Akantu

User's Guide

September 2, 2015 — Version

Contents

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("material.dat", argc, argv);

  // your code
  ...
```

```
  finalize();
}
```

The `initialize` function takes the material file and the program parameters which can be interpreted by **Akantu** in due form. 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 [**?**], Abaqus [**?**] and Diana [**?**]. 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 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.

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
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` $\times$ `spatial_dimension` matrices. The light objects `Matrix` and `Vector` can be used and combined to do most common linear algebra.

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.

2.5.1 Vector & Matrix

The `Array` iterators as presented in the previous section can be shaped as `Vector` or `Matrix`. This objects represent 1^{st} and 2^{nd} 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<N>()` returns the L_N norm defined as $\left(\sum_i |\texttt{A(i)}|^N\right)^{1/N}$. N can take any positive integer value.
   - `A.norm()` is equivalent to `A.norm<L_2>()`
   - `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 $v_1 {v_2}^t$ 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)` $= \boldsymbol{v_i}$ with $\boldsymbol{A}\boldsymbol{v_i} = \lambda_i \boldsymbol{v_i}$ and $\lambda_1 > ... > \lambda_i > ... > \lambda_N$

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

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.

3.1 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).

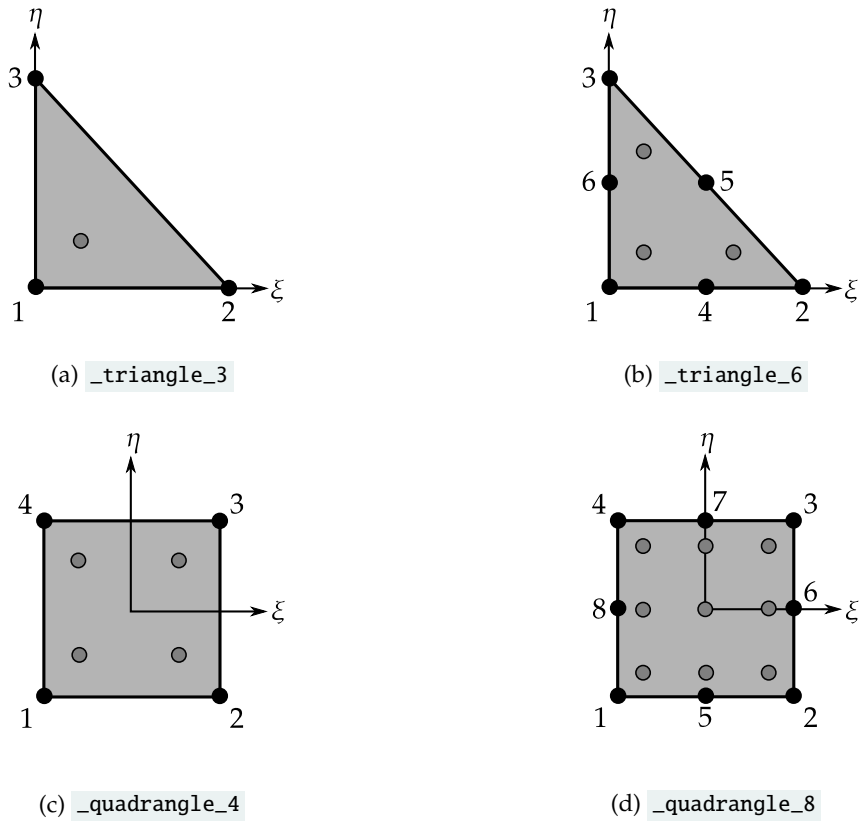
Element type	Order	# nodes	# quad. points
`_segment_2`	linear	2	1
`_segment_3`	quadratic	3	2

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`

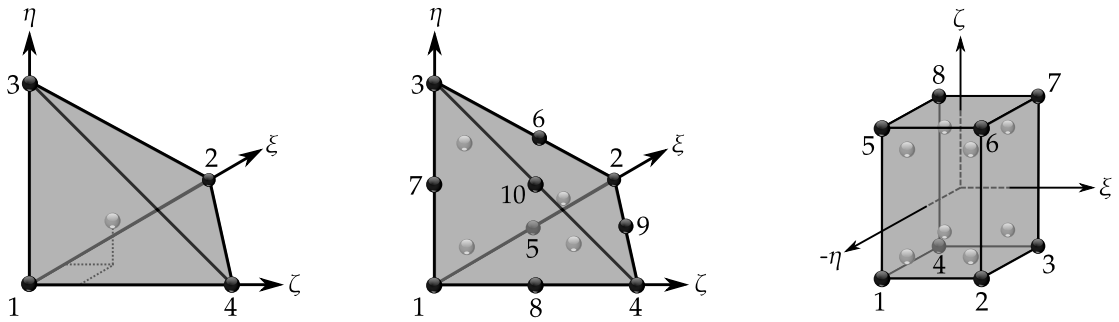
Figure 3.2: Schematic overview of the four 2D element types in **Akantu**. In each element, the node numbering as used in **Akantu** is indicated and also the quadrature points are highlighted (gray circles).

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**.

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.



(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 Cohesive Elements

The cohesive elements that have been implemented in **Akantu** are based on the work of Ortiz and Pandolfi [**?**]. 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 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 4.4.6.

Extrinsic cohesive elements are dynamically inserted between two standard elements when

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

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

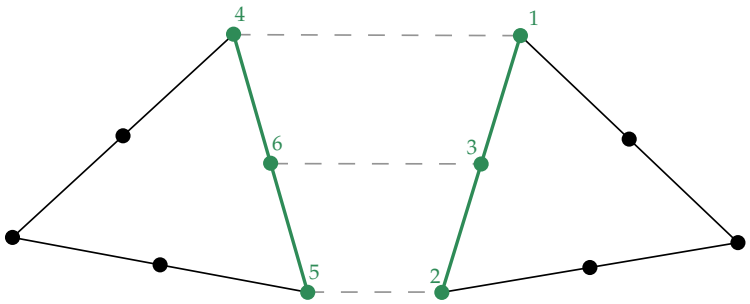


Figure 3.4: Cohesive element in 2D for quadratic triangular elements T6.

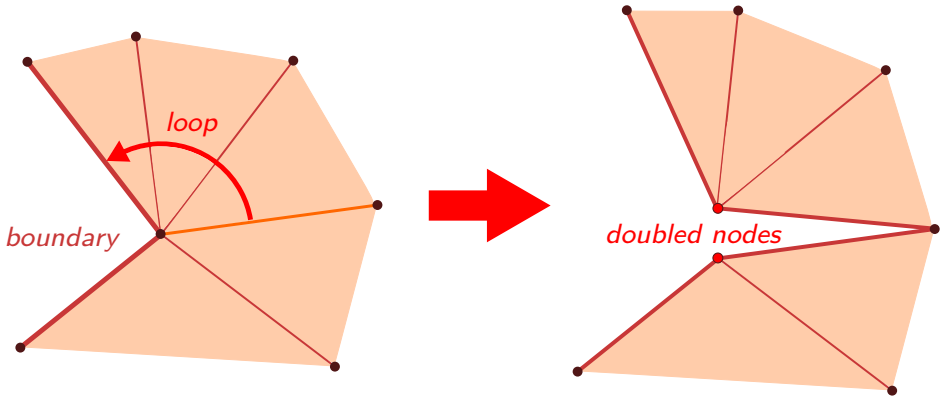


Figure 3.5: Insertion of a cohesive element.

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:

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

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

$$\boldsymbol{U} = \begin{bmatrix} u_0 & v_0 & u_1 & v_1 & u_2 & v_2 & u_3 & v_3 & u_4 & v_4 & u_5 & v_5 \end{bmatrix} \tag{3.3}$$

$$\boldsymbol{A} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} \tag{3.4}$$

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

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).

3.3 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.*

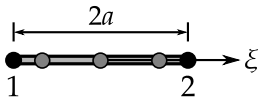


Figure 3.6: Schematic depiction of a Bernoulli beam element (applied to 2D and 3D) in **Akantu**. The node numbering as used in **Akantu** is indicated, and also the quadrature points are highlighted (gray circles).

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 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.

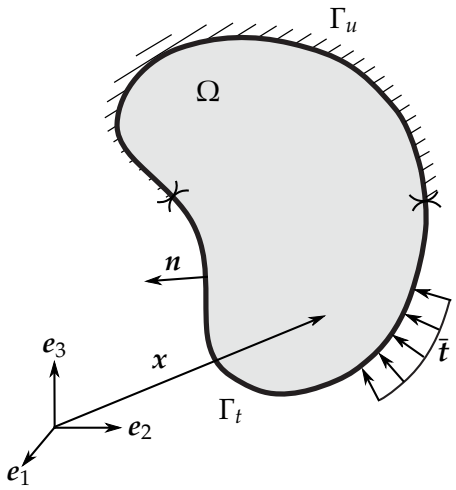


Figure 4.1: Problem domain Ω with boundary in three dimensions. The Dirchelet and the Neumann regions of the boundary are denoted with Γ_u and Γ_t, respecitvely.

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 as shown in the following code:

