AMIE configuration guide

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This document shows how to write initiation files for AMIE. These files can be used to set up variables in simulations without re-compiling the main executable. An example of initiation file usage in AMIE can be found in the main_2d_composite example.

Contents

1 First example

```
# first AMIE configuration file
.sample
..height = 0.1
..width = 0.1
..behaviour
...type = PASTE_BEHAVIOUR
.stepping
..time\_step = 0.1
..number_of_time_steps = 1
.discretization
..sampling_number = 8
..order = LINEAR
.boundary_condition
..condition = FIX_ALONG_XI
..position = LEFT
.boundary_condition
..condition = FIX_ALONG_ETA
..position = BOTTOM
.boundary_condition
..condition = SET_STRESS_ETA
..position = TOP
..value = -1e6
.output
..file_name = output_file
..time_step
...at = ALL
..field = REAL_STRESS_FIELD
..field = STRAIN_FIELD
.export
..file_name = export_mesh_file
..time_step
```

```
...at = ALL
..field = REAL_STRESS_FIELD
..field = STRAIN_FIELD
```

Here is a step-by-step explanation of the content of the file.

1.1 Comment

```
# first AMIE configuration file
```

Everything located on the same line after a # character is considered a comment and will not be accounted for in a simulation. A comment can either start a new line as in the example shown, or be inserted at the end of an existing line.

1.2 Sample definition

```
.sample
..height = 0.1
..width = 0.1
..behaviour
...type = PASTE_BEHAVIOUR
```

Here, we define the box in which the simulation will be carried out. The box is a rectangle of the specified height and width (centered on the point (0,0) if not specified otherwise). The mechanical behaviour of the box is a predefined behaviour corresponding to cement paste.

1.3 Time-stepping parameters

```
.stepping
..time_step = 0.1
..number_of_time_steps = 1
```

Here, we define the number of time steps we want to perform as well as the duration (in days) of each time step.

1.4 Mesh generation parameters

```
.discretization
..sampling_number = 8
..order = LINEAR
```

Here, we define the parameters used to generate the mesh and the subsequent finite element discretization. The mesh will be generated with 8 nodes on each edge of the sample, and we use linear shape functions for the finite element approximation.

1.5 Boundary conditions

```
.boundary_condition
..condition = FIX_ALONG_XI
..position = LEFT
.boundary_condition
..condition = FIX_ALONG_ETA
```

```
..position = BOTTOM
.boundary_condition
..condition = SET_STRESS_ETA
..position = TOP
..value = -1e6
```

Here, we define three boundary conditions. The first condition sets to zero the horizontal displacement (axis XI) of the left edge of the sample. The second conditions sets to zero the vertical displacement (axis ETA) of the bottom edge of the sample. The third condition imposes a stress on the upper edge of the sample. The negative value of the load indicates a compression.

1.6 Output

```
.output
..file_name = output_file
..time_step
...at = ALL
..field = REAL_STRESS_FIELD
..field = STRAIN_FIELD
```

Here, we define that the average real stress and average strain field values will be extracted from the simulation and written in a text file at all time steps of the simulation. This will open a file named output_file and write the following table:

```
0.1 -5.30733 999998 -1015.52 -2.51262e-05 8.37528e-05 -1.09992e-07
```

Each line corresponds to a time step of the simulation. The first column corresponds to the current instant, the three following columns are the three components of the average stress in the sample (ordered as σ_{xx} , σ_{yy} and σ_{xy}), and the three last columns are the three components of the average strain in the sample (ordered as ϵ_{xx} , ϵ_{yy} and ϵ_{xy}).

Note that if output_file already exists, its content will be overwritten.

1.7 Export

```
.export
..file_name = export_mesh_file
..time_step
...at = ALL
..field = REAL_STRESS_FIELD
..field = STRAIN_FIELD
```

Here, we choose to write mesh files containing the deformed state of the sample, as well as the real stress and the strain fields, and that such files will be written at each time step of the simulation. For the present simulation, three files will be generated:

```
export_mesh_file_header
export_mesh_file_1.svg
export_mesh_file_1
```

The header file contains simply a list of all non-SVG files generated. That is:

```
export_mesh_file_1
```

The SVG file contains eight snapshots of the mesh ordered vertically: two for the displacements components, three for the stress components, and three for the strain components.

The last file contains raw information for use of AMIE in-house viewer.

As for the output files, if any of these files already exist, their content will be overwritten.

1.8 Important remarks on file naming

The following remarks apply to any file name called in the configuration file (either as an input or output file):

- Do not use white spaces in the file path. Any white space is ignored during parsing.
- For Windows users, use / as a folder separator instead of \. AMIE does the conversion automatically.

2 Managing inclusions

2.1 First example

```
# example AMIE configuration file with inclusions
.sample
..height = 0.1
..width = 0.1
..behaviour
...type = PASTE_BEHAVIOUR
.stepping
..time\_step = 0.1
..number_of_time_steps = 1
.discretization
..sampling_number = 8
..order = LINEAR
.inclusions
..particle_size_distribution
...type = CONSTANT
...rmax = 0.005
\dotsnumber = 100
..geometry
...type = CIRCLE
..placement
\dotsspacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
.boundary_condition
..condition = FIX_ALONG_XI
..position = LEFT
.boundary_condition
..condition = FIX_ALONG_ETA
..position = BOTTOM
```

```
.boundary_condition
..condition = SET_STRESS_ETA
..position = TOP
..value = -1e6
.output
..file_name = output_file
..time_step
...at = ALL
..field = REAL_STRESS_FIELD
..field = STRAIN_FIELD
.export
..file_name = export_mesh_file
..time_step
...at = ALL
..field = REAL_STRESS_FIELD
..field = STRAIN_FIELD
```

This file is essentially identical to the first, except that the following lines have been added:

```
.inclusions
..particle_size_distribution
...type = CONSTANT
...rmax = 0.008
...number = 100
...fraction = 0.5
..geometry
...type = CIRCLE
..placement
...spacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
```

This defines a set of circular inclusions of a radius of 8 mm each. Inclusions will be generated until either 100 of them have been created, or until they cover at least 50 % of the surface of the sample. They will be randomly placed in the sample with at least 1 mm between each particle. The placement algorithm will try 1000 iterations; any particle not placed in the sample after these 1000 iterations will be left out and ignored. The particles are attributed a predefined mechanical behaviour which corresponds to aggregates used in concrete.

