Akantu

User's Guide

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Contents

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Chapter 1

Introduction

`Akantu` means "little element" in Kinyarwanda, a Bantu language. From now on, it is also an open-source object-oriented *Finite-Element* library with the ambition to be generic and efficient. **`Akantu`** is developed within the LSMS (Computational Solid Mechanics Laboratory, `lsms.epfl.ch`) at the Ecole Polytechnique Federale of Lausanne, Switzerland. The open-source philosophy is important for any scientific software project evolution. The collaboration permitted by shared codes enforces sanity when users (and not only developers) can scrutinize (and possibly criticize) the implementation details.

`Akantu` was born with the vision to associate genericity, robustness and efficiency while benefiting from the open-source visibility. Genericity is necessary to allow the easy exploration of mathematical formulations through algorithmic ideas. Robustness and reliability is naturally expected from any simulation software, even more in the context of parallel computations. In order to achieve these goals, we made noticeable choices in the architecture of **`Akantu`**. First we decided to use the object-oriented paradigm through C++. Then, in order to prevent extra cost associated to virtual function calls, we designed the library as a hybrid architecture with objects at high level layers and vectorization at low level layers. Thus, **`Akantu`** benefits from inheritance and polymorphism mechanisms without the counterpart of having virtual calls within critical loops. This coding philosophy, which was demonstrated to be highly efficient, is innovative in the field of *Finite-Element* software.

This document is appropriate for researchers and engineers willing to use **`Akantu`** in order to perform a finite-element calculation for solid mechanics, structural mechanics, contact mechanics or heat transfer. The solid mechanics solver, which is the most complete and functional part of **`Akantu`**, is presented in details in the remainder of this document.

Chapter 2

Getting Started

2.1 Downloading the Code

The **Akantu** source code can be requested using the form accessible at the URL `http://lsms.epfl.ch/akantu`. There, you will be asked to accept the LGPL license terms.

2.2 Compiling **Akantu**

Akantu is a `cmake` project, so to configure it, you can either follow the usual way:

```
> cd akantu
> mkdir build
> cd build
> ccmake ..
[ Set the options that you need ]
> make
> make install
```

Or, use the `Makefile` we added for your convenience to handle the `cmake` configuration

```
> cd akantu
> make config
> make
> make install
```

All the **Akantu** options are documented in Appendix C.

2.3 Writing a `main` Function

First of all, **Akantu** needs to be initialized. The memory management included in the core library handles the correct allocation and de-allocation of vectors, structures and/or objects. Moreover, in parallel computations, the initialization procedure performs the communication setup. This is achieved by a pair of functions (`initialize` and `finalize`) that are used as follows:

```
#include "aka_common.hh"
#include "..."

using namespace akantu;

int main(int argc, char *argv[]) {
  initialize("input_file.dat", argc, argv);

  // your code
  ...
  finalize();
}
```

The `initialize` function takes the text inpute file and the program parameters which can be parsed by **Akantu** in due form (see 7.1). Obviously it is necessary to include all files needed in main. In this manual all provided code implies the usage of `akantu` as namespace.

2.4 Creating and Loading a Mesh

In its current state, **Akantu** supports three types of meshes: Gmsh [1], Abaqus [2] and Diana [3]. Once a `Mesh` object is created with a given spatial dimension, it can be filled by reading a mesh input file. The method `read` of the class `Mesh` infers the mesh type from the file extension. If a non-standard file extension is used, the mesh type has to be specified.

```
UInt spatial_dimension = 2;
Mesh mesh(spatial_dimension);

// Reading Gmsh files
mesh.read("my_gmsh_mesh.msh");
mesh.read("my_gmsh_mesh", _miot_gmsh);


// Reading Abaqus files
mesh.read("my_abaqus_mesh.inp");
mesh.read("my_abaqus_mesh", _miot_abaqus);

// Reading Diana files
mesh.read("my_diana_mesh.dat");
mesh.read("my_diana_mesh", _miot_diana);
```

The Gmsh reader adds the geometrical and physical tags as mesh data. The physical values are stored as a `UInt` data called `tag_0`, if a string name is provided it is stored as a `std::string` data named `physical_names`. The geometrical tag is stored as a `UInt` data named `tag_1`.

The Abaqus reader stores the `ELSET` in ElementGroups and the `NSET` in NodeGroups. The material assignment can be retrieved from the `std::string` mesh data named `abaqus_material`.

2.5 Using Arrays

Data in **Akantu** can be stored in data containers implemented by the `Array` class. In its most basic usage, the `Array` class implemented in **Akantu** is similar to the `vector` class of the Standard Template Library (STL) for C++. A simple `Array` containing a sequence of `nb_element` values (of a given type) can be generated with:

```
  Array<type> example_array(nb_element);
```

where `type` usually is `Real`, `Int`, `UInt` or `bool`. Each value is associated to an index, so that data can be accessed by typing:

```
  type & val = example_array(index)
```

`Arrays` can also contain tuples of values for each index. In that case, the number of components per tuple must be specified at the `Array` creation. For example, if we want to create an `Array` to store the coordinates (sequences of three values) of ten nodes, the appropriate code is the following:

```
UInt nb_nodes = 10;
UInt spatial_dimension = 3;

Array<Real> position(nb_nodes, spatial_dimension);
```

In this case the x position of the eighth node number will be given by `position(7, 0)` (in C++, numbering starts at 0 and not 1). If the number of components for the sequences is not specified, the default value of 1 is used. Here is a list of some basic operations that can be performed on `Array`:

- `resize(size)` change the size of the `Array`.
- `clear()` set all entries of the `Array` to zero.
- `set(t)` set all entries of the `Array` to `t`.
- `copy(const Array<T> & other)` copy another `Array` into the current one. The two `Array` should have the same number of components.
- `push_back(tuple)` append a tuple with the correct number of components at the end of the `Array`.
- `erase(i) erase the value at the i-th position.`
- `find(value)` search `value` in the current `Array`. Return position index of the first occurence or −1 if not found.
- `storage()` Return the address of the allocated memory of the `Array`.

2.5.1 Arrays iterators

It is very common in **Akantu** to loop over arrays to perform a specific treatment. This ranges from geometric calculation on nodal quantities to tensor algebra (in constitutive laws for example). The `Array` object has the possibility to request iterators in order to make the writing of loops easier and enhance readability. For instance, a loop over the nodal coordinates can be performed like:

```
//accessing the nodal coordinates Array (spatial_dimension components)
Array<Real> nodes = mesh.getNodes();

//creating the iterators
Array<Real>::vector_iterator it  = nodes.begin(spatial_dimension);
Array<Real>::vector_iterator end = nodes.end(spatial_dimension);

for (; it != end; ++it){
  Vector<Real> & coords = (*it);

  //do what you need
  ....

}
```

In that example, each `Vector<Real>` is a geometrical array of size `spatial_dimension` and the iteration is conveniently performed by the `Array` iterator.

The `Array` object is intensively used to store second order tensor values. In that case, it should be specified that the returned object type is a matrix when constructing the iterator. This is done when calling the `begin` function. For instance, assuming that we have a `Array` storing stresses, we can loop over the stored tensors by:

```
//creating the iterators
Array<Real>::matrix_iterator it  = stresses.begin(spatial_dimension,
  spatial_dimension);
Array<Real>::matrix_iterator end = stresses.end(spatial_dimension,
  spatial_dimension);

for (; it != end; ++it){
  Matrix<Real> & stress = (*it);

  //do what you need
  ....

}
```

In that last example, the `Matrix` objects are `spatial_dimension` × `spatial_dimension` matrices. The light objects `Matrix` and `Vector` can be used and combined to do most common linear algebra. If the number of component is 1, it is possible to use a scalar_iterator rather than the vector/matrix one.

In general, a mesh consists of several kinds of elements. Consequently, the amount of data to be stored can differ for each element type. The straightforward example is the connectivity array, namely the sequences of nodes belonging to each element (linear triangular elements have fewer nodes than, say, rectangular quadratic elements etc.). A particular data structure called `ElementTypeMapArray` is provided to easily manage this kind of data. It consists of a group of `Arrays`, each associated to an element type. The following code can retrieve the `ElementTypeMapArray` which stores the connectivity arrays for a mesh:

```
ElementTypeMapArray<UInt> & connectivities = mesh.getConnectivities();
```

Then, the specific array associated to a given element type can be obtained by

```
Array<UInt> & connectivity_triangle = connectivities(_triangle_3);
```

where the first order 3-node triangular element was used in the presented piece of code.

2.5.2 Vector & Matrix

The `Array` iterators as presented in the previous section can be shaped as `Vector` or `Matrix`. This objects represent 1st and 2nd order tensors. As such they come with some functionalities that we will present a bit more into detail in this here.

`Vector<T>`

1. Accessors:

   - `v(i)` gives the i^{th} component of the vector `v`
   - `v[i]` gives the i^{th} component of the vector `v`
   - `v.size()` gives the number of component

2. Level 1: (results are scalars)

   - `v.norm()` returns the geometrical norm (L_2)
   - `v.norm<N>()` returns the L_N norm defined as $\left(\sum_i |\texttt{v(i)}|^N\right)^{1/N}$. N can take any positive integer value. There are also some particular values for the most commonly used norms, `L_1` for the Manhattan norm, `L_2` for the geometrical norm and `L_inf` for the norm infinity.
   - `v.dot(x)` return the dot product of `v` and `x`

- `v.distance(x)` return the geometrical norm of `v` − `x`

3. Level 2: (results are vectors)

   - `v += s`, `v -= s`, `v *= s`, `v /= s` those are element-wise operators that sum, substract, multiply or divide all the component of `v` by the scalar `s`
   - `v += x`, `v -= x` sums or substracts the vector `x` to/from `v`
   - `v.mul(A, x, alpha)` stores the result of $\alpha \boldsymbol{A}\boldsymbol{x}$ in `v`, α is equal to 1 by default
   - `v.solve(A, b)` stores the result of the resolution of the system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ in `v`
   - `v.crossProduct(v1, v2)` computes the cross product of `v1` and `v2` and stores the result in `v`

`Matrix<T>`

1. Accessors:

   - `A(i, j)` gives the component A_{ij} of the matrix `A`
   - `A(i)` gives the i^{th} column of the matrix as a `Vector`
   - `A[k]` gives the k^{th} component of the matrix, matrices are stored in a column major way, which means that to access A_{ij}, $k = i + jM$
   - `A.rows()` gives the number of rows of `A` (M)
   - `A.cols()` gives the number of columns of `A` (N)
   - `A.size()` gives the number of component in the matrix ($M \times N$)

2. Level 1: (results are scalars)

   - `A.norm()` is equivalent to `A.norm<L_2>()`
   - `A.norm<N>()` returns the L_N norm defined as $\left(\sum_i \sum_j |\texttt{A(i,j)}|^N\right)^{1/N}$. N can take any positive integer value. There are also some particular values for the most commonly used norms, `L_1` for the Manhattan norm, `L_2` for the geometrical norm and `L_inf` for the norm infinity.
   - `A.trace()` return the trace of `A`
   - `A.det()` return the determinant of `A`
   - `A.doubleDot(B)` return the double dot product of `A` and `B`, $\boldsymbol{A} : \boldsymbol{B}$

3. Level 3: (results are matrices)

   - `A.eye(s)`, `Matrix<T>::eye(s)` fills/creates a matrix with the $s\boldsymbol{I}$ with $\boldsymbol{I}$ the identity matrix
   - `A.inverse(B)` stores $\boldsymbol{B}^{-1}$ in `A`
   - `A.transpose()` returns $\boldsymbol{A}^t$
   - `A.outerProduct(v1, v2)` stores $\boldsymbol{v_1}\boldsymbol{v_2}^t$ in `A`
   - `C.mul<t_A, t_B>(A, B, alpha)`: stores the result of the product of `A` and codeB time the scalar `alpha` in `C`. `t_A` and `t_B` are boolean defining if `A` and `B` should be transposed or not.

`t_A`	`t_B`	result
false	false	$\boldsymbol{C} = \alpha\boldsymbol{A}\boldsymbol{B}$
false	true	$\boldsymbol{C} = \alpha\boldsymbol{A}\boldsymbol{B}^t$
true	false	$\boldsymbol{C} = \alpha\boldsymbol{A}^t\boldsymbol{B}$
true	true	$\boldsymbol{C} = \alpha\boldsymbol{A}^t\boldsymbol{B}^t$

  - `A.eigs(d, V)` this method computes the eigenvalues and eigenvectors of `A` and store the results in `d` and `V` such that `d(i)` $= \lambda_i$ and `V(i)` $= v_i$ with $Av_i = \lambda_i v_i$ and $\lambda_1 > ... > \lambda_i > ... > \lambda_N$

`Tensor3<T>`

Accessors:

- `t(i, j, k)` gives the component T_{ijk} of the tensor `t`
- `t(k)` gives the k^{th} two-dimensional tensor as a `Matrix`
- `t[k]` gives the k^{th} two-dimensional tensor as a `Matrix`

2.6 Manipulating group of nodes and/or elements

Akantu provides the possibility to manipulate subgroups of elements and nodes. Any `ElementGroup` and/or `NodeGroup` must be managed by a `GroupManager`. Such a manager has the role to associate group objects to names. This is a useful feature, in particular for the application of the boundary conditions, as will be demonstrated in section 4.1.2. To most general group manager is the `Mesh` class which inheritates from the `GroupManager` class.

For instance, the following code shows how to request an element group to a mesh:

```
// request creation of a group of nodes
NodeGroup & my_node_group = mesh.createNodeGroup("my_node_group");
// request creation of a group of elements
ElementGroup & my_element_group = mesh.createElementGroup("my_element_group"
  );

/* fill and use the groups */
```

2.6.1 The NodeGroup object

A group of nodes is stored in `NodeGroup` objects. They are quite simple objects which store the indexes of the selected nodes in a `Array<UInt>`. Nodes are selected by adding them when calling `NodeGroup::add`. For instance you can select nodes having a positive X coordinate with the following code:

```
Array<Real> & nodes = mesh.getNodes();
NodeGroup & group = mesh.createNodeGroup("XpositiveNode");

Array<Real>::const_vector_iterator it  = nodes.begin(spatial_dimension);
Array<Real>::const_vector_iterator end = nodes.end(spatial_dimension);

UInt index = 0;

for (; it != end ; ++it , ++index){
  const Vector<Real> & position = *it;
  if (position(0) > 0) group.add(index);
}
```

2.6.2 The ElementGroup object

A group of elements is stored in `ElementGroup` objects. Since a group can contain elements of various types the `ElementGroup` object stores indexes in a `ElementTypeMapArray<UInt>` object. Then elements can be added to the group by calling `addElement`.

For instance, selecting the elements for which the barycenter of the nodes has a positive X coordinate can be made with:

```
ElementGroup & group = mesh.createElementGroup("XpositiveElement");

Mesh::type_iterator it  = mesh.firstType();
Mesh::type_iterator end = mesh.lastType();

Vector<Real> barycenter(spatial_dimension);

for(; it != end; ++it){
  UInt nb_element  = mesh.getNbElement(*it);
  for(UInt e = 0; e < nb_element; ++e) {
    ElementType type = *it;
    mesh.getBarycenter(e, type, barycenter.storage());
    if (barycenter(0) > 0) group.add(type,e);
  }
}
```

Chapter 3

FEEngine

The `FEEngine` interface is dedicated to handle the finite-element approximations and the numerical integration of the weak form. As we will see in Chapter 4, `Model` creates its own `FEEngine` object so the explicit creation of the object is not required.

3.1 Mathematical Operations

Using the `FEEngine` object, one can compute a interpolation, an integration or a gradient. A simple example is given below.

```
// having a FEEngine object
FEEngine *fem = new FEEngineTemplate<IntegratorGauss,ShapeLagrange>(my_mesh,
                                                                    dim,
                                                                    "my_fem");
// instead of this, a FEEngine object can be get using the model:
// model.getFEEngine()

//compute the gradient
Array<Real> u; //append the values you want
Array<Real> nablauq; //gradient array to be computed
// compute the gradient
fem->gradientOnIntegrationPoints(const Array<Real> &u,
         Array<Real> &nablauq,
         const UInt nb_degree_of_freedom,
         const ElementType & type);

// interpolate
Array<Real> uq; //interpolated array to be computed
// compute the interpolation
fem->interpolateOnIntegrationPoints(const Array<Real> &u,
                                    Array<Real> &uq,
                                    UInt nb_degree_of_freedom,
                                    const ElementType & type);

// interpolated function can be integrated over the elements
Array<Real> int_val_on_elem;
// integrate
fem->integrate(const Array<Real> &uq,
               Array<Real> &int_uq,
               UInt nb_degree_of_freedom,
               const ElementType & type);
```

Another example below shows how to integrate stress and strain fields over elements assigned to a particular material.

```
UInt sp_dim = 3; //spatial dimension
UInt m = 1; //material index of interest
const ElementType type = _tetrahedron_4; //element type

// get the stress and strain arrays associated to the material index m
const Array<Real> & strain_vec = model.getMaterial(m).getGradU(type);
const Array<Real> & stress_vec = model.getMaterial(m).getStress(type);

// get the element filter for the material index
const Array<UInt> & elem_filter = model.getMaterial(m).getElementFilter(type);

// initialize the integrated stress and strain arrays
Array<Real> int_strain_vec(elem_filter.getSize(),
                           sp_dim*sp_dim, "int_of_strain");
Array<Real> int_stress_vec(elem_filter.getSize(),
                           sp_dim*sp_dim, "int_of_stress");

// integrate the fields
model.getFEEngine().integrate(strain_vec, int_strain_vec,
                              sp_dim*sp_dim, type, _not_ghost, elem_filter);
model.getFEEngine().integrate(stress_vec, int_stress_vec,
                              sp_dim*sp_dim, type, _not_ghost, elem_filter);
```

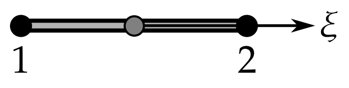
3.2 Elements

The base for every Finite-Elements computation is its mesh and the elements that are used within that mesh. The element types that can be used depend on the mesh, but also on the dimensionality of the problem (1D, 2D or 3D). In **Akantu**, several isoparametric Lagrangian element types are supported (and one serendipity element). Each of these types is discussed in some detail below, starting with the 1D-elements all the way to the 3D-elements. More detailed information (shape function, location of Gaussian quadrature points, and so on) can be found in Appendix A.

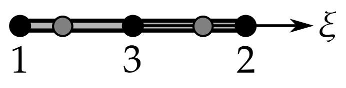
3.2.1 Isoparametric Elements

1D

In **Akantu**, there are two types of isoparametric elements defined in 1D. These element types are called `_segment_2` and `_segment_3`, and are depicted schematically in Figure 3.1. Some of the basic properties of these elements are listed in Table 3.1.



(a) `_segment_2`



(b) `_segment_3`

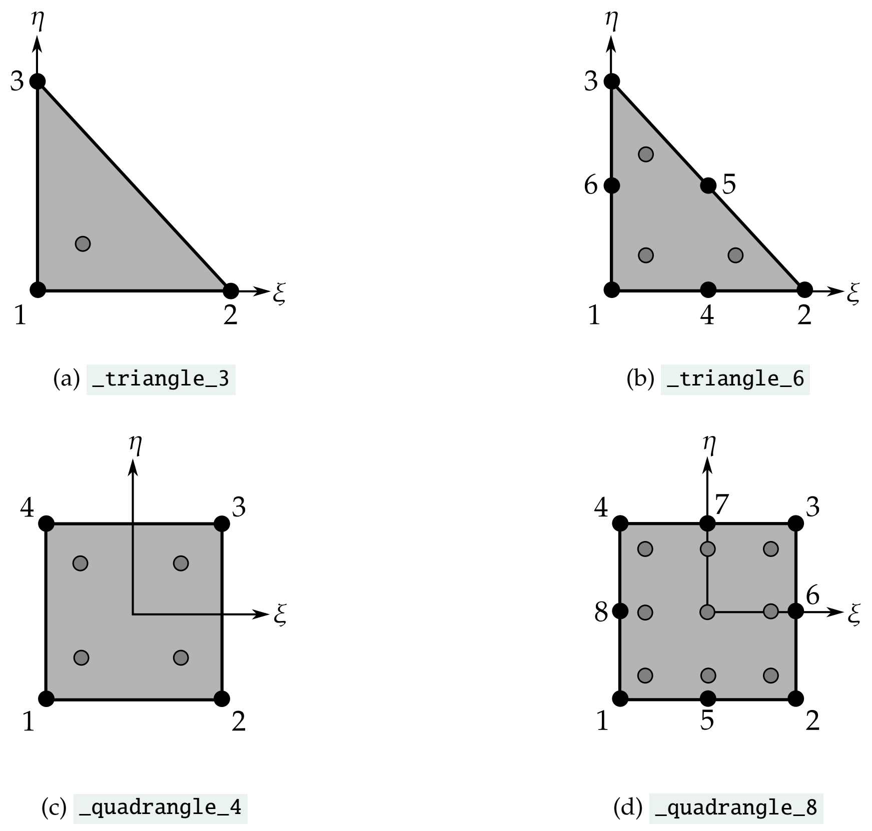
Figure 3.1: Schematic overview of the two 1D element types in **Akantu**. In each element, the node numbering as used in **Akantu** is indicated and also the quadrature points are highlighted (gray circles).

Element type	Order	# nodes	# quad. points
`_segment_2`	linear	2	1
`_segment_3`	quadratic	3	2

Table 3.1: Some basic properties of the two 1D isoparametric elements in **Akantu**.

2D

In **Akantu**, there are four types of isoparametric elements defined in 2D. These element types are called `_triangle_3`, `_triangle_6`, `_quadrangle_4` and `_quadrangle_8`, and all of them are depicted in Figure 3.2. As with the 1D elements, some of the most basic properties of these elements are listed in Table 3.2. It is important to note that the first element is linear, the next two quadratic and the last one cubic. Furthermore, the last element type (`_quadrangle_8`) is not a Lagrangian but a serendipity element.



(a) `_triangle_3` (b) `_triangle_6` (c) `_quadrangle_4` (d) `_quadrangle_8`

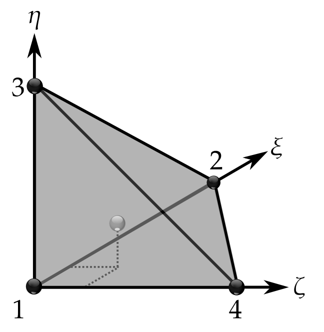
Figure 3.2: Schematic overview of the four 2D element types in **Akantu**. In each element, the node numbering as used in **Akantu** is indicated and also the quadrature points are highlighted (gray circles).

3D

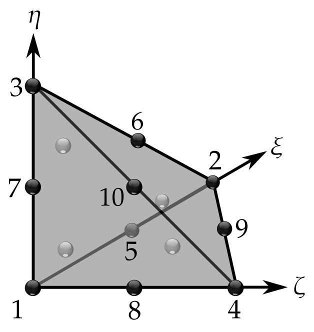
In **Akantu**, there are three types of isoparametric elements defined in 3D. These element types are called `_tetrahedron_4`, `_tetrahedron_10` and `_hexahedron_8`, and all of them are depicted schematically in Figure 3.3. As with the 1D and 2D elements some of the most basic properties of these elements are listed in Table 3.3.

Element type	Order	# nodes	# quad. points
`_triangle_3`	linear	3	1
`_triangle_6`	quadratic	6	3
`_quadrangle_4`	quadratic	4	4
`_quadrangle_8`	cubic	8	9

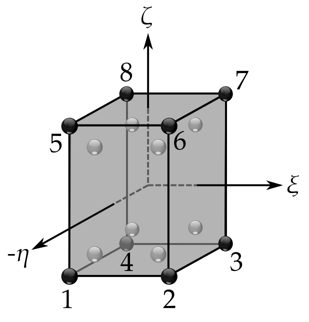
Table 3.2: Some basic properties of the four 2D isoparametric elements in **Akantu**.



(a) `_tetrahedron_4`



(b) `_tetrahedron_10`



(c) `_hexahedron_8`

Figure 3.3: Schematic overview of the three 3D element types in **Akantu**. In each element, the node numbering as used in **Akantu** is indicated and also the quadrature points are highlighted (gray spheres).

Element type	Order	# nodes	# quad. points
`_tetrahedron_4`	linear	4	1
`_tetrahedron_10`	quadratic	10	4
`_hexahedron_8`	cubic	8	8

Table 3.3: Some basic properties of the three 3D isoparametric elements in **Akantu**.

3.2.2 Cohesive Elements

The cohesive elements that have been implemented in **Akantu** are based on the work of Ortiz and Pandolfi [4]. Their main properties are reported in Table 3.4.

Element type	Facet type	Order	# nodes	# quad. points
`_cohesive_1d_2`	`_point_1`	linear	2	1
`_cohesive_2d_4`	`_segment_2`	linear	4	1
`_cohesive_2d_6`	`_segment_3`	quadratic	6	2
`_cohesive_3d_6`	`_triangle_3`	linear	6	1
`_cohesive_3d_12`	`_triangle_6`	quadratic	12	3

Table 3.4: Some basic properties of the cohesive elements in **Akantu**.