```
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 displacement in x-direction
    blocked(i, 1) = true; //block displacement in y-direction
    disp(i, 0) = 0.; //fixed displacement in x-direction
    disp(i, 1)= 0.; //fixed displacement in y-direction
  }
}
```

Figure 4.2: Beam with fixed support.

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`. Boundary conditions 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:

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

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

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

model.applyBC(BC::Dirichlet::IncrementValue(13.0, BC::_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.

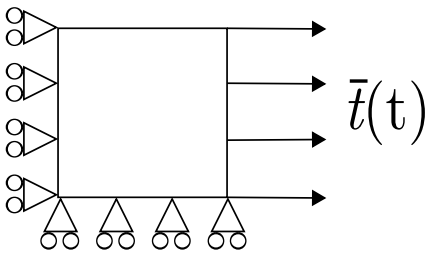


Figure 4.3: Plate on movable supports.

4.1.3 Material Selector

If the user wants to assign different materials to the different finite elements of choice 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 pyhsical 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:

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

where `tag_1` of the mesh file is used as the classifier index and the elements that have index value equal to one will be assigned to the second material in the material file.

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. However, for cohesive elements, it is not possible to assign multiple cohesive materials automatically and user has to write a custom class. **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`. This material selector first checks if an element is a cohesive element or a facet. If there is, then the first cohesive material in the material file is assigned to that element. Otherwise, this material is assigned to the element facet, to which, a cohesive element might be inserted later. Hence, this material selector works for the extrinsic cohesive elements which are dynamically inserted throughout the analysis. If the element of interest is not a cohesive element or an element facet, then `DefaultMaterialSelector` is used by default.

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.

4.1.4 Insertion of Cohesive Elements

Dynamics

As far as dynamic simulations are concerned, cohesive elements are currently compatible only with the explicit time integration scheme (see section 4.3.2). They do not have to be inserted when the mesh is generated but during the simulation. Intrinsic cohesive elements can be introduced at the beginning of the simulation as follows:

```
SolidMechanicsModelCohesive model(mesh);
model.initFull();
model.limitInsertion(_x, -1, 1);
model.insertIntrinsicElements();
```

where the insertion is limited to the facets whose barycenter's x coordinate is in the range $[-1, 1]$. Additional restrictions with respect to y and z directions can be added as well. Similarly the dynamic insertion of extrinsic cohesive elements can be utilized in the following way:

```
SolidMechanicsModelCohesive model(mesh);
model.initFull(SolidMechanicsModelCohesiveOptions(_explicit_lumped_mass,
  true));
model.limitInsertion(_x, -1, 1);
```

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

in which this time the method `limitInsertion` prevents the cohesive elements to be inserted out of the range $[-1, 1]$ in the x direction. In order to check stress and automatically insert elements, it is necessary to call the function `checkCohesiveStress` in the main loop where `solveStep` is:

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

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");
```

Statics

The only cohesive law that is applicable in this case is the exponential one (see section 4.4.6). However unloading-reloading cycles are not supported yet. In this case cohesive elements have to be inserted before creating the `SolidMechanicsModelCohesive` model:

```
Mesh mesh(spatial_dimension);
mesh.read("implicit_mesh.msh");

CohesiveElementInserter inserter(mesh);
inserter.setLimit(_y, 0.9, 1.1);
inserter.insertIntrinsicElements();

SolidMechanicsModelCohesive model(mesh);
model.initFull(SolidMechanicsModelCohesiveOptions(_static));
```

Also in this case the element insertion can be limited to a given range thanks to the method `setLimit`. The first input parameter of this method indicates the direction while the other two indicate the extreme values of the range $[0.9, 1.1]$. In order to compute the energies, the same functions illustrated for dynamics in the last section can be used.

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 or not.

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

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, 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.

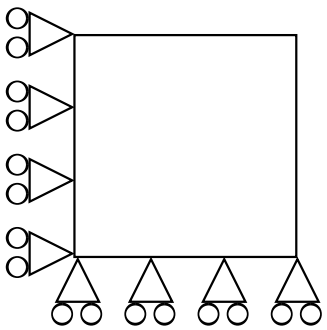


Figure 4.4: Numerical setup

The results of this analysis is depicted in Figure 4.5.

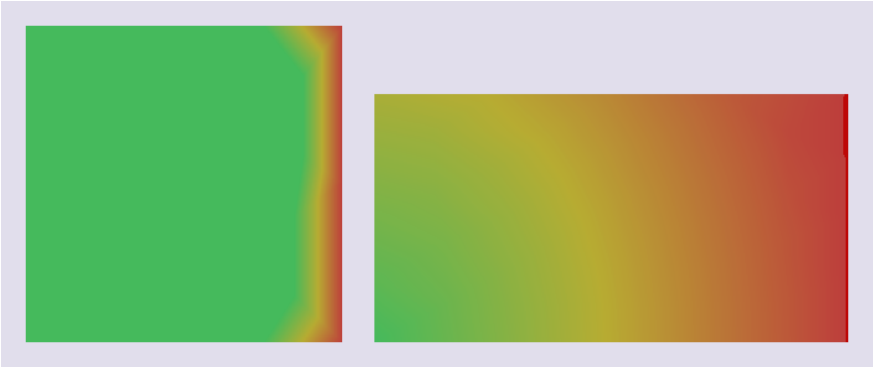


Figure 4.5: Solution of the static analysis. Left: the initial condition, right: the solution (deformation magnified 50 times)

4.3 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 [?] [?] 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:*

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

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, 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:

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

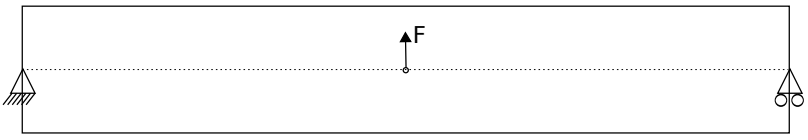


Figure 4.6: Numerical setup

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

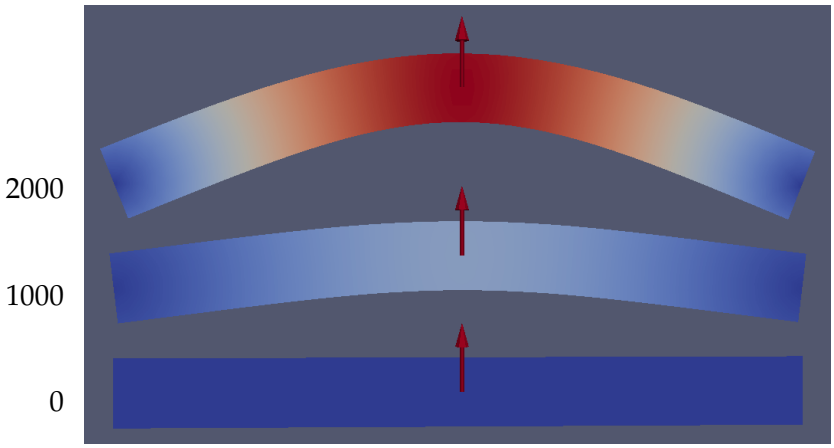


Figure 4.7: Deformed beam at 3 different times (displacement are magnified by a factor 10).

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:

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

The stable time step is defined as:

$$\Delta t_{\text{crit}} = \Delta x \sqrt{\frac{\rho}{2\mu + \lambda}} \tag{4.21}$$

where Δx is a characteristic length (*e.g.*, the inradius in the case of linear triangle element), μ and λ are the first and second Lame's coefficients and ρ is the density. The stable time step corresponds to the time the fastest wave (the compressive wave) needs to travel the characteristic length of the mesh. 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 = 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−β 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 $\dot{\boldsymbol{u}}^{\mathrm{p}}{}_{n+1}$, which will be used later in the method `model.explicitCorr()`. The equations are:

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

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

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

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

  Note: *The internal force $\boldsymbol{f}_{\mathrm{int}\,n+1}$ 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.

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.

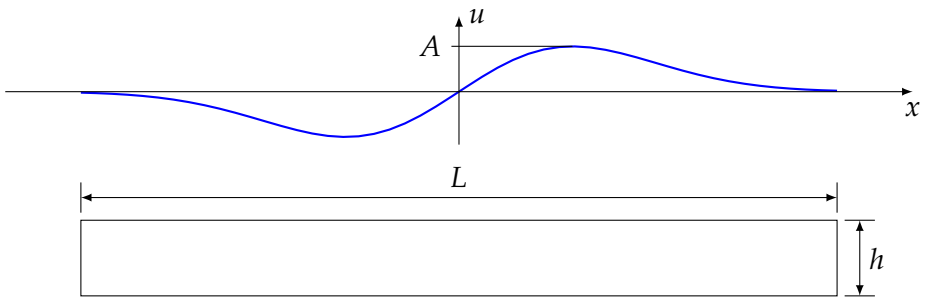


Figure 4.8: Numerical setup

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) in a text file (*e.g.*, material.dat) as follows:

```
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*. For example a non-local constitutive law can be flavored by a weight function. The file needs to be loaded in **Akantu** using the `initialize` method of **Akantu** (as shown in Section 2.3)