AMIE comes with several analytic particle size distributions. Instead of CONSTANT, one of the following curves can be used:

```
...type = BOLOME_A # upper Bolome curve (contains more fine)
...type = BOLOME_B # middle Bolome curve
...type = BOLOME_C # lower Bolome curve (contains more coarse)
...type = BOLOME_D # Bolome curve adapted for mortar
```

2.2 Defining a custom particle size distribution

Custom particle size distribution can be defined in external files, and then imported in AMIE, as in the following example:

```
.inclusions
..particle_size_distribution
...type = FROM_CUMULATIVE_FILE
...file_name = ../examples/data/composite/psd_example.txt
...rmax = 0.008
...number = 100
...fraction = 0.5
..geometry
...type = CIRCLE
..placement
...spacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
```

The file ../examples/data/composite/psd_example.txt contains a two-columns table, the second column being a set of decreasing radii, and the first column the percentage of aggregates with a radius smaller than the current radius. The particle size distribution is then linearly interpolated between these points.

```
100.0 0.008

70.0 0.004

30.0 0.0025

10.0 0.00125

1.0 0.00075

0 0.0005
```

2.3 Importing pre-placed inclusions

If you already have a file containing a list of inclusions with their center and radius, you can easily import the file using the following syntax:

```
.inclusions
..particle_size_distribution
...type = FROM_INCLUSION_FILE
...file_name = ../examples/data/composite/inclusion_example.txt
...number = 5
...column = center_x
...column = center_y
...column = radius
..geometry
...type = CIRCLE
..behaviour
...type = AGGREGATE_BEHAVIOUR
```

Where ../examples/data/composite/inclusion_example.txt contains a table with three columns, the first being the x coordinate of the center of each inclusion, the second the y coordinate, and the third the

radius. The order in which the columns are defined is relevant!

```
0 0 0.008
0.04315 -0.017 0.007
0.025 0.027 0.006
-0.015 -0.001 0.005
-0.015 0.044 0.004
```

Note that since the file already contains the position of the inclusions, we don't need to place them. Therefore the parent inclusions object does not contain a placement object in this specific case.

2.4 Using ellipses

Ellipses can be generated instead of circles using the geometry object:

```
.inclusions
..particle_size_distribution
...type = CONSTANT
...rmax = 0.008
...number = 100
...fraction = 0.5
..geometry
...type = ELLIPSE
...aspect_ratio = 0.7
...orientation = 3.141592
..placement
...spacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
```

This will generate ellipses with an aspect ratio of 0.7, and the same area as a 8mm radius circle. For each ellipse, the angle of the major axis with the horizontal axis XI will be randomly determined to a value between 0 and orientation. Therefore, if orientation = 0, all ellipses will be aligned with the horizontal axis.

Alternatively, ellipses can be imported from a file using the following syntax:

```
.inclusions
..particle_size_distribution
...type = FROM_INCLUSION_FILE
...file_name = ../examples/data/composite/ellipsoidal_inclusion_example.txt
...number = 5
...column = center_x
...column = center_y
...column = radius_a
...column = radius_b
...column = axis_x
...column = axis_y
..geometry
...type = ELLIPSE
```

```
...behaviour
...type = AGGREGATE_BEHAVIOUR
```

Where radius_a and radius_b are the values of the major and minor radii of the ellipses, axis_x and axis_y are coordinates of the direction of the major axis of the ellipse. Therefore, axis_x = 1 and axis_y = 0 define an ellipse aligned with the horizontal axis, while axis_x = 0 and axis_y = 1 define an ellipse aligned with the vertical axis.

2.5 Controlling the placement of inclusions

By default, the inclusions will be placed inside the sample, and so that they do not intersect the edges of the sample. However, it is possible to select a larger (or smaller) box in which to generate the inclusions. For example, this would be used to simulate microstructure from cored concrete. The following example places the inclusions in a slightly larger box:

```
.inclusions
..particle_size_distribution
...type = CONSTANT
...rmax = 0.008
\dotsnumber = 100
\dotsfraction = 0.5
..geometry
...type = CIRCLE
..placement
\dotsspacing = 0.001
...tries = 1000
...box
\dotswidth = 0.11
\dotsheight = 0.11
..behaviour
...type = AGGREGATE_BEHAVIOUR
```

The relative position of the placement box with the sample can also be adjusted by defining its center. The following example will move the placing box to the right side of the sample, leaving the left side empty.

```
...box
...width = 1
...height = 1
...center
....x = 0.5
....y = 0
```

Note that by default, the sample is centered on (0,0), but this can be adjusted with a similar syntax.

When you place the particles in a different box than the sample, the target fraction of inclusions generated corresponds to a fraction of the placement box, and not on the sample itself. Variations can occur depending on the characteristics of your particle size distribution and the relative size of the sample and the placement box.

2.6 Creating several families of inclusions

You can create within the same sample different particles, with different behaviours and different particle sizes distributions. For example, the following code will create two families of inclusions: one set of large inclusions corresponding to aggregates, and a second set of inclusions, with a smaller radius, and a void behaviour (which could for example simulate pores).

```
.inclusions
..particle_size_distribution
...type = CONSTANT
...rmax = 0.008
\dotsnumber = 100
\dotsfraction = 0.4
..geometry
...type = CIRCLE
..placement
\dotsspacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
.inclusions
..particle_size_distribution
...type = CONSTANT
...rmax = 0.001
\dotsnumber = 1000
\dotsfraction = 0.4
..geometry
...type = CIRCLE
..placement
...spacing = 0.0001
...tries = 10000
..behaviour
...type = VOID_BEHAVIOUR
```

The inclusions from the second family are placed after the inclusions in the first family, in the remaining space of the sample. The inclusions of the two families will not overlap nor intersect. Therefore, swapping the position of the second and the first family would yield very different microstructures.

You can define with this method as many families of inclusions as necessary.

2.7 Creating inclusions in inclusions

You can create families of inclusions within an existing family of inclusion with the following syntax:

```
.inclusions
..particle_size_distribution
...type = CONSTANT
...rmax = 0.008
...number = 100
...fraction = 0.4
..geometry
...type = CIRCLE
```

```
..placement
\dotsspacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
..inclusions
...particle_size_distribution
....type = CONSTANT
....rmax = 0.005
\dotsnumber = 1000
\dotsfraction = 0.4
...geometry
....type = CIRCLE
...placement
\dotsspacing = 0.0001
....tries = 10000
...behaviour
....type = VOID_BEHAVIOUR
```

This is very similar to the previous example, except that here the pores will be placed inside the aggregates (and not outside).

You can have several families of inclusions at the same level, and as many embedded families of inclusions as you wish. Structures of the following type are acceptable:

```
.inclusions
# family A placed in the sample
..inclusions
# family B within family A
...inclusions
# family C within family B
...inclusions
# family D within family B
..inclusions
# family E within family A
.inclusions
# family F placed in the sample
```

2.8 Creating concentric inclusions

You can create concentric inclusions inside an existing family of inclusions with the following syntax:

```
.inclusions
# family A
..particle_size_distribution
...type = CONSTANT
...rmax = 0.008
...number = 100
...fraction = 0.4
..geometry
...type = CIRCLE
```

```
..placement
...spacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
..inclusions
# family B within family A
...particle_size_distribution
...type = FROM_PARENT_DISTRIBUTION
...layer_thickness = 0.001
...behaviour
....type = VOID_BEHAVIOUR
```

This will generate one inclusion inside all the inclusions of the family A, with a difference in radius equal to layer_thickness. Inclusions of the family A with a radius lower than layer_thickness will not spawn an inner inclusion.

This feature can also make use of AMIE functions using layer_thickness_function (the x coordinate will be set as the radius of the parent distribution). The definition below is therefore equivalent to the definition above:

```
.inclusions
# family A
..particle_size_distribution
...type = CONSTANT
...rmax = 0.008
\dotsnumber = 100
\dotsfraction = 0.4
..geometry
...type = CIRCLE
..placement
\dotsspacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
..inclusions
# family B within family A
...particle_size_distribution
....type = FROM_PARENT_DISTRIBUTION
....layer_thickness_function = "x 0.005 -"
...behaviour
....type = VOID_BEHAVIOUR
```

2.9 Combining the different techniques

All of the previous features can be combined one with another to generate arbitrarily complex microstructures. However, be mindful of the following:

- Inclusions imported from a pre-generated file (with FROM_INCLUSION_FILE) will be placed even if they overlap or intersect with existing inclusions. However, inclusions placed after the imported family will check overlap and intersection with the pre-generated family.
- Concentric inclusions are not meant to be used with ellipses.

• When placing inclusions in a box different than the sample, the fraction parameter corresponds to a fraction of the placement box, not the sample.

3 Adapting the mesh parameters

The mesh is mostly controlled by the sampling_number in the discretization object, yet further refinement can be achieved.

3.1 Avoid the meshing of the smallest inclusions

Sometimes, meshing the smallest inclusions can yield meshes with elongated elements. This can be avoided by not meshing these inclusions, using the sampling_restiction parameter. This example will not mesh inclusions with less than 4 points along their boundary. Acceptable values are 4, 8 and 16.

```
.discretization
..sampling_number = 8
..order = LINEAR
..sampling_restriction = SAMPLE_RESTRICT_4
```

3.2 Changing the mesh density in specific inclusions

It is possible to modify the mesh density in whole families of inclusions by adding a sampling_factor in the definition of the inclusions. The following example multiplies by two the mesh density in all inclusions defined here.

```
.inclusions
# family A of inclusions ..particle_size_distribution
...type = CONSTANT
...rmax = 0.008
...number = 100
...fraction = 0.5
..geometry
...type = CIRCLE
..placement
...spacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
..sampling_factor = 2
```

sampling_factor is defined only for the current inclusions family. Inclusions from other families still use the non-modified mesh density, including the families of inclusions embedded in the current family.

It is possible to modify the mesh density only for the inclusions which intersects the edges of the sample by using intersection_sampling_factor. The following example will multiply by 3 the mesh density in the inclusions intersecting the edges of the samples, and by 2 the mesh density of the other inclusions.

```
.inclusions
# family A of inclusions ..particle_size_distribution
...type = CONSTANT
...rmax = 0.008
```

```
...number = 100
...fraction = 0.5
..geometry
...type = CIRCLE
..placement
...spacing = 0.001
...tries = 1000
..behaviour
...type = AGGREGATE_BEHAVIOUR
..sampling_factor = 2
..intersection_sampling_factor = 3
```

3.3 Changing the mesh density in the matrix

The mesh density can be changed inside the matrix (that is, outised of any inclusion) by adding a sampling_factor to the main sample of the simulation:

```
.sample
..height = 0.1
..width = 0.1
..behaviour
...type = PASTE_BEHAVIOUR
..sampling_factor = 2
```

4 Defining a time step

The easiest way to manage the time stepping is to use a constant time step. However, two other methods are also available.

4.1 Importing a list of time steps from a file

It is possible to read a text file containing a list of instants at which the simulation will be carried out using the following syntax:

```
.stepping
..list_of_time_steps = ../examples/data/composite/time_steps.txt
```

The series of instants must be strictly increasing; no time step must be equal to 0 (or lower).

4.2 Using a function of time

It is possible to define each time step as a function of the current time and the previous time step:

```
.stepping
..time_step = 0.1
..number_of_time_steps = 10
..next_time_step = "t 0.1 * x +"
```

When declaring such function, use x as the previous time step, and t as previous instant. The example above constructs the following series of $(t_n, \Delta t_n)$:

$$\Delta t_0 = 0.1 \tag{1}$$

$$t_0 = 0 (2)$$

$$\Delta t_{n+1} = \Delta t_n + 0.1 \ t_n \tag{3}$$

$$t_{n+1} = t_n + \Delta t_{n+1} \tag{4}$$

5 Defining boundary conditions

Boundary conditions can either be applied along an edge of the sample (LEFT, RIGHT, BOTTOM and TOP) or on a corner of the sample (BOTTOM_LEFT, BOTTOM_RIGHT, TOP_LEFT and TOP_RIGHT).

5.1 Boundary conditions in displacements

A displacement can be applied using the following syntax:

```
.boundary_condition
..condition = SET_ALONG_ETA
..position = TOP
..value = 0.001
```

Note that the condition FIX_ALONG_XI (respectively ETA) is equivalent to SET_ALONG_XI (respectively ETA) associated with the value 0.

5.2 Boundary conditions in stress

A stress can be applied using the following syntax:

```
.boundary_condition
..condition = SET_STRESS_ETA
..position = TOP
..value = 1e6
```

Stress boundary conditions should not be used on corners, but should be defined along an edge of a sample only.

5.3 Boundary conditions in force

A force can be applied using the following syntax:

```
.boundary_condition
..condition = SET_FORCE_ETA
..position = TOP
..value = 1e6
```

Force boundary conditions should be used on single points (like corners) rather than on surfaces.

5.4 Multiple boundary conditions at the same location

In general, boundary conditions in stress/force and in displacements should not be mixed on the same location (either edge or corner). Also, boundary conditions in stress/force stack, while boundary conditions in displacement on the same axis (XI or ETA) do not: only the latest defined is applied.

5.5 Time-dependent boundary conditions

There are three ways to define a time-dependent boundary condition. The easiest way is to define a rate. The following example will apply a loading rate of 0.1 MPa per day:

```
.boundary_condition
..condition = SET_STRESS_ETA
..position = TOP
..time_evolution
...rate = 1e5
```

One can also define a function of time t. The previous example can be rewritten as follow:

```
.boundary_condition
..condition = SET_STRESS_ETA
..position = TOP
..time_evolution
...function = "1e5 t *"
```

Finally, it is possible to import a file containing the values of the boundary condition at different instants:

```
.boundary_condition
..condition = SET_STRESS_ETA
..position = TOP
..time_evolution
...file_name = ../example/data/composite/time_dependent_load.txt
```

The file must contain two columns, the first being the time, the second the values of the boundary condition. The instants need not be equal to the time steps defined for the simulation. However, be aware that the value of the boundary condition is linearly interpolated between the instants defined in ../example/data/composite/time_dependent_load.txt. The first of the following examples defines a loading ramp, while the second defines a loading step:

```
0 0
1 1e6
2 1e6
0 0
0.99999 0
1 1e6
2 1e6
```

6 Defining behaviours

6.1 Using a pre-defined behaviour

A set of predefined behaviours exist in AMIE to represent common materials found in concrete. These can be used by choosing the appropriate type. The existing materials are listed below:

```
..type = VOID_BEHAVIOUR
..type = PASTE_BEHAVIOUR
..type = AGGREGATE_BEHAVIOUR
..type = ASR_GEL_BEHAVIOUR
..type = CONCRETE_BEHAVIOUR
..type = STEEL_BEHAVIOUR
..type = REBAR_BEHAVIOUR
```

For each of these, it is possible to ignore the default values for some (or all) of the parameters (young_modulus, poisson_ratio, etc) by declaring it again. The list of parameters for each behaviour is listed below with their default values:

```
.behaviour
.type = VOID_BEHAVIOUR

.behaviour
.type = PASTE_BEHAVIOUR
.young_modulus = 12e9
.poisson_ratio = 0.3
.short_term_creep_modulus = 0.3 # defined as a fraction of the elastic modulus
.long_term_creep_modulus = 0.37 # defined as a fraction of the elastic modulus
.tensile_strain_limit = 0.0003
.damage = TRUE
```

The creep properties of the cement paste are ignored if the simulation is not in space-time finite elements (see Using space-time finite elements). The boolean damage can be set to FALSE to run elastic (or viscoelastic) simulations.

```
.behaviour
..type = AGGREGATE_BEHAVIOUR
..young_modulus = 59e9
..poisson_ratio = 0.3
..tensile_strain_limit = 0.0012
..damage = TRUE

.behaviour
..type = ASR_GEL_BEHAVIOUR
..young_modulus = 22e9
..poisson_ratio = 0.18
..imposed_deformation = 0.22

.behaviour
..type = CONCRETE_BEHAVIOUR
..young_modulus = 37e9
..poisson_ratio = 0.3
```

```
..compressive_strength = -37e6
.behaviour
..type = STEEL_BEHAVIOUR
..young_modulus = 210e9
..poisson_ratio = 0.3
..tensile_strength = 276e6
.behaviour
..type = REBAR_BEHAVIOUR
..young_modulus = 59e9
..poisson_ratio = 0.3
..tensile_strength = 57000
```

6.2 Defining an elastic behaviour

A purely elastic behaviour can be defined as in the following example:

```
.behaviour
..type = ELASTICITY
..young_modulus = 10e9
..poisson_ratio = 0.3
```

Alternatively, you can define the material from the bulk and shear moduli. The material defined below is the same as the one defined above:

```
.behaviour
..type = ELASTICITY
..bulk_modulus = 8.3333e9
..poisson_ratio = 3.8461e9
```

However, you cannot mix both definition, and you must define the two selected parameters. You can add an imposed deformation with the following syntax:

```
.behaviour
..type = ELASTICITY_AND_IMPOSED_DEFORMATION
..young_modulus = 10e9
..poisson_ratio = 0.3
..imposed_deformation = 0.0001
```

6.3 Defining an elastic-and-damage behaviour

To use a damaging behaviour, two additional parameters must be set: the first one is a fracture_criterion which defines the failure surface of the material, possibly including its post-peak behaviour. The second one is a damage_model which defines how damage is resolved by AMIE. This can be achieved as in the following example:

```
.behaviour
..type = ELASTICITY_AND_FRACTURE
..young_modulus = 10e9
..poisson_ratio = 0.3
```

```
..fracture_criterion
...type = VON_MISES
...limit_tensile_stress = 1e6
..damage_model
...type = ISOTROPIC_LINEAR_DAMAGE
```

6.4 Defining a fracture criterion

Several types of fracture criteria are available in AMIE. The two mostly used are a Mohr-Coulomb and a Von Mises criteria. The Mohr-Coulomb criterion can furthermore be completed with different descending branches. Example definitions of these criteria are listed below:

```
..fracture_criterion
...type = MOHR_COULOMB
...limit_tensile_strain = 0.001
...limit_compressive_strain = -0.01
..fracture_criterion
...type = LINEAR_SOFTENING_MOHR_COULOMB
...limit_tensile_strain = 0.001 # defines when the damage process starts
...maximum_tensile_strain = 0.002 # defines when the damage process ends
...limit_compressive_strain = -0.01
...maximum_compressive_strain = -0.02
..fracture_criterion
...type = EXPONENTIAL_SOFTENING_MOHR_COULOMB
...limit_tensile_strain = 0.001 # defines when the damage process starts
...maximum_tensile_strain = 0.002 # defines when the damage process ends
...limit_compressive_strain = -0.01
...maximum_compressive_strain = -0.02
..fracture_criterion
...type = VON_MISES
...limit_tensile_stress = 1e6
```

In all cases, the damage follows a non-local definition. The radius of the damage band can be controlled with the parameter material_characteristic_radius as in the following example:

```
...fracture_criterion
...type = VON_MISES
...limit_tensile_stress = 1e6
...material_characteristic_radius = 0.001
```

6.5 Using the Modified Compression Field Theory

The Modified Compressive Field Theory is a specific fracture criterion for reinforced concrete. For this criterion, you need to define the list of rebars present in the material, with the location and diameter of each:

```
...fracture_criterion
...type = MCFT
...limit_compressive_strain = -0.001
```

```
...rebar
....location = 0.001
....diameter = 0.0001
...rebar
....location = 0.005
....diameter = 0.0001
```

As many rebars as required may be defined (including zero).

6.6 Defining a damage model

Two types of damage models can be used. ISOTROPIC_LINEAR_DAMAGE is the default model, and searches for the exact series in which the elements are damaged, and the corresponding damage increment. That is, at each iteration of the damage algorithm a bisection is carried out to find the exact damage increment to apply.

ISOTROPIC_INCREMENTAL_LINEAR_DAMAGE is a similar algorithm, except that it will apply a fixed amount of damage at each iteration. The amount can be fixed using the damage_increment variable:

```
...damage_model
....type = ISOTROPIC_INCREMENTAL_LINEAR_DAMAGE
...damage_increment = 0.01
```

For both damage models, it is possible to define a threshold of damage above which the material will be considered as entirely broken. In the following example, any element which reaches a damage value of 0.6 or higher will be considered as broken and removed from the simulation.

```
..damage_model
...type = ISOTROPIC_INCREMENTAL_LINEAR_DAMAGE
...damage_increment = 0.01
...maximum_damage = 0.6
```

7 Using space-time finite elements

Space-time finite elements are used for visco-elastic analysis of materials def. Several concepts must be defined first before going into the details of the input parameters.

7.1 Additional viscoelastic variables

Space-time finite elements use more unknown than standard finite elements. Indeed, for each dashpot placed in series in the model a new set of viscoelastic displacements is required. For example, the Maxwell model requires one set of additional variables, while a Burger's model requires two.

7.2 Indexed axis

For each set of viscoelastic variables two unknowns (in two dimensions, three for three-dimensional simulations) are necessary: the viscoelastic displacement along the XI axis and the viscoelastic displacement along the ETA axis.

To generalize to an arbitrary number of additional variables, the concept of indexed axis is introduced. One axis is defined for each unknown, and each axis is attributed a positive integer (its index). The two first axes (index 0 and 1) correspond respectively to the displacement along the XI and ETA axis. Then, each

pair of axes corresponds to one pair of viscoelastic displacement. Even indexes correspond to displacements along the XI axis, while odd indexes correspond to displacements along the ETA index.

For example, the correlation between the index of the axes and the displacement of a Burger material is as follow:

Index	Definition
0	Total displacement along the XI axis
1	Total displacement along the ETA axis
2	Internal displacement of the Maxwell dashpot along the XI axis
3	Internal displacement of the Maxwell dashpot along the ETA axis
4	Internal displacement of the Kelvin-Voigt unit along the XI axis
5	Internal displacement of the Kelvin-Voigt unit along the ETA axis

7.3 Boundary conditions

For all boundary conditions, the position of the boundary condition must be complemented with _AFTER. TOP must thus be replaced with TOP_AFTER, LEFT with LEFT_AFTER, etc.

Boundary conditions in stress and in force can be used as previously defined.

Boundary conditions in displacement must use the condition SET_ALONG_INDEXED_AXIS complemented with the index of the axis. Therefore, to set the vertical displacement (which is the axis indexed with 1) equal to 0 on the bottom of the sample one must use:

```
.boundary_condition
..condition = SET_ALONG_INDEXED_AXIS
..position = BOTTOM_AFTER
..value = 0
..axis = 1
```

These two rules must be followed when defining displacement boundary conditions in space-time finite elements:

- If you set the horizontal (respectively vertical) displacement to 0, you must also set all displacements along the even (respectively odd) indexed axes to 0.
- If you set the horizontal (respectively vertical) displacement to a value different than 0, you must leave free the displacements along the other even (respectively odd) indexed axes (that is, no boundary condition related to these axes).

7.4 Behaviours and additional sets of variables

As stated above, each behaviour comes with its own set of additional viscoelastic variables. However, when mixing different behaviours, then you mus make sure that all behaviours have the same number of additional viscoelastic variables. This can be achieved by setting the additional_viscoelastic_variable to the proper number when necessary.

For example, if the matrix is a Burger material (2 sets of viscoelastic variables) and the inclusions an elastic material (no additional set of viscoelastic variables), then the behaviour of the inclusions must be completed with the two missing sets of viscoelastic variables:

```
.sample
# sample description here...
```

```
...behaviour
...type = BURGER
# sample behaviour description here...
.inclusions
# inclusions description here...
..behaviour
...type = ELASTICITY
...additional_viscoelastic_variables = 2
# inclusions behaviour description here...
```

If the inclusions are a Maxwell material (one set of viscoelastic variables), then one set is missing and must be declared:

```
.sample
# sample description here...
..behaviour
...type = BURGER
# sample behaviour description here...
.inclusions
# inclusions description here...
..behaviour
...type = MAXWELL
...additional_viscoelastic_variables = 1
# inclusions behaviour description here...
```

7.5 Using the predefined material behaviours

The predefined PASTE_BEHAVIOUR, AGGREGATE_BEHAVIOUR and ASR_GEL_BEHAVIOUR have each two sets of viscoelastic variables (this cannot be changed, as they are meant to be used together).

The other predefined behaviours (except the VOID_BEHAVIOUR) are not meant to be used with space-time finite elements. The various ELASTICITY behaviour can be used in space-time finite elements, provided the number of additional_viscoelastic_variables is correctly set.

7.6 Defining a viscoelastic material

Different types of viscoelastic materials are available in AMIE. Their definition is summarized here.

VISCOSITY, KELVIN_VOIGT and MAXWELL are the three simplest viscoelastic behaviours. They require three parameters: a young_modulus, a poisson_ratio, and a characteristic_time (in day). The young_modulus/poisson_ratio pair can be replaced with the bulk_modulus/shear_modulus pair. They have no set of viscoelastic variables, except for the MAXWELL model which requires one. Example of a KELVIN_VOIGT material is given here:

```
..behaviour
...type = KELVIN_VOIGT
...young_modulus = 10e9
...poisson_ratio = 0.3
...characteristic_time = 10
```

The Burger material corresponds to a Maxwell unit placed in series with a Kelvin-Voigt unit. It requires two sets of viscoelastic variables, and is defined as follow:

```
..behaviour
...type = BURGER
...maxwell
....young_modulus = 50e9
....poisson_ratio = 0.3
....characteristic_time = 100
...kelvin_voigt
....young_modulus = 10e9
....poisson_ratio = 0.3
....characteristic_time = 10
```

Kelvin-Voigt and Maxwell chains with arbitrary numbers of units can be defined with the GENERALIZED_KELVIN_VOIGT and GENERALIZED_MAXWELL behaviours. These requires as many sets of viscoelastic variables as the number of branch in the chain. The first_branch variable defines the first elastic spring in the chain. An example of generalized Kelvin-Voigt chain with three branches can be found here:

```
..behaviour
...type = GENERALIZED_KELVIN_VOIGT
...first_branch
....young_modulus = 10e9
....poisson_ratio = 0.3
...branch
....young_modulus = 0.1e9
....poisson_ratio = 0.3
....characteristic_time = 10
...branch
....young_modulus = 5e9
....poisson_ratio = 0.3
....characteristic_time = 100
...branch
....young_modulus = 10e9
....poisson_ratio = 0.3
....characteristic_time = 1000
```

7.7 Fracture criterion in space-time finite elements

Space-time finite elements use a different set of fracture criterion. Only the four following criteria are available.

MAXIMUM_TENSILE_STRAIN defines a purely brittle material in which failure occurs when the strain reaches the specified limit_tensile_strain.

```
.fracture_criterion
..type = MAXIMUM_TENSILE_STRAIN
..limit_tensile_strain = 0.001
```

LINEAR_SOFTENING_MAXIMUM_TENSILE_STRAIN defines a material with a linear descending branch in the stress-strain diagram. limit_tensile_strain and limit_tensile_stress indicate the position of the peak, while maximum_tensile_strain indicates the ultimate strain at failure.

```
.fracture_criterion
..type = LINEAR_SOFTENING_MAXIMUM_TENSILE_STRAIN
```

```
..limit_tensile_strain = 0.001
..limit_tensile_stress = 1e6
..maximum_tensile_strain = 0.002
```

MAXIMUM_TENSILE_STRESS defines a pseudo-plastic material in which failure occurs when the stress reaches the specified limit_tensile_stress.

```
.fracture_criterion
..type = MAXIMUM_TENSILE_STRESS
..limit_tensile_stress = 1e6
```

ELLIPSOIDAL_SOFTENING_MAXIMUM_TENSILE_STRESS defines a material which shifts from a MAXIMUM_TENSILE_STRAIN material with a fast loading rate, towards a MAXIMUM_TENSILE_STRESS material with a slow loading rate. The instantaneous_modulus (which corresponds to the apparent modulus of the material with an infinitely fast loading rate) and the relaxed_modulus (apparent modulus with an infinitely slow loading rate) are required as well. The instantaneous_modulus must be strictly higher than the relaxed_modulus.

```
.fracture_criterion
..type = ELLIPSOIDAL_SOFTENING_MAXIMUM_TENSILE_STRESS
..limit_tensile_strain = 0.001
..limit_tensile_stress = 1e6
..instantaneous_modulus = 10e9
..relaxed_modulus = 1e9
```

As for any fracture criteria, these criteria can also have a material_characteristic_radius defined.

7.8 Damage model in space-time finite elements

Only the ISOTROPIC_INCREMENTAL_LINEAR_DAMAGE damage model is available in space-time finite elements. It has an additional parameter, time_tolerance, which indicates with which accuracy the instant at which damage occurs is captured. A small time tolerance indicates a high accuracy. The default value is set to 1e-9.

```
...damage_model
...type = ISOTROPIC_INCREMENTAL_LINEAR_DAMAGE
...damage_increment = 0.01
...time_tolerance = 1e-9
```

8 The generalized logarithmic creep behaviour

This specific behaviour defines a visco-elastic material with imposed deformation. It uses space-time finite elements, so the guidelines of the previous section applies.

8.1 Basic behaviour

The behaviour consists in possibly four parts:

- An elastic behaviour.
- A non-linear visco-elastic behaviour which corresponds to a logarithmic creep curve.
- An imposed deformation (for example, thermal expansion, drying shrinkage, etc).

• A damage behaviour (defined as a pair of a fracture criterion and damage model).

All parts (except the elastic behaviour) are optional, which allows this behaviour to cover a wide range of materials.

8.2 Internal parameters

imposed_deformation

The behaviour relies on a certain number of internal parameters, which might represent for example physical fields (like temperature, relative humidity), material constants (modulus, thermal expansion coefficients, etc), or temporary mathematical variables for ease of calculation. These parameters might be changed dynamically during the simulation (see below).

The parameters are declared with their default values in a parameters object as follow:

```
.behaviour
..type = LOGARITHMIC_CREEP
..parameters
...young_modulus = 10e9
...poisson_ratio = 0.3
...temperature = 293
...thermal_expansion_coefficient = 10e-6
  All LOGARITHMIC_CREEP materials must have the following parameters:
young_modulus
poisson_ratio
  Or alternatively:
bulk_modulus
shear_modulus
  In order to use the logarithmic creep law itself, the material must have the following parameters:
creep_modulus
creep_poisson
creep_characteristic_time
  Or alternatively:
creep_bulk
creep_shear
creep_characteristic_time
  In order to use an imposed deformation, the material ,must have the following parameter:
```

In the current version of AMIE, the internal parameters are not related with the fracture criterion and the damage model. To use damage with a LOGARITHMIC_CREEP behaviour, one must define a fracture_criterion and damage_model as follow:

```
.behaviour
..type = LOGARITHMIC_CREEP
..parameters
# definition of the material parameters
..fracture_criterion
# definition of the fracture criterion
..damage_model
# definition of the damage model
```

8.3 Material laws

The internal parameters defined above are constants, unless appropriate material laws are defined to act upon them. These laws can be used to set variables to a certain value, or to perform specific operations on these variables. Any number of material law can be defined, using the following syntax:

```
.behaviour
..type = LOGARITHMIC_CREEP
..parameters
# definition of the material parameters
..material_law
# definition of first material law
..material_law
# definition of second material law
..material_law
# definition of third material law, etc
```

When doing a time step, AMIE will first apply all the material laws defined, change the mechanical properties of the element accordingly, and then compute the results at that time step.

The material laws will be applied in the order in which they are declared. Therefore, if the material uses a THERMAL_EXPANSION material law without any temperature defined first, no thermal deformation will be occur.

8.4 Predefined material laws

In this section, a few common material laws are defined for ease of use. Their definition include the list of internal parameters required for their proper use.

8.4.1 Thermal expansion

```
..material_law
...type = THERMAL_EXPANSION
...reference_temperature = 293
Requires the following parameters:
```

imposed_deformation
temperature
thermal_expansion_coefficient

$$\alpha = \alpha + k_T (T - T_0) \tag{5}$$

With:

 α : imposed_deformation

 k_T : thermal_expansion_coefficient

T : temperature

 T_0 : reference_temperature

8.4.2 Radiation-induced volumetric expansion

..material_law

...type = RADIATION_INDUCED_VOLUMETRIC_EXPANSION

Requires the following parameters:

imposed_deformation
neutron_fluence
neutron_fluence_correction
radiation_expansion_delay
maximum_radiation_expansion

Applies:

$$\alpha = \alpha + \kappa \, \epsilon_{max} \frac{e^{\delta N} - 1}{\epsilon_{max} + \kappa \, e^{\delta N}} \tag{6}$$

With:

 α : imposed_deformation

 $\kappa \ : \ {\tt radiation_expansion_delay}$ $\epsilon_{max} \ : \ {\tt maximum_radiation_expansion}$ $\delta \ : \ {\tt neutron_fluence_correction}$

N : neutron_fluence

8.4.3 Drying shrinkage

..material_law

...type = DRYING_SHRINKAGE

...reference_relative_humidity = 1.

Requires the following parameters:

imposed_deformation
relative_humidity
drying_shrinkage_coefficient

$$\alpha = \begin{cases} 0 & \text{if } h > h_0 \\ \alpha - k_s(h - h_0) & \text{otherwise} \end{cases}$$
 (7)

With:

 α : imposed_deformation

 k_s : drying_shrinkage_coefficient

h : relative_humidity

 h_0 : reference_relative_humidity

8.4.4 Arrhenius law

- ..material_law
- ...type = ARRHENIUS
- ...parameter_affected = \$parameter
- ...reference_temperature = 293

Requires the following parameters:

temperature
\$parameter
\$parameter_activation_energy

Applies:

$$x = x e^{E_a[1/T - 1/T_0]} (8)$$

With:

x : parameter

 E_a : $parameter_activation_energy$

T : temperature

 T_0 : reference_temperature

8.4.5 Arrhenius law for creep

- ..material_law
- ...type = CREEP_ARRHENIUS
- ...reference_temperature = 293

Requires the following parameters:

temperature
creep_modulus
creep_characteristic_time
creep_activation_energy

$$C = C e^{E_c[1/T - 1/T_0]}$$

$$\eta = \eta e^{E_c[1/T - 1/T_0]}$$
(9)
(10)

$$\eta = \eta e^{E_c[1/T - 1/T_0]} \tag{10}$$

(11)

With:

C : creep_modulus

 η : creep_characteristic_time E_c : creep_activation_energy

T : temperature

 T_0 : reference_temperature

Relative humidity effect on creep

```
..material_law
...type = CREEP_HUMIDITY
```

Requires the following parameters:

relative_humidity creep_modulus creep_humidity_coefficient

Applies:

$$C = C k_h (1 - h) \tag{12}$$

With:

C : creep_modulus

 k_h : creep_humidity_coefficient

h : relative_humidity

8.5 Generic material laws

In this section, generic material laws are described. These laws can be used to formulate various material behaviours.

8.5.1 Extract strain or stress field values

```
..material_law
...type = GET_FIELD
...field = STRAIN_FIELD
```

This law is a utility function to access the values of the common field (displacement, strain, stress, etc). The example above will generate three variables (in two dimensions) strain_field_0, strain_field_1 and strain_field_2 containing the three components of the strain field in the element.

8.5.2 As a function of a single variable

```
..material_law
...type = SIMPLE_DEPENDENT
...input_parameter = $input
...output_parameter = $output
...function = # declare function of x here
...additive = FALSE
```

Requires the following parameters:

\$input
\$output

Applies:

$$\mathcal{Y} = \begin{cases} f(\mathcal{X}) & \text{if additive} = \text{FALSE} \\ \mathcal{Y} + f(\mathcal{X}) & \text{otherwise} \end{cases}$$
 (13)

With:

 \mathcal{X} : \$input \mathcal{Y} : \$ouput

8.5.3 As a linear interpolation of another variable

```
..material_law
```

- ...type = LINEAR_INTERPOLATED
- ...input_parameter = \$input
- ...output_parameter = \$output
- ...file_name = # path to the file containing the interpolation data

Requires the following parameters:

\$input

\$output

Applies:

$$\mathcal{Y} = linear_interpolation(\mathcal{X}) \tag{14}$$

With:

 \mathcal{X} : \$input \mathcal{Y} : \$ouput

The interpolation file must contain two columns, the first being the values of \$input and the second the corresponding values of \$param.

8.5.4 As a function of space and time

```
..material_law
...type = SPACE_TIME_DEPENDENT
...output_parameter = $output
...function = # declare function of x,y,z,t here
...additive = FALSE
```

Requires the following parameters:

\$output

Applies:

$$\mathcal{Y} = \begin{cases} f(x, y, z, t) & \text{if additive} = \text{FALSE} \\ \mathcal{Y} + f(x, y, z, t) & \text{otherwise} \end{cases}$$
 (15)

With:

 \mathcal{Y} : \$output

8.5.5 As a function of multiple variables

```
..material_law
...type = VARIABLE_DEPENDENT
...output_parameter = $output
...x = $input_x
...y = $input_y
...z = $input_z
...t = $input_t
...u = $input_t
...u = $input_u
...v = $input_v
...v = $input_w
...function = # declare function of x,y,z,t,u,v,w here
...additive = FALSE
```

Requires the following parameters:

```
$output
$input_x
$input_y
$input_z
$input_t
$input_u
$input_v
$input_w
```

Applies:

$$\mathcal{Y} = \begin{cases} f(x, y, z, t, u, v, w) & \text{if additive} = \text{FALSE} \\ \mathcal{Y} + f(x, y, z, t, u, v, w) & \text{otherwise} \end{cases}$$
 (16)

With:

 \mathcal{Y} : \$output x : input_x y : input_y z : input_z t : input_t t t : input_u t : input_v t : input_v t : input_w

It is not necessary to define all variables (x, z, y, t, u, v, w). Only those used in f are required. Note that if f is a function of x, y, z or t, and the respective input_x, input_y, input_z or input_t is not declared, then the function uses the actual space-time coordinates of the element.

8.5.6 Time derivative

```
..material_law
...type = TIME_DERIVATIVE
...input_parameter = $input
```

Requires the following parameters:

\$input
\$input_rate

Applies:

$$\mathcal{Y} = \frac{\partial \mathcal{X}}{\partial t} \tag{17}$$

With:

 \mathcal{X} : sinput \mathcal{Y} : $sinput_rate$

8.5.7 Time integral

```
..material_law
...type = TIME_INTEGRAL
...input_parameter = $input
```

Requires the following parameters:

\$input
\$input_integral

$$\mathcal{Y} = \int \mathcal{X} dt \tag{18}$$

With:

 \mathcal{X} : \$input

 \mathcal{Y} : $sinput_integral$

8.5.8 Minimum

```
..material_law
...type = MINIMUM
...output_parameter = $output
...input_parameter = $input_x
...input_parameter = $input_y
...input_parameter = $input_z
```

Requires the following parameters:

\$output

\$input_x

\$input_y

\$input_z

Applies:

$$\mathcal{Y} = \min(x, y, z, \dots) \tag{19}$$

With:

\mathcal{Y} : \$output
x : \$input_x
y : \$input_y
z : \$input_z

This law can accept any number of input_parameter (at least one).

8.5.9 Maximum

```
..material_law
...type = MAXIMUM
...output_parameter = $output
...input_parameter = $input_x
...input_parameter = $input_y
...input_parameter = $input_z
```

Requires the following parameters:

```
\label{eq:continuity} \begin{cases} \texttt{sinput}_x \\ \texttt{sinput}_y \\ \texttt{sinput}_z \end{cases} Applies: \mathcal{Y} = \max(x,y,z,\ldots) \tag{20} With: \begin{aligned} \mathcal{Y} &: & \texttt{soutput} \\ x &: & \texttt{sinput}_x \\ y &: & \texttt{sinput}_y \\ z &: & \texttt{sinput}_z \end{aligned}
```

This law can accept any number of input_parameter (at least one).

8.6 Example

The following example can be used to simulate the serpentine aggregates used in Elleuch's irradiation experiments.

```
.behaviour
..type = LOGARITHMIC_CREEP
# define material parameters
..parameters
...young_modulus = 130e9
...poisson_ratio = 0.2
...imposed_deformation = 0
...temperature = 293
...neutron_fluence = 0
...thermal_expansion_coefficient = 7.5e-6
...radiation_expansion_delay = 84.268
...maximum_radiation_expansion = 0.0972
...neutron_fluence_correction = 0.0099
# define temperature as function of time
..material_law
...type = LINEAR_INTERPOLATED
...input_parameter = t
...output_parameter = temperature
...file_name = ../examples/data/elleuch/temperature_history_g1
# define neutron fluence as function of time
..material_law
...type = LINEAR_INTERPOLATED
...input_parameter = t
...output_parameter = neutron_fluence
...file_name = ../examples/data/elleuch/fluence_history_g1
# apply thermal expansion
```

```
..material_law
...type = THERMAL_EXPANSION
...reference_temperature = 293
# apply radiation-induced expansion
..material_law
...type = RADIATION_INDUCED_VOLUMETRIC_EXPANSION
# apply radiation-induced loss of stiffness
..material_law
...type = LINEAR_INTERPOLATED
...input_parameter = neutron_fluence
...output_parameter = young_modulus
...file_name = ../examples/data/elleuch/aggregate_damage
# damage parameters
..fracture_criterion
...type = MAXIMUM_TENSILE_STRAIN
...limit_tensile_strain = 0.00039
..damage_model
...type = ISOTROPIC_INCREMENTAL_LINEAR_DAMAGE
...damage_increment = 0.01
...time_tolerance = 1e-9
```

9 Future features

The following features might be implemented/corrected at some point in the future.

- The first SVG output file seems to have more fields than required. This is a bug.
- