thesis was to find several frameworks which ease the work with the finite element method. An evaluation of these frameworks was done to select a suitable one for the given task. The evaluation's criteria are presented in this chapter as well as a short description of the studied frameworks.

### 2.1 General Aspects

In preparation of evaluating the frameworks many criteria were created to objectify the search for the most suitable. The individual aspects were as follows:

- **Open Source:** All frameworks under consideration need to be published under the GNU Lesser General Public License or similar license that allows modification and/or redistribution.
- **Parallelization:** In order to accelerate the calculations the framework has to be able to support the widely used Message Passing Interface (MPI).
- **The programming language was chosen to be C++.** Therefore the framework has to be written in this language.
- **Mesh file import:** Common mesh files types like gmsh or xda/xdr must be able to load by the framework. Simultaneously the framework must support finite elements like triangles and quadrilaterals with three and four nodes respectively and be able to handle two dimensional elements defined within three dimensional space.
- **The framework should handle different types of boundary conditions defined in a mesh file.**
- **Built-in solvers:** In order so solve the matrix-vector-system the framework must provide a variety of different iterative solvers.
- **Convenience functions:** To optimize the calculations the framework should make use of functions to get matrix-vector and matrix-matrix products, transpose matrix or sparse-matrices.
- **Accessible and detailed documentation:** In order to guarantee maintainability and expandability the framework has to have a good documentation itself.
- **Up-to-date:** The framework should be well maintained and actively supported by its developers to ensure a long term compatibility with possible new features of the thesis' code
- **The framework should be used by at least a few projects.** This shows the framework's importance and usability.
- **Easy-to-learn syntax and structure:** A rather subjective aspect but an important one. The limited time for the thesis does not allow to study highly complicated structures or semantics. This accompanies the documentation aspect.

## 2.2 Frameworks Overview

The following list contains FEM libraries and frameworks which were evaluated.

### 2.2.1 Feel++

- "Feel++ is a unified C++ implementation of Galerkin methods (finite and spectral element methods) in 1D, 2D and 3D to solve partial differential equations." [Con]
- creation of versatile mathematical kernels allow testing and comparing different techniques and methods in solving problems
- focus on close mathematical abstractions regarding partial differential equations (PDE)
- [PCD<sup>+</sup>12] - imports e.g. gmsh mesh files
- seamlessly parallel with mpi
- currently used in projects at Cemosis (Center for Modeling and Simulation in Strasbourg, France) including fluid structure interactions, high field magnets simulation, or, optical tomography
- actively developed, last major release were on February 2015

### 2.2.2 OOFEM

- [Pat09] - Object Oriented Finite Element Solver (OOFEM) - actively developed with latest release from February 2014
- object oriented architecture; extensible in terms of new element types, boundary conditions or numerical algorithms
  - modules for structural mechanics, transport problems and fluid dynamics
  - focuses on efficient and robust solution to mechanical, transport and fluid problems
  - written in C++ with focus on portability
  - interfaces to various external software libraries like PETSc, ParMETIS, or, ParaView
  - is used in several publications [Pat]

### 2.2.3 GetFEM++

- latest release from July 2015 - framework for solving potentially coupled systems of linear and nonlinear PDE
- written in C++ but provides interfaces to languages like Python and Matlab
- model description that gather the variables, data and terms of a problem and some predefined bricks representing classical models
- easy switching from one method to another due to separation of geometric transformation, integration methods, and, finite element method
- can be used to construct generic finite element codes, where methods and the problem's dimension can be changed very easily
- uses MPI for parallelization, though it is stated that "a certain number of procedures are still remaining sequential" [SPR] - imports e.g. gmsh mesh files
- used in project like IceTools [Jar] (open source model for glaciers), EChem++ [BLSS]

(Problem Solving Environment for Electrochemistry) and SimNIBS [Thi] (software for Simulation of Non-invasive Brain Stimulation)

#### 2.2.4 MFEM

[mfeb] - The Modular Finite Element Method (MFEM) library acts as a toolbox that provides the building blocks for developing finite element algorithms

- it has a wide range of mesh types, e.g. triangular and quadrilateral 2D elements, curved boundary elements or topologically periodic meshes
- supports MPI-based parallelism throughout the library
- variety of built-in solvers
- written in highly portable C++ and extensible due to separation of mesh, finite element and linear algebra abstractions
- hypre library is tightly integrated within MFEM, for example the use of high-performance preconditioners

- The object oriented design of the library as well as the separation of the different parts of the library like the mesh functions, the finite elements, and, the linear algebra, focusing on adapt the code to a variety of applications - use in several publications [mfea]

#### 2.2.5 libMesh

[KPSC06] - actively developed and active user community

- wide variety of mesh file formats to import from (e.g. gmsh, vtk, xda, )
- seamlessly integrated parallel functionality with MPI
- seamlessly interfaces optional external libraries like PETSc or ParMETIS
- complete documentation and documented source code available
- "framework for the numerical simulation of PDE using arbitrary unstructured discretizations on serial and parallel platforms".
- "provide support for adaptive mesh refinement (AMR) computations in parallel"
- supports a variety of 1D, 2D, and 3D geometric and finite element types
- created at The University of Texas at Austin in the CFDLab in March 2002. Contributions have come from developers at the Technische Universität Hamburg-Harburg Institute of Modelling and Computation, CFDLab associates at the PECOS Center at UT-Austin, the Computational Frameworks Group at Idaho National Laboratory, NASA Lyndon B. Johnson Space Center, and MIT.



### 3 Shell Elements

Mathematical fundamentals of shell elements divided into the two parts and the coordinate transformation

#### 3.1 Introduction to Linear Elastic Problems

In the following the fundamental equations of linear elasticity will be considered. Here, the spatial case is used for demonstration, but every lower dimensional problem can easily be derived from it. The following definitions will be used in this thesis:

$$\vec{u}^T = (u \ v \ w) \text{ displacement vector} \quad (1)$$

$$\vec{f}^T = (f_x \ f_y \ f_z) \text{ external force vector} \quad (2)$$

The strains and stresses can either be described in form of tensors  $\underline{\epsilon}$  and  $\underline{\sigma}$ , or as vectors  $\vec{\epsilon}$  and  $\vec{\sigma}$ :

$$\underline{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix}; \underline{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \quad (3)$$

$$\vec{\epsilon}^T = (\epsilon_{xx} \ \epsilon_{yy} \ \epsilon_{zz} \ 2\epsilon_{xy} \ 2\epsilon_{yz} \ 2\epsilon_{zx}); \vec{\sigma}^T = (\sigma_{xx} \ \sigma_{yy} \ \sigma_{zz} \ \sigma_{xy} \ \sigma_{yz} \ \sigma_{zx}) \quad (4)$$

As stated in [Ste15] the relation between displacements and strains is as follows:

$$\underline{\epsilon} = \frac{1}{2} (\nabla \vec{u} + \vec{u} \nabla); \quad \vec{\epsilon} = \underline{L} \vec{u} \quad (5)$$

Equation 5 relates the displacement vector field  $\vec{u}$  with the strain field  $\underline{\epsilon}$ , or  $\vec{\epsilon}$  respectively. Here,  $\underline{L}$  is a differential operator. This strain-displacement relation is also called *kinematic relationship* [Ste15].

In general initial strains can exist inside the material for example due to temperature changes or shrinkage. Such initial strains are denoted  $\vec{\epsilon}_0$  and the stresses will be influenced by the difference between the actual and initial strains. Additionally one could imagine initial residual stresses  $\vec{\sigma}_0$  that can be added to the general equation:

$$\vec{\sigma} = \underline{D} (\vec{\epsilon} - \vec{\epsilon}_0) + \vec{\sigma}_0, \quad (6)$$

where  $\underline{D}$  is the material matrix. In the simplest case of linear elasticity with isotropy,  $\underline{D}$  only contains two parameters, namely the elastic modulus  $E$  (also known as the Young's modulus) and the Poisson's ratio  $\nu$ . The former one defines the relationship between the stress and strain in a material, the latter one results as the quotient of the fraction of expansion and the fraction of compression for small changes. In the following the initial conditions are ignored, resulting in the a simpler form of equation 6:

$$\vec{\sigma} = \underline{D} \vec{\epsilon} \quad (7)$$

For the said isotropic case  $\underline{D}$  results in [ZT00]:

$$\underline{D} = \frac{E}{1 - \nu^2} \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{pmatrix} \quad (8)$$

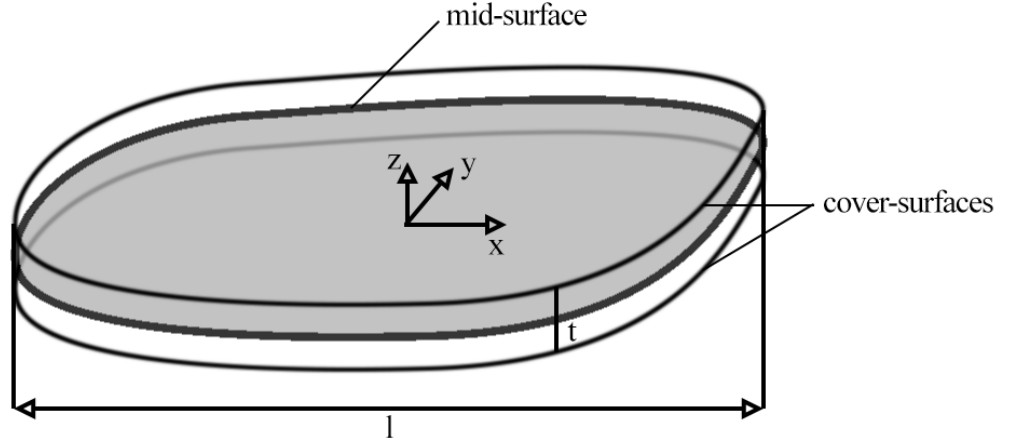


Figure 1: Schematic view of a plane object

## 3.2 Plane Element

First part of shell element: plane part. derivation of this part with two exemplary finite element types

### 3.2.1 Problem Definition

In Figure 1 an object is shown which extends to the  $x$  and  $y$  axis as its primary direction. The extend in  $z$ -direction is smaller and denoted by thickness  $t$ . The mid-surface located in between the top and bottom surface areas has the coordinate  $z = 0$ . Its local  $z$ -axis equals the normal vector of the mid place. Such an object is called *plane* in the following.

There are two different problem definitions regarding plane elements: Plane stress and plane strain. The directions of displacements  $u$  and  $v$  along the orthogonal local  $x$  and  $y$  axis defining its displacement field is a common feature of both problems. Also, both have in common, that only strains and stresses in the  $xy$  plane have to be considered: Instead of nine, only three components remain. While in the case of plane stress all other stress components are zero, in plane strain the stress in direction perpendicular to the  $xy$  plane is non-zero. In this thesis only plane stress will be discussed in further detail. More information about plane strain is given in [ZT00]. The following conditions must be satisfied such that a plane can be in *plane stress* [Ste15]:

- The thickness  $t$  varies only slightly and it must hold:  $t/l \ll 1$ , with  $l$  the extent of the larger side of the plane element.
- The load is applied to the mid place.
- Displacements, strains and stresses are constant across the thickness.

The stress components  $\sigma_{xz}, \sigma_{yz}, \sigma_{zz}$  normal to the surface areas with  $z \pm t/2$  vanish (equals zero). Therefore only the two normal stress components  $\sigma_{xx}$  and  $\sigma_{yy}$  and the transverse stress component  $\sigma_{xy}$  are left non-zero.

Displacements can only occur in x and y direction.  $u$  will be the displacement along x and  $v$  along y. The displacement field  $\vec{u}$  is as follows:

$$\vec{u} = \begin{pmatrix} u(x, y) & v(x, y) \end{pmatrix}^T \quad (9)$$

The vector for the strain components:

$$\vec{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{yy} & 2\epsilon_{xy} \end{pmatrix}^T \quad (10)$$

Sometimes  $2\epsilon_{xy}$  is shortened to  $\gamma_{xy}$  [Ste15]. The vector holding the stress components is similar to that of the strain's vector:

$$\vec{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{yy} & \sigma_{xy} \end{pmatrix}^T \quad (11)$$

The kinematic relationship  $\vec{\epsilon} = \underline{L}\vec{u}$  linking the displacements  $\vec{u}$  with the strains  $\vec{\epsilon}$  at full length:

$$\vec{\epsilon} = \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ 2\epsilon_{xy} \end{pmatrix} = \begin{pmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \underline{L}\vec{u} \quad (12)$$

With the strains known and considering equation 5 one can calculate the stresses  $\vec{\sigma}$ :

$$\vec{\sigma} = \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{pmatrix} = \frac{E}{1-\nu^2} \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{pmatrix} \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ 2\epsilon_{xy} \end{pmatrix} = \underline{D}\vec{\epsilon} = \underline{D}\underline{L}\vec{u} \quad (13)$$

natural boundary conditions in form of nodal forces:  $\vec{F} = \begin{pmatrix} F_x & F_y \end{pmatrix}^T$

The total potential of the plane element problem looks as follows:

$$\Pi = 1/2 \int_V \vec{\epsilon}^T \vec{\sigma} dV - \vec{u}^T \vec{F}, \quad (14)$$

with the first term being the elastic strain energy and the second term the single forces.

### 3.2.2 Tri-3 Plane Element

In section 3.2.1 the plane's functional was derived. Now the focus is on the functional's discretization. Figure 2 shows a general, planar object defined to be placed in the xy-plane. The first discretization step is to divide the object into single triangles approximating the shape of it. This process is called triangulation. Every one of these triangles then represents a finite element with one node at every corner. The finer the triangulation is done the better the object and its boundary are matched by its discrete

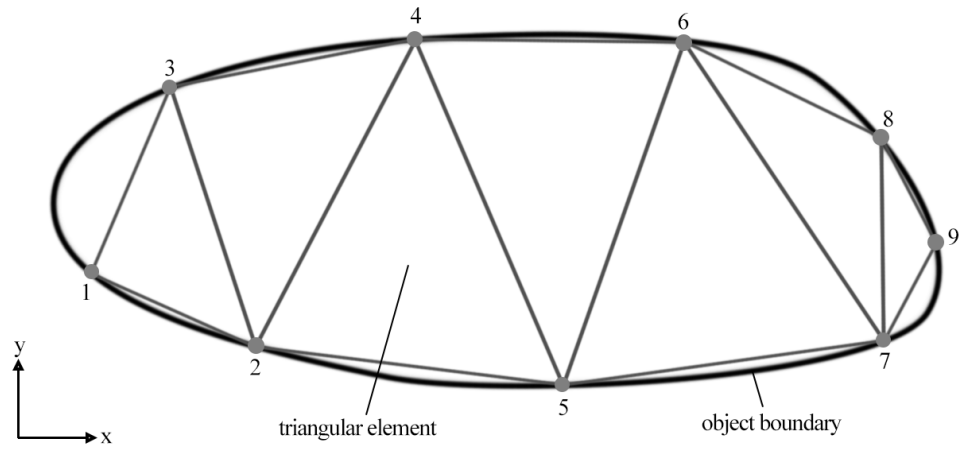


Figure 2: Subdividing plane object with triangular elements

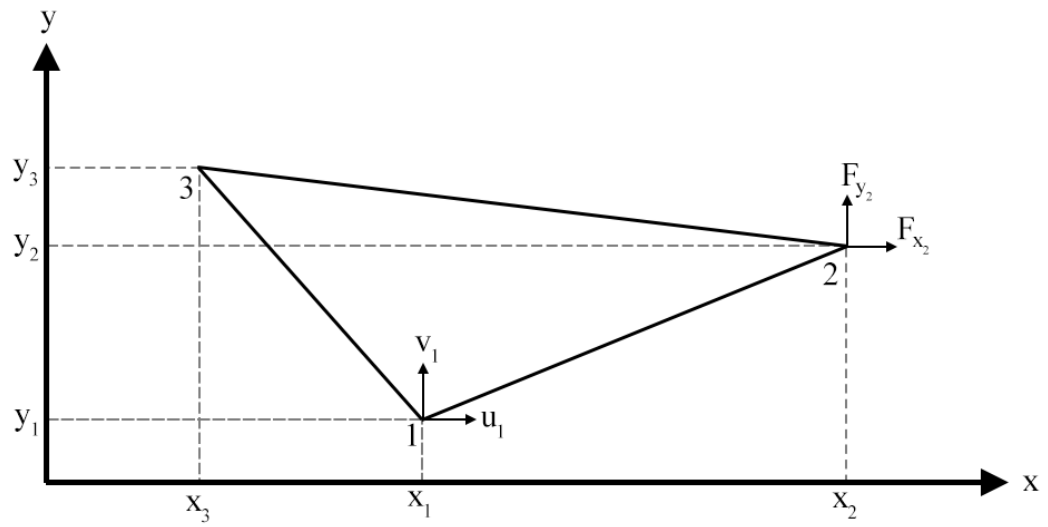


Figure 3: Three node triangular element with its coordinates, nodal displacements and nodal forces

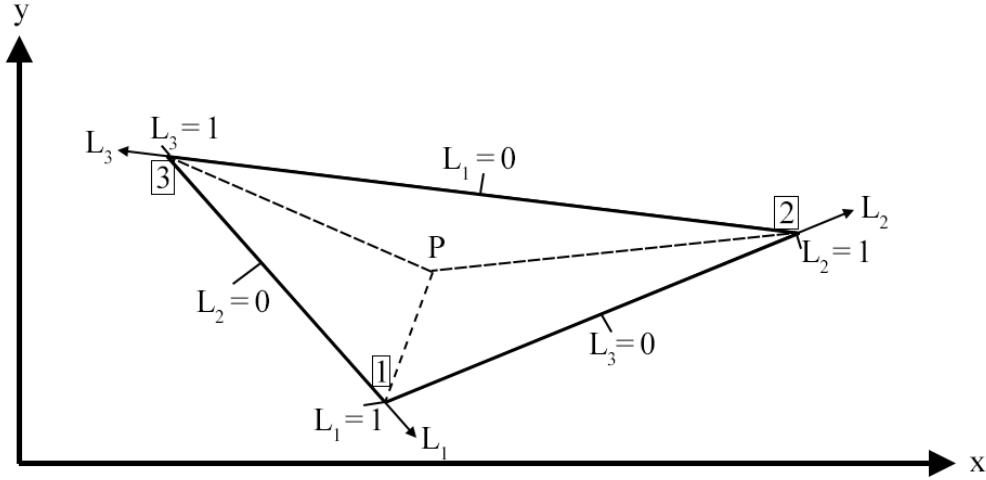


Figure 4: Triangular coordinates  $L_1, L_2, L_3$  and sampling point  $P$  within the triangular element

complement, but also the more finite elements have to be considered in later calculations. One triangular finite element is shown in Figure 3. It is defined by the coordinates  $(x_i, y_i)$  of its three nodes. Since the element is located in the  $xy$ -plane, the  $z$ -coordinate is of no interest and will be ignored. At every node, forces can be applied denoted with  $F_{x_i}$  and  $F_{y_i}$ . Accordingly, every node can be displaced. The movement along the  $x$ -axis is denoted with  $u_i$ , or with  $v_i$  along the  $y$ -axis respectively. Note, that the node numbering is in counter-clockwise direction. This definition will be kept throughout the thesis, and is important to remember when implementing the FEM-code in order to reduce errors. In this thesis only triangles defined by three nodes are discussed. There are many more finite elements forming triangles, such as six node triangles or even seven node triangles. The main difference between these types of elements are the order of shape functions. More details about higher order triangular finite elements can be found in

In the case of a three node triangle the basis functions for the two displacements  $u$  and  $v$  are as follows [Ste15]:

$$u(x, y) = a_0 + a_1 L_1 + a_2 L_2 = \begin{pmatrix} 1 & L_1 & L_2 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \vec{x}^T \vec{a}, \quad (15)$$

$$v(x, y) = a_0 + a_1 L_1 + a_2 L_2 = \begin{pmatrix} 1 & L_1 & L_2 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \vec{x}^T \vec{a}, \quad (16)$$

both defined in triangular coordinates (see figure 4).

To get the unknown coefficients  $a_i$ , values for the triangular coordinates are set. This

creates a system of linear equations:

$$\begin{aligned} u(L_1 = 1, L_2 = 0) &= u_1 \rightarrow u_1 = a_0 + a_1 \\ u(L_1 = 0, L_2 = 1) &= u_2 \rightarrow u_2 = a_0 + a_2 \\ u(L_1 = 0, L_2 = 0) &= u_3 \rightarrow u_3 = a_0 \end{aligned} \quad (17)$$

Alternatively, this could be also done with  $v$ . Written as matrix and vector:

$$\begin{aligned} \underline{A}\vec{a} &= \vec{u} \\ \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} &= \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \end{aligned} \quad (18)$$

Now, inverting matrix  $A$  the coefficients can be found:

$$\vec{a} = \underline{A}^{-1}\vec{u} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & -1 \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \quad (19)$$

If one put equation 19 into 15, or the analogon into 16, the shape functions for the three node triangular finite element will be derived, as described in [Ste15]:

$$\begin{aligned} u &= \vec{x}^T \vec{a} = \vec{x}^T \underline{A}^{-1} \vec{u} = \vec{N}^T \vec{u} \\ \vec{N}^T &= \vec{x}^T \underline{A}^{-1} = \begin{pmatrix} 1 & L_1 & L_2 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & -1 \\ 0 & 1 & -1 \end{pmatrix} \\ &= \begin{pmatrix} L_1 & L_2 & 1 - L_1 - L_2 \end{pmatrix} = \begin{pmatrix} N_1 & N_2 & N_3 \end{pmatrix} \end{aligned} \quad (20)$$

Characteristically for the shape function, as stated in [Ste15], is, that shape function  $N_i$  gets the value 1 at node  $i$  and 0 at the two other nodes. The functions are linear with respect to  $L_1$  and  $L_2$  which can be noticed in equation 20. As stated before, these shape functions are the same for displacement  $u$  and  $v$ . With the knowledge of the displacement values of the element's nodes one can formulate the displacement functions in triangular coordinate notation as follows:

$$\begin{aligned} u &= N_1 u_1 + N_2 u_2 + N_3 u_3 \\ v &= N_1 v_1 + N_2 v_2 + N_3 v_3 \end{aligned} \quad (21)$$

Or in matrix form:

$$\begin{aligned} \vec{\tilde{u}} &= \underline{N}\vec{u} \\ \begin{pmatrix} u \\ v \end{pmatrix} &= \begin{pmatrix} N_1 & 0 & N_2 & 0 & N_3 & 0 \\ 0 & N_1 & 0 & N_2 & 0 & N_3 \end{pmatrix} \begin{pmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \end{pmatrix} \end{aligned} \quad (22)$$

The vector  $\vec{\tilde{u}}$  describes the element's displacements as product of matrix  $\underline{N}$  containing the shape functions and vector  $\vec{u}$  containing the displacements of the single triangle's nodes. Now, one can put equation 22 into 12:

$$\vec{\epsilon} = \underline{L}\vec{\tilde{u}} = \underline{L} \underline{N}\vec{u} = \underline{B}\vec{u} \quad (23)$$

The product of  $\underline{L}$  and  $\underline{N}$  is called *strain-displacement matrix*  $\underline{B}$ . In order to calculate the strain-displacement matrix, one has to assemble the  $\underline{L}$  matrix containing the first partial derivatives of the triangular element. With the chain rule applied, the partial derivatives look as follows:

$$\begin{aligned} \frac{\partial}{\partial L_1} &= \frac{\partial x}{\partial L_1} \frac{\partial}{\partial x} + \frac{\partial y}{\partial L_1} \frac{\partial}{\partial y} \\ \frac{\partial}{\partial L_2} &= \frac{\partial x}{\partial L_2} \frac{\partial}{\partial x} + \frac{\partial y}{\partial L_2} \frac{\partial}{\partial y} \end{aligned} \quad (24)$$

or in matrix notation:

$$\begin{aligned} \tilde{\nabla} &= \underline{J}\nabla \\ \begin{pmatrix} \frac{\partial}{\partial L_1} \\ \frac{\partial}{\partial L_2} \end{pmatrix} &= \begin{pmatrix} \frac{\partial x}{\partial L_1} & \frac{\partial y}{\partial L_1} \\ \frac{\partial x}{\partial L_2} & \frac{\partial y}{\partial L_2} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix}, \end{aligned} \quad (25)$$

where  $\underline{J}$  represents the Jacobian matrix,  $\nabla$  the partial derivatives in Cartesian coordinates and  $\tilde{\nabla}$  the partial derivatives in triangular coordinates. To get the derivatives in Cartesian form the upper equation must be multiplied with the inverse Jacobian matrix  $\underline{J}^{-1}$ :

$$\underline{J}^{-1} = \frac{1}{|\underline{J}|} \begin{pmatrix} \frac{\partial y}{\partial L_2} & -\frac{\partial y}{\partial L_1} \\ -\frac{\partial x}{\partial L_2} & \frac{\partial x}{\partial L_1} \end{pmatrix} \quad (26)$$

The conversion between triangular and Cartesian coordinates can be summarized as follows (see Figure 4 and [Ste15]):

$$\begin{aligned} L_1 + L_2 + L_3 &= 1 \rightarrow L_3 = 1 - L_1 - L_2 \\ x &= x_1 L_1 + x_2 L_2 + x_3 L_3 = (x_1 - x_3)L_1 + (x_2 - x_3)L_2 + x_3 \\ y &= y_1 L_1 + y_2 L_2 + y_3 L_3 = (y_1 - y_3)L_1 + (y_2 - y_3)L_2 + y_3 \end{aligned} \quad (27)$$

Considering equation 27 the Jacobian matrix can now be calculated:

$$\underline{J} = \begin{pmatrix} \frac{\partial x}{\partial L_1} = x_1 - x_3 = x_{13} & \frac{\partial y}{\partial L_1} = y_1 - y_3 = y_{13} \\ \frac{\partial x}{\partial L_2} = x_2 - x_3 = x_{23} & \frac{\partial y}{\partial L_2} = y_2 - y_3 = y_{23} \end{pmatrix} = \begin{pmatrix} x_{13} & y_{13} \\ x_{23} & y_{23} \end{pmatrix} \quad (28)$$

and hence the inverse Jacobian matrix:

$$\underline{J}^{-1} = \frac{1}{2A_{\triangle}} \begin{pmatrix} y_{23} & -y_{13} \\ -x_{23} & x_{13} \end{pmatrix} \quad (29)$$

The determinant of the Jacobian matrix is two times the area of the triangle. With the help of equation 29, 25 can be reorganized

$$\nabla = \underline{J}^{-1} \tilde{\nabla} \quad (30)$$

and this finally yields to the new version of the differential operator  $\underline{L}$  [Ste15]:

$$\underline{L} = \frac{1}{2A_{\Delta}} \begin{pmatrix} y_{23} \frac{\partial}{\partial L_1} - y_{13} \frac{\partial}{\partial L_2} & 0 \\ 0 & -x_{23} \frac{\partial}{\partial L_1} + x_{13} \frac{\partial}{\partial L_2} \\ -x_{23} \frac{\partial}{\partial L_1} + x_{13} \frac{\partial}{\partial L_2} & y_{23} \frac{\partial}{\partial L_1} - y_{13} \frac{\partial}{\partial L_2} \end{pmatrix} \quad (31)$$

Next, the strain-displacement matrix  $\underline{B}$  can be calculated:

$$\begin{aligned} \underline{B} &= \underline{L} \underline{N} \\ &= \frac{1}{2A_{\Delta}} \begin{pmatrix} y_{23} \frac{\partial}{\partial L_1} - y_{13} \frac{\partial}{\partial L_2} & 0 \\ 0 & -x_{23} \frac{\partial}{\partial L_1} + x_{13} \frac{\partial}{\partial L_2} \\ -x_{23} \frac{\partial}{\partial L_1} + x_{13} \frac{\partial}{\partial L_2} & y_{23} \frac{\partial}{\partial L_1} - y_{13} \frac{\partial}{\partial L_2} \end{pmatrix} \\ &\quad \begin{pmatrix} L_1 & 0 & L_2 & 0 & 1 - L_1 - L_2 & 0 \\ 0 & L_1 & 0 & L_2 & 0 & 1 - L_1 - L_2 \end{pmatrix} \\ &= \frac{1}{2A_{\Delta}} \begin{pmatrix} y_{23} & 0 & -y_{13} & 0 & y_{12} & 0 \\ 0 & -x_{23} & 0 & x_{13} & 0 & -x_{12} \\ -x_{23} & y_{23} & x_{13} & -y_{13} & -x_{12} & y_{12} \end{pmatrix} \end{aligned} \quad (32)$$

With  $\underline{B}$  known, one can insert equation 23 into 13 to get the stresses:

$$\vec{\sigma} = \underline{D} \underline{B} \vec{u} \quad (33)$$

Finally, every term of the plane element's functional 14 can be filled with the above discretized terms:

$$\begin{aligned} \Pi &= \frac{1}{2} \int_V \vec{\epsilon}^T \vec{\sigma} dV - \vec{u}^T \vec{F} \\ &= \frac{1}{2} \int_V \vec{u}^T \underline{B}^T \underline{D} \underline{B} \vec{u} dV - \vec{u}^T \vec{F} \\ &= \frac{1}{2} \vec{u}^T \int_V \underline{B}^T \underline{D} \underline{B} dV \vec{u} - \vec{u}^T \vec{F} \\ &= \frac{1}{2} \vec{u}^T \underline{K} \vec{u} - \vec{u}^T \vec{F} \end{aligned} \quad (34)$$

with  $\underline{K}$  the stiffness matrix and  $\vec{F}$  the nodal force vector.

The variation of the functional 34 is as follows [Ste15]:

$$\begin{aligned} \delta \Pi &= \frac{\partial \Pi}{\partial \vec{u}} \delta \vec{u} = 0 \\ &= \frac{1}{2} \delta \vec{u}^T \frac{\partial \vec{u}^T}{\partial \vec{u}^T} \underline{K} \vec{u} + \frac{1}{2} \vec{u}^T \underline{K} \frac{\partial \vec{u}}{\partial \vec{u}} \delta \vec{u} - \delta \vec{u} \frac{\partial \vec{u}^T}{\partial \vec{u}^T} \vec{F} \\ &= \delta \vec{u}^T (\underline{K} \vec{u} - \vec{F}) = 0 \end{aligned} \quad (35)$$



In order to satisfy this equation, the term in between the parenthesis must be zero ( $\delta \vec{u}^T$  can have arbitrary values). This leads to the equilibrium equation of the triangular plane element as described in [Ste15]:

$$\underline{K} \vec{u} = \vec{F} \quad (36)$$

Since the thickness  $t$  of the element is constant per definition, it is  $dV = t \, dA$  and therefore the integral of the stiffness matrix changes to:

$$\underline{K} = t \int_A \underline{B}^T \underline{D} \underline{B} \, dA = t A_{\triangle} \underline{B}^T \underline{D} \underline{B} \quad (37)$$

### 3.2.3 Quad-4 Plane Element

Sometimes it can be beneficial to use quadrilateral elements when describing a mesh. In contrast to triangles which always lie, due to their simple shape, in a plane, quadrilateral can have more complex forms. Such cases include for example: The fourth nodes does not lie in the plane defined by the other three or the shape is not convex. It is difficult to deal with such forms and one could be tempted to restrict the element to have rectangular shapes only, because these are easy to formulate and work with. But they are impractical when complicated geometry is to be modeled, especially if details should be emphasized in fine graduation.

One solution to this problem is the use of isoparametric elements. They can be non-rectangular. The trick is to use reference coordinates which map the physical element into a reference element that is a square. Thus, the physical element can have a more general shape, but a coordinate transformation and numerical integration is needed which brings in more mathematical complexity [CMPW02].

In this section quadrilateral isoparametric elements consisting of four nodes are described, but one can expand it to eight or nine node elements. Figure 5 shows the two abstraction layers: On the left side the original element is shown in physical space, on the right side the reference element is shown. The square has a side length of 2. The coordinate system with the  $\xi$  and  $\eta$  axis has its origin in the center of the square. Also note the numbering of the nodes is again counter-clockwise.

Similarly to the triangular element, interpolating the displacement field as well as the element geometry is done by shape functions. They are defined in reference coordinates. The displacement of a point within the element can be expressed by the displacements at the nodes and shape functions  $\underline{N}$ . Also, the position of that point can be expressed in terms of the (global) nodal positions and shape functions  $\tilde{\underline{N}}$ . The element is called *isoparametric* if  $\underline{N}$  is identical to  $\tilde{\underline{N}}$ . If  $\tilde{\underline{N}}$  is of lower degree than  $\underline{N}$ , the element is called *subparametric* and *superparametric* if it is the other way around [CMPW02].

Every node has two degrees of freedom: A displacement  $u$  along the x-axis and a displacement  $v$  along the y-axis. To find the shape functions it does not matter which variable to choose, so the following basis function was used for  $\phi$  which can either

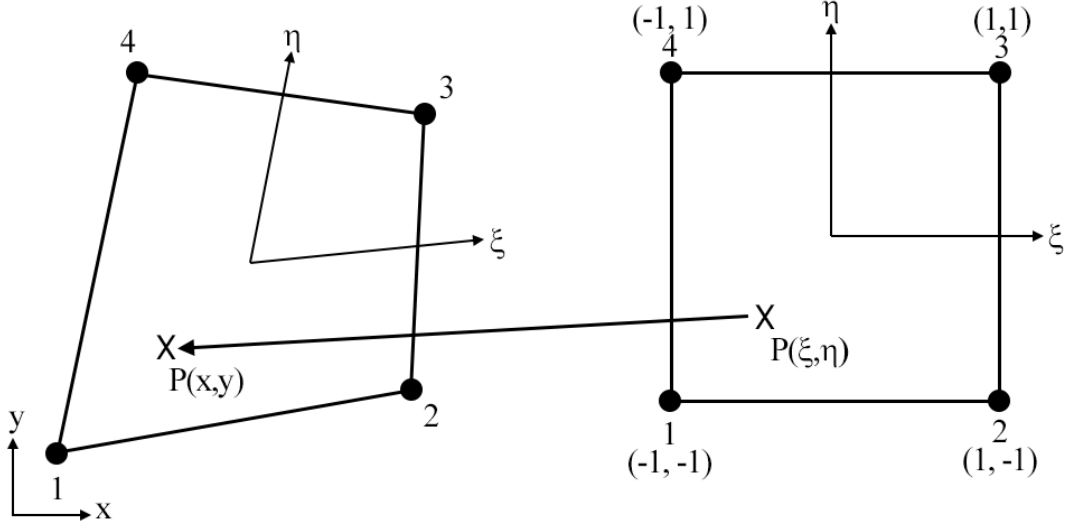


Figure 5: Coordinate transformation of four node quadrilateral element with physical space on the left side and reference space on the right side

represent  $u$  or  $v$  [Ste15]:

$$\phi(\xi, \eta) = a_0 + a_1\xi + a_2\eta + a_3\xi\eta = \begin{pmatrix} 1 & \xi & \eta & \xi\eta \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \vec{x}^T \vec{a} \quad (38)$$

The interpolation conditions at the nodes are as follows:

$$\begin{aligned} \phi(-1, -1) &= \phi_1 \rightarrow \phi_1 = a_0 - a_1 - a_2 + a_3 \\ \phi(1, -1) &= \phi_2 \rightarrow \phi_2 = a_0 + a_1 - a_2 - a_3 \\ \phi(1, 1) &= \phi_3 \rightarrow \phi_3 = a_0 + a_1 + a_2 + a_3 \\ \phi(-1, 1) &= \phi_4 \rightarrow \phi_4 = a_0 - a_1 + a_2 - a_3 \end{aligned} \quad (39)$$

or in matrix notation:

$$\underline{A}\vec{a} = \vec{\phi} \quad \begin{pmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} \quad (40)$$

Inversion of  $\underline{A}$  yields the coefficients  $a_i$ :

$$\vec{a} = \underline{A}^{-1}\vec{\phi} = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} \quad (41)$$

If the last equation is inserted into 38 one gets the shape functions  $\vec{N}$  for the quadrilateral element:

$$\begin{aligned}
\phi &= \vec{x}^T \underline{A}^{-1} \vec{\phi} \\
&= \vec{N}^T \vec{\phi} \\
&= \frac{1}{4} \begin{pmatrix} 1 & \xi & \eta & \xi\eta \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix} \vec{\phi} \\
&= \left( \frac{1}{4}(1-\xi)(1-\eta) \quad \frac{1}{4}(1+\xi)(1-\eta) \quad \frac{1}{4}(1+\xi)(1+\eta) \quad \frac{1}{4}(1-\xi)(1+\eta) \right) \vec{\phi} \quad (42)
\end{aligned}$$

To check the correctness of the four shape function one can evaluate shape function  $i$  with  $\xi\eta$ -coordinates of node  $i$ . It must evaluate to 1 while at any other node coordinate it must be zero. Now, the displacements can be expressed as follows:

$$\vec{u} = \begin{pmatrix} u \\ v \end{pmatrix} = \underline{N} \vec{u} = \begin{pmatrix} N_1 & 0 & N_2 & 0 & N_3 & 0 & N_4 & 0 \\ 0 & N_1 & 0 & N_2 & 0 & N_3 & 0 & N_4 \end{pmatrix} \begin{pmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \\ u_4 \\ v_4 \end{pmatrix} \quad (43)$$

with  $\underline{N}$  being the matrix containing the shape functions and  $\vec{u}$  being the vector of the nodal displacements.

The assembly of the strain-displacement matrix  $\underline{B}$  is more complicated with isoparametric elements. Due to the  $\xi\eta$ -coordinates one cannot easily describe an operator such as  $\partial/\partial x$ . The first step to achieve it, is to formulate a function  $\phi = \phi(\xi, \eta)$ . Like in the derivation on the shape functions  $\phi$  can represent  $u$  or  $v$ . Derivatives with respect to  $\xi$  and  $\eta$  are as follows [CMPW02]:

$$\begin{aligned}
\frac{\partial \phi}{\partial \xi} &= \frac{\partial \phi}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial \phi}{\partial y} \frac{\partial y}{\partial \xi} \\
\frac{\partial \phi}{\partial \eta} &= \frac{\partial \phi}{\partial x} \frac{\partial x}{\partial \eta} + \frac{\partial \phi}{\partial y} \frac{\partial y}{\partial \eta}
\end{aligned} \quad (44)$$

or in matrix notation:

$$\vec{\phi} = \underline{J} \vec{\phi} \quad (45)$$

where  $\underline{J}$  is the Jacobian matrix:

$$\underline{J} = \begin{pmatrix} \sum N_{i,\xi} x_i & \sum N_{i,\xi} y_i \\ \sum N_{i,\eta} x_i & \sum N_{i,\eta} y_i \end{pmatrix} \quad (46)$$

where  $N_{i,j}$  denotes the derivation of the  $i$ -th shape function with respect to  $j$  and  $x_i$  the  $i$ -th component of the  $\vec{x}$  vector. The Jacobian matrix can be written out as follows:

$$\begin{aligned}\underline{J} &= \frac{1}{4} \begin{pmatrix} -(1-\eta) & (1-\eta) & (1+\eta) & -(1+\eta) \\ -(1-\xi) & -(1+\xi) & (1+\xi) & (1-\xi) \end{pmatrix} \begin{pmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \\ x_4 & y_4 \end{pmatrix} \\ &= \begin{pmatrix} (x_{12} + x_{34})\eta - x_{12} + x_{34} & (y_{12} + y_{34})\eta - x_{12} + y_{34} \\ (x_{12} + x_{34})\xi - x_{13} - x_{24} & (y_{12} + y_{34})\xi - y_{13} + y_{24} \end{pmatrix}\end{aligned}\quad (47)$$

Next, equation 45 can be rearranged to get the derivatives with respect to  $x$  and  $y$ :

$$\vec{\phi} = \underline{J}^{-1} \vec{\phi} \quad (48)$$

With the derivatives calculated, the strain-displacement relation 5 can be obtained [CMPW02]:

$$\vec{\epsilon} = \begin{pmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}}_{\underline{L}} \begin{pmatrix} \frac{\partial u}{\partial \xi} \\ \frac{\partial u}{\partial \eta} \\ \frac{\partial v}{\partial \xi} \\ \frac{\partial v}{\partial \eta} \end{pmatrix} \quad (49)$$

$$\begin{pmatrix} \frac{\partial u}{\partial \xi} \\ \frac{\partial u}{\partial \eta} \\ \frac{\partial v}{\partial \xi} \\ \frac{\partial v}{\partial \eta} \end{pmatrix} = \underbrace{\begin{pmatrix} j_{11} & j_{12} & 0 & 0 \\ j_{21} & j_{22} & 0 & 0 \\ 0 & 0 & j_{11} & j_{12} \\ 0 & 0 & j_{21} & j_{22} \end{pmatrix}}_{\underline{\hat{J}}} \begin{pmatrix} \frac{\partial u}{\partial \xi} \\ \frac{\partial u}{\partial \eta} \\ \frac{\partial v}{\partial \xi} \\ \frac{\partial v}{\partial \eta} \end{pmatrix} \quad (50)$$

$$\begin{pmatrix} \frac{\partial u}{\partial \xi} \\ \frac{\partial u}{\partial \eta} \\ \frac{\partial v}{\partial \xi} \\ \frac{\partial v}{\partial \eta} \end{pmatrix} = \underbrace{\begin{pmatrix} N_{1,\xi} & 0N_{2,\xi} & 0 & N_{3,\xi} & 0 & N_{4,\xi} & 0 \\ N_{1,\eta} & 0N_{2,\eta} & 0 & N_{3,\eta} & 0 & N_{4,\eta} & 0 \\ 0 & N_{1,\xi} & 0N_{2,\xi} & 0 & N_{3,\xi} & 0 & N_{4,\xi} \\ 0 & N_{1,\eta} & 0N_{2,\eta} & 0 & N_{3,\eta} & 0 & N_{4,\eta} \end{pmatrix}}_{\underline{\hat{N}}} \begin{pmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \\ u_4 \\ v_4 \end{pmatrix} \quad (51)$$

$$\underline{B} = \underline{L} \underline{\hat{J}} \underline{\hat{N}} \quad (52)$$

where  $j_i$  denotes the  $i$ -th entry in the inverse Jacobian matrix.

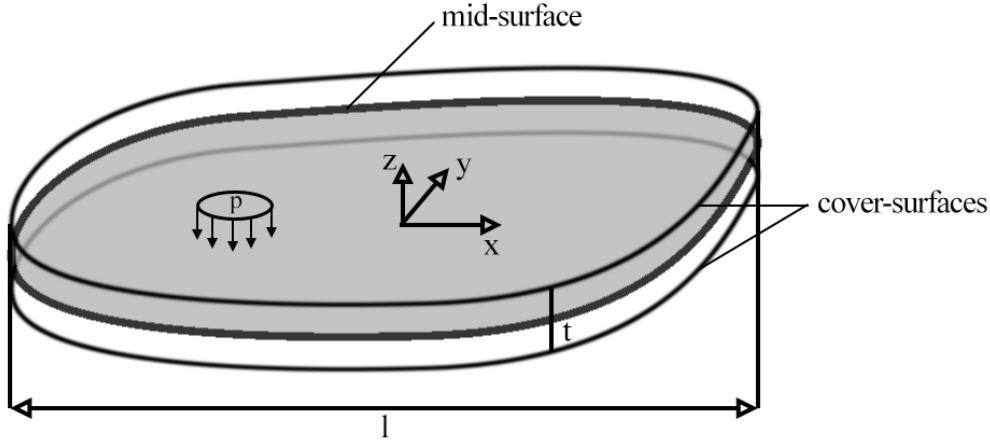


Figure 6: Schematic drawing of a Kirchhoff plate with its main dimension  $l$ , thickness  $t$  and loading  $p$  normal to the mid-surface

Together with the functional equation 34 and the material matrix  $\underline{D}$  13, the stiffness matrix for the quadrilateral isoparametric element can be written as:

$$\underline{K} = \int_V \underline{B}^T \underline{D} \underline{B} dV = t \int_A \underline{B}^T \underline{D} \underline{B} dA = t \int_{-1}^1 \int_{-1}^1 \underline{B}^T \underline{D} \underline{B} |\underline{J}| d\xi d\eta \quad (53)$$

For the four node element a Gaussian quadrature needs 2x2 Gauss integration points to satisfy the above equation [Ste15]. These four points are located at  $\xi_i = \pm \frac{\sqrt{3}}{3}$  and  $\eta_i = \pm \frac{\sqrt{3}}{3}$  with weight factors  $\omega_i = 1$ . The equation for the stiffness matrix can then be written in discretized form as follows:

$$\underline{K} = t \sum_{i=1}^2 \sum_{j=1}^2 \omega_i \omega_j \underline{B}(\xi_i, \eta_j)^T \underline{D} \underline{B}(\xi_i, \eta_j) |\underline{J}(\xi_i, \eta_j)| \quad (54)$$

### 3.3 Plate Bending Element

Second part of shell element: plate part. derivation of this part with two exemplary finite element types

#### 3.3.1 Problem Definition

In contrast to a plane, where the load is located planar with respect to the plane, the load is perpendicular to the mid plane at a plate. Therefore plate element problems are important for supporting structures of bridges or ceilings and floors in buildings, for example. In Figure 6 one can see a generalized plate object. It has a main dimension of  $l$  and a constant thickness  $t$ . With the assumption that  $t \ll l$ , the problem becomes two dimensional and, instead of the whole object, only the middle plane between the two surface areas will be considered. The object has a local coordinate system with its

xy-plane the mid plane and its z-axis perpendicular to this plane. The surface areas are located at  $z = \pm t/2$ . As stated in the beginning, the load is applied in z-direction, i.e. normal to the mid-surface.

In this work Kirchhoff's theory of thin plates is used. For thick plates or laminated plates, the theory of Reissner-Mindlin is more applicable. The main difference is that with Reissner-Mindlin plates one takes the shear deformations into account. Thus, the normal to the mid-surface remains straight but not necessarily perpendicular to it; instead of a Kirchhoff plate: Here, the normal remains normal to the mid-surface even after deformation.

As a short summarize the following conditions must be satisfied for a Kirchhoff plate [Ste15]:

- The thickness  $t$  must be much smaller than the main dimension  $l$ :  $t \ll l$ .
- Straight lines normal to the mid-surface remain straight after deformation.
- Straight lines normal to the mid-surface remain normal to the mid-surface after deformation.
- There is only a small amount of deformation  $w$ , i.e.  $w < t$  and it holds  $w \neq w(z)$ .
- The plate is symmetrical to the mid-surface and changes in thickness must be very small.
- Normal stresses in z-direction  $\sigma_{zz}$  will be neglected.

With [Kle13] and [Ste15] the following displacement terms can be formulated:

$$w = w(x, y) \tag{55}$$

$$u = -z \frac{\partial w}{\partial x} \tag{56}$$

$$v = -z \frac{\partial w}{\partial y} \tag{57}$$

The deformation  $w$  suffices to explain the whole displacement vector. The two derivatives in the equations above describe the torsions around the x- and y-axis.

Similar to the plane element, the Kirchhoff plate element can have a plane strain or

plane stress, respectively [Ste15], i.e. equation 5 can be applied here, too:

$$\begin{aligned}\vec{u} &= \begin{pmatrix} u \\ v \end{pmatrix} = -z \begin{pmatrix} \frac{\partial w}{\partial x} \\ \frac{\partial w}{\partial y} \end{pmatrix} = -z \nabla w \\ \vec{\epsilon} &= \underline{L} \vec{u} = -z \underline{L} \nabla w = -z \vec{\Delta} w = -z \vec{\kappa}\end{aligned}\quad (58)$$

$$\begin{aligned}\vec{\Delta} &= \underline{L} \nabla = \begin{pmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial y} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{\partial^2}{\partial x^2} \\ \frac{\partial^2}{\partial y^2} \\ 2 \frac{\partial^2}{\partial x \partial y} \end{pmatrix} \\ \vec{\kappa} &= \vec{\Delta} w = \begin{pmatrix} \frac{\partial^2 w}{\partial x^2} \\ \frac{\partial^2 w}{\partial y^2} \\ 2 \frac{\partial^2 w}{\partial x \partial y} \end{pmatrix}\end{aligned}\quad (59)$$

Referring [Kle13] ( $\sigma_{zz} = 0, \tau_{xz} = \tau_{yz} = 0$ ), equation 6 can be filled with the above information:

$$\begin{aligned}\vec{\sigma} &= \underline{D} \vec{\epsilon} = -z \underline{D} \vec{\kappa} \\ &= -\frac{Ez}{1-\nu^2} \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{pmatrix} \begin{pmatrix} \kappa_x \\ \kappa_y \\ 2\kappa_{xy} \end{pmatrix}\end{aligned}\quad (60)$$

The integration of the stresses  $\vec{\sigma}$  over the thickness results in the vector of moments  $\vec{M}^T = (M_{xx} \ M_{yy} \ M_{xy})$  [Ste15]:

$$\vec{M} = \int_{-t/2}^{t/2} z \vec{\sigma} dz = - \int_{-t/2}^{t/2} z^2 \underline{D} \vec{\kappa} dz = -\underline{D} \vec{\kappa} \int_{-t/2}^{t/2} z^2 dz = -\frac{t^3}{12} \underline{D} \vec{\kappa} = -\underline{D}_p \vec{\kappa} \quad (61)$$

The above equation relates the moments with the curvatures of the plate. The integrals over the transverse stresses  $\sigma_{xz}$  and  $\sigma_{yz}$  lead to the following shear forces, as described in [Ste15]:

$$\begin{aligned}Q_x &= \int_{-t/2}^{t/2} \sigma_{xz} dz = \int_{-t/2}^{t/2} \sigma_{xz}^{\max} \left( 1 - 4 \left( \frac{z}{t} \right)^2 \right) dz = \frac{2}{3} \sigma_{xz}^{\max} t \\ &= \frac{2}{3} \sigma_{xz}(z=0) t\end{aligned}\quad (62)$$

$$\begin{aligned}Q_y &= \int_{-t/2}^{t/2} \sigma_{yz} dz = \int_{-t/2}^{t/2} \sigma_{yz}^{\max} \left( 1 - 4 \left( \frac{z}{t} \right)^2 \right) dz = \frac{2}{3} \sigma_{yz}^{\max} t \\ &= \frac{2}{3} \sigma_{yz}(z=0) t\end{aligned}\quad (63)$$

The transverse stress is distributed quadratically over the thickness  $t$ , i.e. they have their maximum at  $z = 0$  and vanish at  $z = \pm t/2$ . The equilibrium of forces in  $z$ -direction leads to:

$$\frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} + p = 0 \quad (64)$$

with  $p$  the load applied perpendicular to the mid-surface. Additionally the equilibrium of moments around the x- and y-axis:

$$\begin{aligned}\frac{\partial M_{xx}}{\partial x} + \frac{\partial M_{xy}}{\partial y} + Q_x &= 0 \\ \frac{\partial M_{yy}}{\partial y} + \frac{\partial M_{xy}}{\partial x} + Q_y &= 0\end{aligned}\tag{65}$$

Putting equation 65 into 64 results in:

$$\frac{\partial^2 M_{xx}}{\partial x^2} + \frac{\partial^2 M_{yy}}{\partial y^2} + 2\frac{\partial^2 M_{xy}}{\partial x \partial y} = \vec{\Delta}^T \vec{M} = p\tag{66}$$

Now, one can insert the kinematic equation 59 into equation 61 and then into the equilibrium relation 66:

$$\begin{aligned}\vec{\kappa} &= \vec{\Delta} w \\ \vec{M} &= -\underline{D}_p \vec{\kappa} = -\underline{D}_p \vec{\Delta} w \\ \vec{\Delta}^T \vec{M} &= -\vec{\Delta}^T \underline{D}_p \vec{\Delta} w = p\end{aligned}\tag{67}$$

The last equation leads to the partial differential equation of the plate bending [Kle13]:

$$\frac{\partial^4 w}{\partial x^4} + \frac{\partial^4 w}{\partial y^4} + 2\frac{\partial^4 w}{\partial x^2 \partial y^2} = -\frac{12(1-\nu^2)}{Et^3} p = \frac{p}{k}\tag{68}$$

with  $k$  denoted as *plate stiffness*.

Let  $P$  be a point on the continuous boundary of the plate with a local Cartesian coordinate system as described in [Ste15] (see Figure 7): The  $n$  coordinate is perpendicular to the boundary surface, the  $s$  axis tangential to it. The third axis equals the global z-axis of the plate. There are three essential and three natural boundary conditions defined for  $P$ : The displacement  $w$ , the drills  $\theta_n = \partial w / \partial s$ ,  $\theta_s = -\partial w / \partial n$ , the shear force  $Q_n$  and the moments  $M_{ns}$  and  $M_{nn}$ . Since this leads to an inconsistency with the differential equation above, [Ste15] stated that Kirchhoff introduced new forces:

$$V_n = Q_n - \frac{\partial M_{ns}}{\partial s}\tag{69}$$

With them, only the four conditions for  $w, \theta_s, V_n$  and  $M_{nn}$  occur. The plate can be mounted in different ways:

- clamped:  $w = 0, \theta_s = -\partial w / \partial n = 0$
- simple supported:  $w = 0, M_{nn} = 0$
- symmetrical edge:  $\theta_s = -\partial w / \partial n = 0, V_n = 0$



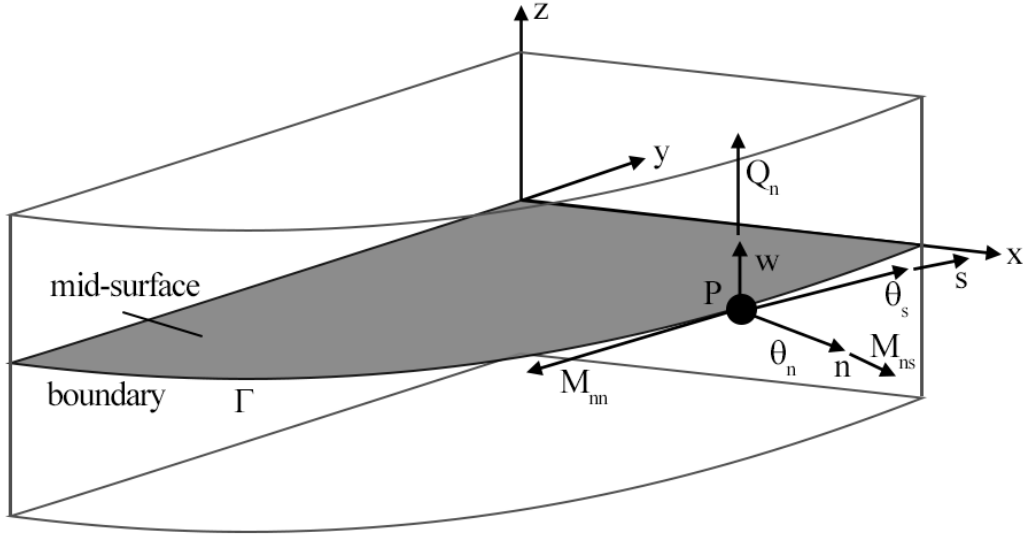


Figure 7: Part of a plate's boundary with its essential and natural boundary conditions

The plate's functional as described in [Ste15] is given below:

$$\frac{1}{2} \int_V \bar{\epsilon}^T \bar{\sigma} dV \quad (70)$$

One can insert equation 58 and 60 into the functional:

$$\frac{1}{2} \int_V \bar{\epsilon}^T \bar{\sigma} dV = \frac{1}{2} \int_V \bar{\kappa}^T \underline{D} \bar{\kappa} z^2 dV = \frac{1}{2} \int_A \bar{\kappa}^T \underline{D}_p \bar{\kappa} dA \quad (71)$$

Together with the potential of the external forces the overall potential of the Kirchhoff plate is:

$$\Pi = \frac{1}{2} \int_A \bar{\kappa}^T \underline{D}_p \bar{\kappa} dA - \int_A p w dA - \int_{\Gamma} (V_n w - M_{nn} \theta_s) d\Gamma \quad (72)$$

Klein [Kle13] states that for the plate element discretization additional conditions must be satisfied. They are: The bending  $w(x, y)$  as well as the normal derivative  $\partial w / \partial n$  at the element's boundary must be continuous to the neighboring elements. This would be the case if the bending and the normal derivative are explicitly determined by the nodal parameters at the border. Further, Klein lists requirements for a plate element ansatz:

- Totality of the displacement approach in order to guarantee good convergence.
- The terms  $1, x, y, x^2, xy, y^2$  should be included to get variable strains, curvatures and rigid body motion.

Steinke [Ste15] expands the requirements as follows:

- Compatibility of the displacement variable at the element's boundary (conformity condition): If the steadiness of the deformation  $w$  and its first derivatives is not satisfied the bending surface between two elements can have a sharp bend at which the elements are overlapping at one side and diverge on the opposite side. If such a behavior is shown, the element is called *non-conforming*.
- Rigid body motions must not create strains and stresses in the element. This requires a constant term in the basis function for the translative part of the motion and a linear term for the rotatory.
- The basis function must provide constant plain strain and plain stress: If the element converges in its size until it becomes a point, a constant state of bending must be describable in this situation. Since the bending is described as second order derivatives of  $w$ , the basis function must include quadratic terms.

The following sections show details of two discretizations of plate elements: A triangular element with three nodes and a quadrilateral element with four nodes.

### 3.3.2 Tri-3 Plate Element

There exists many different types of triangular plate elements, for example Batoz et al. [BBH80], Tocher [Toc63] or Specht [Spe88]. The three node triangular element from [Toc63] has three degrees of freedom (d.o.f.) ( $w, \theta_x, \theta_y$ ) per node. His basis function was a complete cubic polynomial. The term  $xy$  was left out, because the polynomial has one coefficient more than the element has d.o.f. This leads to the problem that no constant state of bending can be described (non-conforming element) and this leads to wrong results at convergence [Ste15]. Therefore, Steinke challenges the practical use of this element. A possible way to use a complete cubic polynomial would be to add another node in the center of mass of the triangle and assign the only degree of freedom  $w$  to it [Ste15]. But the problem of non-conformity persists, as the nodal twists don't suffice to describe the twists along the element's edges, which are quadric. Here, additional nodes on the edges would be needed. To get a conforming element one can choose a basis function with a complete polynomial of order five. It has 21 coefficients and d.o.f. They are distributed as follows: Every node has six d.o.f. ( $w, \partial w / \partial x, \partial w / \partial y, \partial^2 w / \partial x^2, \partial^2 w / \partial y^2, \partial^2 w / \partial x \partial y$ ) and the mid node of every edge gets the degree of freedom  $\partial w / \partial n$ . This results in continuous element edge twists, conformity and convergence. The problem: 21 d.o.f. per element leads to high computational effort and second order derivatives at the boundaries are needed. Hence, Steinke advises against using it in practice [Ste15].

In this work an element from [Spe88] were implemented which is also described in [Ste15]. It has three nodes and also three d.o.f. per node: The deformation  $w$  and the

two twists  $\theta_x$  and  $\theta_y$ . The basis function for the deformation  $w$  is as follows:

$$\begin{aligned}
w = & a_0 L_1 + a_1 L_2 + a_2 L_3 + a_3 L_1 L_2 + a_4 L_2 L_3 + a_5 L_3 L_1 \\
& + a_6 \left( L_2 L_1^2 + \frac{1}{2} L_1 L_2 L_3 (3(1 - \mu_3) L_1 - (1 + 3\mu_3) L_2 + (1 + 3\mu_3) L_3) \right) \\
& + a_7 \left( L_3 L_2^2 + \frac{1}{2} L_1 L_2 L_3 (3(1 - \mu_1) L_2 - (1 + 3\mu_1) L_3 + (1 + 3\mu_1) L_1) \right) \\
& + a_8 \left( L_1 L_3^2 + \frac{1}{2} L_1 L_2 L_3 (3(1 - \mu_2) L_3 - (1 + 3\mu_2) L_1 + (1 + 3\mu_2) L_2) \right)
\end{aligned} \tag{73}$$

with

$$\begin{aligned}
\mu_1 &= \frac{S_{21} - S_{31}}{S_{32}} \\
\mu_2 &= \frac{S_{32} - S_{21}}{S_{31}} \\
\mu_3 &= \frac{S_{31} - S_{32}}{S_{21}}
\end{aligned} \tag{74}$$

$$\begin{aligned}
S_{32} &= x_{32}^2 + y_{32}^2 \\
S_{31} &= x_{31}^2 + y_{31}^2 \\
S_{21} &= x_{21}^2 + y_{21}^2
\end{aligned} \tag{75}$$

$S_{ij}$  denoted the square of the length of the edge between node  $i$  and  $j$ . This can be written in vector form:

$$\begin{aligned}
w &= \vec{x}^T \vec{a} \\
\vec{x} &= \begin{pmatrix} L_1 \\ L_2 \\ L_3 \\ L_1 L_2 \\ L_2 L_3 \\ L_3 L_1 \\ \left( L_2 L_1^2 + \frac{1}{2} L_1 L_2 L_3 (3(1 - \mu_3) L_1 - (1 + 3\mu_3) L_2 + (1 + 3\mu_3) L_3) \right) \\ \left( L_3 L_2^2 + \frac{1}{2} L_1 L_2 L_3 (3(1 - \mu_1) L_2 - (1 + 3\mu_1) L_3 + (1 + 3\mu_1) L_1) \right) \\ \left( L_1 L_3^2 + \frac{1}{2} L_1 L_2 L_3 (3(1 - \mu_2) L_3 - (1 + 3\mu_2) L_1 + (1 + 3\mu_2) L_2) \right) \end{pmatrix} \\
\vec{a}^T &= (a_0 \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \quad a_7 \quad a_8)
\end{aligned} \tag{76}$$

The twists  $\theta_x$  and  $\theta_y$  are yet described in Cartesian coordinates. They must be transformed into triangular coordinates with the help of equation 25:

$$\vec{\theta} = \begin{pmatrix} \theta_x \\ \theta_y \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \nabla w = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \underline{J}^{-1} \tilde{\nabla} \vec{x}^T \vec{a} = \underline{G} \vec{a} \tag{77}$$

with  $\underline{J}^{-1}$  the inverse Jacobian matrix and  $\tilde{\nabla}$  the nabla operator in triangular coordinates. The matrix  $\underline{G}$ :

$$\underline{G} = \frac{1}{2A_{\Delta}} \begin{pmatrix} x_{32} & x_{13} \\ y_{32} & y_{13} \end{pmatrix} \begin{pmatrix} \frac{\partial x_1}{\partial L_1} & \frac{\partial x_2}{\partial L_1} & \dots & \frac{\partial x_9}{\partial L_1} \\ \frac{\partial x_1}{\partial L_2} & \frac{\partial x_2}{\partial L_2} & \dots & \frac{\partial x_9}{\partial L_2} \end{pmatrix} \quad (78)$$

Next, the interpolation conditions at the three nodes for the three unknowns can be set (cf. Figure 4). Following the notation of [Ste15]:

$$\underbrace{\begin{pmatrix} \vec{x}^T(1,0) \\ G_1(1,0) \\ G_2(1,0) \\ \vec{x}^T(0,1) \\ G_1(0,1) \\ G_2(0,1) \\ \vec{x}^T(0,0) \\ G_1(0,0) \\ G_2(0,0) \end{pmatrix}}_{\underline{A}} \vec{a} = \underbrace{\begin{pmatrix} w_1 \\ \theta_{x_1} \\ \theta_{y_1} \\ w_2 \\ \theta_{x_2} \\ \theta_{y_2} \\ w_3 \\ \theta_{x_3} \\ \theta_{y_3} \end{pmatrix}}_{\vec{w}} \quad (79)$$

where  $\underline{G}_i$  is the  $i$ -th row of matrix  $\underline{G}$ . The unknown coefficients  $a_i$  can be computed by inverting the matrix  $\underline{A}$ :  $\vec{a} = \underline{A}^{-1}\vec{w}$ :

$$\underline{A}^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & y_{12} & x_{21} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & y_{23} & x_{32} \\ 1 & y_{31} & x_{13} & 0 & 0 & 0 & -1 & 0 & 0 \\ 2 & y_{21} & x_{12} & -2 & y_{21} & x_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & y_{32} & x_{23} & -2 & y_{32} & x_{23} \\ -2 & y_{13} & x_{31} & 0 & 0 & 0 & 2 & y_{13} & x_{31} \end{pmatrix} \quad (81)$$

where  $x_{ij}$  and  $y_{ij}$  denotes the differences of the node's coordinates  $x_i - x_j$  and  $y_i - y_j$ . Now, the coefficients can be inserted into equation 76:

$$w = \vec{x}^T \vec{a} = \vec{x}^T \underline{A}^{-1} \vec{w} = \vec{N}^T \vec{w} \quad (82)$$

The vector  $\vec{N}$  containing the shape functions  $N_i$  can then be calculated as follows:

$$\vec{N} = \left( \underline{A}^{-1} \right)^T \vec{x} \quad (83)$$

Since the shape functions following a pattern, due to the regular order in the matrix  $\underline{A}^{-1}$ , one can summarize the nine shape functions into three groups; one for every node:

$$N_i = \begin{cases} \chi_i - \chi_{i+3} + \chi_{k+3} + 2(\chi_{i+6} - \chi_{k+6}) & \text{for d.o.f. } w \\ -y_{ki}(\chi_{k+6} - \chi_{k+3}) + y_{ji}\chi_{i+6} & \text{for d.o.f. } \theta_x \\ x_{ki}(\chi_{k+6} - \chi_{k+3}) - x_{ji}\chi_{i+6} & \text{for d.o.f. } \theta_y \end{cases} \quad (84)$$

The variables  $\chi_i$  denotes the  $i$ -th component of the vector  $\vec{\chi}$ , the indexes  $i, j, k$  under  $\chi$  are cyclic permutations of 1, 2, 3.  $x_{ij}$  and  $y_{ij}$  denote the coordinate differences  $x_i - x_j$  and  $y_i - y_j$ . The index under  $N$  is incremented in such a way, that  $N_1, N_4, N_7$  describes the d.o.f.  $w$ ,  $N_2, N_5, N_8$  describes the d.o.f.  $\theta_x$  and  $N_3, N_6, N_9$  describes the d.o.f.  $\theta_y$ . Similar to the plane elements, one can check the correctness of the shape functions by evaluating them at the triangular coordinates of the three triangle's nodes. For example, shape function  $N_7$  will evaluate to 1 for the coordinates  $(L_1 = 0, L_2 = 0)$  (node 3) and will be zero for  $(L_1 = 1, L_2 = 0)$  (node 1) and  $(L_1 = 0, L_2 = 1)$  (node 2).

The displacement-strain relation 58 introduced for the plate element contains an operator living in the Cartesian space. It has to be converted into triangular coordinates. With equation 30 ( $\nabla = \underline{J}^{-1}\tilde{\nabla}$ ) one can describe a second order derivative operator  $\Delta$ :

$$\Delta = \nabla \nabla^T = \underline{J}^{-1} \tilde{\nabla} \left( \underline{J}^{-1} \tilde{\nabla} \right)^T = \underline{J}^{-1} \tilde{\nabla} \tilde{\nabla}^T \left( \underline{J}^{-1} \right)^T = \underline{J}^{-1} \tilde{\Delta} \left( \underline{J}^{-1} \right)^T \quad (85)$$

$$\Delta = \begin{pmatrix} \frac{\partial^2}{\partial x^2} & \frac{\partial^2}{\partial x \partial y} \\ \frac{\partial^2}{\partial y \partial x} & \frac{\partial^2}{\partial y^2} \end{pmatrix} \rightarrow \vec{\Delta} = \begin{pmatrix} \frac{\partial^2}{\partial x^2} \\ \frac{\partial^2}{\partial y^2} \\ 2 \frac{\partial^2}{\partial x \partial y} \end{pmatrix}$$

$$\vec{\Delta} = \frac{1}{4A_{\Delta}^2} \begin{pmatrix} y_{32}^2 & y_{31}^2 & y_{23}y_{31} \\ x_{32}^2 & x_{31}^2 & x_{13}x_{32} \\ 2x_{32}y_{23} & 2x_{13}y_{31} & x_{32}y_{31} + x_{31}y_{32} \end{pmatrix} \begin{pmatrix} \frac{\partial^2}{\partial L_1^2} \\ \frac{\partial^2}{\partial L_2^2} \\ 2 \frac{\partial^2}{\partial L_1 \partial L_2} \end{pmatrix}$$

$$\vec{\Delta} = \underline{Y} \tilde{\Delta} \quad (86)$$

Next, equation 58 can be rewritten for triangular coordinates:

$$\vec{\epsilon} = -z \vec{\Delta} w = -z \underline{Y} \tilde{\Delta} w = -z \vec{\kappa} \quad (87)$$

And additionally, with the help of equation 82, this yields a new version of equation 59:

$$\vec{\kappa} = \vec{\Delta} w = \underline{Y} \tilde{\Delta} \vec{N}^T \vec{w} = \underline{Y} \tilde{B} \vec{w} = \underline{B} \vec{w} \quad (88)$$

$$\tilde{B} = \tilde{\Delta} \vec{N}^T = \begin{pmatrix} \frac{\partial^2 N_1}{\partial L_1^2} & \frac{\partial^2 N_2}{\partial L_1^2} & \dots & \frac{\partial^2 N_9}{\partial L_1^2} \\ \frac{\partial^2 N_1}{\partial L_2^2} & \frac{\partial^2 N_2}{\partial L_2^2} & \dots & \frac{\partial^2 N_9}{\partial L_2^2} \\ 2 \frac{\partial^2 N_1}{\partial L_1 \partial L_2} & 2 \frac{\partial^2 N_2}{\partial L_1 \partial L_2} & \dots & 2 \frac{\partial^2 N_9}{\partial L_1 \partial L_2} \end{pmatrix} \quad (89)$$

With the help of equation 88, the first term (denoted as  $\Pi_1$ ) of the plate element's functional 72 can be written out:

$$\begin{aligned} \Pi_1 &= \frac{1}{2} \int_A \vec{\kappa}^T \underline{D}_p \vec{\kappa} \, dA \\ &= \frac{1}{2} \vec{w}^T \int_A \underline{B}^T \underline{D}_p \underline{B} \, dA \vec{w} \\ &= \frac{1}{2} \vec{w}^T \underline{K} \vec{w} \end{aligned} \quad (90)$$

where  $\underline{K}$  describes the stiffness matrix for the three node triangular plate element. The stiffness matrix must be integrated in triangular coordinates. This will be done by a Gaussian quadrature with the Gauss points located at:  $(L_{1_1} = 1/6, L_{2_1} = 1/6), (L_{1_2} = 2/3, L_{2_2} = 1/6), (L_{1_3} = 1/6, L_{2_3} = 2/3)$  and weights  $\omega_i = 1/6$  for all three points. For an exact integration one would accumulate four sampling points, but [Ste15] states that this leads to an element, that is too stiff; with only three samplings a more natural element results.

$$\underline{K} = 2A_{\Delta} \sum_{i=1}^3 \omega_i \underline{B}^T(L_{1_i}, L_{2_i}) \underline{D}_p \underline{B}(L_{1_i}, L_{2_i}) \quad (91)$$

The plate's functional 72 has two more terms including the surface load  $p$  and edge loads  $V_n$ . These two can now be written as follows (see also [Ste15]):

$$\int_A p w dA = \vec{w}^T \vec{F}_p = \vec{w}^T p \int_A \vec{N} dA = 2\vec{w}^T A_{\Delta} p \int_0^1 \left( \int_0^{1-L_1} \vec{N} dL_2 \right) dL_1 \quad (92)$$

where  $\vec{F}_p$  is a  $1 \times 9$  vector containing forces and moments emerging from the surface load  $p$ . As an example, an edge load  $V_n$  is applied to edge  $S_{13}$ . This can be described as follows [Ste15]:

$$\int_{\Gamma_V} V_n w d\Gamma = \int_{\Gamma_V} V_n \vec{w}^T \vec{N}(L_2 = 0) d\Gamma \quad (93)$$

with  $d\Gamma = S_{13} dL_1$ . With  $V_n$  being constant all over the edge:

$$\int_{\Gamma_V} V_n \vec{w}^T \vec{N}(L_2 = 0) d\Gamma = \vec{w}^T S_{13} V_n \int_0^1 \vec{N} dL_1 = \vec{w}^T \vec{F}_v \quad (94)$$

The edge load applies forces and moments contained in  $\vec{F}_v$  to the nodes forming that edge. The above equation can be applied to every other edge.

### 3.3.3 Quad-4 Plate Element

The element implemented in this work is the so-called *DKQ* element, introduced by Batoz et al. [BT82]. It is a four node, 12 degrees-of-freedom quadrilateral element for thin plates. It is based on a generalization of the *Discrete Kirchhoff Triangular* (DKT) element which is a three node, 9 d.o.f. triangular element. Like the triangular element of the previous section, the DKQ element's nodes have all three degrees of freedom: The displacement  $w$  and the rotations  $\theta_x$  and  $\theta_y$  around the element's local  $x$ - and  $y$ -axis. Figure 8 shows an example of such an element.

The formulation of the DKQ element by Batoz et al. [BT82] uses the discrete Kirchhoff technique. It is based on the discretization of the strain energy and neglects the transverse shear energy. This results in the following functional:

$$\Pi = \frac{1}{2} \int_A \vec{\kappa}^T \underline{D}_p \vec{\kappa} dA \quad (95)$$

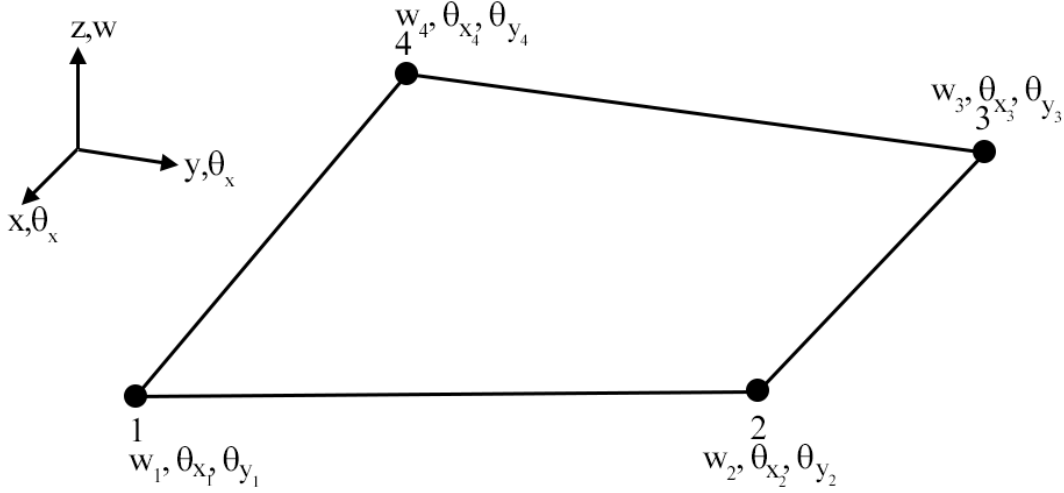


Figure 8: 12 node quadrilateral plate element DQK

where  $\underline{D}_p$  is the material matrix as defined previously (equation 61) and  $\vec{\kappa}$  denotes:

$$\vec{\kappa} = \begin{pmatrix} \frac{\partial \beta_x}{\partial x} \\ \frac{\partial \beta_y}{\partial y} \\ \frac{\partial \beta_x}{\partial y} + \frac{\partial \beta_y}{\partial x} \end{pmatrix} \quad (96)$$

$\beta_i$  is the rotation of the normal to the undeformed mid-surface in  $x$ - $z$ -plane and  $y$ - $z$ -plane, respectively. For  $\Pi$  only  $C^0$  continuity is required [BT82]. Further, Batoz et al. states that  $\beta_x$  and  $\beta_y$  must be related to  $w$  in such a way, that the final element satisfies the following requirements:

- The nodal variables must be  $w$ ,  $\theta_x$  and  $\theta_y$  with respect to  $x$  and  $y$  at the four element's nodes ( $\theta_x = \partial w / \partial y$ ,  $\theta_y = -\partial w / \partial x$ )
- The Kirchhoff boundary conditions must be satisfied.

Two incomplete cubic polynomial expressions define  $\beta_x$  and  $\beta_y$ :

$$\beta_x = \sum_{i=1}^8 N_i \beta_{x_i} \quad (97)$$

$$\beta_y = \sum_{i=1}^8 N_i \beta_{y_i} \quad (98)$$

$N_i(\xi, \eta)$  are here the shape functions with isoparametric coordinates  $\xi$  and  $\eta$ . They are the same as of the eight node Serendipity element, described for example in [ZT00] and seen in Figure 9. The shape functions of this element are achieved by products of linear

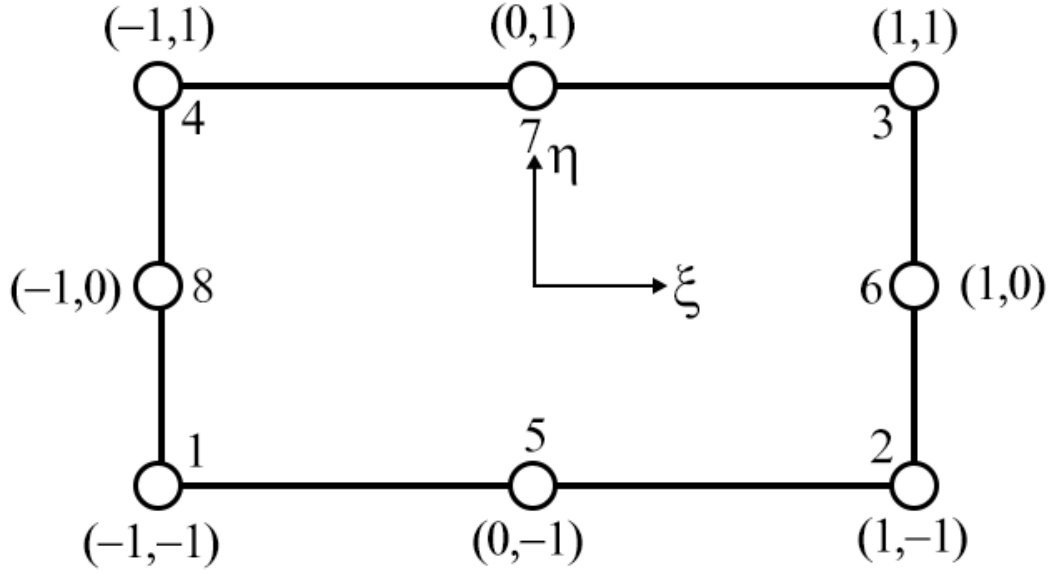


Figure 9: lange Unter-Überschrift

lagrangian polynomials of the form  $\frac{1}{4}(\xi + 1)(\eta + 1)$ . For the eight node element the following shape functions result:

$$\begin{aligned}
 N_1(\xi, \eta) &= \frac{1}{4}(1 - \xi)(1 - \eta)(-\xi - \eta - 1) \\
 N_2(\xi, \eta) &= \frac{1}{4}(1 + \xi)(1 - \eta)(\xi - \eta - 1) \\
 N_3(\xi, \eta) &= \frac{1}{4}(1 + \xi)(1 + \eta)(\xi + \eta - 1) \\
 N_4(\xi, \eta) &= \frac{1}{4}(1 - \xi)(1 + \eta)(-\xi + \eta - 1) \\
 N_5(\xi, \eta) &= \frac{1}{2}(1 - \xi^2)(1 - \eta) \\
 N_6(\xi, \eta) &= \frac{1}{2}(1 + \xi)(1 - \eta^2) \\
 N_7(\xi, \eta) &= \frac{1}{2}(1 - \xi^2)(1 + \eta) \\
 N_8(\xi, \eta) &= \frac{1}{2}(1 - \xi)(1 - \eta^2)
 \end{aligned}$$

$\beta_{x_i}$  and  $\beta_{y_i}$  are transitory nodal variables at the four nodes and mid-sides of the element. Next, Batoz et al. described the Kirchhoff assumptions at the corner nodes (cf. Figure 9 for the following):

$$\begin{pmatrix} \beta_{x_i} + \partial w / \partial x_i \\ \beta_{y_i} + \partial w / \partial y_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad i = 1, 2, 3, 4 \quad (99)$$



and at the mid-nodes:

$$\beta_{s_k} + \partial w / \partial s_k = 0, \quad k = 5, 6, 7, 8 \quad (100)$$

where  $s$  denotes the coordinate along the element boundary and  $\partial w / \partial s_k$  is the derivative of the displacement  $w$  with respect to the mid-node  $k$ :

$$\frac{\partial w}{\partial s_k} = -\frac{3}{2l_{ij}}(w_i - w_j) - \frac{1}{4} \left( \frac{\partial w}{\partial s_i} + \frac{\partial w}{\partial s_j} \right) \quad (101)$$

with  $k = 5, 6, 7, 8$  being the mid-node of side  $ij = 12, 23, 34, 41$  and  $l_{ij}$  denotes the length of side  $ij$ .  $\beta_n$  varies linearly along the sides:

$$\beta_{n_k} = \frac{1}{2} (\beta_{n_i} + \beta_{n_j}) - \frac{1}{2} \left( \frac{\partial w}{\partial n_i} + \frac{\partial w}{\partial n_j} \right) \quad (102)$$

with  $k$  same as before.  $\beta_x$  and  $\beta_y$  can be rewritten as follows:

$$\beta_x = H^x(\vec{\xi}, \eta)^T \vec{w} \quad (103)$$

$$\beta_y = H^y(\vec{\xi}, \eta)^T \vec{w} \quad (104)$$

$$\vec{w}^T = (w_1 \quad \theta_{x_1} \quad \theta_{y_1} \quad w_2 \quad \theta_{x_2} \quad \theta_{y_2} \quad w_3 \quad \theta_{x_3} \quad \theta_{y_3})$$

with

$$\begin{aligned} \vec{H}^x{}^T &= (H_1^x \quad \dots \quad H_{12}^x) \\ H_{[1,4,7,10]}^x &= \frac{3}{2} (a_{[5,6,7,8]} N_{[5,6,7,8]} - a_{[8,5,6,7]} N_{[8,5,6,7]}) \\ H_{[2,5,8,11]}^x &= b_{[5,6,7,8]} N_{[5,6,7,8]} + b_{[8,5,6,7]} N_{[8,5,6,7]} \\ H_{[3,6,9,12]}^x &= N_{[1,2,3,4]} - c_{[5,6,7,8]} N_{[5,6,7,8]} - c_{[8,5,6,7]} N_{[8,5,6,7]} \\ \vec{H}^y{}^T &= (H_1^y \quad \dots \quad H_{12}^y) \\ H_{[1,4,7,10]}^y &= \frac{3}{2} (d_{[5,6,7,8]} N_{[5,6,7,8]} - d_{[8,5,6,7]} N_{[8,5,6,7]}) \\ H_{[2,5,8,11]}^y &= -N_{[1,2,3,4]} + e_{[5,6,7,8]} N_{[5,6,7,8]} + e_{[8,5,6,7]} N_{[8,5,6,7]} \\ H_{[3,6,9,12]}^y &= -b_{[5,6,7,8]} N_{[5,6,7,8]} - b_{[8,5,6,7]} N_{[8,5,6,7]} \end{aligned}$$

The function notation  $H_{[i,j,k,l]}^x$  groups four functions together. The first function of the group gets the first index of the squared brackets, the second function the second index,

and so on. The coefficients  $a, b, c, d$  and  $e$  are as follows:

$$\begin{aligned} a_k &= -\frac{x_{ij}}{l_{ij}^2} \\ b_k &= \frac{3}{4} \frac{x_{ij} y_{ij}}{l_{ij}^2} \\ c_k &= \frac{\frac{x_{ij}^2}{4} - \frac{y_{ij}^2}{2}}{l_{ij}^2} \\ d_k &= -\frac{y_{ij}}{l_{ij}^2} \\ e_k &= \frac{\frac{y_{ij}^2}{4} - \frac{x_{ij}^2}{2}}{l_{ij}^2} \end{aligned}$$

where  $k = 5, 6, 7, 8$  for the sides  $ij = 12, 23, 34, 41$ ,  $x_{ij} = x_i - x_j$ ,  $y_{ij} = y_i - y_j$  and  $l_{ij}^2 = x_{ij}^2 + y_{ij}^2$ . For more details about the derivation of these coefficients and functions  $H^x$  and  $H^y$  see Batoz et al. [BT82].

Next, the Jacobian matrix  $\underline{J}$  can be assembled, that is:

$$\underline{J} = \frac{1}{4} \begin{pmatrix} (x_{12} + x_{34})\eta - x_{12} + x_{34} & (y_{12} + y_{34})\eta - x_{12} + y_{34} \\ (x_{12} + x_{34})\xi - x_{13} - x_{24} & (y_{12} + y_{34})\xi - y_{13} + y_{24} \end{pmatrix} = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix} \quad (105)$$

With its determinant and inverse:

$$|\underline{J}| = J_{11}J_{22} - J_{12}J_{21} \quad (106)$$

$$\underline{J}^{-1} = \frac{1}{|\underline{J}|} \begin{pmatrix} J_{22} & -J_{12} \\ -J_{21} & J_{11} \end{pmatrix} = \begin{pmatrix} j_{11} & j_{12} \\ j_{21} & j_{22} \end{pmatrix} \quad (107)$$

The strain-displacement matrix can now be obtained:

$$\underline{B} = \begin{pmatrix} \vec{H}_x^x \\ \vec{H}_y^y \\ \vec{H}_y^x + \vec{H}_x^y \end{pmatrix} = \begin{pmatrix} j_{11} & j_{12} & 0 & 0 \\ 0 & 0 & j_{21} & j_{22} \\ j_{21} & j_{22} & j_{11} & j_{12} \end{pmatrix} \begin{pmatrix} \vec{H}_\xi^x \\ \vec{H}_\eta^x \\ \vec{H}_\xi^y \\ \vec{H}_\eta^y \end{pmatrix} \quad (108)$$

The expressions  $vec H_\xi^x, \vec{H}_\eta^x, \vec{H}_\xi^y$  and  $\vec{H}_\eta^y$  are vectors containing the derivatives of the corresponding components of the vectors  $\vec{H}^x$  and  $\vec{H}^y$  with respect to  $\xi$  and  $\eta$ , respectively. And the matrix  $\underline{B}$  can then be inserted into the displacement-strain relation, like equation 88:

$$\vec{\kappa} = \underline{B}\vec{w} \quad (109)$$

Next,  $\vec{\kappa} = \underline{B}\vec{w}$  can be used in the functional to get the first term like equation 90:

$$\begin{aligned}\Pi_1 &= \frac{1}{2} \int_A \vec{\kappa}^T \underline{D}_p \vec{\kappa} \, dA \\ &= \frac{1}{2} \vec{w}^T \int_A \underline{B}^T \underline{D}_p \underline{B} \, dA \vec{w} \\ &= \frac{1}{2} \vec{w}^T \underline{K} \vec{w}\end{aligned}$$

with the stiffness matrix of the DKQ element  $\underline{K}$ :

$$\begin{aligned}\underline{K} &= \int_A \underline{B}^T \underline{D}_p \underline{B} \, dA \\ &= \int_{-1}^1 \int_{-1}^1 \underline{B}^T \underline{D}_p \underline{B} \, |\underline{J}| \, d\xi d\eta\end{aligned}\tag{110}$$

The stiffness matrix can be numerically integration with a  $2 \times 2$  Gaussian integration scheme. Batoz et al. states that four sampling points are enough, although a  $3 \times 3$  point scheme would be necessary for exact integration on a rectangular element [BT82]. Those four sampling points are located at  $\xi_i = \pm \frac{\sqrt{3}}{3}$  and  $\eta_i = \pm \frac{\sqrt{3}}{3}$  with weight factor  $\omega_i = 1$  equivalent to all four. The equation for the stiffness matrix can then be written in discretized form as follows:

$$\underline{K} = \sum_{i=1}^2 \sum_{j=1}^2 \omega_i \omega_j \underline{B}(\xi_i, \eta_j)^T \underline{D}_p \underline{B}(\xi_i, \eta_j) |\underline{J}(\xi_i, \eta_j)|\tag{111}$$

When all nodal values  $\vec{w}$  are known, the moments  $\vec{M}$  at point  $(x, y)$  in the element can be calculated:

$$\vec{M}(x, y) = \underline{D}_p \underline{B}(x, y) \vec{w}\tag{112}$$

with

$$\vec{M} = \begin{pmatrix} M_x \\ M_y \\ M_{xy} \end{pmatrix}\tag{113}$$

### 3.4 Coordinate Transformation

The nodes and elements in the mesh are defined in a global three dimensional coordinate system. The elements need to be transformed into a two dimensional local coordinate system in order to be able to calculate their local stiffness matrices. This local stiffness matrix must then be transformed back into the global system before adding it to the global stiffness matrix. This section describes the building of the transformation matrix, that will be used in the following section for the addressed transformation steps. First the transformation of an arbitrary triangle defined in 3D space is described.

Given a triangle with vertices  $\vec{A} = (a_x, a_y, a_z)^T$ ,  $\vec{B} = (b_x, b_y, b_z)^T$  and  $\vec{C} = (c_x, c_y, c_z)^T$  ordered in counter-clockwise direction, as shown in Figure 10. Let  $\vec{u}$  be the vector from

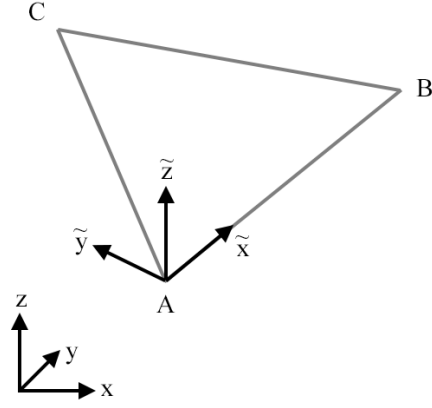


Figure 10: Arbitrary triangle with nodes A, B and C, defined in global  $xyz$  coordinate system. After transformation a new, local,  $\tilde{x}\tilde{y}\tilde{z}$  coordinate system with node A in its origin, is created.

node  $\vec{A}$  to  $\vec{B}$  and  $\vec{v}$  be the vector from node  $\vec{A}$  to  $\vec{C}$ :

$$\begin{aligned}\vec{u} &= \vec{B} - \vec{A} = \begin{pmatrix} b_x - a_x & b_y - a_y & b_z - a_z \end{pmatrix}^T \\ \vec{v} &= \vec{C} - \vec{A} = \begin{pmatrix} c_x - a_x & c_y - a_y & c_z - a_z \end{pmatrix}^T\end{aligned}$$

First local unit vector:

$$\vec{\tilde{x}} = \frac{1}{|\vec{u}|} \vec{u}$$

Second local unit vector:

$$\begin{aligned}\vec{\tilde{z}} &= \vec{u} \times \vec{v} \\ \vec{\tilde{z}} &\leftarrow \frac{1}{|\vec{\tilde{z}}|} \vec{\tilde{z}}\end{aligned}$$

Third local unit vector:

$$\vec{\tilde{y}} = \vec{\tilde{z}} \times \vec{\tilde{x}}$$

Define transformation matrix  $\underline{T}$  as follows:

$$\underline{T} = \begin{pmatrix} \vec{\tilde{x}}^T \\ \vec{\tilde{y}}^T \\ \vec{\tilde{z}}^T \end{pmatrix} = \begin{pmatrix} \tilde{x}_x & \tilde{x}_y & \tilde{x}_z \\ \tilde{y}_x & \tilde{y}_y & \tilde{y}_z \\ \tilde{z}_x & \tilde{z}_y & \tilde{z}_z \end{pmatrix} \quad (114)$$

Assembly of element's stiffness matrix needs partial derivatives. In order to get these derivatives with less computational effort, every triangle can be translated in such a way, that node  $\vec{A}$  lies in the global origin before transforming it to local coordinates. Node  $\vec{A}$

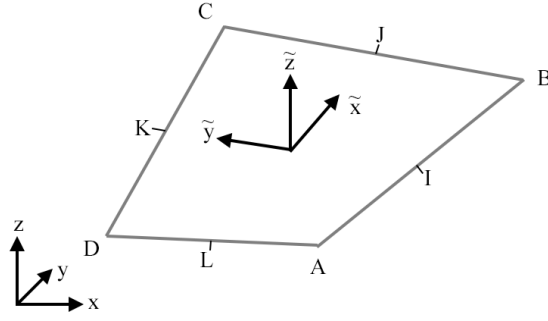


Figure 11: Quadrilateral with nodes A, B, C and D, defined in global  $xyz$  coordinate system. After transformation a new, local,  $\tilde{x}\tilde{y}\tilde{z}$  coordinate system is created.

stays at (0, 0, 0) coordinates which then simplifies getting the derivatives (see section ??). It follows:

$$\begin{aligned}\vec{A} &= \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}^T \\ \vec{B} &= \begin{pmatrix} \tilde{b}_x & 0 & 0 \end{pmatrix}^T \\ \vec{C} &= \begin{pmatrix} \tilde{c}_x & \tilde{c}_y & 0 \end{pmatrix}^T\end{aligned}$$

Node  $\vec{A}$  will not be changed by the transformation with  $\underline{T}$ ,  $\vec{B}$  will be projected onto the local  $x$ -axis that is defined to be the normalized vector between  $\vec{A}$  and  $\vec{B}$ . Node  $\vec{C}$  will be projected onto the local  $xy$ -plane. One can see that the  $z$ -component vanishes by transforming into local space, thus generating the wished two dimensional local space.

The other element described in this work is the quadrilateral. Let an arbitrary quadrilateral be given with vertices  $\vec{A} = (a_x, a_y, a_z)^T$ ,  $\vec{B} = (b_x, b_y, b_z)^T$ ,  $\vec{C} = (c_x, c_y, c_z)^T$ ,  $\vec{D} = (d_x, d_y, d_z)^T$  ordered in counter-clockwise direction, cf. Figure 11. Next, let  $\vec{I}$  be the midpoint of edge  $\overline{AB}$ :

$$\vec{I} = \vec{A} + \frac{1}{2} (\vec{B} - \vec{A})$$

Analogously let  $\vec{J}$ ,  $\vec{K}$  and  $\vec{L}$  be the midpoints of the edges  $\overline{BC}$ ,  $\overline{CD}$  and  $\overline{DA}$ :

$$\begin{aligned}\vec{J} &= \vec{B} + \frac{1}{2} (\vec{C} - \vec{B}) \\ \vec{K} &= \vec{C} + \frac{1}{2} (\vec{D} - \vec{C}) \\ \vec{L} &= \vec{D} + \frac{1}{2} (\vec{A} - \vec{D})\end{aligned}$$

Let then  $\vec{u}$  be the vector from node  $\vec{L}$  to  $\vec{J}$  and  $\vec{v}$  be the vector from node  $\vec{I}$  to  $\vec{K}$ :

$$\begin{aligned}\vec{u} &= \vec{J} - \vec{L} = \begin{pmatrix} j_x - l_x & j_y - l_y & j_z - l_z \end{pmatrix}^T \\ \vec{v} &= \vec{K} - \vec{I} = \begin{pmatrix} k_x - i_x & k_y - i_y & k_z - i_z \end{pmatrix}^T\end{aligned}$$

First local unit vector:

$$\vec{x} = \frac{1}{|\vec{u}|} \vec{u}$$

Second local unit vector:

$$\begin{aligned} \vec{z} &= \vec{u} \times \vec{v} \\ \vec{z} &\leftarrow \frac{1}{|\vec{z}|} \vec{z} \end{aligned}$$

Third local unit vector:

$$\vec{y} = \vec{z} \times \vec{x}$$

Define transformation matrix  $T$  as follows:

$$\underline{T} = \begin{pmatrix} \vec{x}^T \\ \vec{y}^T \\ \vec{z}^T \end{pmatrix} = \begin{pmatrix} \vec{x}_x & \vec{x}_y & \vec{x}_z \\ \vec{y}_x & \vec{y}_y & \vec{y}_z \\ \vec{z}_x & \vec{z}_y & \vec{z}_z \end{pmatrix} \quad (115)$$

Remark: In order to transform a quadrilateral element from 3D to a local two dimensional space, the nodes of the original element must all be situated on a common plane. Otherwise such a transformation cannot be performed. Such shaped quadrilaterals cannot be used as shell elements.

### 3.5 Shell Element

Shell elements combine the potential of both, plane and plate elements. Every time a thin walled structure like a car body, dome structure or container with multiaxial pressures is to be simulated, shell elements provide a good solution. In this work only the so-called flat shell elements are described and used in the implementation. Details about curved shell elements, shells of revolution and general shells can be found in Cook et al. [CMPW02].

Flat shell elements have a state of bending and membrane stress that can be described by superposition of the plane and plate element [Kle13]. Figure 12 shows the superposition of plane and plate elements to a flat shell element. The degrees of freedom of plane and plate at every node are combined at the node of the shell element. Obviously the plane and plate element must be of the same finite element's type, for example three node triangular or eight node quadrilateral.

The plane has displacements  $u$  and  $v$  with dedicated forces  $F_x$  and  $F_y$ . The plate has the deformation  $w$  with assigned normal force  $F_z$  and the two twists  $\theta_x$  and  $\theta_y$  with assigned moments  $M_x$  and  $M_y$ . Through the linking of the elements the shell element node has now five natural degrees of freedom. An additional twist around the local z-axis  $\theta_z$  will be introduced [Ste15], increasing the number to six degrees of freedom per node. In vector notation the resulting displacement vector  $\vec{u}_i$  of a shell element's node

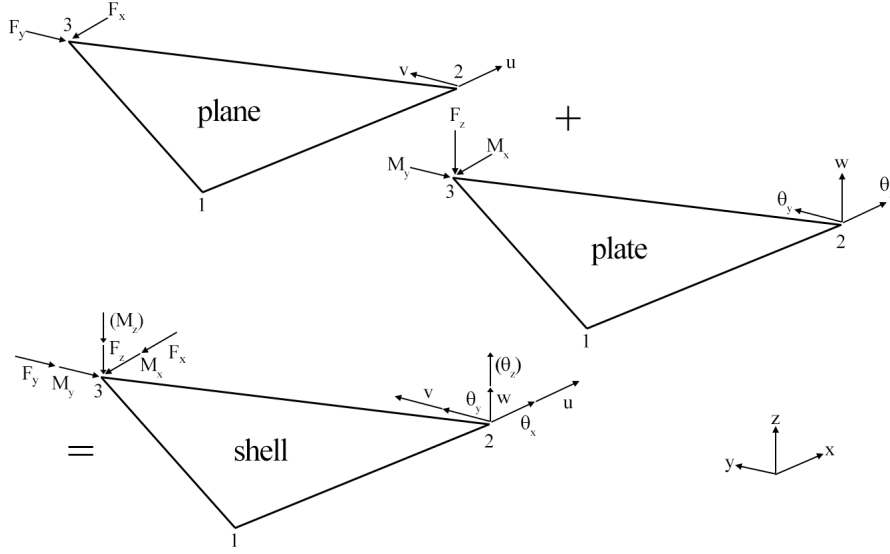


Figure 12: Creation of a triangular flat shell element by superimposing a triangular plane and a triangular plate element. The elements are described in the same local coordinate system with their degrees of freedom shown exemplary at one node per element.

$i$  is:

$$\vec{u} = \underbrace{\begin{pmatrix} u \\ v \\ w \\ \theta_x \\ \theta_y \\ \theta_z \end{pmatrix}}_{\text{shell}} = \underbrace{\begin{pmatrix} u \\ v \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}}_{\text{plane}} + \underbrace{\begin{pmatrix} 0 \\ 0 \\ w \\ \theta_x \\ \theta_y \\ 0 \end{pmatrix}}_{\text{plate}} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \theta_z \end{pmatrix} \quad (116)$$

$$(117)$$

For the two different finite elements in this work - the three node triangular element and the four node quadrilateral element - the stiffness matrix for the shell element is described by a block matrix of either  $3 \times 3$  submatrices for the triangular case or  $4 \times 4$  submatrices for the quadrilateral. The following equation shows the latter case as example:

$$\underline{K} \vec{u} = \vec{F}$$

$$\begin{pmatrix} \underline{K}_{11} & \underline{K}_{12} & \underline{K}_{13} & \underline{K}_{14} \\ \underline{K}_{21} & \underline{K}_{22} & \underline{K}_{23} & \underline{K}_{24} \\ \underline{K}_{31} & \underline{K}_{32} & \underline{K}_{33} & \underline{K}_{34} \\ \underline{K}_{41} & \underline{K}_{42} & \underline{K}_{43} & \underline{K}_{44} \end{pmatrix} \begin{pmatrix} \vec{u}_1 \\ \vec{u}_2 \\ \vec{u}_3 \\ \vec{u}_4 \end{pmatrix} = \begin{pmatrix} \vec{F}_1 \\ \vec{F}_2 \\ \vec{F}_3 \\ \vec{F}_4 \end{pmatrix} \quad (118)$$

where the vectors  $\vec{u}_i$  are the same as in equation 116. The single submatrices  $\underline{K}_{ij}$  of  $\underline{K}$  were created by the superposition of the stiffness matrices of the plane and the plate:

$$\underline{K}_{ij} = \left( \hat{K}_{ij} \right)_m + \left( \hat{K}_{ij} \right)_p \quad (119)$$

The submatrix  $\underline{K}_{ij}$  has the following structure:

$$\begin{array}{c} \begin{array}{c|c} \begin{array}{cccccc} \underline{u} & \underline{v} & \underline{w} & \underline{\theta}_x & \underline{\theta}_y & \underline{\theta}_z \end{array} \\ \left( \begin{array}{cccccc} \circ & \circ & 0 & 0 & 0 & 0 \\ \circ & \circ & 0 & 0 & 0 & 0 \\ 0 & 0 & \star & \star & \star & 0 \\ 0 & 0 & \star & \star & \star & 0 \\ 0 & 0 & \star & \star & \star & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right) \end{array} & \begin{array}{c} |u \\ |v \\ |w \\ |\theta_x \\ |\theta_y \\ |\theta_z \end{array} & = & \begin{array}{c|c} \begin{array}{cccccc} \underline{u} & \underline{v} & \underline{w} & \underline{\theta}_x & \underline{\theta}_y & \underline{\theta}_z \end{array} \\ \left( \begin{array}{cccccc} \circ & \circ & 0 & 0 & 0 & 0 \\ \circ & \circ & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right) \end{array} & \begin{array}{c} |u \\ |v \\ |w \\ |\theta_x \\ |\theta_y \\ |\theta_z \end{array} & + & \begin{array}{c|c} \begin{array}{cccccc} \underline{u} & \underline{v} & \underline{w} & \underline{\theta}_x & \underline{\theta}_y & \underline{\theta}_z \end{array} \\ \left( \begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \star & \star & \star & 0 \\ 0 & 0 & \star & \star & \star & 0 \\ 0 & 0 & \star & \star & \star & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right) \end{array} & \begin{array}{c} |u \\ |v \\ |w \\ |\theta_x \\ |\theta_y \\ |\theta_z \end{array} \end{array} \quad (120)$$

$\left( \hat{K}_{ij} \right)_m$  describes the submatrix of the stiffness matrix of the plane element for node  $i$  and  $j$  and is marked with the  $\circ$ -symbol,  $\left( \hat{K}_{ij} \right)_p$  describes the corresponding matrix part of the plate element's stiffness matrix and is symbolized with a  $\star$ . The degree of freedom  $\theta_z$  does not exist in both, the plane and the plate element, and were introduced with the shell element. Therefore  $(\underline{K}_{ij})_{66}$  is zero. The sixth degree of freedom is necessary because the missing stiffness regarding a rotation around the axis normal to the element could produce singularities in the overall stiffness matrix. This happens for example, if all neighboring elements of a node lie in the same plane, i.e. they are coplanar. A singularity can lead to a non-solvable system, so this case needs to be excluded [Ste15]. One way is to introduce this sixth degree of freedom and give it a value that is so small that it does not influence the displacements and stresses too much. The number of this values varies: Werkle suggests a value of 1/10000 of the smallest diagonal entry of  $\underline{K}_{ij}$  [Wer95], where Ibrahimbegovic et al. suggests 1/1000 of the smallest diagonal entry of  $\underline{K}_{ij}$ . The value must be small, but big enough to prevent the singularities. Since this value is an approximation, one has to modify it, if the solution is not as expected or one cannot get a solution at all due to the addressed singularities.

The stiffness matrix for the shell element was constructed in a local coordinate system as described in section ??, ?? and ??. The overall stiffness matrix containing information about all elements need to be described in a global coordinate system. Before the element stiffness matrix is added to the global stiffness matrix, it has to be transformed from local to global. This can be achieved by transforming the single blocks of  $\underline{K}$  from equation 118 with the relation:

$$\check{\underline{K}}_{ij} \vec{u}_j = \vec{F}_i \quad (121)$$

where “ $\sim$ ” denotes that the matrix and vector are represented in local coordinates. With the help of the transformation matrix  $\underline{\hat{T}}$ , the globally described displacement vector  $\vec{u}_j$



and load vector  $\vec{F}_i$  can be represented in local coordinates:

$$\check{\vec{u}}_j = \underline{\tilde{T}} \vec{u}_j \quad (122)$$

$$\check{\vec{F}}_i = \underline{\tilde{T}} \vec{F}_i \quad (123)$$

Since the load vector is to be defined in a global coordinate system and the resulting displacements are to be defined globally, too, equation 121 will be multiplied by  $\underline{\tilde{T}}^T$  from left:

$$\underline{\tilde{T}}^T \check{\underline{K}}_{ij} \underline{\tilde{T}} \vec{u}_j = \underline{\tilde{T}}^T \underline{\tilde{T}} \vec{F}_i = \vec{F}_i \quad (124)$$

Hence, the two vectors will be represented in global coordinates and only the local element stiffness matrix need to be transformed. The addressed  $6 \times 6$  transformation matrix  $\underline{\tilde{T}}$  is made up of the  $3 \times 3$  transformation matrix  $\underline{T}$  from section ??:

$$\underline{\tilde{T}} = \begin{pmatrix} \underline{T} & 0 \\ 0 & \underline{T} \end{pmatrix} \quad (125)$$

In order to get the local element stiffness matrix  $\underline{K}$  transformed to the global coordinate system, one has to transform the single submatrices  $\underline{K}_{ij}$  as follows:

$$\underline{K}_{ij} = \underline{\tilde{T}}^T \check{\underline{K}}_{ij} \underline{\tilde{T}} \quad (126)$$

for  $1 \leq i, j \leq 3$  in the case of the triangular element and  $1 \leq i, j, \leq 4$  for the quadrilateral element, respectively.

## 4 FEM Code Implementation

contains development of the program code with focus on the assembly of the system and its solving, the process of parallelization

### 4.1 Introduction to libMesh

The libMesh finite element library was started as part of the Ph.D. work of Benjamin Kirk [Kir07]. It is a tool for numerical simulation of partial differential equations on serial and parallel platforms and uses the finite element method. Major goals are to provide data structures and algorithms for applications that need implicit numerical methods, parallel computing, adaptive mesh refinement techniques, or, a combination of them. Further, it simplifies many programming details for the user, such as: Reading the mesh from file, initialize data structures, solving the discretized system, and, writing out the results [KPS13].

LibMesh allows discretization of one, two and three dimensional problems using several geometric element types, including: Edges, quadrilaterals, triangles, tetrahedra, hexahedra, pyramids, prisms and some infinite elements of quadrilaterals or hexahedra. Finite elements include traditional first and second order Lagrange, as well as arbitrary order hierarchical bases, and Nédélec elements of first type.

Mesh partitioning is available in libMesh through interfaces to several external packages, but also some internal partitioning algorithms are provided: Linear and centroid partitioner as examples of internal algorithms, Metis and ParMetis [KK98] as examples for external partitioner. In addition to these two, libMesh includes interfaces to solver libraries such as PETSc [pet] and LAPACK [las]. Thus, libMesh provides several linear equation solvers such as GMRES, CG, Bi-CGSTAB, QMR, and preconditioners like Jacobi, incomplete LU factorization and incomplete Cholesky factorization. The choice of an appropriate solver and preconditioner is made by the user at runtime.

A wide variety of mesh formats are supported by libMesh to facilitate use of complex geometries. The following is an incomplete list of supported input and output formats: Nemesis, TetGen, I-deas Universal UNV, AVS's ASCII UCD, Visualization Toolkit VTK, libMesh formats XDR/XDA, ExodusII, GMSH, LANL's General Mesh Viewer GMV, GnuPlot (only output), Matlab (only input) [KPS13].

An example program using the libMesh library would look like listing 1.

Listing 1: Example libMesh program

```
1 #include "libmesh/libmesh.h"
2 #include "libmesh/additional_libmesh_components"
3
4 using namespace libMesh;
5
6 void assemble_something(EquationSystems& es, const std::string& system_name);
7
8 int main (int argc, char** argv)
9 {
```

```

10  LibMeshInit (int argc, char** argv);
11
12  Mesh mesh( init.comm() );
13
14  // mesh generation via MeshTools::Generation::build... or mesh import from file via
    mesh.read(std::string filename)
15
16  EquationSystems es(mesh);
17
18  LinearImplicitSystem& system = es.add_system<LinearImplicitSystem> ("example_system");
19
20  system.add_variable ("a", FIRST);
21  system.add_variable ("b", SECOND, LAGRANGE);
22
23  system.attach_assemble_function (assemble_something);
24
25  es.init();
26
27  system.solve();
28
29  VTKIO (mesh).write_equation_systems ("out.pvtu", es);
30
31  return 0;
32 }

```

In fact, this is the base construction of nearly every libMesh program. It starts with including libMesh components that are needed by the program, e.g. *mesh.h*, *equation\_systems.h*, *fe.h*. Then, the library needs to be initialized (line 10). This is necessary because it may depend on a number of other external libraries like MPI and PETSc that require initialization before use. On the other hand, if the **LibMeshInit** object goes out of scope, the other libraries are finalized automatically by libMesh. Next, a mesh is created (lines 12-14) on the default MPI communicator (even if the program is executed single-threaded). The mesh can either be read from file or created by internal mesh generation tools. In line 16 an equation systems object is created. It can contain multiple different systems. Here, only one linear implicit system is added to the object (line 16). Each system can contain multiple variables of different approximation orders (see lines 20/21). Many systems require a user-defined function that will assemble the (linear) system (lines 6 and 23). Now, the data structures for equation system must be initialized which is done in line 25. The solving of the systems is done in line 27 of the code. This one line of code calls the assemble function defined earlier and invokes the default numerical solver. If the external library PETSc is installed, the solver can be controlled from the command line by the user. After solving the system, the solution can be written to file; here, for example, the results are written to a VTK-formatted plot file (line 29).

## 4.2 Implementation Details

details about the implementation with the libmesh FEM framework

- short overview: stand-alone-version: gets input parameters from user and mesh file and produces results stored in output file

### 4.2.1 Initialization

- loading of parameters: which parameters are needed by the user
  - poisson's ratio  $\nu$  required, no default value
  - elastic modulus  $E$  required, no default value
  - mesh thickness  $t$  required, no default value
  - debugging messages, default false
  - mesh file required, no default file, type msh oder xda, xdr, see next section for more details
  - output file, if not given, no output is made
- special parameters for petsc:
  - solver-type
  - preconditioner-type

### 4.2.2 Mesh file import

- wie sieht mesh file aus, was muss definiert sein:
  - vertices mit coordinates
  - elements
  - boundary conditions
- beispiel im libmesh-format xda
- welche typen werden akzeptiert: xda, gmsh implementiert; weitere als erweiterung denkbar
- welche ids für bcs müssen verwendet werden: auflistung der bc-id und ihre bedeutung
  - 0: clamped/simple supported
  - 1: simply supported/clamped
  - 2: inner node, part of preCICE interface region (only used by preCICE coupled variant)
  - 20: same as 0 but additionally part of preCICE interface region (only used...)
  - 21: same as 1 but additionally part of preCICE ...
- especially for standalone-case: force file
  - structure with short example matching the mesh-example
  - entries defined in global coordinate system like vertices, too

### 4.2.3 System setup

- setting up libmesh
  - LinearImplicitSystem, erklärung aus doxygen
  - 6 variablen erstellen
  - set boundary condition types, DirichletBoundary class
- nochmal auf theorieteil eingehen

### 4.2.4 Matrix and vector assembly

- material matrices: D\_m und D\_p
- creation of local and global stiffness matrix
- integral with gauss-quadrature
- read corresponding entry from force array and set it in the right-hand-side vector
- storing already processed nodes with unordered\_set-structure

### 4.2.5 Solving the system

- solving part is just one line. calls the assemble-function and the defined solver (e.g. if PETSc is installed)
- which settings are possible (error-eps, #iters)
- build\_solution\_vector

### 4.2.6 Output

- for standalone-version output as exodus2-file
- exodus2 can be read by ParaView, parallel vtk-output is not supported by libMesh
  - according to the user command line parameter, output file is written to specified file or not at all

## 4.3 Parallelization with MPI

additional steps to make the code ready for multi process execution with MPI

### 4.3.1 libMesh requirements

grundsätzlich ist zum lösen des gleichungssystem mit mehreren prozessen petsc als externe lib notwendig

#### **4.3.2 Partitioning the mesh**

am mesh muss nichts verändert werden, da libmesh automatisch eine partitionierung des meshes vornimmt (kann aber verbessert werden)

#### **4.3.3 Local elements**

grundsätzlich sorgt libMesh dafür, dass jeder prozessor nur zugriff auf "seine" element, knoten usw. hat. Das wird hier wichtig mit änderungen an den iteratoren usw.

#### **4.3.4 Assembly changes**

damit rhs korrekt gesetzt wird muss über die prozessgrenzen hinweg klar sein, ob knoten bereits bearbeitet wurde oder nicht. wie das gelöst wurde kommt hier rein

## **5 Coupling with preCICE**

### **5.1 Introduction to coupling**

### **5.2 Introduction to preCICE**

short introduction what preCICE is

### **5.3 Coupling methods**

siehe paper

### **5.4 Implementation**

"modification" of the code to work with preCICE

## 6 Validation

The code was tested with several problems to validate its correctness and state where and why there are differing results to the existing (commercial) FEM codes

### 6.1 Test A: Membrane Displacement with Tri-3

Sprungbrett bestehend aus 8 Elementen; links fest eingespannt, rechts Kraft in y-Richtung an beiden Randknoten

Sprungbrett bestehend aus 32 Elementen in Fischgrätmuster angeordnet; selbe BCs aber andere Kraftwerte

test\_c.xda, test\_d.xda - beides korrekt

### 6.2 Test B: Membrane Displacement with Quad-4

Sprungbrett bestehend aus 3 Elementen mit BC wie in Test A aber einzelne Kraft auf oberen rechten Knoten in neg. y-Richtung

selbes Mesh wie in test\_d.xda nur eben mit 16 Elementen. Selbe BCs, selbe Kraftwerte

test\_e.xda, test\_f.xda - beides korrekt

### 6.3 Test C: Plate Displacement with Tri-3

Platte an allen 4 Seiten eingespannt. Einzelne Kraft im Zentrum in neg. z-Richtung

Alternativ mit anderen Parametern test\_g

test\_a\_triN.xda, test\_g\_triAB\_N.xda - korrekt, noch nicht getestet

### 6.4 Test D: Plate Displacement with Quad-4

Selbes mesh wie Test C nur eben mit Quadelementen

test\_a\_quadN.xda, test\_g\_quad\_N.xda - korrekt, noch nicht getestet

### 6.5 Test E: Shell Displacement with Tri-3

Ein H-Trägerbalken. Am einen Ende fest eingespannt. Am anderen Ende wird oben eine Kraft am äußeren Knoten in den Balken hinein in flacher Ebene gegeben, gleichzeitig wird unten an der gegenüberliegenden Seite eine Kraft in entgegengesetzter Richtung gegeben

test\_j\_tri.xda - korrekt

### 6.6 Test F: Shell Displacement with Quad-4

Gleich wie Test E nur eben Quadelemente

test\_j\_quad.xda - korrekt



### **6.7 Test G: Convergence (increasing number of elements)**

??? theoretisch mit Test C/D bereits durchführbar mit  $N=2,4,8,16,32,64,128$

### **6.8 Test H: MPI (increasing number of processes)**

??? theoretisch alle Tests, z.B. E/F mit Prozessoranzahl = 1,2,4,8,16. In dem Fall ist natürlich die Zeit interessant und ob die Ergebnisse jeweils alle gleich sind

### **6.9 Test I: Coupling with preCICE**

???

## 7 Conclusion

What does my code do, what problems arose, what problems persist, what does my code cannot do, where are opportunities for extensions, etc.

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## **Erklärung**

Ich versichere, diese Arbeit selbstständig verfasst zu haben. Ich habe keine anderen als die angegebenen Quellen benutzt und alle wörtlich oder sinngemäß aus anderen Werken übernommene Aussagen als solche gekennzeichnet. Weder diese Arbeit noch wesentliche Teile daraus waren bisher Gegenstand eines anderen Prüfungsverfahrens. Ich habe diese Arbeit bisher weder teilweise noch vollständig veröffentlicht. Das elektronische Exemplar stimmt mit allen eingereichten Exemplaren überein.

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Ort, Datum, Unterschrift