```
initialize("material.dat", argc, argv);
```

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 material 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 can be substituted with any number. Currently **Akantu** is can reproduce always the same distribution when the seed is specified *only* in serial.

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.

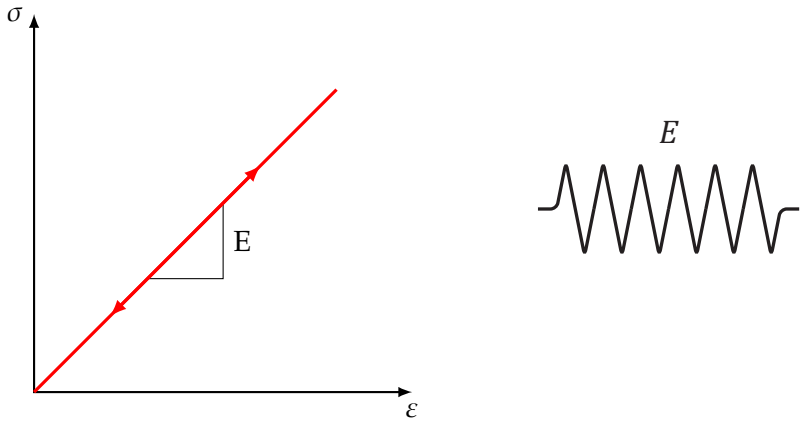
4.4.1 Elasticity

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



(a) (b)

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

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

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

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:

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

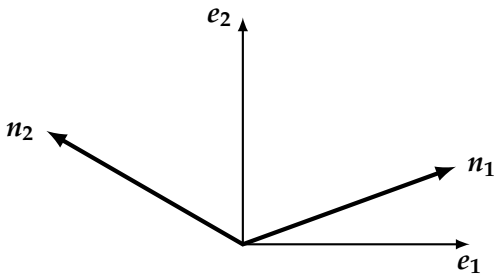


Figure 4.10: Material basis

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:

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

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

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

(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 poison 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.

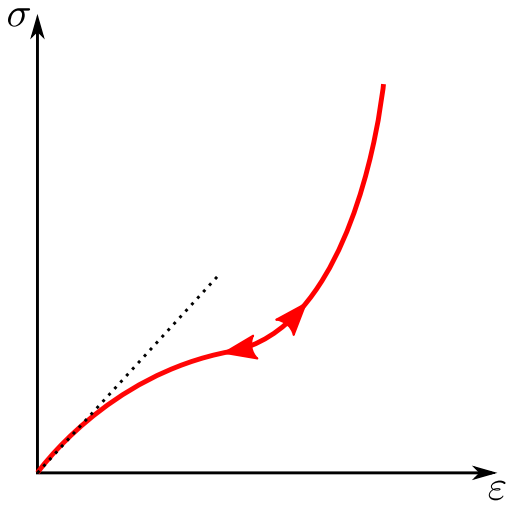


Figure 4.11: Neo-hookean Stress-strain curve.

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 [**?**].

The strain energy stored in the material is given by:

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

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 ($\boldsymbol{F} = \nabla_X \boldsymbol{x}$): $J = \det(\boldsymbol{F})$. 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 (σ) should be computed through the second Piola-Kirchhoff stress tensor $\boldsymbol{S}$:

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

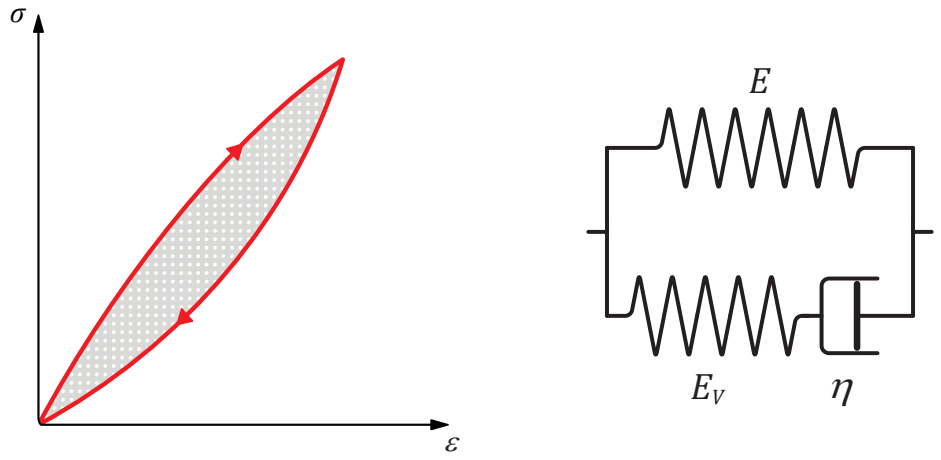
Finally the second Piola-Kirchhoff stress tensor is given by:

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

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



(a) (b)

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.

10.3 of [**?**]) 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` (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

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

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

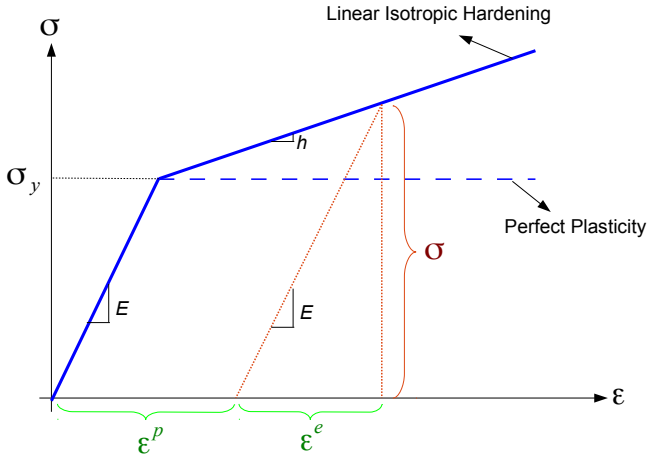


Figure 4.13: Stress-strain curve for the small-deformation plasticity with linear isotropic hardening.

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.

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

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

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

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

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 $\frac{\boldsymbol{\sigma}^{\text{tr}}}{\sigma_{\text{eff}}}$ 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:

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

6. Update the variables:

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

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

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 [**?**, **?**]. 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 [**?**] is a behavioral model to represent damage evolution in concrete. The governing variable in this damage law is the equivalent strain $\varepsilon_{\text{eq}} = \sqrt{< \boldsymbol{\varepsilon} >_+ : < \boldsymbol{\varepsilon} >_+}$, with $< . >_+$ the positive part of the tensor. The damage the is defined as:

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

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

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

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

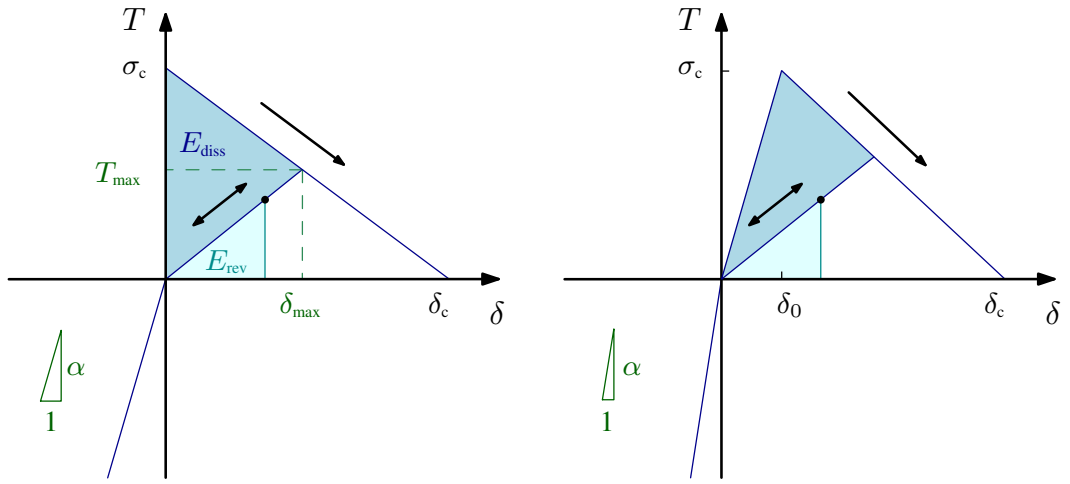
With κ_0 the damage threshold, A_t and B_t the damage parameter in traction, A_c and B_c the damage parameter in compression, β is the shear parameter. α_t is the coupling parameter between traction and compression, the ε_i are the eigenstrain and the $\varepsilon_{\text{nd}\, i}$ are the eigenvalues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

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

4.4.6 Cohesive laws

Linear Irreversible Law (B.10)

Akantu includes the Snozzi-Molinari [**?**] linear irreversible cohesive law (see Figure 4.14). It is an extension to the Camacho-Ortiz [**?**] 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



(a) Linear (b) Bilinear

Figure 4.14: Irreversible cohesive laws for explicit simulations.

is introduced:

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

where $G_{c,I}$ and $G_{c,II}$ 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:

$$\boldsymbol{T} = \left(\frac{\beta^2}{\kappa}\Delta_t \boldsymbol{t} + \Delta_n \boldsymbol{n}\right)\frac{\sigma_c}{\delta}\left(1 - \frac{\delta}{\delta_c}\right) = \hat{\boldsymbol{T}}\,\frac{\sigma_c}{\delta}\left(1 - \frac{\delta}{\delta_c}\right) \tag{4.70}$$

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 $\boldsymbol{\Delta}$, 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/`.

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 [**?**]. 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 δ_{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

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

where δ_f is a material parameter. 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.

Exponential Cohesive Law (B.11)

Ortiz and Pandolfi proposed this cohesive law in 1999 [**?**]. 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

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

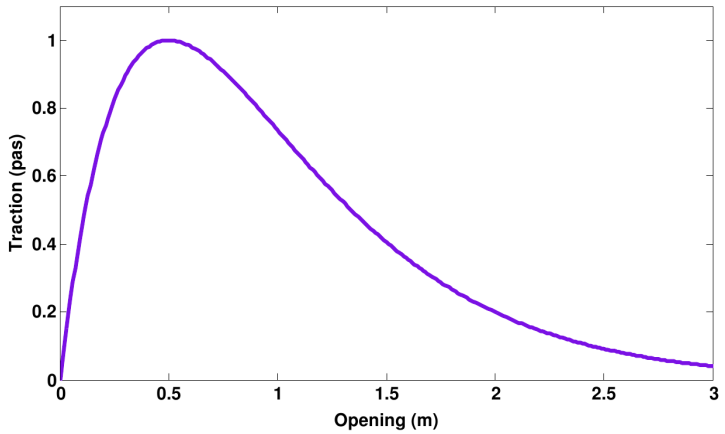


Figure 4.15: Exponential cohesive law

4.5 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:

$$\boldsymbol{\sigma} = \lambda \text{tr}(\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon} \tag{4.84}$$

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:

$$\boldsymbol{K} = \int \boldsymbol{B}^T \boldsymbol{D}(\boldsymbol{\varepsilon})\boldsymbol{B} \tag{4.85}$$

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.*

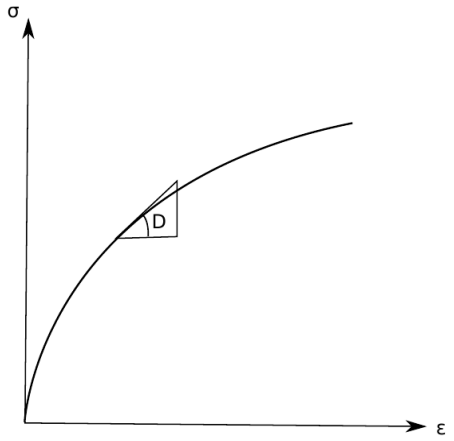


Figure 4.16: Tangent to the stress-strain curve.

- `getStableTimeStep`: The stable time step should be calculated based on (4.21) for the conditionally stable methods. This function depends on the longitudinal wave speed which changes for different materials and strains. Therefore, the value of this velocity should be defined in this method for each new material.

Note: *In case of need, the calculation of the longitudinal and shear wave speeds can be done in separate functions (* `getPushWaveSpeed` *and* `getShearWaveSpeed`*). Therefore, the first function can be called for calculation of the stable time step.*

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`.

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 [**?**]. 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`.

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.

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

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

where $\boldsymbol{K}$ is the global stiffness matrix, $\boldsymbol{u}$ the generalized displacement vector and $\boldsymbol{f}_{\text{ext}}$ 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 $\boldsymbol{f}_{\text{ext}}$ 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 $q = 6\,\text{kN}\,\text{m}^{-1}$, moment $\bar{M} = 3.6\,\text{kN}\,\text{m}$, moments of inertia $I_1 = 250\,000\,\text{cm}^4$ and $I_2 = 128\,000\,\text{cm}^4$ and lengths $L_1 = 10\,\text{m}$ and $L_2 = 8\,\text{m}$. The resulting rotations at node two and three are $\varphi_2 = 0.001\,167$ and $\varphi_3 = -0.000\,771$.

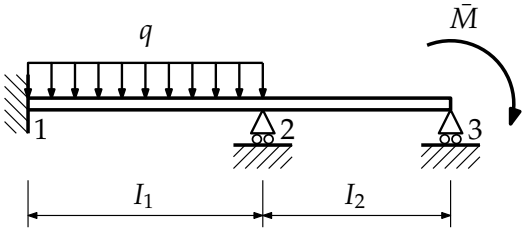


Figure 5.1: 2D beam example

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

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()
```

where a material file name has to be provided. 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 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* [**?**].

- 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 $8940\,kg/m^3$, a conductivity of $401\,W\,m^{-1}\,K^{-1}$ and a specific heat capacity of $385\,J\,K^{-1}\,kg^{-1}$. The time step used is $0.12\,s$.

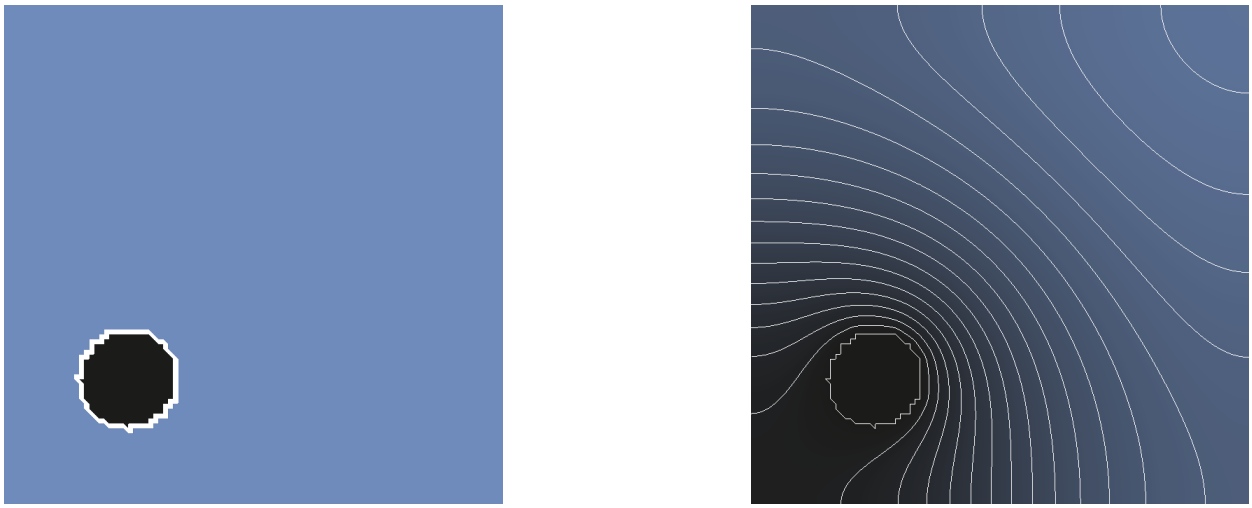


Figure 6.1: Initial temperature field (left) and after 15000 time steps = 30 minutes (right). The lines represent iso-surfaces.

Chapter 7

Input/Output

7.1 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` [?], `ViSit` [?] or `Mayavi` [?].

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");
...

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 2^{nd} 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 2^{nd} 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).

The user can also register external fields which have the same mesh as the mesh from the model as support. To do this, an object of type `Field` has to be created.

- For nodal fields :

```
Vector<T> vect(nb_nodes, nb_component);
Field field = new DumperIOHelper::NodalField<T>(vect));
model.addDumpFieldExternal("my_field", field);
```

- For elemental fields :

```
ElementTypeMapArray<T> arr;
Field field = new DumperIOHelper::ElementalField<T>(arr,
  spatial_displacement));
```

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

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

```
model.addDumpFieldExternal("my_field", field);
```

7.2 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");
```

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** [?] 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);
}
```

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

Contact

9.1 Implicit Contact Solver

The contact formulation corresponds to the augmented-Lagrangian method [**?**], which seeks to minimize the following energy functional between two bodies with contact interface $\Gamma_c^{(1)}$:

$$\Pi^{al}(\boldsymbol{u}, \lambda_N) := \sum_{i=1}^{2} \Pi^{(i)}(\boldsymbol{u}^{(i)}) + \int_{\Gamma_c^{(1)}} \left[\frac{1}{2\epsilon_N} \langle \lambda_N + \epsilon_N g \rangle^2 - \frac{1}{2\epsilon_N} \lambda_N^2 \right] d\Gamma, \tag{9.1}$$

where $\Pi^{(i)}$ corresponds to the energy functional of the i-th body in contact, which is a function of the displacement field $\boldsymbol{u}$ and the Lagrangian multiplier λ_N. In the equation above, ϵ_N is a penalty parameter, g the contact gap function, and $\langle \cdot \rangle$ the Macaulay bracket.

The solution procedure seeks to make the equation above stationary with respect to both $\boldsymbol{u}$ and λ_N:

$$\begin{aligned} 0 &= D_{\boldsymbol{u}} \Pi^{al} \cdot \boldsymbol{w} = G^{int,ext}(\boldsymbol{u}, \boldsymbol{w}) + \int_{\Gamma_c^{(1)}} \langle \lambda_N + \epsilon_N g \rangle \, \delta g \, d\Gamma \qquad \forall \boldsymbol{w} \in \mathcal{V} \\ 0 &= D_{\lambda} \Pi^{al} \cdot q_N = \frac{1}{\epsilon_N} \int_{\Gamma_c^{(1)}} \left[\langle \lambda_N + \epsilon_N g \rangle - \lambda_N \right] q_N \, d\Gamma \qquad \forall q_N \in \mathcal{M} \end{aligned} \tag{9.2}$$

A solution is then found by using Uzawa's method, for which we solve for $\boldsymbol{u}^{(k)}$, with $\lambda_N^{(k)}$ fixed:

$$G^{int,ext}(\boldsymbol{u}^{(k)}, \boldsymbol{w}) + \int_{\Gamma_c^{(1)}} \left\langle \lambda_N^{(k)} + \epsilon_N g(\boldsymbol{u}^{(k)}) \right\rangle \delta g \, d\Gamma = 0 \qquad \forall \boldsymbol{w} \in \mathcal{V}, \tag{9.3}$$

followed by an update of the multipliers on $\Gamma_c^{(1)}$:

$$\lambda_N^{(k+1)} = \left\langle \lambda_N^{(k)} + \epsilon_N g(\boldsymbol{u}^{(k)}) \right\rangle. \tag{9.4}$$

It is worth noting that the results of the implicit contact resolution depend largely on the choice of the penalty parameter ϵ_N. Depending on this parameter, the computational time needed to obtain a converged solution can be increased dramatically, or a convergence solution could not even be obtained at all.

The code provides a flag that allows the user to rely on an automatic value of ϵ_N for each slave node. Yet, this value should be used as a reference only, since for some problems it is actually overestimated and convergence cannot be obtained.

9.1.1 Implementation

In **Akantu**, the object that handles the implicit contact can be found in `implicit_contact_manager.hh`. The object that handles the implicit contact resolution stage is the class template

```
template <int dim, class model_type> struct ContactData;
```

This object takes the command line parameters during construction, which can be used to set up the behavior during contact resolution. The object can take the following parameters (default values in brackets):

-e	[auto]	Penalty parameter for augmented-Lagrangian formulation
-alpha	[1]	Multiplier for values of the penalty parameter
-utol	[0.001]	Tolerance used for multipliers in the Uzawa method
-ntol	[0.001]	Tolerance used in the Newton-Raphson inner convergence loop
-usteps	[100]	Maximum number of steps allowed in the Uzawa loop
-nsteps	[100]	Maximum number of steps allowed in the Newton-Raphson loop

Also, the following flags can be given to the command line

-dump	Dumping within Newton iterations
-v	Verbose output

The `ContactData` object stores the state of the contact mechanics simulation. The state is contained within the following variables:

`sm_`	slave-master map
`multipliers_`	Lagrange multiplier map
`areas_`	slave areas map
`penalty_`	penalty parameter map
`gaps_`	gap function map
`model_`	reference to solid mechanics model
`multiplier_dumper_`	structures used to dump multipliers
`pressure_dumper_`	structures used to dump pressure
`options_`	options map
`flags_`	flags map
`uiter_`, `niter_`	Uzawa and Newton iteration counters

The interface of the `ContactData` object contains three methods to solve for each contact step, which is overloaded depending on the parameters passed. Their signatures are as follows

```
void solveContactStep();

void solveContactStep(search_type *search);

template <class PostAssemblyFunctor>
void solveContactStep(search_type *search, const PostAssemblyFunctor& fn);
}
```

The second method allows the user to provide a pointer to an object that is used to search slave-master pairs. This can be done, for example, when due to the deformed configuration current slave-master pairs are no longer valid. The last method in the snippet above allows the user to provide a functor that is called after the assembly of the contact contributions to the stiffness matrix and the force vector. The last takes place within the method `computeTangentAndResidual()`.

Hertz Example

Here we outline, step by step, the use of the implicit contact solver to obtain the solution of Hertzian contact. The complete implementation can be found in `examples/contact/hertz_3D.cc`.

The following class is used as the object that will perform the search for new contact elements when a slave node is found to lie outside its master element. The class derives from a `SearchBase` class, and implements the virtual method `search`.

```
struct Assignator : public ContactData<3,SolidMechanicsModel>::SearchBase {
  typedef Point <3> point_type;
```

```
  typedef SolidMechanicsModel model_type;
  typedef ModelElement <model_type> master_type;

  model_type &model_;

  Assignator(model_type& model) : model_(model) {}

  virtual int search(const Real *ptr) {
    point_type p(ptr);

    ElementGroup &rs = model_.getMesh().getElementGroup("rigid_surface");

    for (ElementGroup::type_iterator tit = rs.firstType(); tit != rs.lastType
    (); ++tit)
      for (ElementGroup::const_element_iterator it = rs.element_begin(*tit);
           it != rs.element_end(*tit); ++it) {
        master_type m(model_, _triangle_3, *it);
        if (point_has_projection_to_triangle(p, m.point <3>(0), m.point <3>(1)
    , m.point <3>(2))) {
          return m.element;
        }
      }
    return -1;
  }
};
```

The first thing we do in the main file is to add some type definitions:

```
int main(int argc, char *argv[]) {

  // set dimension
  static const UInt dim = 3;

  // type definitions
  typedef Point <dim> point_type;
  typedef BoundingBox <dim> bbox_type;
  typedef SolidMechanicsModel model_type;
  typedef ModelElement <model_type> master_type;
  typedef ContactData <dim, model_type> contact_type;

  typedef std::chrono::high_resolution_clock clock;
  typedef std::chrono::seconds seconds;
```

We initialize the library, create a mesh, and set the solid mechanics model up:

```
  initialize("steel.dat", argc, argv);

  // create mesh
  Mesh mesh(dim);

  // read mesh
  mesh.read("hertz_3D.msh");

  // create model
  model_type model(mesh);
  SolidMechanicsModelOptions opt(_static);

  // initialize material
```

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

Then we create the contact data, which can be used to solve the contact problem. Note that some of the parameters required by the contact object can be coded in the implementation file (these can also be passed as arguments).

```
// create data structure that holds contact data
contact_type cd(argc, argv, model);

// optimal value of penalty multiplier
cd[Alpha] = 0.05;
cd[Uzawa_tol] = 1.e-2;
cd[Newton_tol] = 1.e-2;
```

Next we find the area that corresponds to each slave node. For this we use the fact that if we apply a unit distributed load over the contact surface, the resulting force vector at each slave node has magnitude that is equal to the area.

```
// get physical names from Gmsh file
mesh.createGroupsFromMeshData <std::string>("physical_names");

// get areas for the nodes of the circle
// this is done by applying a unit pressure to the contact surface elements
model.applyBC(BC::Neumann::FromHigherDim(Matrix <Real>::eye(3, 1.)), "
  contact_surface");
Array <Real>& areas = model.getForce();

// loop over contact surface nodes and store node areas
ElementGroup &eg = mesh.getElementGroup("contact_surface");
cout << "- Adding areas to slave nodes. " << endl;
for (auto nit = eg.node_begin(); nit != eg.node_end(); ++nit) {
  // compute area contributing to the slave node
  Real a = 0.;
  for (UInt i = 0; i < dim; ++i)
    a += pow(areas(*nit, i), 2.);
  cd.addArea(*nit, sqrt(a));
}

// set force value to zero
areas.clear();
```

Note that we clear the force vector after the assignment of areas.
In the next step we prescribe the boundary conditions that do not change in time:

```
// apply boundary conditions for the rigid plane
model.applyBC(BC::Dirichlet::FixedValue(0., BC::_x), "bottom_body");
model.applyBC(BC::Dirichlet::FixedValue(0., BC::_y), "bottom_body");
model.applyBC(BC::Dirichlet::FixedValue(0., BC::_z), "bottom_body");

// block z-disp in extreme points of top surface
model.getBoundary()(1, 2) = true;
model.getBoundary()(2, 2) = true;

// block x-disp in extreme points of top surface
model.getBoundary()(3, 0) = true;
model.getBoundary()(4, 0) = true;
```

Next we add the slave-master pairs for the analysis. We use a bounding box to consider only a fraction of the slave nodes in the model. Those slave nodes that are not within the bounding box are not considered in the analysis:

```
// set-up bounding box to include slave nodes that lie inside it
Real l1 = 1.;
Real l2 = 0.2;
Real l3 = 1.;
point_type c1(-l1 / 2, -l2 / 2, -l3 / 2);
point_type c2(l1 / 2,  l2 / 2,  l3 / 2);
bbox_type bb(c1, c2);

// search policy for slave-master pairs
Assignator a(model);


// loop over nodes in contact surface to create contact elements
cout << "- Adding slave-master pairs" << endl;
for (auto nit = cs.node_begin(); nit != cs.node_end(); ++nit) {
  point_type p(&coords(*nit));

  // ignore slave node if it doesn't lie within the bounding box
  if (!(bb & p))
    continue;

  int el = a.search(&coords(*nit));
  if (el != -1)
    cd.addPair(*nit, master_type(model, _triangle_3, el));
}
```

We then start the loop over displacement increments, and at each step we call solveContactStep and save the displacement, resulting force, and maximum pressure, in an array that will be used to print the results at the end of the simulation:

```
const size_t steps = 30;
Real data[3][steps]; // store results for printing
Real step = 0.001;  // top displacement increment
size_t k = 0;

for (Real delta = 0; delta <= step * steps; delta += step) {
  // apply displacement to the top surface of the half-sphere
  model.applyBC(BC::Dirichlet::FixedValue(-delta, BC::_y), "top_surface");

  // solve contact step, this method also dumps Paraview files
  cd.solveContactStep(&a);

  data[0][k] = delta;
  data[1][k] = cd.getForce();
  data[2][k] = cd.getMaxPressure();
  ++k;
}
```

The last portion of the output of code above is as follows:

```
  Disp.         Force  Max pressure
     0             0             0
 0.001          1.29     6.068e+04
```

0.002	6.702e+06	6.78e+09
0.003	1.832e+07	9.453e+09
0.004	3.349e+07	1.091e+10
0.005	5.2e+07	1.171e+10
0.006	7.211e+07	1.298e+10
0.007	9.377e+07	1.481e+10
0.008	1.183e+08	1.624e+10
0.009	1.41e+08	1.616e+10
0.01	1.7e+08	1.688e+10
0.011	1.963e+08	1.678e+10
0.012	2.263e+08	1.758e+10
0.013	2.581e+08	1.805e+10
0.014	2.907e+08	1.821e+10
0.015	3.244e+08	1.877e+10
0.016	3.593e+08	1.954e+10
0.017	4.051e+08	2.131e+10
0.018	4.317e+08	2.115e+10
0.019	4.823e+08	2.201e+10
0.02	5.237e+08	2.315e+10
0.021	5.639e+08	2.379e+10
0.022	6.058e+08	2.405e+10
0.023	6.483e+08	2.485e+10
0.024	6.917e+08	2.536e+10
0.025	7.363e+08	2.854e+10
0.026	7.681e+08	3.099e+10
0.027	8.332e+08	3.291e+10
0.028	8.577e+08	3.399e+10
0.029	9.281e+08	3.426e+10

The following figure shows the deformed state of the half-sphere at the end of the simulation, together with the contact pressure distribution:

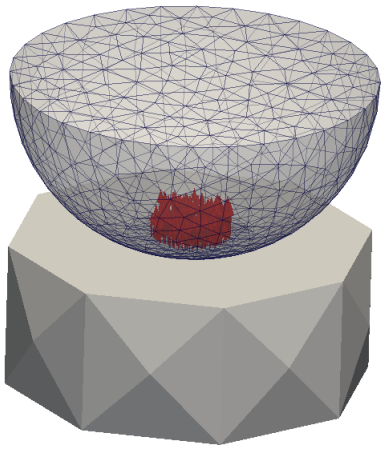


Figure 9.1: State of pressure and deformation at the end of the simulation of the example of Hertz in 3D.

Appendix A

Shape Functions

Schmatic overview of all the element types defined in **Akantu** is described in Chapter 3. 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 Chapter 3.

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. $(\xi\ ,\ \eta\ ,\ \zeta)$	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. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(\frac{1}{4}\ ,\ \frac{1}{4}\ ,\ \frac{1}{4}\right)$
Weight	$\frac{1}{6}$

A.3.2 Tetrahedron 10

Element properties

Node (i)	Coord. $(\xi\ ,\ \eta\ ,\ \zeta)$	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. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(\frac{(5-\sqrt{5})}{20}\ ,\ \frac{(5-\sqrt{5})}{20}\ ,\ \frac{(5-\sqrt{5})}{20}\right)$	$\left(\frac{(5+3\sqrt{5})}{20}\ ,\ \frac{(5-\sqrt{5})}{20}\ ,\ \frac{(5-\sqrt{5})}{20}\right)$
Weight	1/24	1/24
Coord. $(\xi\ ,\ \eta\ ,\ \zeta)$	$\left(\frac{(5-\sqrt{5})}{20}\ ,\ \frac{(5+3\sqrt{5})}{20}\ ,\ \frac{(5-\sqrt{5})}{20}\right)$	$\left(\frac{(5-\sqrt{5})}{20}\ ,\ \frac{(5-\sqrt{5})}{20}\ ,\ \frac{(5+3\sqrt{5})}{20}\right)$
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

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

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 (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
- `S`: (*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: 4.4.6
Parameters:

- `sigma_c`: (*Real*) Critical stress σ_c
- `delta_c`: (*Real*) Critical displacement δ_c
- `beta`: (*Real*) β parameter
- `G_c`: (*Real*) Mode I fracture energy
- `kappa`: (*Real*) κ parameter
- `penalty`: (*Real*) penalty coefficient α

B.10 Cohesive bilinear

Keyword: `cohesive_bilinear`
Description here: 4.4.6
Parameters:

- `sigma_c`: (*Real*) Critical stress σ_c
- `delta_c`: (*Real*) Critical displacement δ_c
- `beta`: (*Real*) β parameter
- `G_c`: (*Real*) Mode I fracture energy
- `kappa`: (*Real*) κ parameter
- `penalty`: (*Real*) Penalty coefficient α
- `delta_0`: (*Real*) Elastic limit displacement δ_0

B.11 Cohesive exponential

Keyword: `cohesive_exponential`
Description here: 4.4.6
Parameters:

- `sigma_c`: (*Real*) Critical stress σ_c
- `delta_c`: (*Real*) Critical displacement δ_c
- `beta`: (*Real*) β parameter

B.12 Cohesive linear fatigue

Keyword: `cohesive_linear_fatigue`
Description here: 4.4.6
Parameters:

- `sigma_c`: (*Real*) Critical stress σ_c
- `delta_c`: (*Real*) Critical displacement δ_c
- `beta`: (*Real*) β parameter
- `G_c`: (*Real*) Mode I fracture energy
- `kappa`: (*Real*) κ parameter
- `penalty`: (*Real*) penalty coefficient α
- `delta_f`: (*Real*) Characteristic opening displacement δ_f

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.

To have the complete documentation you should compile it in your build folder by activating the option `AKANTU_DOCUMENTATION_MANUAL`