Cohesive element insertion can be either realized at the beginning of the simulation or it can be carried out dynamically during the simulation. The first approach is called *intrinsic*, the second

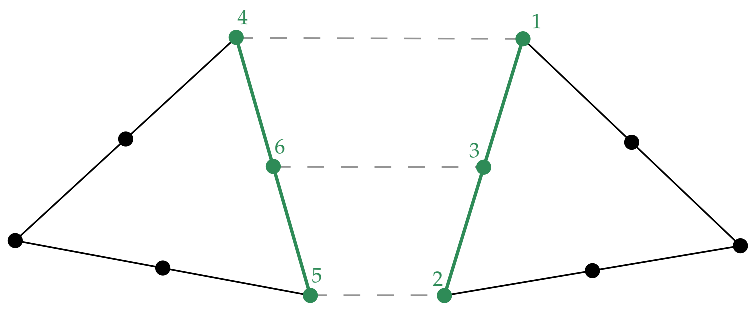


Figure 3.4: Cohesive element in 2D for quadratic triangular elements T6.

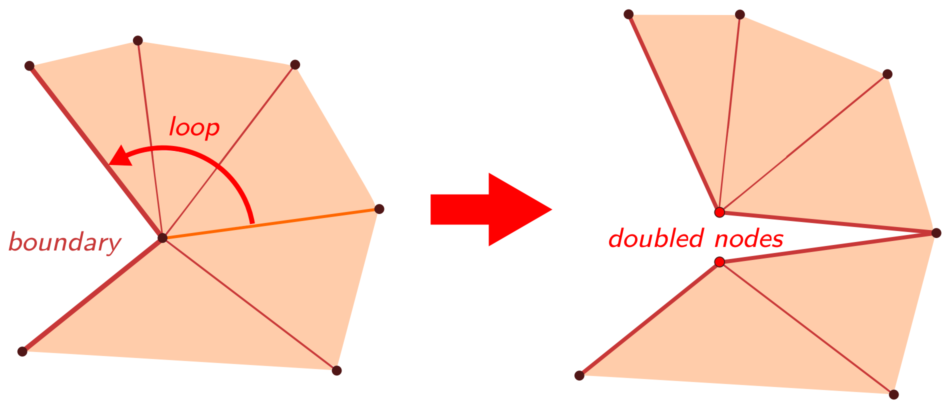


Figure 3.5: Insertion of a cohesive element.

one *extrinsic*. When an element is present from the beginning, a bilinear or exponential cohesive law should be used instead of a linear one. A bilinear law works exactly like a linear one except for an additional parameter δ_0 separating an initial linear elastic part from the linear irreversible one. For additional details concerning cohesive laws see Section 4.5.

Extrinsic cohesive elements are dynamically inserted between two standard elements when

$$\sigma_{\mathrm{eff}} > \sigma_{\mathrm{c}} \quad \text{with} \quad \sigma_{\mathrm{eff}} = \sqrt{\sigma_{\mathrm{n}}^2 + \frac{\tau^2}{\beta^2}} \tag{3.1}$$

in which σ_{n} is the tensile normal traction and τ the resulting tangential one (Figure 3.5).

For the static analysis of the structures containing cohesive elements, the stiffness of the cohesive elements should also be added to the total stiffness of the structure. Considering a 2D quadratic cohesive element as that in Figure 3.4, the opening displacement along the mid-surface can be written as:

$$\boldsymbol{\Delta}(s) = [\![\boldsymbol{u}]\!]\,\boldsymbol{N}(s) = \begin{bmatrix} u_3 - u_0 & u_4 - u_1 & u_5 - u_2 \\ v_3 - v_0 & v_4 - v_1 & v_5 - v_2 \end{bmatrix} \begin{bmatrix} N_0(s) \\ N_1(s) \\ N_2(s) \end{bmatrix} = \mathbf{N}^{\mathrm{k}}\boldsymbol{A}\boldsymbol{U} = \boldsymbol{P}\boldsymbol{U} \tag{3.2}$$

The $\boldsymbol{U}$, $\boldsymbol{A}$ and $\boldsymbol{N}^{\mathrm{k}}$ are as following:

$$\boldsymbol{U} = \left[\begin{array}{cccccccccccc} u_0 & v_0 & u_1 & v_1 & u_2 & v_2 & u_3 & v_3 & u_4 & v_4 & u_5 & v_5 \end{array} \right] \tag{3.3}$$

$$\boldsymbol{A} = \left[\begin{array}{cccccccccccc} 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \end{array} \right] \tag{3.4}$$

$$\boldsymbol{N}^{\mathrm{k}} = \begin{bmatrix} N_0(s) & 0 & N_1(s) & 0 & N_2(s) & 0 \\ 0 & N_0(s) & 0 & N_1(s) & 0 & N_2(s) \end{bmatrix} \tag{3.5}$$

The consistent stiffness matrix for the element is obtained as

$$\boldsymbol{K} = \int_{S_0} \boldsymbol{P}^{\mathrm{T}} \frac{\partial \boldsymbol{T}}{\partial \delta} \boldsymbol{P} \, \mathrm{d}S_0 \tag{3.6}$$

where $\boldsymbol{T}$ is the cohesive traction and δ the opening displacement (for more details check Section 3.4).

3.2.3 Structural Elements

Bernoulli Beam Elements

These elements allow to compute the displacements and rotations of structures constituted by Bernoulli beams. **Akantu** defines them for both 2D and 3D problems respectively in the element types `_bernoulli_beam_2` and `_bernoulli_beam_3`. A schematic depiction of a beam element is shown in Figure 3.6 and some of its properties are listed in Table 3.5.

Note: *Beam elements are of mixed order: the axial displacement is linearly interpolated while transverse displacements and rotations use cubic shape functions.*

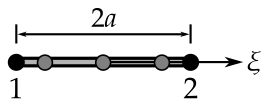


Figure 3.6: Schematic depiction of a Bernoulli beam element (applied to 2D and 3D) in **Akantu**. The node numbering as used in **Akantu** is indicated, and also the quadrature points are highlighted (gray circles).

Element type	Dimension	# nodes	# quad. points	# d.o.f.
`_bernoulli_beam_2`	2D	2	3	6
`_bernoulli_beam_3`	3D	2	3	12

Table 3.5: Some basic properties of the beam elements in **Akantu**

Chapter 4

Solid Mechanics Model

The solid mechanics model is a specific implementation of the `Model` interface dedicated to handle the equations of motion or equations of equilibrium. The model is created for a given mesh. It will create its own `FEEngine` object to compute the interpolation, gradient, integration and assembly operations. A `SolidMechanicsModel` object can simply be created like this:

```
SolidMechanicsModel model(mesh);
```

where `mesh` is the mesh for which the equations are to be solved. A second parameter called `spatial_dimension` can be added after `mesh` if the spatial dimension of the problem is different than that of the mesh.

This model contains at least the following six `Arrays`:

blocked_dofs contains a Boolean value for each degree of freedom specifying whether that degree is blocked or not. A Dirichlet boundary condition can be prescribed by setting the **blocked_dofs** value of a degree of freedom to `true`. A Neumann boundary condition can be applied by setting the **blocked_dofs** value of a degree of freedom to `false`. The **displacement**, **velocity** and **acceleration** are computed for all degrees of freedom for which the **blocked_dofs** value is set to `false`. For the remaining degrees of freedom, the imposed values (zero by default after initialization) are kept.

displacement contains the displacements of all degrees of freedom. It can be either a computed displacement for free degrees of freedom or an imposed displacement in case of blocked ones ($\boldsymbol{u}$ in the following).

velocity contains the velocities of all degrees of freedom. As **displacement**, it contains computed or imposed velocities depending on the nature of the degrees of freedom ($\dot{\boldsymbol{u}}$ in the following).

acceleration contains the accelerations of all degrees of freedom. As **displacement**, it contains computed or imposed accelerations depending on the nature of the degrees of freedom ($\ddot{\boldsymbol{u}}$ in the following).

force contains the external forces applied on the nodes ($\boldsymbol{f}_{\text{ext}}$ in the following).

residual contains the difference between external and internal forces. On blocked degrees of freedom, **residual** contains the support reactions. ($\boldsymbol{r}$ in the following). It should be mentioned that at equilibrium **residual** should be zero on free degrees of freedom.

Some examples to help to understand how to use this model will be presented in the next sections.

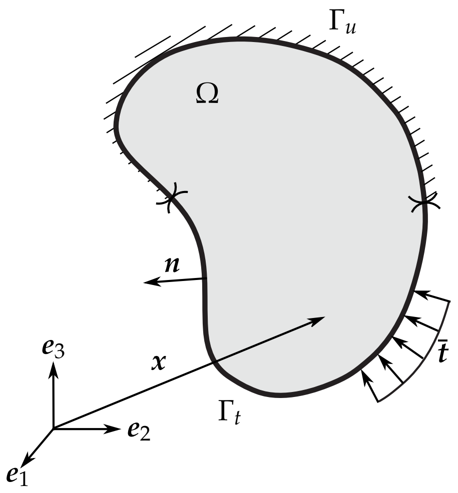


Figure 4.1: Problem domain Ω with boundary in three dimensions. The Dirchelet and the Neumann regions of the boundary are denoted with Γ_u and Γ_t, respecitvely.

4.1 Model Setup

4.1.1 Setting Initial Conditions

For a unique solution of the equations of motion, initial displacements and velocities for all degrees of freedom must be specified:

$$\boldsymbol{u}(t = 0) = \boldsymbol{u}_0 \tag{4.1}$$

$$\dot{\boldsymbol{u}}(t = 0) = \boldsymbol{v}_0 \tag{4.2}$$

The solid mechanics model can be initialized as follows:

```
model.initFull()
```

This function initializes the internal arrays and sets them to zero. Initial displacements and velocities that are not equal to zero can be prescribed by running a loop over the total number of nodes. Here, the initial displacement in x-direction and the initial velocity in y-direction for all nodes is set to 0.1 and 1, respectively.

```
Array<Real> & disp = model.getDisplacement();
Array<Real> & velo = model.getVelocity();
for (UInt i = 0; i < mesh.getNbNodes(); ++i) {
  disp(i, 0) = 0.1;
  velo(i, 1) = 1.;
}
```

4.1.2 Setting Boundary Conditions

This section explains how to impose Dirichlet or Neumann boundary conditions. A Dirichlet boundary condition specifies the values that the displacement needs to take for every point x at the boundary (Γ_u) of the problem domain (Fig. 4.1):

$$\boldsymbol{u} = \bar{\boldsymbol{u}} \quad \forall \boldsymbol{x} \in \Gamma_u \tag{4.3}$$

A Neumann boundary condition imposes the value of the gradient of the solution at the boundary Γ_t of the problem domain (Fig. 4.1):

$$\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n} = \bar{\boldsymbol{t}} \quad \forall \boldsymbol{x} \in \Gamma_t \tag{4.4}$$

Different ways of imposing these boundary conditions exist. A basic way is to loop over nodes or elements at the boundary and apply local values. A more advanced method consists of using the notion of the boundary of the mesh. In the following both ways are presented.

Starting with the basic approach, as mentioned, the Dirichlet boundary conditions can be applied by looping over the nodes and assigning the required values. Figure 4.2 shows a beam with a fixed support on the left side. On the right end of the beam, a load is applied. At the fixed support, the displacement has a given value. For this example, the displacements in both the x and the y-direction are set to zero. Implementing this displacement boundary condition is similar to the implementation of initial displacement conditions described above. However, in order to impose a displacement boundary condition for all time steps, the corresponding nodes need to be marked as boundary nodes using the function `blocked`. While, in order to impose a load on the right side, the nodes are not marked. The detail codes are shown as follows:

```
Array<bool> & blocked = model.getBlockedDOFs();
const Array<Real> & pos = mesh.getNodes();

UInt nb_nodes = mesh.getNbNodes();

for (UInt i = 0; i < nb_nodes; ++i) {
  if(Math::are_float_equal(pos(i, 0), 0)) {
    blocked(i, 0) = true; //block dof in x-direction
    blocked(i, 1) = true; //block dof in y-direction
    disp(i, 0) = 0.; //fixed displacement in x-direction
    disp(i, 1)= 0.; //fixed displacement in y-direction
  } else if (Math::are_float_equal(pos(i, 10), 0)) {
    blocked(i, 0) = false; //unblock dof in x-direction
    forces(i, 0) = 10.; //force in x-direction
  }
}
```

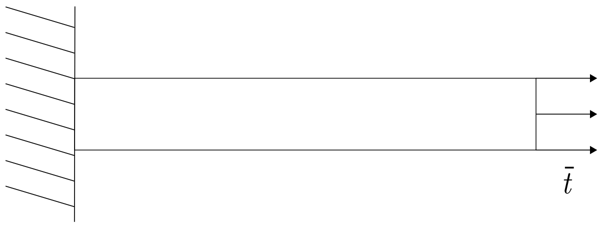


Figure 4.2: Beam with fixed support and load.

For the more advanced approach, one needs the notion of a boundary in the mesh. Therefore, the boundary should be created before boundary condition functors can be applied. Generally the boundary can be specified from the mesh file or the geometry. For the first case, the function `createGroupsFromMeshData` is called. This function can read any types of mesh data which are provided in the mesh file. If the mesh file is created with Gmsh, the function takes one input strings which is either `tag_0`, `tag_1` or `physical_names`. The first two tags are assigned by Gmsh to each element which shows the physical group that they belong to. In Gmsh, it is also possible to consider strings for different groups of elements. These elements can be separated by giving a string `physical_names` to the function `createGroupsFromMeshData`:

```
mesh.createGroupsFromMeshData<std::string>("physical_names").
```

Boundary conditions support can also be created from the geometry by calling `createBoundaryGroupFromGeometry`. This function gathers all the elements on the boundary of the geometry.

To apply the required boundary conditions, the function `applyBC` needs to be called on a `SolidMechanicsModel`. This function gets a Dirichlet or Neumann functor and a string which specifies the desired boundary on which the boundary conditions is to be applied. The functors specify the type of conditions to apply. Three built-in functors for Dirichlet exist: `FlagOnly, FixedValue,` and `IncrementValue`. The functor `FlagOnly` is used if a point is fixed in a given direction. Therefore, the input parameter to this functor is only the fixed direction. The `FixedValue` functor is used when a displacement value is applied in a fixed direction. The `IncrementValue` applies an increment to the displacement in a given direction. The following code shows the utilization of three functors for the top, bottom and side surface of the mesh which were already defined in the Gmsh file:

```
model.applyBC(BC::Dirichlet::FixedValue(13.0, _y), "Top");

model.applyBC(BC::Dirichlet::FlagOnly(_x), "Bottom");

model.applyBC(BC::Dirichlet::IncrementValue(13.0, _x), "Side");
```

To apply a Neumann boundary condition, the applied traction or stress should be specified before. In case of specifying the traction on the surface, the functor `FromTraction` of Neumann boundary conditions is called. Otherwise, the functor `FromStress` should be called which gets the stress tensor as an input parameter.

```
Array<Real> surface_traction(3);
surface_traction(0)=0.0;
surface_traction(1)=0.0;
surface_traction(2)=-1.0;

Matrix<Real> surface_stress(3, 3, 0.0);
surface_stress(0,0)=0.0;
surface_stress(1,1)=0.0;
surface_stress(2,2)=-1.0;

model.applyBC(BC::Neumann::FromTraction(surface_traction), "Bottom");

model.applyBC(BC::Neumann::FromStress(surface_stress), "Top");
```

If the boundary conditions need to be removed during the simulation, a functor is called from the Neumann boundary condition to free those boundary conditions from the desired boundary.

```
 model.applyBC(BC::Neumann::FreeBoundary(), "Side");
```

User specified functors can also be implemented. A full example for setting both initial and boundary conditions can be found in `examples/boundary_conditions.cc`. The problem solved in this example is shown in Fig. 4.3. It consists of a plate that is fixed with movable supports on the left and bottom side. On the right side, a traction, which increases linearly with the number of time steps, is applied. The initial displacement and velocity in x-direction at all free nodes is zero and two respectively.

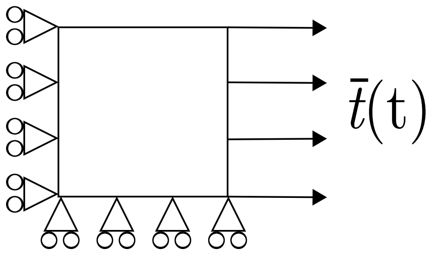


Figure 4.3: Plate on movable supports.

As it is mentioned in Section 2.6, node and element groups can be used to assign the boundary conditions. A generic example is given below with a Dirichlet boundary condition.

```
// create a node group
NodeGroup & node_group = mesh.createNodeGroup("nodes_fix");

/*
fill the node group with the nodes you want
*/

// create an element group using the existing node group
mesh.createElementGroupFromNodeGroup("el_fix", "nodes_fix",
  spatial_dimension-1);

// boundary condition can be applied using the element group name
model.applyBC(BC::Dirichlet::FixedValue(0.0, _x), "el_fix");
```

4.1.3 Material Selector

If the user wants to assign different materials to different finite elements groups in **Akantu**, a material selector has to be used. By default, **Akantu** assigns the first valid material in the material file to all elements present in the model (regular continuum materials are assigned to the regular elements and cohesive materials are assigned to cohesive elements or element facets).

To assign different materials to specific elements, mesh data information such as tag information or specified physical names can be used. `MeshDataMaterialSelector` class uses this information to assign different materials. With the proper physical name or tag name and index, different materials can be assigned as demonstrated in the examples below.

```
MeshDataMaterialSelector<std::string> * mat_selector;
mat_selector = new MeshDataMaterialSelector<std::string>("physical_names",
  model);
model.setMaterialSelector(*mat_selector);
```

In this example the physical names specified in a GMSH geometry file will by used to match the material names in the input file.

Another example would be to use the first (`tag_0`) or the second (`tag_1`) tag associated to each elements in the mesh:

```
MeshDataMaterialSelector<UInt> * mat_selector;
mat_selector = new MeshDataMaterialSelector<UInt>("tag_1", model,
  first_index);
model.setMaterialSelector(*mat_selector);
```

where `first_index` (default is 1) is the value of `tag_1` that will be associated to the first material in the material input file. The following values of the tag will be associated with the following materials.

There are four different material selectors pre-defined in **Akantu**. `MaterialSelector` and `DefaultMaterialSelector` is used to assign a material to regular elements by default. For the regular elements, as in the example above, `MeshDataMaterialSelector` can be used to assign different materials to different elements.

Apart from the **Akantu**'s default material selectors, users can always develop their own classes in the main code to tackle various multi-material assignment situations.

For cohesive material, **Akantu** has a pre-defined material selector to assign the first cohesive material by default to the cohesive elements which is called `DefaultMaterialCohesiveSelector` and it inherits its properties from `DefaultMaterialSelector`. Multiple cohesive materials can be assigned using mesh data information (for more details, see 4.1.4).

4.1.4 Insertion of Cohesive Elements

Cohesive elements are currently compatible only with static simulation and dynamic simulation with an explicit time integration scheme (see section 4.3.2). They do not have to be inserted when the mesh is generated (intrinsic) but can be added during the simulation (extrinsic). At any time during the simulation, it is possible to access the following energies with the relative function:

```
Real Ed = model.getEnergy("dissipated");
Real Er = model.getEnergy("reversible");
Real Ec = model.getEnergy("contact");
```

A new model have to be call in a very similar way that the solid mechanics model:

```
SolidMechanicsModelCohesive model(mesh);
model.initFull(SolidMechanicsModelCohesiveOptions(_explicit_lumped_mass,
  true));
```

Extrinsic approach

The dynamic insertion of extrinsic cohesive elements should be initialized in the following way:

```
model.updateAutomaticInsertion();
```

During the simulation, stress has to be checked along each facet in order to insert cohesive elements where the stress criterion is reached. This check is performed by calling the method `checkCohesiveStress`, as example before each step resolution:

```
model.checkCohesiveStress();
model.solveStep();
```

In case the extrinsic cohesive method is used in the implicit solution scheme, the cohesive elements are inserted one by one, starting from the highest locally stressed element (more precisely, the most stressed element per material type is inserted). When a cohesive element is inserted, the new equilibrated solution of the last incremental step is sought. Then, the method `checkCohesiveStress` is called again to check if new cohesive elements have to be inserted. When the insertion is terminated, the solution of the incremental loading step is stored, and the simulation can advance to the next incremental loading step. This procedure is managed by the function `solveStepCohesive` (for more details see 4.2)

The area where stresses are checked and cohesive elements inserted can be limited using the method `limitInsertion` during initialization. As example, to limit insertion in the range $[-1.5, 1.5]$ in the x direction:

```
model.limitInsertion(_x, -1.5, 1.5);
model.updateAutomaticInsertion();
```

Additional restrictions with respect to y and z directions can be added as well.

Intrinsic approach

Intrinsic cohesive elements are inserted in the mesh with the method `insertIntrinsicElements`. Similarly, the range of insertion can me limited with `limitInsertion`. As example with a static simulation,

```
model.limitInsertion(_x, -1.5, 1.5);
model.insertIntrinsicElements();
```

Mesh data information becomes vital to the insertion of cohesive elements along surface with more sophisticated geometry or when multiple cohesive materials are wanted. To do so, cohesive elements can be inserted along a specific group of surface elements identified in a GMSH geometry file. This can be achieved with the material selector (see section 4.1.3), in the input file specify the name of these physical groups in the corresponding cohesive materials, and call these material in the *mesh parameters* section. As example, with two physical surfaces named *weak_interface* and *strong_interface* defined in the GMSH geometry file:

```
...
  material cohesive_constitutive_law [
     name = weak_interface
     sigma_c = value
     ...
  ]
  material cohesive_constitutive_law [
     name = strong_interface
     sigma_c = value
     ...
  ]
  mesh parameters [
      cohesive_surfaces = weak_interface,strong_interface
  ]
```

In this case, there is no need to call `insertIntrinsicElements` anymore since the insertion of cohesive elements along physical surfaces is performed automatically during `initFull` call.

4.2 Static Analysis

The `SolidMechanicsModel` class can handle different analysis methods, the first one being presented is the static case. In this case, the equation to solve is

$$\boldsymbol{K}\boldsymbol{u} = \boldsymbol{f}_{\text{ext}} \tag{4.5}$$

where $\boldsymbol{K}$ is the global stiffness matrix, $\boldsymbol{u}$ the displacement vector and $\boldsymbol{f}_{\text{ext}}$ the vector of external forces applied to the system.

To solve such a problem, the static solver of the `SolidMechanicsModel` object is used. First, a model has to be created and initialized. To create the model, a mesh (which can be read from a file) is needed, as explained in Section 2.4. Once an instance of a `SolidMechanicsModel` is obtained, the easiest way to initialize it is to use the `initFull` method by giving the `SolidMechanicsModelOptions`. These options specify the type of analysis to be performed and whether the materials should be initialized with `initMaterials` or not.

```
SolidMechanicsModel model(mesh);
model.initFull(SolidMechanicsModelOptions(_static, false));
```

Here, a static analysis is chosen by passing the argument `_static` to the method. By default, the Boolean for no initialization of the materials is set to false, so that they are initialized during the `initFull`. The method `initFull` also initializes all appropriate vectors to zero. Once the model is created and initialized, the boundary conditions can be set as explained in Section 4.1.2. Boundary conditions will prescribe the external forces for some free degrees of freedom $\boldsymbol{f}_{\text{ext}}$ and displacements for some others. At this point of the analysis, the function `solveStep` can be called:

```
model.solveStep<_scm_newton_raphson_tangent_modified, _scc_residual>(1e-4, 1);
```

This function is templated by the solving method and the convergence criterion and takes two arguments: the tolerance and the maximum number of iterations (100 by default), which are 1×10^{-4} and 1 for this example. The modified Newton-Raphson method is chosen to solve the system. In this method, the equilibrium equation (4.5) is modified in order to apply a Newton-

Raphson convergence algorithm:

$$\begin{aligned} \boldsymbol{K}^{i+1}\delta\boldsymbol{u}^{i+1} &= \boldsymbol{r} && (4.6)\\ &= \boldsymbol{f}_{\text{ext}} - \boldsymbol{f}_{\text{int}} && (4.7)\\ &= \boldsymbol{f}_{\text{ext}} - \boldsymbol{K}^{i}\boldsymbol{u}^{i} && (4.8)\\ \boldsymbol{u}^{i+1} &= \boldsymbol{u}^{i} + \delta\boldsymbol{u}^{i+1}\ , \end{aligned}$$

where $\delta\boldsymbol{u}$ is the increment of displacement to be added from one iteration to the other, and i is the Newton-Raphson iteration counter. By invoking the `solveStep` method in the first step, the global stiffness matrix $\boldsymbol{K}$ from Equation (4.5) is automatically assembled. A Newton-Raphson iteration is subsequently started, $\boldsymbol{K}$ is updated according to the displacement computed at the previous iteration and one loops until the forces are balanced (`_scc_residual`), *i.e.*, $||\boldsymbol{r}|| <$ `_scc_residual`. One can also iterate until the increment of displacement is zero (`_scc_increment`) which also means that the equilibrium is found. For a linear elastic problem, the solution is obtained in one iteration and therefore the maximum number of iterations can be set to one. But for a non-linear case, one needs to iterate as long as the norm of the residual exceeds the tolerance threshold and therefore the maximum number of iterations has to be higher, e.g. 100:

```
model.solveStep<_scm_newton_raphson_tangent_modified,_scc_residual>(1e-4, 100)
```

At the end of the analysis, the final solution is stored in the **displacement** vector. A full example of how to solve a static problem is presented in the code `examples/static/static.cc`. This example is composed of a 2D plate of steel, blocked with rollers on the left and bottom sides as shown in Figure 4.4. The nodes from the right side of the sample are displaced by 0.01% of the length of the plate.

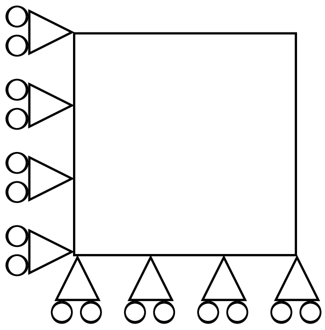


Figure 4.4: Numerical setup

The results of this analysis is depicted in Figure 4.5.

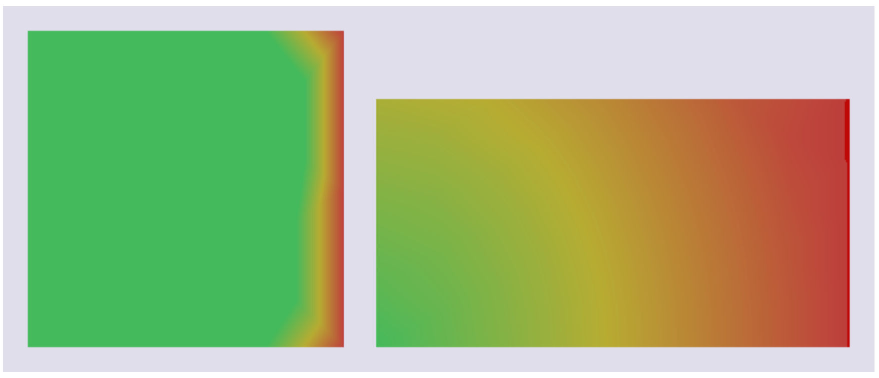


Figure 4.5: Solution of the static analysis. Left: the initial condition, right: the solution (deformation magnified 50 times)

4.2.1 Static implicit analysis with dynamic insertion of cohesive elements

In order to solve problems with the extrinsic cohesive method in the static implicit solution scheme, the function `solveStepCohesive` has to be used:

```
model.solveStepCohesive<_scm_newton_raphson_tangent, _scc_increment>(1e-13,
    error, 25, false, 1e5, true);
```

in which the arguments are: tolerance, error, max_iteration, load_reduction, tol_increase_factor, do_not_factorize. This function, first applies the Newton-Raphson procedure to solve the problem. Then, it calls the method `checkCohesiveStress` to check if cohesive elements have to be inserted. Since the approach is implicit, only one element is added, the most stressed one (see Section 4.1.4). After insertion, the Newton-Raphson procedure is applied again to solve the same incremental loading step, with the new inserted cohesive element. The procedure loops in this way since no new cohesive elements have to be inserted. At that point, the solution is saved, and the simulation can advance to the next incremental loading step. In case the convergence is not reached, the obtained solution is not saved and the simulation return to the main file with the error given by the solution saved in the argument of the function *error*. In this way, the user can intervene in the simulation in order to find anyhow convergence. A possibility is, for instance, to reduce the last incremental loading step. The variable *load_reduction* can be used to identify if the load has been already reduced or not. At the same time, with the variable *tol_increase_factor* it is possible to increase the tolerance by a factor defined by the user in the main file, in order to accept a solution even with an error bigger than the tolerance set at the beginning. It is possible to increase the tolerance only in the phase of loading reduction, i.e., when load_reduction = true. A not converged solution is never saved. In case the convergence is not reached even after the loading reduction procedure, the displacement field is not updated and remains the one of the last converged incremental steps. Also, cohesive elements are inserted only if convergence is reached. An example of the extrinsic cohesive method in the static implicit solution scheme is presented in `examples/cohesive_element/cohesive_extrinsic_implicit`.

4.3 Dynamic Methods

Different ways to solve the equations of motion are implemented in the solid mechanics model. The complete equations that should be solved are:

$$\boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{C}\dot{\boldsymbol{u}} + \boldsymbol{K}\boldsymbol{u} = \boldsymbol{f}_{\text{ext}}\,, \tag{4.9}$$

where $\boldsymbol{M}$, $\boldsymbol{C}$ and $\boldsymbol{K}$ are the mass, damping and stiffness matrices, respectively.

In the previous section, it has already been discussed how to solve this equation in the static case, where $\ddot{\boldsymbol{u}} = \dot{\boldsymbol{u}} = 0$. Here the method to solve this equation in the general case will be presented. For this purpose, a time discretization has to be specified. The most common discretization method in solid mechanics is the Newmark-β method, which is also the default in **Akantu**.

For the Newmark-β method, (4.9) becomes a system of three equations (see [5] [6] for more details):

$$\boldsymbol{M}\ddot{\boldsymbol{u}}_{n+1} + \boldsymbol{C}\dot{\boldsymbol{u}}_{n+1} + \boldsymbol{K}\boldsymbol{u}_{n+1} = \boldsymbol{f}_{\text{ext}\,n+1} \tag{4.10}$$

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + (1-\alpha)\,\Delta t\dot{\boldsymbol{u}}_n + \alpha\Delta t\dot{\boldsymbol{u}}_{n+1} + \left(\frac{1}{2}-\alpha\right)\Delta t^2\ddot{\boldsymbol{u}}_n \tag{4.11}$$

$$\dot{\boldsymbol{u}}_{n+1} = \dot{\boldsymbol{u}}_n + (1-\beta)\,\Delta t\ddot{\boldsymbol{u}}_n + \beta\Delta t\ddot{\boldsymbol{u}}_{n+1} \tag{4.12}$$

In these new equations, $\ddot{\boldsymbol{u}}_n$, $\dot{\boldsymbol{u}}_n$ and $\boldsymbol{u}_n$ are the approximations of $\ddot{\boldsymbol{u}}(t_n)$, $\dot{\boldsymbol{u}}(t_n)$ and $\boldsymbol{u}(t_n)$. Equation (4.10) is the equation of motion discretized in space (finite-element discretization), and equations (4.11) and (4.12) are discretized in both space and time (Newmark discretization). The α and β parameters determine the stability and the accuracy of the algorithm. Classical values for α and β are usually $\beta = 1/2$ for no numerical damping and $0 < \alpha < 1/2$.

α	Method ($\beta = 1/2$)	Type
0	central difference	explicit
1/6	Fox-Goodwin (royal road)	implicit
1/3	Linear acceleration	implicit
1/2	Average acceleration (trapezoidal rule)	implicit

The solution of this system of equations, (4.10)-(4.12) is split into a predictor and a corrector system of equations. Moreover, in the case of a non-linear equations, an iterative algorithm such as the Newton-Raphson method is applied. The system of equations can be written as:

1. *Predictor:*

$$\boldsymbol{u}^0_{n+1} = \boldsymbol{u}_n + \Delta t \dot{\boldsymbol{u}}_n + \frac{\Delta t^2}{2} \ddot{\boldsymbol{u}}_n \tag{4.13}$$

$$\dot{\boldsymbol{u}}^0_{n+1} = \dot{\boldsymbol{u}}_n + \Delta t \ddot{\boldsymbol{u}}_n \tag{4.14}$$

$$\ddot{\boldsymbol{u}}^0_{n+1} = \ddot{\boldsymbol{u}}_n \tag{4.15}$$

2. *Solve:*

$$\left(c\boldsymbol{M} + d\boldsymbol{C} + e\boldsymbol{K}^i_{n+1}\right) \boldsymbol{w} = \boldsymbol{f}_{\text{ext}\, n+1} - \boldsymbol{f}_{\text{int}\, n+1}^{\ i} - \boldsymbol{C}\dot{\boldsymbol{u}}^i_{n+1} - \boldsymbol{M}\ddot{\boldsymbol{u}}^i_{n+1} = \boldsymbol{r}^i_{n+1} \tag{4.16}$$

3. *Corrector:*

$$\ddot{\boldsymbol{u}}^{i+1}_{n+1} = \ddot{\boldsymbol{u}}^i_{n+1} + c\boldsymbol{w} \tag{4.17}$$

$$\dot{\boldsymbol{u}}^{i+1}_{n+1} = \dot{\boldsymbol{u}}^i_{n+1} + d\boldsymbol{w} \tag{4.18}$$

$$\boldsymbol{u}^{i+1}_{n+1} = \boldsymbol{u}^i_{n+1} + e\boldsymbol{w} \tag{4.19}$$

where i is the Newton-Raphson iteration counter and c, d and e are parameters depending on the method used to solve the equations

	$\boldsymbol{w}$	e	d	c
in acceleration	$\delta\ddot{\boldsymbol{u}}$	$\alpha\beta\Delta t^2$	$\beta\Delta t$	1
in velocity	$\delta\dot{\boldsymbol{u}}$	$\frac{1}{\beta}\Delta t$	1	$\alpha\Delta t$
in displacement	$\delta\boldsymbol{u}$	1	$\frac{1}{\alpha}\Delta t$	$\frac{1}{\alpha\beta}\Delta t^2$

4.3.1 Implicit Time Integration

To solve a problem with an implicit time integration scheme, first a `SolidMechanicsModel` object has to be created and initialized. Then the initial and boundary conditions have to be set. Everything is similar to the example in the static case (Section 4.2), however, in this case the implicit dynamic scheme is selected at the initialization of the model.

```
SolidMechanicsModel model(mesh);
model.initFull(SolidMechanicsModelOptions(_implicit_dynamic));
/*Boundary conditions see Section~4.1.2 */
```

Because a dynamic simulation is conducted, an integration time step Δt has to be specified. In the case of implicit simulations, **Akantu** implements a trapezoidal rule by default. That is to say $\alpha = 1/2$ and $\beta = 1/2$ which is unconditionally stable. Therefore the value of the time step can be chosen arbitrarily within reason.

```
model.setTimeStep(time_step);
```

Since the system has to be solved for a given amount of time steps, the method `solveStep()`, (which has already been used in the static example in Section 4.2), is called inside a time loop:

```
/// time loop
Real time = 0.;
for (UInt s = 1; time <max_time; ++s, time += time_step) {
  model.solveStep<_scm_newton_raphson_tangent_modified,_scc_increment>(1e-12,
    100);
}
```

An example of solid mechanics with an implicit time integration scheme is presented in `examples/implicit/implicit_dynamic.cc`. This example consists of a 3D beam of 10 m × 1 m × 1 m blocked on one side and is on a roller on the other side. A constant force of 5 kN is applied in its middle. Figure 4.6 presents the geometry of this case. The material used is a fictitious linear elastic material with a density of 1000 kg m^{-3}, a Young's Modulus of 120 MPa and Poisson's ratio of 0.3. These values were chosen to simplify the analytical solution.

An approximation of the dynamic response of the middle point of the beam is given by:

$$u\left(\frac{L}{2},t\right) = \frac{1}{\pi^4}\left(1 - cos\left(\pi^2 t\right) + \frac{1}{81}\left(1 - cos\left(3^2\pi^2 t\right)\right) + \frac{1}{625}\left(1 - cos\left(5^2\pi^2 t\right)\right)\right) \tag{4.20}$$

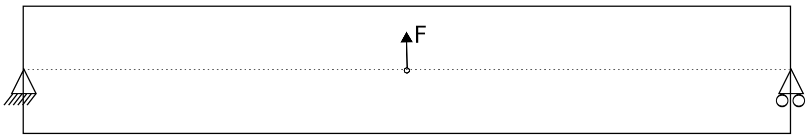


Figure 4.6: Numerical setup

Figure 4.7 presents the deformed beam at 3 different times during the simulation: time steps 0, 1000 and 2000.

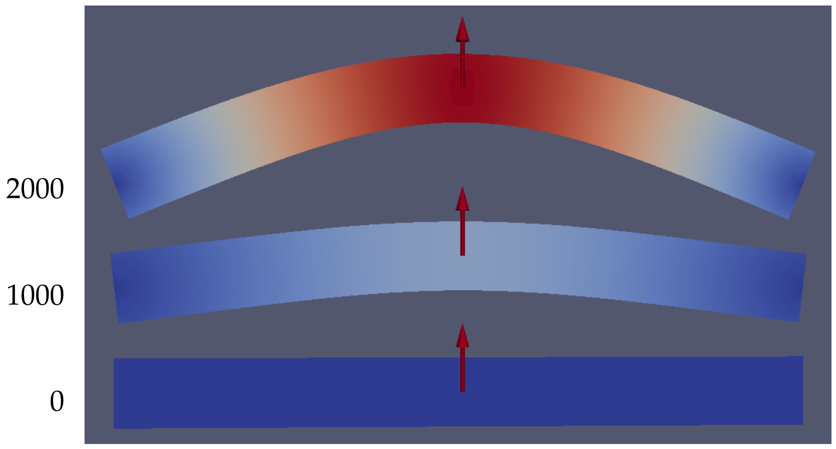


Figure 4.7: Deformed beam at 3 different times (displacement are magnified by a factor 10).

4.3.2 Explicit Time Integration

The explicit dynamic time integration scheme is based on the Newmark-β scheme with $\alpha = 0$ (see equations 4.10-4.12). In **Akantu**, β is defaults to $\beta = 1/2$, see section 4.3.

The initialization of the simulation is similar to the static and implicit dynamic version. The model is created from the `SolidMechanicsModel` class. In the initialization, the explicit scheme is selected using the `_explicit_lumped_mass` constant.

```
SolidMechanicsModel model(mesh);
model.initFull(SolidMechanicsModelOptions(_explicit_lumped_mass));
```

Note: *Writing* `model.initFull()` *or* `model.initFull(SolidMechanicsModelOptions());` *is equivalent to use the* `_explicit_lumped_mass` *keyword, as this is the default case.*

The explicit time integration scheme implemented in **Akantu** uses a lumped mass matrix $\boldsymbol{M}$ (reducing the computational cost). This matrix is assembled by distributing the mass of each element onto its nodes. The resulting $\boldsymbol{M}$ is therefore a diagonal matrix stored in the **mass** vector of the model.

The explicit integration scheme is conditionally stable. The time step has to be smaller than the stable time step which is obtained in **Akantu** as follows:

```
critical_time_step = model.getStableTimeStep();
```

The stable time step corresponds to the time the fastest wave (the compressive wave) needs to travel the characteristic length of the mesh:

$$\Delta t_{\text{crit}} = \frac{\Delta x}{c} \tag{4.21}$$

where Δx is a characteristic length (*e.g.*, the inradius in the case of linear triangle element) and c is the celerity of the fastest wave in the material. It is generally the compressive wave of celerity $c = \sqrt{\frac{2\mu+\lambda}{\rho}}$, μ and λ are the first and second Lame's coefficients and ρ is the density. However, it is recommended to impose a time step that is smaller than the stable time step, for instance, by multiplying the stable time step by a safety factor smaller than one.

```
const Real safety_time_factor = 0.8;
Real applied_time_step = critical_time_step * safety_time_factor;
model.setTimeStep(applied_time_step);
```

The initial displacement and velocity fields are, by default, equal to zero if not given specifically by the user (see 4.1.1).

Like in implicit dynamics, a time loop is used in which the displacement, velocity and acceleration fields are updated at each time step. The values of these fields are obtained from the Newmark$-\beta$ equations with $\beta = 1/2$ and $\alpha = 0$. In **Akantu** these computations at each time step are invoked by calling the function `solveStep`:

```
for (UInt s = 1; (s-1)*applied_time_step < total_time; ++s) {
  model.solveStep();
}
```

The method `solveStep` wraps the four following functions:

- `model.explicitPred()` allows to compute the displacement field at $t+1$ and a part of the velocity field at $t+1$, denoted by $\dot{\boldsymbol{u}}^{\text{p}}{}_{n+1}$, which will be used later in the method `model.explicitCorr()`. The equations are:

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + \Delta t \dot{\boldsymbol{u}}_n + \frac{\Delta t^2}{2} \ddot{\boldsymbol{u}}_n \tag{4.22}$$

$$\dot{\boldsymbol{u}}^{\text{p}}{}_{n+1} = \dot{\boldsymbol{u}}_n + \Delta t \ddot{\boldsymbol{u}}_n \tag{4.23}$$

- `model.updateResidual()` and `model.updateAcceleration()` compute the acceleration increment $\delta\ddot{\boldsymbol{u}}$:

$$\left(\boldsymbol{M} + \frac{1}{2}\Delta t \boldsymbol{C}\right)\delta\ddot{\boldsymbol{u}} = \boldsymbol{f}_{\text{ext}} - \boldsymbol{f}_{\text{int}\,n+1} - \boldsymbol{C}\dot{\boldsymbol{u}}_n - \boldsymbol{M}\ddot{\boldsymbol{u}}_n \tag{4.24}$$

  Note: *The internal force $\boldsymbol{f}_{\text{int}\,n+1}$ is computed from the displacement $\boldsymbol{u}_{n+1}$ based on the constitutive law.*

- `model.explicitCorr()` computes the velocity and acceleration fields at $t+1$:

$$\dot{\boldsymbol{u}}_{n+1} = \dot{\boldsymbol{u}}^{\mathrm{P}}{}_{n+1} + \frac{\Delta t}{2}\delta\ddot{\boldsymbol{u}} \tag{4.25}$$

$$\ddot{\boldsymbol{u}}_{n+1} = \ddot{\boldsymbol{u}}_n + \delta\ddot{\boldsymbol{u}} \tag{4.26}$$

The use of an explicit time integration scheme is illustrated by the example:
`examples/explicit/explicit_dynamic.cc`
This example models the propagation of a wave in a steel beam. The beam and the applied displacement in the x direction are shown in Figure 4.8.

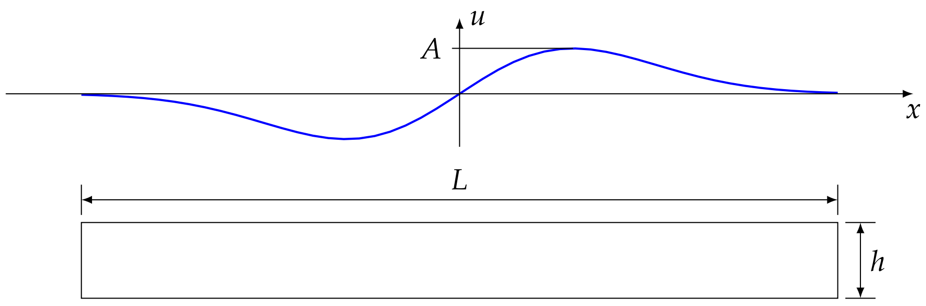


Figure 4.8: Numerical setup

The length and height of the beam are $L = 10\,\mathrm{m}$ and $h = 1\,\mathrm{m}$, respectively. The material is linear elastic, homogeneous and isotropic (density: $7800\,\mathrm{kg\,m^{-3}}$, Young's modulus: 210 GPa and Poisson's ratio: 0.3). The imposed displacement follow a Gaussian function with a maximum amplitude of $A = 0.01\,\mathrm{m}$. The potential, kinetic and total energies are computed. The safety factor is equal to 0.8.

4.4 Constitutive Laws

In order to compute an element's response to deformation, one needs to use an appropriate constitutive relationship. The constitutive law is used to compute the element's stresses from the element's strains.

In the finite-element discretization, the constitutive formulation is applied to every quadrature point of each element. When the implicit formulation is used, the tangent matrix has to be computed.

The chosen materials for the simulation have to be specified in the mesh file or, as an alternative, they can be assigned using the `element_material` vector. For every material assigned to the problem one has to specify the material characteristics (constitutive behavior and material properties) using the text input file (see 7.1.3).
In order to conveniently store values at each quadrature in a material point **Akantu** provides a special data structure, the `InternalField`. The internal fields are inheriting from the `ElementTypeMapArray`. Furthermore, it provides several functions for initialization, auto-resizing and auto removal of quadrature points.

Sometimes it is also desired to generate random distributions of internal parameters. An example might be the critical stress at which the material fails. To generate such a field, in the text input file, a random quantity needs be added to the base value:

```
sigma_c = base
sigma_c = base uniform [min, max]
sigma_c = base weibull [λ, m]
```

All parameters are real numbers. For the uniform distribution, minimum and maximum values have to be specified. Random parameters are defined as a *base* value to which we add a random number that follows the chosen distribution.

The *Uniform* distribution is gives a random values between in $[min, max)$. The *Weibull* distribution is characterized by the following cumulative distribution function:

$$F(x) = 1 - e^{-(x/\lambda)^m} \tag{4.27}$$

which depends on m and λ, which are the shape parameter and the scale parameter. These random distributions are different each time the code is executed. In order to obtain always the same one, it possible to manually set the *seed* that is the number from which these pseudo-random distributions are created. This can be done by adding the following line to the input file *outside* the material parameters environments:

```
seed = 1.0
```

where the value 1.0 can be substituted with any number. Currently **Akantu** can reproduce always the same distribution when the seed is specified *only* in serial. The value of the *seed* can be also specified directly in the code (for instance in the main file) with the command:

```
RandGenerator:: seed(1.0)
```

The same command, with empty brackets, can be used to check the value of the *seed* used in the simulation.

The following sections describe the constitutive models implemented in **Akantu**. In Appendix B a summary of the parameters for all materials of **Akantu** is provided.

4.4.1 Elasticity

The elastic law is a commonly used constitutive relationship that can be used for a wide range of engineering materials (*e.g.*, metals, concrete, rock, wood, glass, rubber, etc.) provided that the strains remain small (*i.e.*, small deformation and stress lower than yield strength).

The elastic laws are often expressed as $\boldsymbol{\sigma} = \boldsymbol{C} : \boldsymbol{\varepsilon}$ with where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\boldsymbol{\varepsilon}$ represents the infinitesimal strain tensor and $\boldsymbol{C}$ is the elastic modulus tensor.

Linear isotropic (B.1)

The linear isotropic elastic behavior is described by Hooke's law, which states that the stress is linearly proportional to the applied strain (material behaves like an ideal spring), as illustrated in Figure 4.9. The equation that relates the strains to the displacements is: point) from the displacements as follows:

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left[\nabla_0 \boldsymbol{u} + \nabla_0 \boldsymbol{u}^T\right] \tag{4.28}$$

where $\boldsymbol{\varepsilon}$ represents the infinitesimal strain tensor, $\nabla_0 \boldsymbol{u}$ the displacement gradient tensor according to the initial configuration. The constitutive equation for isotropic homogeneous media can be expressed as:

$$\boldsymbol{\sigma} = \lambda \mathrm{tr}(\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon} \tag{4.29}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor (λ and μ are the the first and second Lame's coefficients).

In Voigt notation this correspond to

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix} \tag{4.30}$$

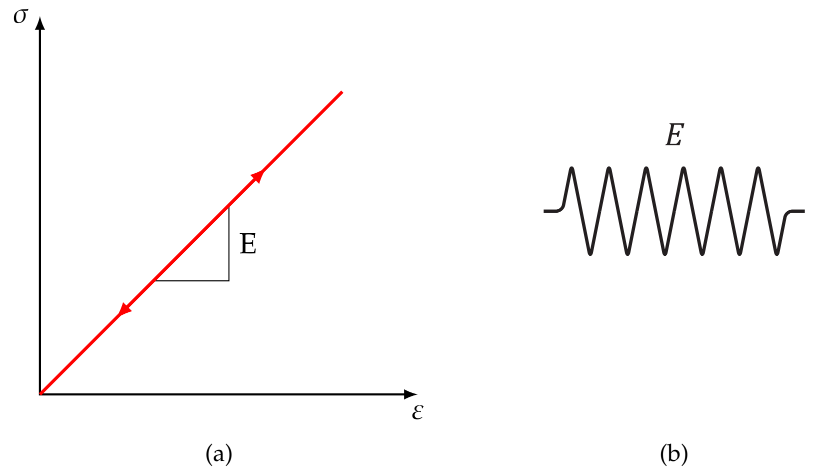


Figure 4.9: (a) Stress-strain curve for elastic material and (b) schematic representation of Hooke's law, denoted as a spring.

Linear anisotropic (B.2)

This formulation is not sufficient to represent all elastic material behavior. Some materials have characteristic orientation that have to be taken into account. To represent this anisotropy a more general stress-strain law has to be used. For this we define the elastic modulus tensor as follow:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{21} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{31} & c_{32} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{41} & c_{42} & c_{43} & c_{44} & c_{45} & c_{46} \\ c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & c_{56} \\ c_{61} & c_{62} & c_{63} & c_{64} & c_{65} & c_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix} \tag{4.31}$$

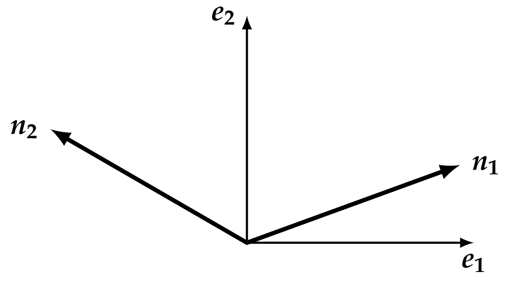


Figure 4.10: Material basis

To simplify the writing of input files the $\boldsymbol{C}$ tensor is expressed in the material basis. And this basis as to be given too. This basis $\Omega_{\text{mat}} = \{\boldsymbol{n}_1, \boldsymbol{n}_2, \boldsymbol{n}_3\}$ is used to define the rotation $R_{ij} = \boldsymbol{n}_j.\boldsymbol{e}_i$. And $\boldsymbol{C}$ can be rotated in the global basis $\Omega = \{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ as follow:

$$\boldsymbol{C}_\Omega = \boldsymbol{R}_1 \boldsymbol{C}_{\Omega_{\text{mat}}} \boldsymbol{R}_2 \tag{4.32}$$

$$\boldsymbol{R}_1 = \begin{bmatrix} R_{11}R_{11} & R_{12}R_{12} & R_{13}R_{13} & R_{12}R_{13} & R_{11}R_{13} & R_{11}R_{12} \\ R_{21}R_{21} & R_{22}R_{22} & R_{23}R_{23} & R_{22}R_{23} & R_{21}R_{23} & R_{21}R_{22} \\ R_{31}R_{31} & R_{32}R_{32} & R_{33}R_{33} & R_{32}R_{33} & R_{31}R_{33} & R_{31}R_{32} \\ R_{21}R_{31} & R_{22}R_{32} & R_{23}R_{33} & R_{22}R_{33} & R_{21}R_{33} & R_{21}R_{32} \\ R_{11}R_{31} & R_{12}R_{32} & R_{13}R_{33} & R_{12}R_{33} & R_{11}R_{33} & R_{11}R_{32} \\ R_{11}R_{21} & R_{12}R_{22} & R_{13}R_{23} & R_{12}R_{23} & R_{11}R_{23} & R_{11}R_{22} \end{bmatrix} \tag{4.33}$$

$$\boldsymbol{R}_2 = \begin{bmatrix} R_{11}R_{11} & R_{21}R_{21} & R_{31}R_{31} & R_{21}R_{31} & R_{11}R_{31} & R_{11}R_{21} \\ R_{12}R_{12} & R_{22}R_{22} & R_{32}R_{32} & R_{22}R_{32} & R_{12}R_{32} & R_{12}R_{22} \\ R_{13}R_{13} & R_{23}R_{23} & R_{33}R_{33} & R_{23}R_{33} & R_{13}R_{33} & R_{13}R_{23} \\ R_{12}R_{13} & R_{22}R_{23} & R_{32}R_{33} & R_{22}R_{33} & R_{12}R_{33} & R_{12}R_{23} \\ R_{11}R_{13} & R_{21}R_{23} & R_{31}R_{33} & R_{21}R_{33} & R_{11}R_{33} & R_{11}R_{23} \\ R_{11}R_{12} & R_{21}R_{22} & R_{31}R_{32} & R_{21}R_{32} & R_{11}R_{32} & R_{11}R_{22} \end{bmatrix} \tag{4.34}$$

$$\tag{4.35}$$

Linear orthotropic (B.3)

A particular case of anisotropy is when the material basis is orthogonal in which case the elastic modulus tensor can be simplified and rewritten in terms of 9 independents material parameters.

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{22} & c_{23} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & \text{sym.} & & & c_{55} & 0 \\ & & & & & c_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix} \tag{4.36}$$

$$c_{11} = E_1(1-\nu_{23}\nu_{32})\Gamma \qquad c_{22} = E_2(1-\nu_{13}\nu_{31})\Gamma \qquad c_{33} = E_3(1-\nu_{12}\nu_{21})\Gamma \tag{4.37}$$

$$c_{12} = E_1(\nu_{21}-\nu_{31}\nu_{23})\Gamma = E_2(\nu_{12}-\nu_{32}\nu_{13})\Gamma \tag{4.38}$$

$$c_{13} = E_1(\nu_{31}-\nu_{21}\nu_{32})\Gamma = E_2(\nu_{13}-\nu_{21}\nu_{23})\Gamma \tag{4.39}$$

$$c_{23} = E_2(\nu_{32}-\nu_{12}\nu_{31})\Gamma = E_3(\nu_{23}-\nu_{21}\nu_{13})\Gamma \tag{4.40}$$

$$c_{44} = \mu_{23} \qquad c_{55} = \mu_{13} \qquad c_{66} = \mu_{12} \tag{4.41}$$

$$\Gamma = \frac{1}{1-\nu_{12}\nu_{21}-\nu_{13}\nu_{31}-\nu_{32}\nu_{23}-2\nu_{21}\nu_{32}\nu_{13}} \tag{4.42}$$

The Poisson ratios follow the rule $\nu_{ij} = \nu_{ji}E_i/E_j$.

4.4.2 Neo-Hookean (B.4)

The hyperelastic Neo-Hookean constitutive law results from an extension of the linear elastic relationship (Hooke's Law) for large deformation. Thus, the model predicts nonlinear stress-strain behavior for bodies undergoing large deformations.

As illustrated in Figure 4.11, the behavior is initially linear and the mechanical behavior is very close to the corresponding linear elastic material. This constitutive relationship, which accounts for compressibility, is a modified version of the one proposed by Ronald Rivlin [7].

The strain energy stored in the material is given by:

$$\Psi(\boldsymbol{C}) = \frac{1}{2}\lambda_0 (\ln J)^2 - \mu_0 \ln J + \frac{1}{2}\mu_0 (\text{tr}(\boldsymbol{C}) - 3) \tag{4.43}$$

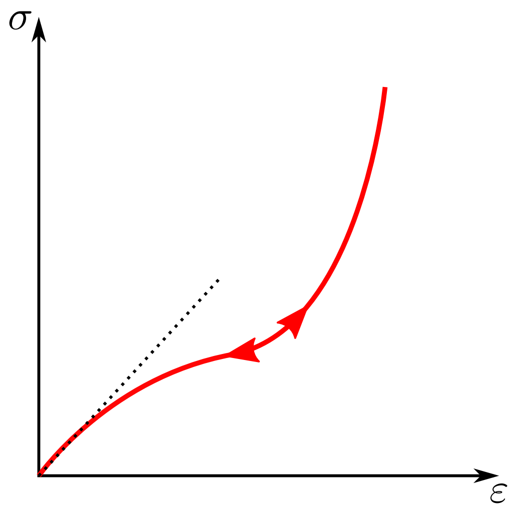


Figure 4.11: Neo-hookean Stress-strain curve.

where λ_0 and μ_0 are, respectively, Lamé's first parameter and the shear modulus at the initial configuration. J is the jacobian of the deformation gradient ($\boldsymbol{F} = \nabla_{\boldsymbol{X}} \boldsymbol{x}$): $J = \det(\boldsymbol{F})$. Finally $\boldsymbol{C}$ is the right Cauchy-Green deformation tensor.

Since this kind of material is used for large deformation problems, a finite deformation framework should be used. Therefore, the Cauchy stress ($\boldsymbol{\sigma}$) should be computed through the second Piola-Kirchhoff stress tensor $\boldsymbol{S}$:

$$\boldsymbol{\sigma} = \frac{1}{J} \boldsymbol{F} \boldsymbol{S} \boldsymbol{F}^T \tag{4.44}$$

Finally the second Piola-Kirchhoff stress tensor is given by:

$$\boldsymbol{S} = 2\frac{\partial \Psi}{\partial \boldsymbol{C}} = \lambda_0 \ln J \boldsymbol{C}^{-1} + \mu_0 \left(\boldsymbol{I} - \boldsymbol{C}^{-1} \right) \tag{4.45}$$

The parameters to indicate in the material file are the same as those for the elastic case: `E` (Young's modulus), `nu` (Poisson's ratio).

4.4.3 Visco-Elasticity (B.5)

Visco-elasticity is characterized by strain rate dependent behavior. Moreover, when such a material undergoes a deformation it dissipates energy. This dissipation results in a hysteresis loop in the stress-strain curve at every loading cycle (see Figure 4.12a). In principle, it can be applied to many materials, since all materials exhibit a visco-elastic behavior if subjected to particular conditions (such as high temperatures). The standard rheological linear solid model (see Sections 10.2 and 10.3 of [8]) has been implemented in **Akantu**. This model results from the combination of a spring mounted in parallel with a spring and a dashpot connected in series, as illustrated in Figure 4.12b. The advantage of this model is that it allows to account for creep or stress relaxation. The equation that relates the stress to the strain is (in 1D):

$$\frac{d\varepsilon(t)}{dt} = (E + E_V)^{-1} \cdot \left[\frac{d\sigma(t)}{dt} + \frac{E_V}{\eta}\sigma(t) - \frac{EE_V}{\eta}\varepsilon(t) \right] \tag{4.46}$$

where η is the viscosity. The equilibrium condition is unique and is attained in the limit, as $t \to \infty$. At this stage, the response is elastic and depends on the Young's modulus E. The mandatory parameters for the material file are the following: `rho` (density), `E` (Young's modulus), `nu`

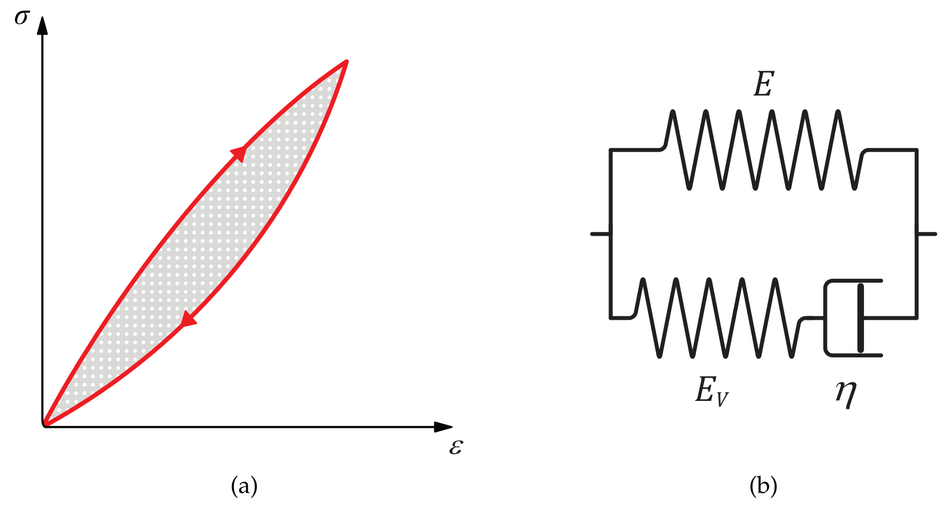


Figure 4.12: (a) Characteristic stress-strain behavior of a visco-elastic material with hysteresis loop and (b) schematic representation of the standard rheological linear solid visco-elastic model.

(Poisson's ratio), `Plane_Stress` (if set to zero plane strain, otherwise plane stress), `eta` (dashpot viscosity) and `Ev` (stiffness of the viscous element).

Note that the current standard linear solid model is applied only on the deviatoric part of the strain tensor. The spheric part of the strain tensor affects the stress tensor like an linear elastic material.

4.4.4 Small-Deformation Plasticity (B.6)

The small-deformation plasticity is a simple plasticity material formulation which accounts for the additive decomposition of strain into elastic and plastic strain components. This formulation is applicable to infinitesimal deformation where the additive decomposition of the strain is a valid approximation. In this formulation, plastic strain is a shearing process where hydrostatic stress has no contribution to plasticity and consequently plasticity does not lead to volume change. Figure 4.13 shows the linear strain hardening elasto-plastic behavior according to the additive decomposition of strain into the elastic and plastic parts in infinitesimal deformation as

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p \tag{4.47}$$

$$\boldsymbol{\sigma} = 2G(\boldsymbol{\varepsilon}^e) + \lambda \operatorname{tr}(\boldsymbol{\varepsilon}^e)\boldsymbol{I} \tag{4.48}$$

In this class, the von Mises yield criterion is used. In the von Mises yield criterion, the yield is independent of the hydrostatic stress. Other yielding criteria such as Tresca and Gurson can be easily implemented in this class as well.

In the von Mises yield criterion, the hydrostatic stresses have no effect on the plasticity and consequently the yielding occurs when a critical elastic shear energy is achieved.

$$f = \sigma_{\text{eff}} - \sigma_y = \left(\frac{3}{2}\boldsymbol{\sigma}^{\text{tr}} : \boldsymbol{\sigma}^{\text{tr}}\right)^{\frac{1}{2}} - \sigma_y(\boldsymbol{\varepsilon}^p) \tag{4.49}$$

$$f < 0 \quad \text{Elastic deformation,} \qquad f = 0 \quad \text{Plastic deformation} \tag{4.50}$$

where σ_y is the yield strength of the material which can be function of plastic strain in case of hardening type of materials and $\boldsymbol{\sigma}^{\text{tr}}$ is the deviatoric part of stress given by

$$\boldsymbol{\sigma}^{\text{tr}} = \boldsymbol{\sigma} - \frac{1}{3}\operatorname{tr}(\boldsymbol{\sigma})\boldsymbol{I} \tag{4.51}$$

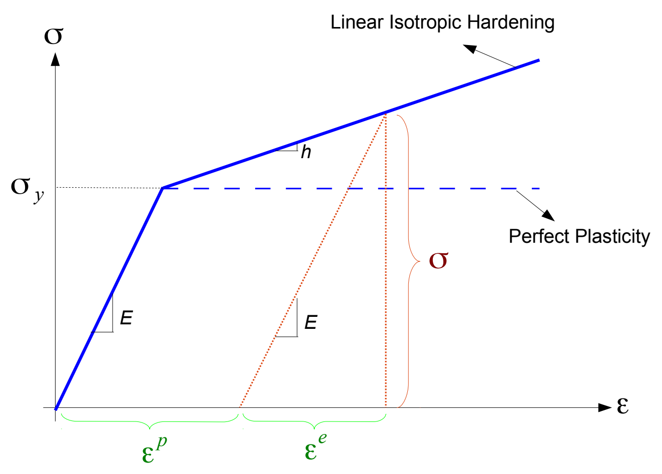


Figure 4.13: Stress-strain curve for the small-deformation plasticity with linear isotropic hardening.

After yielding ($f = 0$), the normality hypothesis of plasticity determines the direction of plastic flow which is normal to the tangent to the yielding surface at the load point. Then, the tensorial form of the plastic constitutive equation using the von Mises yielding criterion (see equation 4.34) may be written as

$$\Delta\boldsymbol{\varepsilon}^p = \Delta p \frac{\partial f}{\partial \boldsymbol{\sigma}} = \frac{3}{2}\Delta p \frac{\boldsymbol{\sigma}^{\text{tr}}}{\sigma_{\text{eff}}} \tag{4.52}$$

In these expressions, the direction of the plastic strain increment (or equivalently, plastic strain rate) is given by $\frac{\sigma^{\text{tr}}}{\sigma_{\text{eff}}}$ while the magnitude is defined by the plastic multiplier Δp. This can be obtained using the *consistency condition* which impose the requirement for the load point to remain on the yielding surface in the plastic regime.

Here, we summarize the implementation procedures for the small-deformation plasticity with linear isotropic hardening:

1. Compute the trial stress:

$$\boldsymbol{\sigma}^{\text{tr}} = \boldsymbol{\sigma}_t + 2G\Delta\boldsymbol{\varepsilon} + \lambda\,\text{tr}(\Delta\boldsymbol{\varepsilon})\boldsymbol{I} \tag{4.53}$$

2. Check the Yielding criteria:

$$f = (\frac{3}{2}\boldsymbol{\sigma}^{\text{tr}} : \boldsymbol{\sigma}^{\text{tr}})^{1/2} - \sigma_y(\boldsymbol{\varepsilon}^p) \tag{4.54}$$

3. Compute the Plastic multiplier:

$$d\Delta p = \frac{\sigma_{eff}^{tr} - 3G\Delta P^{(k)} - \sigma_y^{(k)}}{3G + h} \tag{4.55}$$

$$\Delta p^{(k+1)} = \Delta p^{(k)} + d\Delta p \tag{4.56}$$

$$\sigma_y^{(k+1)} = (\sigma_y)_t + h\Delta p \tag{4.57}$$

4. Compute the plastic strain increment:

$$\Delta\boldsymbol{\varepsilon}^p = \frac{3}{2}\Delta p \frac{\boldsymbol{\sigma}^{\text{tr}}}{\sigma_{\text{eff}}} \tag{4.58}$$

5. Compute the stress increment:

$$\Delta\boldsymbol{\sigma} = 2G(\Delta\boldsymbol{\varepsilon} - \Delta\boldsymbol{\varepsilon}^p) + \lambda \mathrm{tr}(\Delta\boldsymbol{\varepsilon} - \Delta\boldsymbol{\varepsilon}^p)\boldsymbol{I} \tag{4.59}$$

6. Update the variables:

$$\boldsymbol{\varepsilon}^p = \boldsymbol{\varepsilon}^p_t + \Delta\boldsymbol{\varepsilon}^p \tag{4.60}$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_t + \Delta\boldsymbol{\sigma} \tag{4.61}$$

We use an implicit integration technique called *the radial return method* to obtain the plastic multiplier. This method has the advantage of being unconditionally stable, however, the accuracy remains dependent on the step size. The plastic parameters to indicate in the material file are: σ_y (Yield stress) and `h` (Hardening modulus). In addition, the elastic parameters need to be defined as previously mentioned: `E` (Young's modulus), `nu` (Poisson's ratio).

4.4.5 Damage

In the simplified case of a linear elastic and brittle material, isotropic damage can be represented by a scalar variable d, which varies from 0 to 1 for no damage to fully broken material respectively. The stress-strain relationship then becomes:

$$\boldsymbol{\sigma} = (1 - d)\,\boldsymbol{C} : \boldsymbol{\varepsilon}$$

where $\boldsymbol{\sigma}$, $\boldsymbol{\varepsilon}$ are the Cauchy stress and strain tensors, and $\boldsymbol{C}$ is the elastic stiffness tensor. This formulation relies on the definition of an evolution law for the damage variable. In **Akantu**, many possibilities exist and they are listed below.

Marigo (B.7)

This damage evolution law is energy based as defined by Marigo [9,10]. It is an isotropic damage law.

$$Y = \frac{1}{2}\boldsymbol{\varepsilon} : \boldsymbol{C} : \boldsymbol{\varepsilon} \tag{4.62}$$

$$F = Y - Y_d - Sd \tag{4.63}$$

$$d = \begin{cases} \min\left(\frac{Y-Y_d}{S},\ 1\right) & \text{if } F > 0 \\ \text{unchanged} & \text{otherwise} \end{cases} \tag{4.64}$$

In this formulation, Y is the strain energy release rate, Y_d the rupture criterion and S the damage energy. The non-local version of this damage evolution law is constructed by averaging the energy Y.

Mazars (B.8)

This law introduced by Mazars [11] is a behavioral model to represent damage evolution in concrete. This model does not rely on the computation of the tangent stiffness, the damage is directly evaluated from the strain.

The governing variable in this damage law is the equivalent strain $\varepsilon_{\mathrm{eq}} = \sqrt{<\boldsymbol{\varepsilon}>_+ : <\boldsymbol{\varepsilon}>_+}$, with $< . >_+$ the positive part of the tensor. This part is defined in the principal coordinates (I, II, III) as

$\varepsilon_{\text{eq}} = \sqrt{<\boldsymbol{\varepsilon_I}>_+^2 + <\boldsymbol{\varepsilon_{II}}>_+^2 + <\boldsymbol{\varepsilon_{III}}>_+^2}$. The damage is defined as:

$$D = \alpha_t^\beta D_t + (1-\alpha_t)^\beta D_c \tag{4.65}$$

$$D_t = 1 - \frac{\kappa_0(1-A_t)}{\varepsilon_{\text{eq}}} - A_t \exp^{-B_t(\varepsilon_{\text{eq}}-\kappa_0)} \tag{4.66}$$

$$D_c = 1 - \frac{\kappa_0(1-A_c)}{\varepsilon_{\text{eq}}} - A_c \exp^{-B_c(\varepsilon_{\text{eq}}-\kappa_0)} \tag{4.67}$$

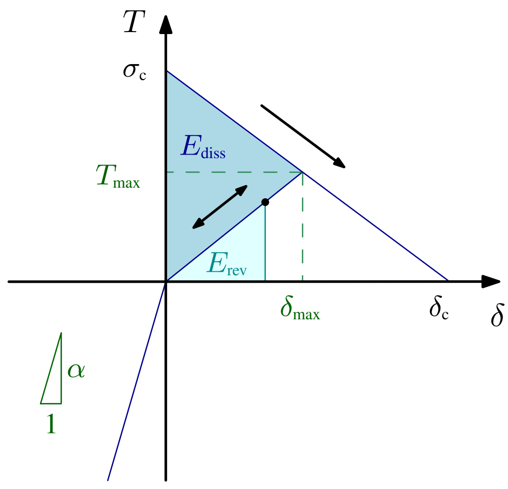
$$\alpha_t = \frac{\sum_{i=1}^3 <\varepsilon_i>_+ \varepsilon_{\text{nd}\,i}}{\varepsilon_{\text{eq}}^2} \tag{4.68}$$

With κ_0 the damage threshold, A_t and B_t the damage parameter in traction, A_c and B_c the damage parameter in compression, β is the shear parameter. α_t is the coupling parameter between traction and compression, the ε_i are the eigenstrain and the $\varepsilon_{\text{nd}\,i}$ are the eigenvalues of the strain if the material were undamaged.

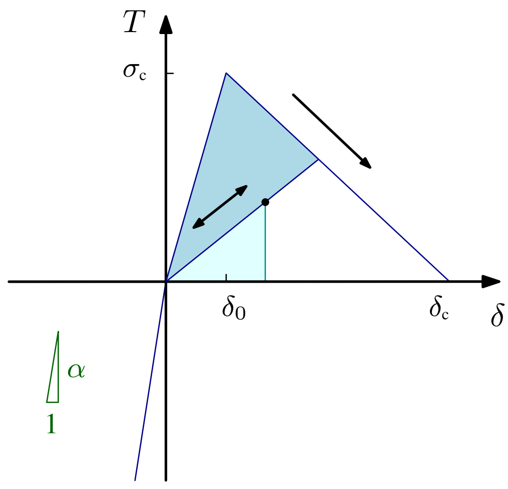
The coefficients A and B are the post-peak asymptotic value and the decay shape parameters.

4.5 Cohesive Constitutive laws

4.5.1 Linear Irreversible Law (B.10)



(a) Linear



(b) Bilinear

Figure 4.14: Irreversible cohesive laws for explicit simulations.

Akantu includes the Snozzi-Molinari [12] linear irreversible cohesive law (see Figure 4.14). It is an extension to the Camacho-Ortiz [13] cohesive law in order to make dissipated fracture energy path-dependent. The concept of free potential energy is dropped and a new independent parameter κ is introduced:

$$\kappa = \frac{G_{\text{c,II}}}{G_{\text{c,I}}} \tag{4.69}$$

where $G_{\text{c,I}}$ and $G_{\text{c,II}}$ are the necessary works of separation per unit area to open completely a cohesive zone under mode I and mode II, respectively. Their model yields to the following equation for cohesive tractions $\boldsymbol{T}$ in case of crack opening δ:

$$\boldsymbol{T} = \left(\frac{\beta^2}{\kappa}\Delta_\text{t}\boldsymbol{t} + \Delta_\text{n}\boldsymbol{n}\right)\frac{\sigma_\text{c}}{\delta}\left(1 - \frac{\delta}{\delta_\text{c}}\right) = \hat{\boldsymbol{T}}\frac{\sigma_\text{c}}{\delta}\left(1 - \frac{\delta}{\delta_\text{c}}\right) \tag{4.70}$$

where σ_c is the material strength along the fracture, δ_c the critical effective displacement after which cohesive tractions are zero (complete decohesion), Δ_t and Δ_n are the tangential and normal components of the opening displacement vector $\mathbf{\Delta}$, respectively. The parameter β is a weight that indicates how big the tangential opening contribution is. The effective opening displacement is:

$$\delta = \sqrt{\frac{\beta^2}{\kappa^2}\Delta_t^2 + \Delta_n^2} \tag{4.71}$$

In case of unloading or reloading $\delta < \delta_{max}$, tractions are calculated as:

$$T_n = \Delta_n \frac{\sigma_c}{\delta_{max}}\left(1 - \frac{\delta_{max}}{\delta_c}\right) \tag{4.72}$$

$$T_t = \frac{\beta^2}{\kappa}\Delta_t \frac{\sigma_c}{\delta_{max}}\left(1 - \frac{\delta_{max}}{\delta_c}\right) \tag{4.73}$$

so that they vary linearly between the origin and the maximum attained tractions. As shown in Figure 4.14, in this law, the dissipated and reversible energies are:

$$E_{diss} = \frac{1}{2}\sigma_c \, \delta_{max} \tag{4.74}$$

$$E_{rev} = \frac{1}{2} T \, \delta \tag{4.75}$$

Moreover, a damage parameter D can be defined as:

$$D = \min\left(\frac{\delta_{max}}{\delta_c}, 1\right) \tag{4.76}$$

which varies from 0 (undamaged condition) and 1 (fully damaged condition). This variable can only increase because damage is an irreversible process. A simple penalty contact model has been incorporated in the cohesive law so that normal tractions can be returned in case of compression:

$$T_n = \alpha \Delta_n \quad \text{if } \Delta_n < 0 \tag{4.77}$$

where α is a stiffness parameter that defaults to zero. The relative contact energy is equivalent to reversible energy but in compression.

The material name of the linear decreasing cohesive law is `material_cohesive_linear` and its parameters with their respective default values are:

- `sigma_c`: 0
- `delta_c`: 0
- `beta`: 0
- `G_c`: 0
- `kappa`: 1
- `penalty`: 0

where `G_c` corresponds to $G_{c,I}$. A random number generator can be used to assign a random σ_c to each facet following a given distribution (see Section 4.4). Only one parameter between `delta_c` and `G_c` has to be specified. For random σ_c distributions, the chosen parameter of these two is kept fixed and the other one is varied.

The bilinear constitutive law works exactly the same way as the linear one, except for the additional parameter `delta_0` that by default is zero. Two examples for the extrinsic and intrinsic cohesive elements and also an example to assign different properties to intergranular and transgranular cohesive elements can be found in the folder `examples/cohesive_element/`.

4.5.2 Linear Cohesive Law with Friction (B.11)

This law represents a variation of the linear irreversible cohesive of the previous section, which adds friction. The friction behavior is approximated with an elasto-plastic law, which relates the friction force to the relative sliding between the two faces of the cohesive element. The slope of the elastic branch is called *penalty_for_friction*, and is defined by the user, together with the friction coefficient, as a material property. The friction contribution evolves with the damage of the cohesive law: it is null when the damage is zero, and it becomes maximum when the damage is equal to one. This is done by defining a current value of the friction coefficient (mu) that increases linearly with the damage, up to the value of the friction coefficient defined by the user. The yielding plateau of the friction law is given by the product of the current friction coefficient and the local compression stress acting in the cohesive element. Such an approach is equivalent to a node-to-node contact friction. Its accuracy is acceptable only for small displacements.

The material name of the linear cohesive law with friction is `material_cohesive_linear_friction`. Its additional parameters with respect to those of the linear cohesive law without friction, with the respective default values, are:

- `mu`: 0
- `penalty_for_friction`: 0

4.5.3 Linear Cohesive Law with Fatigue (B.12)

This law represents a variation of the linear irreversible cohesive law of the previous section, that removes the hypothesis of elastic unloading-reloading cycles. With this law, some energy is dissipated also during unloading and reloading with hysteresis. The implementation follows the work of [14]. During the unloading-reloading cycle, the traction increment is computed as

$$\dot{T} = \begin{cases} K^- \, \dot{\delta} & \text{if } \dot{\delta} < 0 \\ K^+ \, \dot{\delta} & \text{if } \dot{\delta} > 0 \end{cases} \tag{4.78}$$

where $\dot{\delta}$ and $\dot{T}$ are respectively the effective opening displacement and the cohesive traction increments with respect to time, while K^- and K^+ are respectively the unloading and reloading incremental stiffness. The unloading path is linear and results in an unloading stiffness

$$K^- = \frac{T_{\max}}{\delta_{\max}} \tag{4.79}$$

where $T_{\max}$ and $\delta_{\max}$ are the maximum cohesive traction and the effective opening displacement reached during the precedent loading phase. The unloading stiffness remains constant during the unloading phase. On the other hand the reloading stiffness increment $\dot{K}^+$ is calculated as

$$\dot{K}^+ = \begin{cases} -K^+ \, \dot{\delta}/\delta_{\mathrm{f}} & \text{if } \dot{\delta} > 0 \\ (K^+ - K^-) \, \dot{\delta}/\delta_{\mathrm{f}} & \text{if } \dot{\delta} < 0 \end{cases} \tag{4.80}$$

where δ_{f} is a material parameter (refer to [15] for more details). During unloading the stiffness K^+ tends to K^-, while during reloading K^+ gets decreased at every time step. If the cohesive traction during reloading exceeds the upper limit given by equation (4.70), it is recomputed following the behavior of the linear decreasing cohesive law for crack opening.

4.5.4 Exponential Cohesive Law (B.13)

Ortiz and Pandolfi proposed this cohesive law in 1999 [4]. The traction-opening equation for this law is as follows:

$$T = e\sigma_c \frac{\delta}{\delta_c} e^{-\delta/\delta_c} \tag{4.81}$$

This equation is plotted in Figure 4.15. The term $\partial \boldsymbol{T}/\partial\delta$ of equation (3.6) after the necessary derivation can expressed as

$$\frac{\partial \boldsymbol{T}}{\partial\delta} = \hat{\boldsymbol{T}} \otimes \frac{\partial(T/\delta)}{\partial\delta}\frac{\hat{\boldsymbol{T}}}{\delta} + \frac{T}{\delta}\left[\beta^2 \boldsymbol{I} + \left(1-\beta^2\right)(\boldsymbol{n}\otimes\boldsymbol{n})\right] \tag{4.82}$$

where

$$\frac{\partial(T/\delta)}{\partial\delta} = \begin{cases} -e\frac{\sigma_c}{\delta_c^2}e^{-\delta/\delta_c} & if \delta \geq \delta_{max} \\ 0 & if \delta < \delta_{max}, \delta_n > 0 \end{cases} \tag{4.83}$$

As regards the behavior in compression, two options are available: a contact penalty approach with stiffness following the formulation of the exponential law and a contact penalty approach with constant stiffness. In the second case, the stiffness is defined as a function of the tangent of the exponential law at the origin.

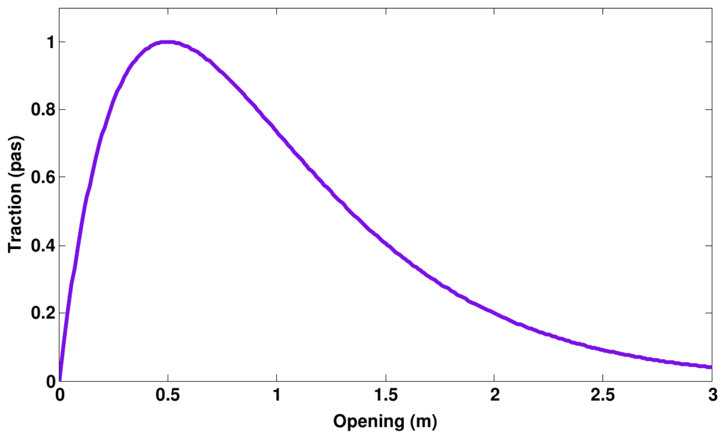


Figure 4.15: Exponential cohesive law

4.6 Non-Local Constitutive Laws

Continuum damage modeling of quasi-brittle materials undergo significant softening after the onset of damage. This fast growth of damage causes a loss of ellipticity of partial differential equations of equilibrium. Therefore, the numerical simulation results won't be objective anymore, because the dissipated energy will depend on mesh size used in the simulation. One way to avoid this effect is the use of non-local damage formulations. In this approach a local quantity such as the strain is replaced by its non-local average, where the size of the domain, over which the quantitiy is averaged, depends on the underlying material microstructure. **Akantu** provides non-local versions of many constitutive laws for damage. Examples are for instance the material Mazar and the material Marigo, that can be used in a non-local context. In order to use the corresponding non-local formulation the user has to define the non-local material he wishes to use in the text input file:

```
material constitutive_law_non_local [
   name = material_namerho = value...]
```

where *constitutive_law_non_local* is the name of the non-local constitutive law, *e.g. marigo_non_local*. In addition to the material the non-local neighborhood, that should be used for the averaging process needs to be defined in the material file as well:

```
non_local neighborhood_name  weight_function_type [
   radius = value
```

```
    ...
    weight_function weight_parameter [
      damage_limit = value
      ...
    ]
]
```

for the non-local averaging, *e.g. base_wf*, followed by the properties of the non-local neighborhood, such as the radius, and the weight function parameters. It is important to notice that the non-local neighborhood must have the same name as the material to which the neighborhood belongs! The following two sections list the non-local constitutive laws and different type of weight functions available in **Akantu**.

4.6.1 Non-local constitutive laws

Let us consider a body having a volume V and a boundary Γ. The stress-strain relation for a non-local damage model can be described as follows:

$$\boldsymbol{\sigma} = (1 - \bar{d})\boldsymbol{D} : \boldsymbol{\epsilon} \tag{4.84}$$

with $\boldsymbol{D}$ the elastic moduli tensor, σ the stress tensor, ϵ the strain tensor and $\bar{d}$ the non-local damage variable. Note that this stres-strain relationship is similar to the relationship defined in Damage model except $\bar{d}$. The non-local damage model can be extended to the damage constitutive laws: Marigo (Section 4.4.5) and Mazars (Section 4.4.5).

The non-local damage variable $\bar{d}$ is defined as follows:

$$\bar{d}(\boldsymbol{x}) = \int_V W(\boldsymbol{x}, \boldsymbol{y}) d(\boldsymbol{y}) dV(\boldsymbol{y}) \tag{4.85}$$

with $W(\boldsymbol{x}, \boldsymbol{y})$ the weight function which averages local damage variables to describe the non-local interactions. A list of available weight functions and its functionalities in **Akantu** are explained in the next section.

4.6.2 Non-local weight functions

The available weight functions in **Akantu** are follows:

- *base_weight_function*: This weight function averages local damage variables by using a bell-shape function on spatial dimensions.
- *damaged_weight_function*: A linear-shape weight function is applied to average local damage variables. Its slope is determined by damage variables. For example, the damage variables for an element which is highly damaged are averaged over large spatial dimension (linear function including a small slope).
- *remove_damaged_weight_function*: This weight function averages damage values by using a bell-shape function as *base_weight_function*, but excludes elements which are fully damaged.
- *remove_damaged_with_damage_rate_weight_function*: A bell-shape function is applied to average local damage variables for elements having small damage rates.
- *stress_based_weight_function*: Non local integral takes stress states, and use the states to construct weight function: an ellipsoid shape. Detailed explanations of this weight function are given in Giry et al.: Stress-based nonlocal damage model IJSS, 48, 2011.

4.7 Adding a New Constitutive Law

There are several constitutive laws in **Akantu** as described in the previous Section 4.4. It is also possible to use a user-defined material for the simulation. These materials are referred to as local materials since they are local to the example of the user and not part of the **Akantu** library. To define a new local material, two files (`material_XXX.hh` and `material_XXX.cc`) have to be provided where `XXX` is the name of the new material. The header file `material_XXX.hh` defines the interface of your custom material. Its implementation is provided in the `material_XXX.cc`. The new law must inherit from the `Material` class or any other existing material class. It is therefore necessary to include the interface of the parent material in the header file of your local material and indicate the inheritance in the declaration of the class:

```
/* ---------------------------------------------------------------------- */
#include "material.hh"
/* ---------------------------------------------------------------------- */

#ifndef __AKANTU_MATERIAL_XXX_HH__
#define __AKANTU_MATERIAL_XXX_HH__

__BEGIN_AKANTU__

class MaterialXXX : public Material {

/// declare here the interface of your material

};
```

In the header file the user also needs to declare all the members of the new material. These include the parameters that a read from the material input file, as well as any other material parameters that will be computed during the simulation and internal variables.

In the following the example of adding a new damage material will be presented. In this case the parameters in the material will consist of the Young's modulus, the Poisson coefficient, the resistance to damage and the damage threshold. The material will then from these values compute its Lamé coefficients and its bulk modulus. Furthermore, the user has to add a new internal variable `damage` in order to store the amount of damage at each quadrature point in each step of the simulation. For this specific material the member declaration inside the class will look as follows:

```
class LocalMaterialDamage : public Material {

/// declare constructors/destructors here

/// declare methods and accessors here

  /* -------------------------------------------------------------------- */
  /* Class Members                                                        */
  /* -------------------------------------------------------------------- */

  AKANTU_GET_MACRO_BY_ELEMENT_TYPE_CONST(Damage, damage, Real);
private:

  /// the young modulus
  Real E;

  /// Poisson coefficient
  Real nu;
  /// First Lame coefficient
  Real lambda;

  /// Second Lame coefficient (shear modulus)
  Real mu;

  /// resistance to damage
  Real Yd;

  /// damage threshold
  Real Sd;

  /// Bulk modulus
  Real kpa;

  /// damage internal variable
  InternalField<Real> damage;

};
```

In order to enable to print the material parameters at any point in the user's example file using the standard output stream by typing:

```
for (UInt m = 0; m  < model.getNbMaterials(); ++m)
  std::cout << model.getMaterial(m) << std::endl;
```

the standard output stream operator has to be redefined. This should be done at the end of the header file:

```
class LocalMaterialDamage : public Material {

  /// declare here the interace of your material

}:
/* -------------------------------------------------------------------- */
/* inline functions                                                     */
/* -------------------------------------------------------------------- */
/// standard output stream operator
inline std::ostream & operator <<(std::ostream & stream, const
    LocalMaterialDamage & _this)
{
  _this.printself(stream);
  return stream;
}
```

However, the user still needs to register the material parameters that should be printed out. The registration is done during the call of the constructor. Like all definitions the implementation of the constructor has to be written in the `material_XXX.cc` file. However, the declaration has to be provided in the `material_XXX.hh` file:

```
class LocalMaterialDamage : public Material {
  /* ------------------------------------------------------------------ */
  /* Constructors/Destructors                                           */
  /* ------------------------------------------------------------------ */
public:

  LocalMaterialDamage(SolidMechanicsModel & model, const ID & id = "");
};
```

The user can now define the implementation of the constructor in the `material_XXX.cc` file:

```
/* -------------------------------------------------------------------------- */
#include "local_material_damage.hh"
#include "solid_mechanics_model.hh"

__BEGIN_AKANTU__

/* -------------------------------------------------------------------------- */
LocalMaterialDamage::LocalMaterialDamage(SolidMechanicsModel & model,
           const ID & id)  :
  Material(model, id),
  damage("damage", *this) {
  AKANTU_DEBUG_IN();

  this->registerParam("E", E, 0., _pat_parsable, "Young's modulus");
  this->registerParam("nu", nu, 0.5, _pat_parsable, "Poisson's ratio");
  this->registerParam("lambda", lambda, _pat_readable, "First Lame coefficient
    ");
  this->registerParam("mu", mu, _pat_readable, "Second Lame coefficient");
  this->registerParam("kapa", kpa, _pat_readable, "Bulk coefficient");
  this->registerParam("Yd", Yd,   50., _pat_parsmod);
  this->registerParam("Sd", Sd, 5000., _pat_parsmod);

  damage.initialize(1);

  AKANTU_DEBUG_OUT();
}
```

During the intializer list the reference to the model and the material id are assigned and the constructor of the internal field is called. Inside the scope of the constructor the internal values have to be initialized and the parameters, that should be printed out, are registered with the function: `registerParam`:

```
void registerParam(name of the parameter (key in the material file),
       member variable,
       default value (optional parameter),
       access permissions,
       description);
```

The available access permissions are as follows:

- `_pat_internal`: Parameter can only be output when the material is printed.
- `_pat_writable`: User can write into the parameter. The parameter is output when the material is printed.
- `_pat_readable`: User can read the parameter. The parameter is output when the material is printed.
- `_pat_modifiable`: Parameter is writable and readable.
- `_pat_parsable`: Parameter can be parsed, *i.e.* read from the input file.
- `_pat_parsmod`: Parameter is modifiable and parsable.

In order to implement the new constitutive law the user needs to specify how the additional material parameters, that are not defined in the input material file, should be calculated. Furthermore, it has to be defined how stresses and the stable time step should be computed for the new local material. In the case of implicit simulations, in addition, the computation of the tangent stiffness needs to be defined. Therefore, the user needs to redefine the following functions of the parent material:

```
void initMaterial();

// for explicit and implicit simulations void
computeStress(ElementType el_type, GhostType ghost_type = _not_ghost);

// for implicit simulations
void computeTangentStiffness(const ElementType & el_type,
           Array<Real> & tangent_matrix,
           GhostType ghost_type = _not_ghost);

// for explicit and implicit simulations
Real getStableTimeStep(Real h, const Element & element);
```

In the following a detailed description of these functions is provided:

- `initMaterial`: This method is called after the material file is fully read and the elements corresponding to each material are assigned. Some of the frequently used constant parameters are calculated in this method. For example, the Lamé constants of elastic materials can be considered as such parameters.

- `computeStress`: In this method, the stresses are computed based on the constitutive law as a function of the strains of the quadrature points. For example, the stresses for the elastic material are calculated based on the following formula:

  $$\sigma = \lambda \mathrm{tr}(\varepsilon)\boldsymbol{I} + 2\mu\varepsilon \tag{4.86}$$

  Therefore, this method contains a loop on all quadrature points assigned to the material using the two macros:

  `MATERIAL_STRESS_QUADRATURE_POINT_LOOP_BEGIN`

  `MATERIAL_STRESS_QUADRATURE_POINT_LOOP_END`

  ```
  MATERIAL_STRESS_QUADRATURE_POINT_LOOP_BEGIN(element_type);

  // sigma <- f(grad_u)

  MATERIAL_STRESS_QUADRATURE_POINT_LOOP_END;
  ```

  Note: *The strain vector in* **Akantu** *contains the values of* $\nabla\boldsymbol{u}$, *i.e. it is really the* displacement gradient,

- `computeTangentStiffness`: This method is called when the tangent to the stress-strain curve is desired (see Fig 4.16). For example, it is called in the implicit solver when the stiffness matrix for the regular elements is assembled based on the following formula:

  $$\boldsymbol{K} = \int \boldsymbol{B}^T \boldsymbol{D}(\varepsilon)\boldsymbol{B} \tag{4.87}$$

  Therefore, in this method, the `tangent` matrix ($\boldsymbol{D}$) is computed for a given strain.

  Note: *The* `tangent` *matrix is a* 4^{th} *order tensor which is stored as a matrix in Voigt notation.*

- `getCelerity`: The stability criterion of the explicit integration scheme depend on the fastest wave celerity (4.21). This celerity depend on the material, and therefore the value of this velocity should be defined in this method for each new material. By default, the fastest wave speed is the compressive wave whose celerity can be defined in `getPushWaveSpeed`.

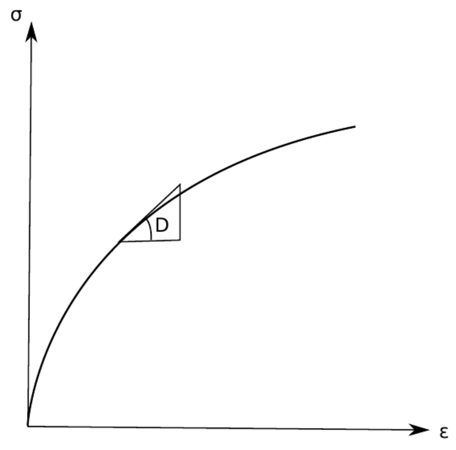


Figure 4.16: Tangent to the stress-strain curve.

Once the declaration and implementation of the new material has been completed, this material can be used in the user's example by including the header file:

```
#include "material_XXX.hh"
```

For existing materials, as mentioned in Section 4.4, by default, the materials are initialized inside the method `initFull`. If a local material should be used instead, the initialization of the material has to be postponed until the local material is registered in the model. Therefore, the model is initialized with the boolean for skipping the material initialization equal to true:

```
/// model initialization
model.initFull(SolidMechanicsModelOptions(_explicit_lumped_mass,true));
```

Once the model has been initialized, the local material needs to be registered in the model:

```
model.registerNewCustomMaterials<XXX>("name_of_local_material");
```

Only at this point the material can be initialized:

```
model.initMaterials();
```

A full example for adding a new damage law can be found in `examples/new_material`.

4.7.1 Adding a New Non-Local Constitutive Law

In order to add a new non-local material we first have to add the local constitutive law in **Akantu** (see above). We can then add the non-local version of the constitutive law by adding the two files (`material_XXX_non_local.hh` and `material_XXX_non_local.cc`) where `XXX` is the name of the corresponding local material. The new law must inherit from the two classes, non-local parent class, such as the `MaterialNonLocal` class, and from the local version of the constitutive law, *i.e.* `MaterialXXX`. It is therefore necessary to include the interface of those classes in the header file of your custom material and indicate the inheritance in the declaration of the class:

```
/* -------------------------------------------------------------------------- */
#include "material_non_local.hh" // the non-local parent
#include "material_XXX.hh"
/* -------------------------------------------------------------------------- */

#ifndef __AKANTU_MATERIAL_XXX_HH__
#define __AKANTU_MATERIAL_XXX_HH__

__BEGIN_AKANTU__
```

```
class MaterialXXXNonLocal : public MaterialXXX,
                            public MaterialNonLocal {

/// declare here the interface of your material

};
```

As members of the class we only need to add the internal fields to store the non-local quantities, which are obtained from the averaging process:

```
/* ---------------------------------------------------------------------------
    */
/* Class members
    */
/* ---------------------------------------------------------------------------
    *
protected:
  InternalField<Real> grad_u_nl;
```

The following four functions need to be implemented in the non-local material:

```
  /// initialization of the material
  void initMaterial();
  /// loop over all element and invoke stress computation
  virtual void computeNonLocalStresses(GhostType ghost_type);
  /// compute stresses after local quantities have been averaged
  virtual void computeNonLocalStress(ElementType el_type, GhostType ghost_type
    )
  /// compute all local quantities
  void computeStress(ElementType el_type, GhostType ghost_type);
```

In the intialization of the non-local material we need to register the local quantity for the averaging process. In our example the internal field *grad_u_nl* is the non-local counterpart of the gradient of the displacement field (*grad_u_nl*):

```
  void MaterialXXXNonLocal::initMaterial() {
    MaterialXXX::initMaterial();
    MaterialNonLocal::initMaterial();
    /// register the non-local variable in the manager
    this->model->getNonLocalManager().registerNonLocalVariable(this->grad_u.
    getName(), this->grad_u_nl.getName(), spatial_dimension *
    spatial_dimension);

}
```

The function to register the non-local variable takes as parameters the name of the local internal field, the name of the non-local counterpart and the number of components of the field we want to average. In the *computeStress* we now need to compute all the quantities we want to average. We can then write a loop for the stress computation in the function *computeNonLocalStresses* and then provide the constitutive law on each integration point in the function *computeNonLocalStress*.

Chapter 5

Structural Mechanics Model

Static structural mechanics problems can be handled using the class `StructuralMechanicsModel`. So far, **Akantu** provides 2D and 3D Bernoulli beam elements [16]. This model is instantiated for a given `Mesh`, as for the `SolidMechanicsModel`. The model will create its own `FEEngine` object to compute the interpolation, gradient, integration and assembly operations. The `StructuralMechanicsModel` constructor is called in the following way:

```
StructuralMechanicsModel model(mesh, spatial_dimension);
```

where `mesh` is a `Mesh` object defining the structure for which the equations of statics are to be solved, and `spatial_dimension` is the dimensionality of the problem. If `spatial_dimension` is omitted, the problem is assumed to have the same dimensionality as the one specified by the mesh.

Note 1: *Dynamic computations are not supported to date.*

Note 2: *Structural meshes are created and loaded as described in Section 2.4 with* `MeshIOMSHStruct` *instead of* `MeshIOMSH`*:*

```
akantu::MeshIOMSHStruct mesh_io;
mesh_io.read("structural_mesh.msh", beams);
```

This model contains at least the following `Arrays`:

blocked_dofs contains a Boolean value for each degree of freedom specifying whether that degree is blocked or not. A Dirichlet boundary condition can be prescribed by setting the **blocked_dofs** value of a degree of freedom to `true`. The **displacement** is computed for all degrees of freedom for which the **blocked_dofs** value is set to `false`. For the remaining degrees of freedom, the imposed values (zero by default after initialization) are kept.

displacement_rotation contains the generalized displacements (*i.e.* displacements and rotations) of all degrees of freedom. It can be either a computed displacement for free degrees of freedom or an imposed displacement in case of blocked ones ($\boldsymbol{u}$ in the following).

force_moment contains the generalized external forces (forces and moments) applied to the nodes ($\boldsymbol{f}_{\text{ext}}$ in the following).

residual contains the difference between the generalized external and internal forces and moments. On the blocked degrees of freedom, **residual** contains the support reactions ($\boldsymbol{r}$ in the following). It should be mentioned that, at equilibrium, **residual** should be zero on the free degrees of freedom.

An example to help understand how to use this model will be presented in the next section.

5.1 Model Setup

5.1.1 Initialization

The easiest way to initialize the structural mechanics model is:

```
model.initFull();
```

The method `initFull` computes the shape functions, initializes the internal vectors mentioned above and allocates the memory for the stiffness matrix, unlike the solid mechanics model, its default argument is `_static`.

Material properties are defined using the `StructuralMaterial` structure described in Table 5.1. Such a definition could, for instance, look like

```
StructuralMaterial mat1;
mat.E=3e10;
mat.I=0.0025;
mat.A=0.01;
```

Field	Description
`E`	Young's modulus
`A`	Cross section area
`I`	Second cross sectional moment of inertia (for 2D elements)
`Iy`	`I` around beam y–axis (for 3D elements)
`Iz`	`I` around beam z–axis (for 3D elements)
`GJ`	Polar moment of inertia of beam cross section (for 3D elements)

Table 5.1: Material properties for structural elements defined in the class `StructuralMaterial`.

Materials can be added to the model's `element_material` vector using

```
model.addMaterial(mat1);
```

They are successively numbered and then assigned to specific elements.

```
for (UInt i = 0; i < nb_element_mat_1; ++i) {
   model.getElementMaterial(_bernoulli_beam_2)(i,0) = 1;
 }
```

5.1.2 Setting Boundary Conditions

As explained before, the Dirichlet boundary conditions are applied through the array **blocked_dofs**. Two options exist to define Neumann conditions. If a nodal force is applied, it has to be directly set in the array **force_momentum**. For loads distributed along the beam length, the method `computeForcesFromFunction` integrates them into nodal forces. The method takes as input a function describing the distribution of loads along the beam and a functor `BoundaryFunctionType` specifing if the function is expressed in the local coordinates (`_bft_traction_local`) or in the global system of coordinates (`_bft_traction`).

```
 static void lin_load(double * position, double * load,
          Real * normal, UInt surface_id){
  memset(load,0,sizeof(Real)*3);
  load[1] = position[0]*position[0]-250;
}
int main(int argc, char *argv[]){
...
model.computeForcesFromFunction<_bernoulli_beam_2>(lin_load,
                                                _bft_traction_local);
...}
```

5.2 Static Analysis

The `StructuralMechanicsModel` class can perform static analyses of structures. In this case, the equation to solve is the same as for the `SolidMechanicsModel` used for static analyses

$$\boldsymbol{K}\boldsymbol{u} = \boldsymbol{f}_{\mathbf{ext}} \,, \tag{5.1}$$

where $\boldsymbol{K}$ is the global stiffness matrix, $\boldsymbol{u}$ the generalized displacement vector and $\boldsymbol{f}_{\mathbf{ext}}$ the vector of generalized external forces applied to the system.

To solve such a problem, the static solver of the `StructuralMechanicsModel` object is used. First a model has to be created and initialized.

```
StructuralMechanicsModel model(mesh);
model.initFull();
```

- `model.initFull` initializes all internal vectors to zero.

Once the model is created and initialized, the boundary conditions can be set as explained in Section 5.1.2. Boundary conditions will prescribe the external forces or moments for the free degrees of freedom $\boldsymbol{f}_{\mathbf{ext}}$ and displacements or rotations for the others. To completely define the system represented by equation (5.1), the global stiffness matrix $\boldsymbol{K}$ must be assembled.

```
model.assembleStiffnessMatrix();
```

The computation of the static equilibrium is performed using the same Newton-Raphson algorithm as described in Section 4.2.

Note: *To date,* `StructuralMechanicsModel` *handles only constitutively and geometrically linear problems, the algorithm is therefore guaranteed to converge in two iterations.*

```
model.updateResidual();
model.solve();
```

- `model.updateResidual` assembles the internal forces and removes them from the external forces.
- `model.solve` solves the Equation (5.1). The **increment** vector of the model will contain the new increment of displacements, and the **displacement_rotation** vector is also updated to the new displacements.

At the end of the analysis, the final solution is stored in the **displacement_rotation** vector. A full example of how to solve a structural mechanics problem is presented in the code `examples/structural_mechanics/bernoulli_beam_2_example.cc`. This example is composed of a 2D beam, clamped at the left end and supported by two rollers as shown in Figure 5.1. The problem is defined by the applied load $q = 6\,\mathrm{kN\,m^{-1}}$, moment $\bar{M} = 3.6\,\mathrm{kN\,m}$, moments of inertia $I_1 = 250\,000\,\mathrm{cm}^4$ and $I_2 = 128\,000\,\mathrm{cm}^4$ and lengths $L_1 = 10\,\mathrm{m}$ and $L_2 = 8\,\mathrm{m}$. The resulting rotations at node two and three are $\varphi_2 = 0.001\,167$ and $\varphi_3 = -0.000\,771$.

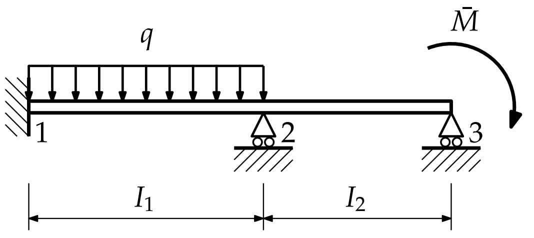


Figure 5.1: 2D beam example

Chapter 6

Heat Transfer Model

The heat transfer model is a specific implementation of the `Model` interface dedicated to handle the dynamic heat equation.

6.1 Theory

The strong form of the dynamic heat equation can be expressed as

$$\rho c_v \dot{T} + \nabla \cdot \boldsymbol{\kappa} \nabla T = b \tag{6.1}$$

with T the scalar temperature field, c_v the specific heat capacity, ρ the mass density, $\boldsymbol{\kappa}$ the conductivity tensor, and b the heat generation per unit of volume. The discretized weak form with a finite number of elements is

$$\forall i \quad \sum_j \left(\int_\Omega \rho c_v N_j N_i d\Omega \right) \dot{T}_j - \sum_j \left(\int_\Omega \boldsymbol{\kappa} \nabla N_j \nabla N_i d\Omega \right) T_j = - \int_\Gamma N_i \boldsymbol{q} \cdot \boldsymbol{n} d\Gamma + \int_\Omega b N_i d\Omega \tag{6.2}$$

with i and j the node indices, $\boldsymbol{n}$ the normal field to the surface $\Gamma = \partial\Omega$. To simplify, we can define the capacity and the conductivity matrices as

$$C_{ij} = \int_\Omega \rho c_v N_j N_i d\Omega \qquad \text{and} \qquad K_{ij} = - \int_\Omega \boldsymbol{\kappa} \nabla N_j \nabla N_i d\Omega \tag{6.3}$$

and the system to solve can be written

$$\boldsymbol{C} \cdot \dot{\boldsymbol{T}} = \boldsymbol{Q}^{\text{ext}} - \boldsymbol{K} \cdot \boldsymbol{T} \,, \tag{6.4}$$

with $\boldsymbol{Q}^{\text{ext}}$ the consistent heat generated.

6.2 Using the Heat Transfer Model

A material file name has to be provided during initialization. Currently, the `HeatTransferModel` object uses dynamic analysis with an explicit time integration scheme. It can simply be created like this

```
HeatTransferModel model(mesh, spatial_dimension);
```

while an existing mesh has been used (see 2.4). Then the model object can be initialized with:

```
model.initFull()
```

This function will load the material properties, and allocate / initialize the nodes and element `Array`s More precisely, the heat transfer model contains 4 `Arrays`:

temperature contains the nodal temperature T (zero by default after the initialization).

temperature_rate contains the variations of temperature $\dot{T}$ (zero by default after the initialization).

blocked_dofs contains a Boolean value for each degree of freedom specifying whether the degree is blocked or not. A Dirichlet boundary condition (T_d) can be prescribed by setting the **blocked_dofs** value of a degree of freedom to `true`. The **temperature** and the **temperature_rate** are computed for all degrees of freedom where the **blocked_dofs** value is set to `false`. For the remaining degrees of freedom, the imposed values (zero by default after initialization) are kept.

residual contains the difference between external and internal heat generations. The **residual** contains the supported heat reactions ($\boldsymbol{R} = \boldsymbol{Q}^{ext} - \boldsymbol{K} \cdot \boldsymbol{T}$) on the nodes that the temperature imposed.

Only a single material can be specified on the domain. A material text file (*e.g.*, material.dat) provides the material properties as follows:

```
heat name_material [
capacity = XXX
density = XXX
conductivity = [XXX ... XXX]
]
```

where the `capacity` and `density` are scalars, and the `conductivity` is specified as a 3×3 tensor.

6.2.1 Explicit Dynamic

The explicit time integration scheme in **Akantu** uses a lumped capacity matrix $\boldsymbol{C}$ (reducing the computational cost, see Chapter 4). This matrix is assembled by distributing the capacity of each element onto its nodes. Therefore, the resulting $\boldsymbol{C}$ is a diagonal matrix stored in the `capacity Array` of the model.

```
model.assembleCapacityLumped();
```

Note: *Currently, only the explicit time integration with lumped capacity matrix is implemented within* ***Akantu****.*

The explicit integration scheme is *Forward Euler* [5].

- Predictor: $\boldsymbol{T}_{n+1} = \boldsymbol{T}_n + \Delta t \dot{\boldsymbol{T}}_n$
- Update residual: $\boldsymbol{R}_{n+1} = \left(\boldsymbol{Q}^{ext}_{\boldsymbol{n+1}} - \boldsymbol{K}\boldsymbol{T}_{n+1}\right)$
- Corrector : $\dot{\boldsymbol{T}}_{n+1} = \boldsymbol{C}^{-1}\boldsymbol{R}_{n+1}$

The explicit integration scheme is conditionally stable. The time step has to be smaller than the stable time step, and it can be obtained in **Akantu** as follows:

```
time_step = model.getStableTimeStep();
```

The stable time step is defined as:

$$\Delta t_{\text{crit}} = 2\Delta x^2 \frac{\rho c_v}{\| \boldsymbol{\kappa} \|^{\infty}} \tag{6.5}$$

where Δx is the characteristic length (*e.g.*, the inradius in the case of linear triangle element), ρ is the density, $\boldsymbol{\kappa}$ is the conductivity tensor, and c_v is the specific heat capacity. It is necessary to impose a time step which is smaller than the stable time step, for instance, by multiplying the stable time step by a safety factor smaller than one.

```
const Real safety_time_factor = 0.1;
Real applied_time_step = time_step * safety_time_factor;
model.setTimeStep(applied_time_step);
```

The following loop allows, for each time step, to update the `temperature`, `residual` and `temperature_rate` fields following the previously described integration scheme.

```
for (UInt s = 1; (s-1)*applied_time_step < total_time; ++s) {
  model.explicitPred();
  model.updateResidual();
  model.explicitCorr();
}
```

An example of explicit dynamic heat propagation is presented in
`examples/heat_transfer/explicit_heat_transfer.cc`.
This example consists of a square 2D plate of 1 m^2 having an initial temperature of 100 K everywhere but a none centered hot point maintained at 300 K. Figure 6.1 presents the geometry of this case. The material used is a linear fictitious elastic material with a density of 8940 $\mathrm{kg/m}^3$, a conductivity of 401 $\mathrm{W\,m^{-1}\,K^{-1}}$ and a specific heat capacity of 385 $\mathrm{J\,K^{-1}\,kg^{-1}}$. The time step used is 0.12 s.

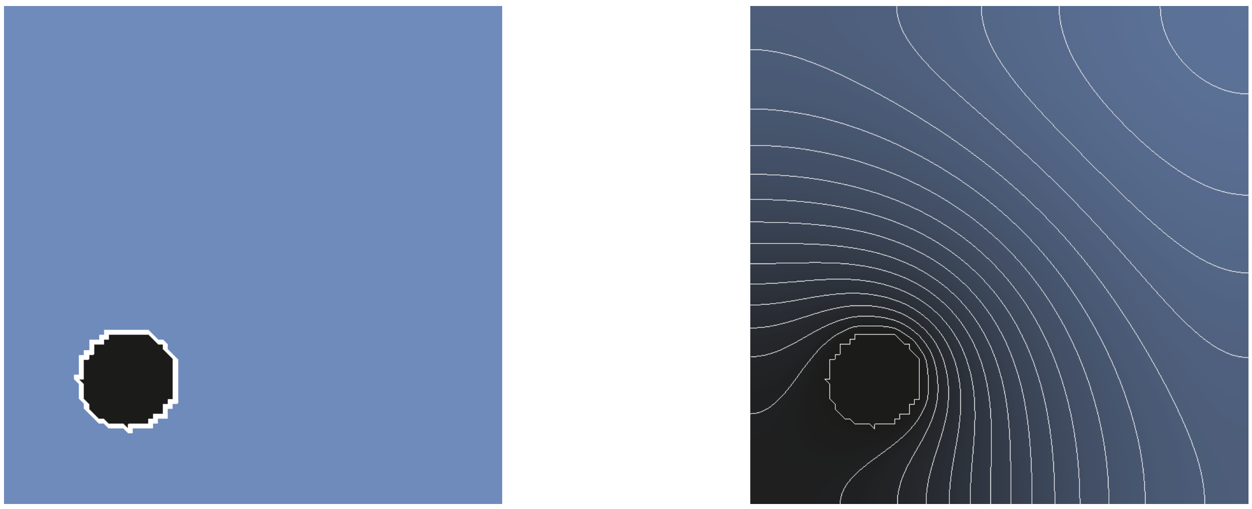


Figure 6.1: Initial temperature field (left) and after 15000 time steps = 30 minutes (right). The lines represent iso-surfaces.

Chapter 7

Input/Output

7.1 Input file

The text input file of a simulation should be precised using the method `initialize` which will instantiate the static `Parser` object of **Akantu**. This section explains how to manipulate `Parser` objects to input data in **Akantu**.

```
int main(int argc, char *argv[]) {
  initialize("input_files.dat", argc, argv);
  ...
```

7.1.1 Akantu Parser

Akantu file parser has a tree organization.

- `Parser`, the root of the tree, can be accessed using

  ```
  Parser & parser = getStaticParser();
  ```

- `ParserSection`, branch of the tree, contains map a of sub-sections (`SectionType`, `ParserSection`) and a `ParserSection *` pointing to the parent section. The user section of the input file can directly be accessed by

  ```
  const ParserSection & usersect = getUserParser();
  ```

- `ParserParameter`, the leaf of the tree, carries data of the input file which can be casted to the correct type with

  ```
  Real mass = usersect.getParameter("mass");
  ```

  or used directly within an expression

  ```
  Real dead_weight = 9.81 * usersect.getParameterValue<Real>("mass");
  ```

7.1.2 Grammar

The structure of text input files consists of different sections containing a list of parameters. As example, the file parsed in the previous section will look like

```
user parameters [
   mass = 10.5
]
```

Basically every standard arithmetic operations can be used inside of input files as well as the constant `pi` and `e` and the exponent operator `^`. Operations between `ParserParameter` are also possible with the convention that only parameters of the current and the parent sections are available. `Vector` and `Matrix` can also be read according to the `NumPy` [17] writing convention (a.e. cauchy_stress_tensor = [[σ_{xx}, σ_{xy}],[σ_{yx},σ_{yy}]]). An example illustrating how to parse the following input file can be found in `example\io\parser\example_parser.cc`.

```
user parameters [
   spatial_dimension = 2
   mesh_file = swiss_cheese.msh
   inner_holes = holes
   outter_crust = crust
   lactostatic_p = 30e3
   stress = [[lactostatic_p,0],[0,lactostatic_p]]
   max_nb_iterations = 100
   precision = 1e-9
]
```

7.1.3 Material section

The input file should also be used to specify material characteristics (constitutive behavior and material properties). The dedicated material section is then read by `initFull` method of `SolidMechanicsModel` which initializes the different materials specified with the following convention:

```
material constitutive_law <optional flavor> [
   name = value
   rho = value
   ...
]
```

where *constitutive_law* is the adopted constitutive law, followed by the material properties listed one by line in the bracket (*e.g.*, `name` and density `rho`). Some constitutive laws can also have an *optional flavor*. More information can be found in sections relative to material constitutive laws 4.4 or in Appendix B.

7.2 Output data

7.2.1 Generic data

In this chapter, we address ways to get the internal data in human-readable formats. The models in **Akantu** handle data associated to the mesh, but this data can be split into several `Arrays`. For example, the data stored per element type in a `ElementTypeMapArray` is composed of as many `Array`s as types in the mesh.

In order to get this data in a visualization software, the models contain a object to dump `VTK` files. These files can be visualized in software such as `ParaView` [18], `ViSit` [19] or `Mayavi` [20].

The internal dumper of the model can be configured to specify which data fields are to be written. This is done with the `addDumpField` method. By default all the files are generated in a folder called `paraview/`

```
model.setBaseName("output"); // prefix for all generated files

model.addDumpField("displacement");
model.addDumpField("stress");
...
```

key	type	support
displacement	Vector<Real>	nodes
mass	Vector<Real>	nodes
velocity	Vector<Real>	nodes
acceleration	Vector<Real>	nodes
force	Vector<Real>	nodes
residual	Vector<Real>	nodes
increment	Vector<Real>	nodes
blocked_dofs	Vector<bool>	nodes
partitions	Real	elements
material_index	variable	elements
strain	Matrix<Real>	quadrature points
Green strain	Matrix<Real>	quadrature points
principal strain	Vector<Real>	quadrature points
principal Green strain	Vector<Real>	quadrature points
grad_u	Matrix<Real>	quadrature points
stress	Matrix<Real>	quadrature points
Von Mises stress	Real	quadrature points
material_index	variable	quadrature points

Table 7.1: List of dumpable fields for `SolidMechanicsModel`.

```
model.dump()
```

The fields are dumped with the number of components of the memory. For example, in 2D, the memory has `Vector`s of 2 components, or the 2nd order tensors with 2×2 components. This memory can be dealt with `addDumpFieldVector` which always dumps `Vector`s with 3 components or `addDumpFieldTensor` which dumps 2nd order tensors with 3×3 components respectively. The routines `addDumpFieldVector` and `addDumpFieldTensor` were introduced because of `ParaView` which mostly manipulate 3D data.

Those fields which are stored by quadrature point are modified to be seen in the `VTK` file as elemental data. To do this, the default is to average the values of all the quadrature points.

The list of fields depends on the models (for `SolidMechanicsModel` see table 7.1).

7.2.2 Cohesive elements' data

Cohesive elements and their relative data can be easily dumped thanks to a specific dumper contained in `SolidMechanicsModelCohesive`. In order to use it, one has just to add the string `"cohesive elements"` when calling each method already illustrated. Here is an example on how to dump displacement and damage:

```
model.setBaseNameToDumper("cohesive elements", "cohesive_elements_output");
model.addDumpFieldVectorToDumper("cohesive elements", "displacement");
model.addDumpFieldToDumper("cohesive elements", "damage");
...

model.dump("cohesive elements");
```

Fragmentation data

Whenever the `SolidMechanicsModelCohesive` is used, it is possible to dump additional data about the fragments that get formed in the simulation both in serial and parallel. This task is carried out by the `FragmentManager` class, that takes care of computing the following quantities for each fragment:

- index;
- mass;
- moments of inertia;
- velocity;
- number of elements.

These computations can be realized at once by calling the function `computeAllData`, or individually by calling the other public functions of the class. The data can be dumped to be visualized in Paraview, or can be accessed within the simulation. An example of usage is:

```
FragmentManager fragment_manager(model);
fragment_manager.buildAllData();
...

model.addDumpField("fragments");       // this field contains the indices
model.addDumpField("fragments mass");
model.addDumpField("moments of inertia");
model.addDumpField("elements per fragment");
...

for (UInt step = 1; step <= total_steps; ++step) {
  ...

  fragment_manager.buildAllData();
  model.dump();
}
...

const Array<Real> & fragment_velocities = fragment_manager.getVelocity();
...
```

At the end of this example the velocities of the fragments are accessed with a reference to a `const Array<Real>`. The size of this array is the number of fragments, and its number of components is the spatial dimension in this case.

7.2.3 Advanced dumping

Arbitrary fields

In addition to the predetermined fields from the models and materials, the user can add any data to a dumper as long as the support is the same. That is to say data that have the size of the full mesh on if the dumper is dumping the mesh, or of the size of an element group if it is a filtered dumper.

For this the easiest is to use the “external” fields register functions

The simple case force nodal and elemental data are to pass directly the data container itself if it as the good size.

- For nodal fields :

```
Array<T> nodal_data(nb_nodes, nb_component);
...
model.addDumpFieldExternal("my_field", nodal_data);
```

- For elemental fields :

  ```
  ElementTypeMapArray<T> elem_data;
  ...
  model.addDumpFieldExternal("my_field", elem_data);
  ```

If some changes have to be applied on the data as for example a padding for `ParaView` vectors, this can be done by using the field interface.

```
model.addDumpFieldExternal(const std::string & field_name,
                           dumper::Field * field);
```

An example of code presenting this interface is present in the `examples/io/dumper`. This interface is part of the `Dumpable` class from which the `Mesh` inherits.

Creating a new dumper

You can also create you own dumpers, **Akantu** uses a third-party library in order to write the output files, `IOHelper`. **Akantu** supports the `ParaView` format and a Text format defined by `IOHelper`.

This two files format are handled by the classes `DumperParaview` and `DumperText`.

In order to use them you can instantiate on of this object in your code. This dumper have a simple interface. You can register a mesh `registerMesh`, `registerFilteredMesh` or a field, `registerField`.

An example of code presenting this low level interface is present in the `examples/io/dumper`. The different types of `Field` that can be created are present in the source folder `src/io/dumper`.

Chapter 8

Parallel Computation

This section explains how to launch a parallel computation. The strategy adopted by **Akantu** uses a mesh partitioning where elements are mapped to processors. Mesh partitions are then distributed to available processors by adequate routines as will be described below. The sequence of additional operations to be performed by the user are:

- Initializing the parallel context
- Partitioning the mesh
- Distributing mesh partitions

After these steps, the `Model` object proceeds with the interprocess communication automatically without the user having to explicitly take care of them. In what follows we show how it works on a `SolidMechanics` model.

8.1 Initializing the Parallel Context

The user must initialize **Akantu** by forwarding the arguments passed to the program by using the function `initialize`, and close **Akantu** instances at the end of the program by calling the `finalize` function.

Note: *This step does not change from the sequential case as it was stated in Section 2.3. It only gives a additional motivation in the parallel/MPI context.*

The `initialize` function builds a `StaticCommunicator` object responsible for handling the interprocess communications later on. The `StaticCommunicator` can, for instance, be used to ask the total number of declared processors available for computations as well as the process rank through the functions `getNbProc` and `whoAmI` respectively.

An example of the initializing sequence and basic usage of the `StaticCommunicator` is:

```
int main(int argc, char *argv[])
{
  initialize("material.dat", argc, argv);

  StaticCommunicator & comm = StaticCommunicator::getStaticCommunicator();
  Int psize = comm.getNbProc();
  Int prank = comm.whoAmI();

  ...

  finalize();
}
```

8.2 Partitioning the Mesh

The mesh is partitioned after the correct initialization of the processes playing a role in the computation. We assume that a `Mesh` object is constructed as presented in Section 2.4. Then a partition must be computed by using an appropriate mesh partitioner. At present time, the only partitioner available is `MeshPartitionScotch` which implements the function `partitionate` using the **Scotch** [21] program. This is achieved by the following code

```
Mesh mesh(spatial_dimension);
MeshPartition * partition = NULL;

if(prank == 0) {
  mesh.read("my_mesh.msh");
  partition = new MeshPartitionScotch(mesh, spatial_dimension);
  partition->partitionate(psize);
}
```

The algorithm that partition the mesh needs the generation of a random distribution of values. Therefore, in order to run several time a simulation with the same partition of the mesh, the *seed* has to be set manually. This can be done either by adding the following line to the input file *outside* the material parameters environments:

```
seed = 1.0
```

where the value 1.0 can be substituted with any number, or by setting it directly in the code with the command:

```
RandGenerator:: seed(1.0)
```

The latter command, with empty brackets, can be used to check the value of the *seed* used in the simulation.

Note: *Only the processor of rank* 0 *should load the mesh file to partition it. Nevertheless, the* `Mesh` *object must by declared for all processors since the mesh distribution will store mesh pieces to that object.*

8.3 Distributing Mesh Partitions

The distribution of the mesh is done automatically by the `SolidMechanicsModel` through the `initParallel` method. Thus, after creating a `SolidMechanicsModel` with our mesh as the initial parameter, the `initParallel` method must be called receiving the partition as a parameter.

```
SolidMechanicsModel model(mesh);
model.initParallel(partition);
```

After that point, everything remains as in the sequential case from the user point of view. This allows the user to care only about his simulation without concern for the parallelism.

An example of an explicit dynamic 2D bar in compression in a parallel context can be found in `examples/parallel_2d`.

8.4 Launching a Parallel Program

Using **MPI** a parallel run can be launched from a shell using the command

```
mpirun -np #procs program_name parameter1 parameter2 ...
```

Chapter 9

Python interface

Akantu as a python interface which allows to implement a finite element case entirely in the Python language. The interface is currently in beta version and bugs (including memory leaks) can be expected.

The philosophy of the python wrappers is that it should follow, as much as possible, the C++ interface. This is made possible thanks to the software which can port C++ interfaces to Python. However, the possibilities of the Python language have some restrictions which do not allow the concept of template. For this reason the templated classes and methods are currently hardly supported in the Akantu Python interface (some are, but without any warranty that the interface shall not change in a near future).

In order to use the python interface you want to import the `akantu` module which is possibly located in directory where you built or where you installed **Akantu**. The easiest way is to source the file `akantu_environement.sh` in your terminal environment:

```
source AKANTU_BUILD_DIR/akantu_environement.sh
```

or for an installed akantu version:

```
source AKANTU_INSTALL_DIR/share/akantuVERSION/akantu_environement.sh
```

Then, you can create a Python script, like `script.py` which starts with:

```
import akantu
```

Then, you can write the initialization sequence just like for the C++ case:

```
akantu.initialize('materials.dat') spatial_dimension = 2

mesh = akantu.Mesh(spatial_dimension) mesh.read('mesh.msh')
model = akantu.SolidMechanicsModel(mesh)
model.initFull(akantu.SolidMechanicsModelOptions(akantu._static))
```

Then for the dumpers declaration:

```
model.setBaseName("example") model.addDumpFieldVector("displacement")
model.addDumpFieldVector("force") model.addDumpField("boundary")
model.addDumpField("strain") model.addDumpField("stress")
model.addDumpField("blocked_dofs")
```

The **Akantu** arrays can be retrieved at all time. For convenience there is an automatic trans-typing operator which allows to use **Akantu** Array, Vectors and Matrix as mere **Numpy**s.

```
displacement = model.getDisplacement()
```

There is no copy made and the **Numpy** vectors are wrapped around **Akantu**'s memory pool.

```
displacement[:,:] = 1.
displacement[0,1] = 10.
```

Also to assign an entire vector to another the '[]' operator must be used:

```
result = numpy.linspace(0.,1.,100)

# This works
displacement[:] = result[:]
# This does not
displacement = result
```

Then you can solve the problem for instance with:

```
model.solveStaticDisplacement(1e-10,2);
```

And dump to Paraview:

```
model.dump()
```

Do not forget to finalize at the end of the script:

```
akantu.finalize()
```

Finally the python script can be launched with:

```
python ./script.py
```

Warning! : We recall once more that the Python interface is in **beta** state and is provided only for its nice services: it avoids recompilation of akantu when coding the main function. Several preliminary examples are provided in the `examples` directory where it is described how to specify boundary conditions and also constitutive behavior.

Appendix A

Shape Functions

Schmatic overview of all the element types defined in **Akantu** is described in Section 3.2. In this appendix, more detailed information (shape function, location of Gaussian quadrature points, and so on) of each of these types is listed. For each element type, the coordinates of the nodes are given in the isoparametric frame of reference, together with the shape functions (and their derivatives) on these respective nodes. Also all the Gaussian quadrature points within each element are assigned (together with the weight that is applied on these points). The graphical representations of all the element types can be found in Section 3.2.

A.1 1D-Shape Functions

A.1.1 Segment 2

Element properties

Node (i)	Coord. (ξ)	Shape function (N_i)	Derivative ($\partial N_i/\partial \xi$)
1	-1	$\frac{1}{2}(1-\xi)$	$-\frac{1}{2}$
2	1	$\frac{1}{2}(1+\xi)$	$\frac{1}{2}$

Gaussian quadrature points

Coord. (ξ)	0
Weight	2

A.1.2 Segment 3

Element properties

Node (i)	Coord. (ξ)	Shape function (N_i)	Derivative ($\partial N_i/\partial \xi$)
1	-1	$\frac{1}{2}\xi(\xi-1)$	$\xi-\frac{1}{2}$
2	1	$\frac{1}{2}\xi(\xi+1)$	$\xi+\frac{1}{2}$
3	0	$1-\xi^2$	-2ξ

Gaussian quadrature points

Coord. (ξ)	$-1/\sqrt{3}$	$1/\sqrt{3}$
Weight	1	1

A.2 2D-Shape Functions

A.2.1 Triangle 3

Element properties

Node (i)	Coord. $(\xi\,,\,\eta)$	Shape function (N_i)	Derivative $(\partial N_i/\partial\xi\,,\,\partial N_i/\partial\eta)$
1	$(0\,,\,0)$	$1-\xi-\eta$	$(-1\,,\,-1)$
2	$(1\,,\,0)$	ξ	$(1\,,\,0)$
3	$(0\,,\,1)$	η	$(0\,,\,1)$

Gaussian quadrature points

Coord. $(\xi\,,\,\eta)$	$\left(\frac{1}{3}\,,\,\frac{1}{3}\right)$
Weight	1

A.2.2 Triangle 6

Element properties

Node (i)	Coord. $(\xi\,,\,\eta)$	Shape function (N_i)	Derivative $(\partial N_i/\partial\xi\,,\,\partial N_i/\partial\eta)$
1	$(0\,,\,0)$	$-(1-\xi-\eta)(1-2(1-\xi-\eta))$	$(1-4(1-\xi-\eta)\,,\,1-4(1-\xi-\eta))$
2	$(1\,,\,0)$	$-\xi(1-2\xi)$	$(4\xi-1\,,\,0)$
3	$(0\,,\,1)$	$-\eta(1-2\eta)$	$(0\,,\,4\eta-1)$
4	$\left(\frac{1}{2}\,,\,0\right)$	$4\xi(1-\xi-\eta)$	$(4(1-2\xi-\eta)\,,\,-4\xi)$
5	$\left(\frac{1}{2}\,,\,\frac{1}{2}\right)$	$4\xi\eta$	$(4\eta\,,\,4\xi)$
6	$\left(0\,,\,\frac{1}{2}\right)$	$4\eta(1-\xi-\eta)$	$(-4\eta\,,\,4(1-\xi-2\eta))$

Gaussian quadrature points

Coord. $(\xi\,,\,\eta)$	$\left(\frac{1}{6}\,,\,\frac{1}{6}\right)$	$\left(\frac{2}{3}\,,\,\frac{1}{6}\right)$	$\left(\frac{1}{6}\,,\,\frac{2}{3}\right)$
Weight	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$

A.2.3 Quadrangle 4

Element properties

Node (i)	Coord. $(\xi\,,\,\eta)$	Shape function (N_i)	Derivative $(\partial N_i/\partial\xi\,,\,\partial N_i/\partial\eta)$
1	$(-1\,,\,-1)$	$\frac{1}{4}(1-\xi)(1-\eta)$	$\left(-\frac{1}{4}(1-\eta)\,,\,-\frac{1}{4}(1-\xi)\right)$
2	$(1\,,\,-1)$	$\frac{1}{4}(1+\xi)(1-\eta)$	$\left(\frac{1}{4}(1-\eta)\,,\,-\frac{1}{4}(1+\xi)\right)$
3	$(1\,,\,1)$	$\frac{1}{4}(1+\xi)(1+\eta)$	$\left(\frac{1}{4}(1+\eta)\,,\,\frac{1}{4}(1+\xi)\right)$
4	$(-1\,,\,1)$	$\frac{1}{4}(1-\xi)(1+\eta)$	$\left(-\frac{1}{4}(1+\eta)\,,\,\frac{1}{4}(1-\xi)\right)$

Gaussian quadrature points

$(\xi\,,\,\eta)$	$\left(-\frac{1}{\sqrt{3}}\,,\,-\frac{1}{\sqrt{3}}\right)$	$\left(\frac{1}{\sqrt{3}}\,,\,-\frac{1}{\sqrt{3}}\right)$	$\left(\frac{1}{\sqrt{3}}\,,\,\frac{1}{\sqrt{3}}\right)$	$\left(-\frac{1}{\sqrt{3}}\,,\,\frac{1}{\sqrt{3}}\right)$
Weight	1	1	1	1

A.2.4 Quadrangle 8

Element properties

Node (i)	Coord. $(\xi\,,\,\eta)$	Shape function (N_i)	Derivative $(\partial N_i/\partial\xi\,,\,\partial N_i/\partial\eta)$
1	$(-1\,,\,-1)$	$\frac{1}{4}(1-\xi)(1-\eta)(-1-\xi-\eta)$	$\left(\frac{1}{4}(1-\eta)(2\xi+\eta)\,,\,\frac{1}{4}(1-\xi)(\xi+2\eta)\right)$
2	$(1\,,\,-1)$	$\frac{1}{4}(1+\xi)(1-\eta)(-1+\xi-\eta)$	$\left(\frac{1}{4}(1-\eta)(2\xi-\eta)\,,\,-\frac{1}{4}(1+\xi)(\xi-2\eta)\right)$
3	$(1\,,\,1)$	$\frac{1}{4}(1+\xi)(1+\eta)(-1+\xi+\eta)$	$\left(\frac{1}{4}(1+\eta)(2\xi+\eta)\,,\,\frac{1}{4}(1+\xi)(\xi+2\eta)\right)$
4	$(-1\,,\,1)$	$\frac{1}{4}(1-\xi)(1+\eta)(-1-\xi+\eta)$	$\left(\frac{1}{4}(1+\eta)(2\xi-\eta)\,,\,-\frac{1}{4}(1-\xi)(\xi-2\eta)\right)$
5	$(0\,,\,-1)$	$\frac{1}{2}(1-\xi^2)(1-\eta)$	$\left(-\xi(1-\eta)\,,\,-\frac{1}{2}(1-\xi^2)\right)$
6	$(1\,,\,0)$	$\frac{1}{2}(1+\xi)(1-\eta^2)$	$\left(\frac{1}{2}(1-\eta^2)\,,\,-\eta(1+\xi)\right)$
7	$(0\,,\,1)$	$\frac{1}{2}(1-\xi^2)(1+\eta)$	$\left(-\xi(1+\eta)\,,\,\frac{1}{2}(1-\xi^2)\right)$
8	$(-1\,,\,0)$	$\frac{1}{2}(1-\xi)(1-\eta^2)$	$\left(-\frac{1}{2}(1-\eta^2)\,,\,-\eta(1-\xi)\right)$

Gaussian quadrature points

Coord. $(\xi\,,\,\eta)$	$(0,0)$	$\left(\sqrt{\frac{3}{5}}\,,\,\sqrt{\frac{3}{5}}\right)$	$\left(-\sqrt{\frac{3}{5}}\,,\,\sqrt{\frac{3}{5}}\right)$	$\left(-\sqrt{\frac{3}{5}}\,,\,-\sqrt{\frac{3}{5}}\right)$	$\left(\sqrt{\frac{3}{5}}\,,\,-\sqrt{\frac{3}{5}}\right)$
Weight	64/81	25/81	25/81	25/81	25/81
Coord. $(\xi\,,\,\eta)$	$\left(0,\,\sqrt{\frac{3}{5}}\right)$	$\left(-\sqrt{\frac{3}{5}}\,,\,0\right)$	$\left(0,\,-\sqrt{\frac{3}{5}}\right)$	$\left(\sqrt{\frac{3}{5}}\,,\,0\right)$	
Weight	40/81	40/81	40/81	40/81	

A.3 3D-Shape Functions

A.3.1 Tetrahedron 4

Element properties

Node (i)	Coord. (ξ, η, ζ)	Shape function (N_i)	Derivative $(\partial N_i/\partial\xi, \partial N_i/\partial\eta, \partial N_i/\partial\zeta)$
1	$(0, 0, 0)$	$1-\xi-\eta-\zeta$	$(-1, -1, -1)$
2	$(1, 0, 0)$	ξ	$(1, 0, 0)$
3	$(0, 1, 0)$	η	$(0, 1, 0)$
4	$(0, 0, 1)$	ζ	$(0, 0, 1)$

Gaussian quadrature points

Coord. (ξ, η, ζ)	$\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$
Weight	$\frac{1}{6}$

A.3.2 Tetrahedron 10

Element properties

Node (i)	Coord. (ξ, η, ζ)	Shape function (N_i)	Derivative $(\partial N_i/\partial\xi, \partial N_i/\partial\eta, \partial N_i/\partial\zeta)$
1	$(0, 0, 0)$	$(1-\xi-\eta-\zeta)(1-2\xi-2\eta-2\zeta)$	$(4\xi+4\eta+4\zeta-3,$ $4\xi+4\eta+4\zeta-3,$ $4\xi+4\eta+4\zeta-3)$
2	$(1, 0, 0)$	$\xi(2\xi-1)$	$(4\xi-1, 0, 0)$
3	$(0, 1, 0)$	$\eta(2\eta-1)$	$(0, 4\eta-1, 0)$
4	$(0, 0, 1)$	$\zeta(2\zeta-1)$	$(0, 0, 4\zeta-1)$
5	$\left(\frac{1}{2}, 0, 0\right)$	$4\xi(1-\xi-\eta-\zeta)$	$(4-8\xi-4\eta-4\zeta, -4\xi, -4\xi)$
6	$\left(\frac{1}{2}, \frac{1}{2}, 0\right)$	$4\xi\eta$	$(4\eta, 4\xi, 0)$
7	$\left(0, \frac{1}{2}, 0\right)$	$4\eta(1-\xi-\eta-\zeta)$	$(-4\eta, 4-4\xi-8\eta-4\zeta, -4\eta)$
8	$\left(0, 0, \frac{1}{2}\right)$	$4\zeta(1-\xi-\eta-\zeta)$	$(-4\zeta, -4\zeta, 4-4\xi-4\eta-8\zeta)$
9	$\left(\frac{1}{2}, 0, \frac{1}{2}\right)$	$4\xi\zeta$	$(4\zeta, 0, 4\xi)$
10	$\left(0, \frac{1}{2}, \frac{1}{2}\right)$	$4\eta\zeta$	$(0, 4\zeta, 4\eta)$

Gaussian quadrature points

Coord. (ξ, η, ζ)	$\left(\frac{(5-\sqrt{5})}{20}, \frac{(5-\sqrt{5})}{20}, \frac{(5-\sqrt{5})}{20}\right)$	$\left(\frac{(5+3\sqrt{5})}{20}, \frac{(5-\sqrt{5})}{20}, \frac{(5-\sqrt{5})}{20}\right)$
Weight	1/24	1/24
Coord. (ξ, η, ζ)	$\left(\frac{(5-\sqrt{5})}{20}, \frac{(5+3\sqrt{5})}{20}, \frac{(5-\sqrt{5})}{20}\right)$	$\left(\frac{(5-\sqrt{5})}{20}, \frac{(5-\sqrt{5})}{20}, \frac{(5+3\sqrt{5})}{20}\right)$
Weight	1/24	1/24

A.3.3 Hexahedron 8

Element properties

Node (i)	Coord. $(\xi\,,\,\eta\,,\,\zeta)$	Shape function (N_i)	Derivative $(\partial N_i/\partial\xi\,,\,\partial N_i/\partial\eta\,,\,\partial N_i/\partial\zeta)$
1	$(-1\,,-1\,,-1)$	$\frac{1}{8}(1-\xi)(1-\eta)(1-\zeta)$	$\left(-\frac{1}{8}(1-\eta)(1-\zeta)\,,\,-\frac{1}{8}(1-\xi)(1-\zeta)\,,\,-\frac{1}{8}(1-\xi)(1-\eta)\right)$
2	$(1\,,-1\,,-1)$	$\frac{1}{8}(1+\xi)(1-\eta)(1-\zeta)$	$\left(\frac{1}{8}(1-\eta)(1-\zeta)\,,\,-\frac{1}{8}(1+\xi)(1-\zeta)\,,\,-\frac{1}{8}(1+\xi)(1-\eta)\right)$
3	$(1\,,1\,,-1)$	$\frac{1}{8}(1+\xi)(1+\eta)(1-\zeta)$	$\left(\frac{1}{8}(1+\eta)(1-\zeta)\,,\,\frac{1}{8}(1+\xi)(1-\zeta)\,,\,-\frac{1}{8}(1+\xi)(1+\eta)\right)$
4	$(-1\,,1\,,-1)$	$\frac{1}{8}(1-\xi)(1+\eta)(1-\zeta)$	$\left(-\frac{1}{8}(1+\eta)(1-\zeta)\,,\,\frac{1}{8}(1-\xi)(1-\zeta)\,,\,-\frac{1}{8}(1-\xi)(1+\eta)\right)$
5	$(-1\,,-1\,,1)$	$\frac{1}{8}(1-\xi)(1-\eta)(1+\zeta)$	$\left(-\frac{1}{8}(1-\eta)(1+\zeta)\,,\,-\frac{1}{8}(1-\xi)(1+\zeta)\,,\,\frac{1}{8}(1-\xi)(1-\eta)\right)$
6	$(1\,,-1\,,1)$	$\frac{1}{8}(1+\xi)(1-\eta)(1+\zeta)$	$\left(\frac{1}{8}(1-\eta)(1+\zeta)\,,\,-\frac{1}{8}(1+\xi)(1+\zeta)\,,\,\frac{1}{8}(1+\xi)(1-\eta)\right)$
7	$(1\,,1\,,1)$	$\frac{1}{8}(1+\xi)(1+\eta)(1+\zeta)$	$\left(\frac{1}{8}(1+\eta)(1+\zeta)\,,\,\frac{1}{8}(1+\xi)(1+\zeta)\,,\,\frac{1}{8}(1+\xi)(1+\eta)\right)$
8	$(-1\,,1\,,1)$	$\frac{1}{8}(1-\xi)(1+\eta)(1+\zeta)$	$\left(-\frac{1}{8}(1+\eta)(1+\zeta)\,,\,\frac{1}{8}(1-\xi)(1+\zeta)\,,\,\frac{1}{8}(1-\xi)(1+\eta)\right)$

Gaussian quadrature points

$(\xi\,,\,\eta\,,\,\zeta)$	$\left(-\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}}\right)$	$\left(\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}}\right)$	$\left(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}}\right)$	$\left(-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}}\right)$
Weight	1	1	1	1
$(\xi\,,\,\eta\,,\,\zeta)$	$\left(-\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}}\right)$	$\left(\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}}\right)$	$\left(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}}\right)$	$\left(-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}}\right)$
Weight	1	1	1	1

A.3.4 Pentahedron 6

Element properties

Node (i)	Coord. $(\xi\,,\,\eta\,,\,\zeta)$	Shape function (N_i)	Derivative $(\partial N_i/\partial\xi\,,\,\partial N_i/\partial\eta\,,\,\partial N_i/\partial\zeta)$
1	$(-1\,,1\,,0)$	$\frac{1}{2}(1-\xi)\eta$	$\left(-\frac{1}{2}\eta\,,\,\frac{1}{2}(1-\xi)\,,\,0.0\right)$
2	$(-1\,,0\,,1)$	$\frac{1}{2}(1-\xi)\zeta$	$\left(-\frac{1}{2}\zeta\,,\,0.0\,,\,\frac{1}{2}(1-\xi)\right)$
3	$(-1\,,0\,,0)$	$\frac{1}{2}(1-\xi)(1-\eta-\zeta)$	$\left(-\frac{1}{2}(1-\eta-\zeta)\,,\,-\frac{1}{2}(1-\xi)\,,\,-\frac{1}{2}(1-\xi)\right)$
4	$(1\,,1\,,0)$	$\frac{1}{2}(1+\xi)\eta$	$\left(\frac{1}{2}\eta\,,\,\frac{1}{2}(1+\xi)\,,\,0.0\right)$
5	$(1\,,0\,,1)$	$\frac{1}{2}(1+\xi)\zeta$	$\left(\frac{1}{2}\zeta\,,\,0.0\,,\,\frac{1}{2}(1+\xi)\right)$
6	$(1\,,0\,,0)$	$\frac{1}{2}(1+\xi)(1-\eta-\zeta)$	$\left(\frac{1}{2}(1-\eta-\zeta)\,,\,-\frac{1}{2}(1+\xi)\,,\,-\frac{1}{2}(1+\xi)\right)$

Gaussian quadrature points

$(\xi\,,\,\eta\,,\,\zeta)$	$\left(-\frac{1}{\sqrt{3}},0.5,0.5\right)$	$\left(-\frac{1}{\sqrt{3}},0.0,0.5\right)$	$\left(-\frac{1}{\sqrt{3}},0.5,0.0\right)$	$\left(\frac{1}{\sqrt{3}},0.5,0.5\right)$	$\left(\frac{1}{\sqrt{3}},0.0,0.5\right)$	$\left(\frac{1}{\sqrt{3}},0.5,0.0\right)$
Weight	1/6	1/6	1/6	1/6	1/6	1/6

A.3.5 Hexahedron 20

Element properties

Node (i)	Coord. (ξ , η , ζ)	Shape function (N_i)
1	(−1 , −1 , −1)	$\frac{1}{8}(1-\xi)(1-\eta)(1-\zeta)(-2-\xi-\eta-\zeta)$
2	(1 , −1 , −1)	$\frac{1}{8}(1+\xi)(1-\eta)(1-\zeta)(-2+\xi-\eta-\zeta)$
3	(1 , 1 , −1)	$\frac{1}{8}(1+\xi)(1+\eta)(1-\zeta)(-2+\xi+\eta-\zeta)$
4	(−1 , 1 , −1)	$\frac{1}{8}(1-\xi)(1+\eta)(1-\zeta)(-2-\xi+\eta-\zeta)$
5	(−1 , −1 , 1)	$\frac{1}{8}(1-\xi)(1-\eta)(1+\zeta)(-2-\xi-\eta+\zeta)$
6	(1 , −1 , 1)	$\frac{1}{8}(1+\xi)(1-\eta)(1+\zeta)(-2+\xi-\eta+\zeta)$
7	(1 , 1 , 1)	$\frac{1}{8}(1+\xi)(1+\eta)(1+\zeta)(-2+\xi+\eta+\zeta)$
8	(−1 , 1 , 1)	$\frac{1}{8}(1-\xi)(1+\eta)(1+\zeta)(-2-\xi+\eta+\zeta)$
9	(0 , −1 , −1)	$\frac{1}{4}(1-\xi^2)(1-\eta)(1-\zeta)$
10	(1 , 0 , −1)	$\frac{1}{4}(1+\xi)(1-\eta^2)(1-\zeta)$
11	(0 , 1 , −1)	$\frac{1}{4}(1-\xi^2)(1+\eta)(1-\zeta)$
12	(−1 , 0 , −1)	$\frac{1}{4}(1-\xi)(1-\eta^2)(1-\zeta)$
13	(−1 , −1 , 0)	$\frac{1}{4}(1-\xi)(1-\eta)(1-\zeta^2)$
14	(1 , −1 , 0)	$\frac{1}{4}(1+\xi)(1-\eta)(1-\zeta^2)$
15	(1 , 1 , 0)	$\frac{1}{4}(1+\xi)(1+\eta)(1-\zeta^2)$
16	(−1 , 1 , 0)	$\frac{1}{4}(1-\xi)(1+\eta)(1-\zeta^2)$
17	(0 , −1 , 1)	$\frac{1}{4}(1-\xi^2)(1-\eta)(1+\zeta)$
18	(1 , 0 , 1)	$\frac{1}{4}(1+\xi)(1-\eta^2)(1+\zeta)$
19	(0 , 1 , 1)	$\frac{1}{4}(1-\xi^2)(1+\eta)(1+\zeta)$
20	(−1 , 0 , 1)	$\frac{1}{4}(1-\xi)(1-\eta^2)(1+\zeta)$

Element properties

Node (i)	Derivative $(\partial N_i/\partial\xi\ ,\ \partial N_i/\partial\eta\ ,\ \partial N_i/\partial\zeta)$
1	$\left(\ \frac{1}{4}\left(\xi+\frac{1}{2}(\eta+\zeta+1)\right)(\eta-1)(\zeta-1)\ ,\ \frac{1}{4}\left(\eta+\frac{1}{2}(\xi+\zeta+1)\right)(\xi-1)(\zeta-1)\ ,\ \frac{1}{4}\left(\zeta+\frac{1}{2}(\xi+\eta+1)\right)(\xi-1)(\eta-1)\ \right)$
2	$\left(\ \frac{1}{4}\left(\xi-\frac{1}{2}(\eta+\zeta+1)\right)(\eta-1)(\zeta-1)\ ,\ -\frac{1}{4}\left(\eta-\frac{1}{2}(\xi-\zeta-1)\right)(\xi+1)(\zeta-1)\ ,\ -\frac{1}{4}\left(\zeta-\frac{1}{2}(\xi-\eta-1)\right)(\xi+1)(\eta-1)\ \right)$
3	$\left(\ -\frac{1}{4}\left(\xi+\frac{1}{2}(\eta-\zeta-1)\right)(\eta+1)(\zeta-1)\ ,\ -\frac{1}{4}\left(\eta+\frac{1}{2}(\xi-\zeta-1)\right)(\xi+1)(\zeta-1)\ ,\ \frac{1}{4}\left(\zeta-\frac{1}{2}(\xi+\eta-1)\right)(\xi+1)(\eta+1)\ \right)$
4	$\left(\ -\frac{1}{4}\left(\xi-\frac{1}{2}(\eta-\zeta-1)\right)(\eta+1)(\zeta-1)\ ,\ \frac{1}{4}\left(\eta-\frac{1}{2}(\xi+\zeta+1)\right)(\xi-1)(\zeta-1)\ ,\ -\frac{1}{4}\left(\zeta+\frac{1}{2}(\xi-\eta+1)\right)(\xi-1)(\eta+1)\ \right)$
5	$\left(\ -\frac{1}{4}\left(\xi+\frac{1}{2}(\eta-\zeta+1)\right)(\eta-1)(\zeta+1)\ ,\ -\frac{1}{4}\left(\eta+\frac{1}{2}(\xi-\zeta+1)\right)(\xi-1)(\zeta+1)\ ,\ \frac{1}{4}\left(\zeta-\frac{1}{2}(\xi+\eta+1)\right)(\xi-1)(\eta-1)\ \right)$
6	$\left(\ -\frac{1}{4}\left(\xi-\frac{1}{2}(\eta-\zeta+1)\right)(\eta-1)(\zeta+1)\ ,\ \frac{1}{4}\left(\eta-\frac{1}{2}(\xi+\zeta-1)\right)(\xi+1)(\zeta+1)\ ,\ -\frac{1}{4}\left(\zeta+\frac{1}{2}(\xi-\eta-1)\right)(\xi+1)(\eta-1)\ \right)$
7	$\left(\ \frac{1}{4}\left(\xi+\frac{1}{2}(\eta+\zeta-1)\right)(\eta+1)(\zeta+1)\ ,\ \frac{1}{4}\left(\eta+\frac{1}{2}(\xi+\zeta-1)\right)(\xi+1)(\zeta+1)\ ,\ \frac{1}{4}\left(\zeta+\frac{1}{2}(\xi+\eta-1)\right)(\xi+1)(\eta+1)\ \right)$
8	$\left(\ \frac{1}{4}\left(\xi-\frac{1}{2}(\eta+\zeta-1)\right)(\eta+1)(\zeta+1)\ ,\ -\frac{1}{4}\left(\eta-\frac{1}{2}(\xi-\zeta+1)\right)(\xi-1)(\zeta+1)\ ,\ -\frac{1}{4}\left(\zeta-\frac{1}{2}(\xi-\eta+1)\right)(\xi-1)(\eta+1)\ \right)$
9	$\left(\ -\frac{1}{2}\xi(\eta-1)(\zeta-1)\ ,\ -\frac{1}{4}(\xi^2-1)(\zeta-1)\ ,\ -\frac{1}{4}(\xi^2-1)(\eta-1)\ \right)$
10	$\left(\ \frac{1}{4}(\eta^2-1)(\zeta-1)\ ,\ \frac{1}{2}\eta(\xi+1)(\zeta-1)\ ,\ \frac{1}{4}(\xi+1)(\eta^2-1)\ \right)$
11	$\left(\ \frac{1}{2}\xi(\eta+1)(\zeta-1)\ ,\ \frac{1}{4}(\xi^2-1)(\zeta-1)\ ,\ \frac{1}{4}(\xi^2-1)(\eta+1)\ \right)$
12	$\left(\ -\frac{1}{4}(\eta^2-1)(\zeta-1)\ ,\ -\frac{1}{2}\eta(\xi-1)(\zeta-1)\ ,\ -\frac{1}{4}(\xi-1)(\eta^2-1)\ \right)$
13	$\left(\ -\frac{1}{4}(\eta-1)(\zeta^2-1)\ ,\ -\frac{1}{4}(\xi-1)(\zeta^2-1)\ ,\ -\frac{1}{2}\zeta(\xi-1)(\eta-1)\ \right)$
14	$\left(\ \frac{1}{4}(\eta-1)(\zeta^2-1)\ ,\ \frac{1}{4}(\xi+1)(\zeta^2-1)\ ,\ \frac{1}{2}\zeta(\xi+1)(\eta-1)\ \right)$
15	$\left(\ -\frac{1}{4}(\eta+1)(\zeta^2-1)\ ,\ -\frac{1}{4}(\xi+1)(\zeta^2-1)\ ,\ -\frac{1}{2}\zeta(\xi+1)(\eta+1)\ \right)$
16	$\left(\ \frac{1}{4}(\eta+1)(\zeta^2-1)\ ,\ \frac{1}{4}(\xi-1)(\zeta^2-1)\ ,\ \frac{1}{2}\zeta(\xi-1)(\eta+1)\ \right)$
17	$\left(\ \frac{1}{2}\xi(\eta-1)(\zeta+1)\ ,\ \frac{1}{4}(\xi^2-1)(\zeta+1)\ ,\ \frac{1}{4}(\xi^2-1)(\eta-1)\ \right)$
18	$\left(\ -\frac{1}{4}(\eta^2-1)(\zeta+1)\ ,\ -\frac{1}{2}\eta(\xi+1)(\zeta+1)\ ,\ -\frac{1}{4}(\xi+1)(\eta^2-1)\ \right)$
19	$\left(\ -\frac{1}{2}\xi(\eta+1)(\zeta+1)\ ,\ -\frac{1}{4}(\xi^2-1)(\zeta+1)\ ,\ -\frac{1}{4}(\xi^2-1)(\eta+1)\ \right)$
20	$\left(\ \frac{1}{4}(\eta^2-1)(\zeta+1)\ ,\ \frac{1}{2}\eta(\xi-1)(\zeta+1)\ ,\ \frac{1}{4}(\xi-1)(\eta^2-1)\ \right)$

Gaussian quadrature points

Coord. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(-\sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}\right)$	$\left(-\sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}, 0\right)$	$\left(-\sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}\right)$	$\left(-\sqrt{\frac{3}{5}}, 0, -\sqrt{\frac{3}{5}}\right)$
Weight	125/729	200/729	125/729	200/729
Coord. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(-\sqrt{\frac{3}{5}}, 0, 0\right)$	$\left(-\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}}\right)$	$\left(-\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}\right)$	$\left(-\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}, 0\right)$
Weight	320/729	200/729	125/729	200/729
Coord. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(-\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}\right)$	$\left(0, -\sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}\right)$	$\left(0, -\sqrt{\frac{3}{5}}, 0\right)$	$\left(0, -\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}\right)$
Weight	125/729	200/729	320/729	200/729
Coord. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(0, 0, -\sqrt{\frac{3}{5}}\right)$	$(0, 0, 0)$	$\left(0, 0, \sqrt{\frac{3}{5}}\right)$	$\left(0, \sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}\right)$
Weight	320/729	512/729	320/729	200/729
Coord. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(0, \sqrt{\frac{3}{5}}, 0\right)$	$\left(0, \sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}\right)$	$\left(\sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}\right)$	$\left(\sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}, 0\right)$
Weight	320/729	200/729	125/729	200/729
Coord. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(\sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}\right)$	$\left(\sqrt{\frac{3}{5}}, 0, -\sqrt{\frac{3}{5}}\right)$	$\left(\sqrt{\frac{3}{5}}, 0, 0\right)$	$\left(\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}}\right)$
Weight	125/729	200/729	320/729	200/729
Coord. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}, -\sqrt{\frac{3}{5}}\right)$	$\left(\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}, 0\right)$	$\left(\sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}, \sqrt{\frac{3}{5}}\right)$	
Weight	125/729	200/729	125/729	

A.3.6 Pentahedron 15

Element properties

Node (i)	Coord. $(\xi\,,\,\eta\,,\,\zeta)$	Shape function (N_i)
1	$(-1\,,\,1\,,\,0)$	$\frac{1}{2}\eta\,(1-\xi)\,(2\eta-2-\xi)$
2	$(-1\,,\,0\,,\,1)$	$\frac{1}{2}\zeta\,(1-\xi)\,(2\zeta-2-\xi)$
3	$(-1\,,\,0\,,\,0)$	$\frac{1}{2}\,(\xi-1)\,(1-\eta-\zeta)\,(\xi+2\eta+2\zeta)$
4	$(1\,,\,1\,,\,0)$	$\frac{1}{2}\eta\,(1+\xi)\,(2\eta-2+\xi)$
5	$(1\,,\,0\,,\,1)$	$\frac{1}{2}\zeta\,(1+\xi)\,(2\zeta-2+\xi)$
6	$(1\,,\,0\,,\,0)$	$\frac{1}{2}\,(-\xi-1)\,(1-\eta-\zeta)\,(-\xi+2\eta+2\zeta)$
7	$(-1\,,\,0.5\,,\,0.5)$	$2\eta\zeta\,(1-\xi)$
8	$(-1\,,\,0\,,\,0.5)$	$2\zeta\,(1-\eta-\zeta)\,(1-\xi)$
9	$(-1\,,\,0.5\,,\,0)$	$2\eta\,(1-\xi)\,(1-\eta-\zeta)$
10	$(0\,,\,1\,,\,0)$	$\eta\,(1-\xi^2)$
11	$(0\,,\,0\,,\,1)$	$\zeta\,(1-\xi^2)$
12	$(0\,,\,0\,,\,0)$	$(1-\xi^2)\,(1-\eta-\zeta)$
13	$(1\,,\,0.5\,,\,0.5)$	$2\eta\zeta\,(1+\xi)$
14	$(1\,,\,0\,,\,0.5)$	$2\zeta\,(1+\xi)\,(1-\eta-\zeta)$
15	$(1\,,\,0.5\,,\,0)$	$2\eta\,(1+\xi)\,(1-\eta-\zeta)$

Element properties

Node (i)	Derivative ($\partial N_i/\partial\xi$, $\partial N_i/\partial\eta$, $\partial N_i/\partial\zeta$)
1	$\left(\frac{1}{2}\eta(2\xi-2\eta+1),\ -\frac{1}{2}(\xi-1)(4\eta-\xi-2),\ 0.0\right)$
2	$\left(\frac{1}{2}\zeta(2\xi-2\zeta+1),\ 0.0,\ -\frac{1}{2}(\xi-1)(4\zeta-\xi-2)\right)$
3	$\left(-\frac{1}{2}(2\xi+2\eta+2\zeta-1)(\eta+\zeta-1),\ -\frac{1}{2}(\xi-1)(4\eta+\xi+2(2\zeta-1)),\ -\frac{1}{2}(\xi-1)(4\zeta+\xi+2(2\eta-1))\right)$
4	$\left(\frac{1}{2}\eta(2\xi+2\eta-1),\ \frac{1}{2}(\xi+1)(4\eta+\xi-2),\ 0.0\right)$
5	$\left(\frac{1}{2}\zeta(2\xi+2\zeta-1),\ 0.0,\ \frac{1}{2}(\xi+1)(4\zeta+\xi-2)\right)$
6	$\left(-\frac{1}{2}(\eta+\zeta-1)(2\xi-2\eta-2\zeta+1),\ \frac{1}{2}(\xi+1)(4\eta-\xi+2(2\zeta-1)),\ \frac{1}{2}(\xi+1)(4\zeta-\xi+2(2\eta-1))\right)$
7	$(-2\eta\zeta,\ -2(\xi-1)\zeta,\ -2(\xi-1)\eta)$
8	$(2\zeta(\eta+\zeta-1),\ 2\zeta-(\xi-1),\ 2(\xi-1)(2\zeta+\eta-1))$
9	$(2\eta(\eta+\zeta-1),\ 2(2\eta+\zeta-1)(\xi-1),\ 2\eta(\xi-1))$
10	$(-2\xi\eta,\ -(\xi^2-1),\ 0.0)$
11	$(-2\xi\zeta,\ 0.0,\ -(\xi^2-1))$
12	$(2\xi(\eta+\zeta-1),\ (\xi^2-1),\ (\xi^2-1))$
13	$(2\eta\zeta,\ 2\zeta(\xi+1),\ 2\eta(\xi+1))$
14	$(-2\zeta(\eta+\zeta-1),\ -2\zeta(\xi+1),\ -2(\xi+1)(2\zeta+\eta-1))$
15	$(-2\eta(\eta+\zeta-1),\ -2(2\eta+\zeta-1)(\xi+1),\ -2\eta(\xi+1))$

Gaussian quadrature points

Coord. (ξ , η , ζ)	$\left(-\frac{1}{\sqrt{3}},\ \frac{1}{3},\ \frac{1}{3}\right)$	$\left(-\frac{1}{\sqrt{3}},\ 0.6,\ 0.2\right)$	$\left(-\frac{1}{\sqrt{3}},\ 0.2,\ 0.6\right)$	$\left(-\frac{1}{\sqrt{3}},\ 0.2,\ 0.2\right)$
Weight	-27/96	25/96	25/96	25/96
Coord. (ξ , η , ζ)	$\left(\frac{1}{\sqrt{3}},\ \frac{1}{3},\ \frac{1}{3}\right)$	$\left(\frac{1}{\sqrt{3}},\ 0.6,\ 0.2\right)$	$\left(\frac{1}{\sqrt{3}},\ 0.2,\ 0.6\right)$	$\left(\frac{1}{\sqrt{3}},\ 0.2,\ 0.2\right)$
Weight	-27/96	25/96	25/96	25/96

Appendix B

Material parameters

B.1 Linear elastic isotropic

Keyword: `elastic`
Description here: 4.4.1
Parameters:

- `rho`: (*Real*) Density
- `E`: (*Real*) Young's modulus
- `nu`: (*Real*) Poisson's ratio
- `Plane_Stress`: (*bool*) Plane stress simplification (only 2D problems)

B.2 Linear elastic anisotropic

Keyword: `elastic_anisotropic`
Description here: 4.4.1
Parameters:

- `rho`: (*Real*) Density
- `n1`: (*Vector<Real>*) Direction of the main material axis
- `n2`: (*Vector<Real>*) Direction of the second material axis (if applicable)
- `n3`: (*Vector<Real>*) Direction of the third material axis (if applicable)
- `C..`: (*Real*) Coefficient ij of the material tensor C (all the 36 values in Voigt notation can be entered .)

B.3 Linear elastic orthotropic

Keyword: `elastic_orthotropic`
Description here: 4.4.1
Parameters:

- `rho`: (*Real*) Density
- `n1`: (*Vector<Real>*) Direction of the main material axis
- `n2`: (*Vector<Real>*) Direction of the second material axis (if applicable)
- `n3`: (*Vector<Real>*) Direction of the third material axis (if applicable)
- `E1`: (*Real*) Young's modulus (n1)
- `E2`: (*Real*) Young's modulus (n2)
- `E3`: (*Real*) Young's modulus (n3)
- `nu12`: (*Real*) Poisson's ratio (12)
- `nu13`: (*Real*) Poisson's ratio (13)
- `nu23`: (*Real*) Poisson's ratio (23)

- `G12`: (*Real*) Shear modulus (12)
- `G13`: (*Real*) Shear modulus (13)
- `G23`: (*Real*) Shear modulus (23)

B.4 Neohookean (finite strains)

Keyword: `neohookean`
Description here: 4.4.2
Parameters:

- `rho`: (*Real*) Density
- `E`: (*Real*) Young's modulus
- `nu`: (*Real*) Poisson's ratio
- `Plane_Stress`: (*bool*) Plane stress simplification : false = plane strain, true = plane stress (default: false) (only 2D problems)

B.5 Standard linear solid

Keyword: `sls_deviatoric`
Description here: 4.4.3
Parameters:

- `rho`: (*Real*) Density
- `E`: (*Real*) Young's modulus
- `nu`: (*Real*) Poisson's ratio
- `Plane_Stress`: (*bool*) Plane stress simplification (only 2D problems)
- `Eta`: (*Real*) Viscosity
- `Ev`: (*Real*) Stiffness of the viscous element

B.6 Elasto-plastic linear isotropic hardening

Keyword: `plastic_linear_isotropic_hardening`
Description here: 4.4.4
Parameters:

- `rho`: (*Real*) Density
- `E`: (*Real*) Young's modulus
- `nu`: (*Real*) Poisson's ratio
- `h`: (*Real*) Hardening modulus
- `sigma_y`: (*Real*) Yielding stress

B.7 Damage: Marigo

Keyword: `marigo`
Description here: 4.4.5
Parameters:

- `rho`: (*Real*) Density
- `E`: (*Real*) Young's modulus
- `nu`: (*Real*) Poisson's ratio
- `Plane_Stress`: (*bool*) Plane stress simplification (only 2D problems)
- `Yd`: (*Random*) Rupture criterion
- `Sd`: (*Real*) Damage Energy

B.8 Damage: Mazars

Keyword: `mazars`
Description here: 4.4.5
Parameters:

- `rho`: (*Real*) Density
- `E`: (*Real*) Young's modulus
- `nu`: (*Real*) Poisson's ratio
- `At`: (*Real*) Traction post-peak asymptotic value
- `Bt`: (*Real*) Traction decay shape
- `Ac`: (*Real*) Compression post-peak asymptotic value
- `Bc`: (*Real*) Compression decay shape
- `K0`: (*Real*) Damage threshold
- `beta`: (*Real*) Shear parameter

B.9 Cohesive linear

Keyword: `cohesive_linear`
Description here: 4.5.1
Parameters:

- `sigma_c`: (*Real*) Critical stress σ_c
  Either G_c and kappa or, G_cI and G_cII or delta_c have to be specified
- `G_c`: (*Real*) Mode I fracture energy
- `kappa`: (*Real*) $\kappa = G\_cII/G\_cI$ parameter (default 1)
- `delta_c`: (*Real*) Critical displacement δ_c
- `beta`: (*Real*) β parameter (default 1)
- `penalty`: (*Real*) penalty coefficient for compression α (optional; default 0)
- `volume_s & m_s`: (*Reals*) optional; to adapt statistical distribution following [22]
- `contact_after_breaking`: (*bool*) Activation of contact when the elements are fully damaged (default false)
- `max_quad_stress_insertion`: (*bool*) Insertion of cohesive element when stress is high enough just on one quadrature point (default false)

B.10 Cohesive bilinear

Keyword: `cohesive_bilinear`
Description here: 4.5.1
Parameters:

- `sigma_c`: (*Real*) Critical stress σ_c
- `delta_0`: (*Real*) Elastic limit displacement δ_0
  Either G_c and kappa or, G_cI and G_cII or delta_c have to be specified
- `G_c`: (*Real*) Mode I fracture energy
- `kappa`: (*Real*) $\kappa = G\_cII/G\_cI$ parameter (default 1)
- `delta_c`: (*Real*) Critical displacement δ_c
- `beta`: (*Real*) β parameter (default 1)
- `penalty`: (*Real*) Penalty coefficient for compression α (optional; default 0)

B.11 Cohesive linear with friction

Keyword: `cohesive_linear_friction`
Description here: 4.5.2
Parameters:

- `sigma_c`: (*Real*) Critical stress σ_c
  Either G_c and kappa or, G_cI and G_cII or delta_c have to be specified
- `G_c`: (*Real*) Mode I fracture energy
- `kappa`: (*Real*) $\kappa = G\_cII/G\_cI$ parameter (default 1)
- `delta_c`: (*Real*) Critical displacement δ_c
- `beta`: (*Real*) β parameter (default 1)
- `penalty`: (*Real*) Penalty coefficient for compression α (optional; default 0)
- `volume_s & m_s`: (*Reals*) optional; to adapt statistical distribution following [22]
- `contact_after_breaking`: (*bool*) Activation of contact when the elements are fully damaged (default false)
- `max_quad_stress_insertion`: (*bool*) Insertion of cohesive element when stress is high enough just on one quadrature point (default false)
- `mu`: (*Real*) Maximum attainable value of the friction coefficient, μ (default 0)
- `penalty_for_friction`: (*Real*) Penalty parameter for the elasto-plastic friction law (default 0)

B.12 Cohesive linear fatigue

Keyword: `cohesive_linear_fatigue`
Description here: 4.5.3
Parameters:

- `sigma_c`: (*Real*) Critical stress σ_c
- `delta_c`: (*Real*) Critical displacement δ_c
- `beta`: (*Real*) β parameter (default 1)
- `G_c`: (*Real*) Mode I fracture energy
- `kappa`: (*Real*) κ parameter (default 1)
- `penalty`: (*Real*) penalty coefficient α (optional, default 0)
- `delta_f`: (*Real*) Characteristic opening displacement δ_f (see [15])

B.13 Cohesive exponential

Keyword: `cohesive_exponential`
Description here: 4.5.4
Parameters:

- `sigma_c`: (*Real*) Critical stress σ_c
- `delta_c`: (*Real*) Displacement at the peak traction δ_c
- `beta`: (*Real*) β parameter (default 1)
- `exponential_penalty`: (*Bool*) parameter to activate contact penalty following the exponential law (default true)
- `contact_tangent`: (*Real*) ratio of the contact tangent over the initial exponential tangent (to be defined if exponential_penalty is false; default 1.0)

Appendix C

Package dependencies

During the configuration, `cmake` offers several **Akantu** options which have dependencies with each other or with external packages and software. Each of these are described in details now.

AKANTU_USE_BOOST Akantu uses Boost header only for preprocessor and Spirit Under Ubuntu (14.04 LTS) the installation can be performed using the commands:

```
> sudo apt-get install libboost
```

AKANTU_COHESIVE_ELEMENT This package activates the cohesive elements engine within Akantu. It depends on:

- A fortran compiler.
- An implementation of BLAS/LAPACK.

Dependencies: *AKANTU_USE_LAPACK*

AKANTU_CORE This package is the core engine of **Akantu**. It depends on:

- A C++ compiler (GCC >= 4, or Intel).
- The cross-platform, open-source CMake build system.
- The Boost C++ portable libraries.
- The zlib compression library.

Under Ubuntu (14.04 LTS) the installation can be performed using the commands:

```
> sudo apt-get install cmake libboost-dev zlib1g-dev g++
```

Under Mac OS X the installation requires the following steps:

- Install Xcode
- Install the command line tools.
- Install the MacPorts project which allows to automatically download and install opensource packages.

Then the following commands should be typed in a terminal:

```
> sudo port install cmake gcc48 boost
```

AKANTU_CORE_CXX11 This option activates some features of the C++11 standard. This is usable with GCC>=4.7 or Intel>=13.

AKANTU_DAMAGE_NON_LOCAL This package activates the non local damage feature of AKANTU *Dependencies*: *AKANTU_USE_LAPACK*

AKANTU_DOCUMENTATION_MANUAL This package alows to compile the user manual in the build folder `build/doc/manual/manual.pdf`. Under Ubuntu (14.04 LTS), the installation of the dependencies can be performed using the following command:

```
> sudo apt-get install install rubber texlive texlive-science texlive-latex-
  extra
```

AKANTU_HEAT_TRANSFER This package activates the heat transfer model within Akantu. It has no additional dependencies.

AKANTU_IMPLICIT This package activates the sparse solver necessary to solve implicitely static/dynamic finite element problems. It depends on:

- MUMPS, a parallel sparse direct solver.
- Scotch, a graph partitioner.

Dependencies: *AKANTU_USE_SCOTCH AKANTU_USE_MUMPS*

AKANTU_USE_IOHELPER This package activates the IOHelper facilities withing Akantu. This is mandatory if you want to be able to output Paraview files as well as any Dumper within Akantu.

AKANTU_USE_LAPACK This package provides access to a LAPACK implementation. Under Ubuntu (14.04 LTS), the installation can be performed using the following command:

```
> sudo apt-get install libatlas-base-dev
```

AKANTU_USE_MPI This is a meta package providing access to MPI. Under Ubuntu (14.04 LTS) the installation can be performed using the commands:

```
> sudo apt-get install libopenmpi-dev
```

Under Mac OS X the installation requires the following steps:

```
> sudo port install mpich-devel
```

Dependencies: *AKANTU_USE_SCOTCH*

AKANTU_USE_MUMPS This package enables the MUMPS parallel direct solver for sparce matrices. This is necessary to solve static or implicit problems. Under Ubuntu (14.04 LTS) the installation can be performed using the commands:

```
> sudo apt-get install libmumps-seq-dev # for sequential
> sudo apt-get install libmumps-dev     # for parallel
```

Under Mac OS X the installation requires the following steps:

```
> sudo port install mumps
```

If you activate the advanced option AKANTU_USE_THIRD_PARTY_MUMPS the make system of akantu can automatically compile MUMPS. For this you will have to download MUMPS from `http://mumps.enseeiht.fr/` or `http://graal.ens-lyon.fr/MUMPS` and place it in `<akantu source>/third-party`

AKANTU_USE_NUMPY This package allows to wrap Akantu arrays to numpy arrays Under Ubuntu (14.04 LTS) the installation can be performed using the commands:

```
> sudo apt-get install python-numpy
```

AKANTU_PARALLEL This option activates the parallel features of AKANTU. *Dependencies*: *AKANTU_USE_MPI AKANTU_USE_SCOTCH AKANTU_USE_SCOTCH*

AKANTU_PYTHON_INTERFACE This package enables the python interface of Akantu. It relies on swig3.0 to generate the code Under Ubuntu (14.04 LTS) the installation can be performed using the commands:

```
> sudo apt-get install swig3.0
```

Dependencies: *AKANTU_USE_PYTHONLIBS AKANTU_USE_NUMPY AKANTU_CORE_CXX11*

AKANTU_USE_PYTHONLIBS This package is a dependency of the python interface Under Ubuntu (14.04 LTS) the installation can be performed using the commands:

```
> sudo apt-get install libpython2.7-dev
```

Dependencies: *AKANTU_USE_NUMPY*

AKANTU_USE_SCOTCH This package enables the use the Scotch library in order to perform a graph partitioning leading to the domain decomposition used within **Akantu** Under Ubuntu (14.04 LTS) the installation can be performed using the commands:

```
> sudo apt-get install libscotch-dev
```

If you activate the advanced option AKANTU_USE_THIRD_PARTY_SCOTCH the make system of akantu can automatically compile Scotch. If the automated download fails due to a SSL access not supported by your version of CMake please download the file scotch_5.1.12b_esmumps.tar.gz and then place it in the directory `<akantu source>/third-party`

AKANTU_STRUCTURAL_MECHANICS This package activates the compilation for the Structural Mechanics engine of Akantu *Dependencies*: *AKANTU_IMPLICIT AKANTU_USE_SCOTCH AKANTU_USE_MUMPS*

AKANTU_TRACTION-AT-SPLIT-NODE-CONTACT TODO: No Documentation in package.cmake looking for the sequence:

```
\package_declare_documentation(
  traction-at-split-node-contact
  "documentation text"
  )
```

Dependencies: *AKANTU_USE_IOHELPER*

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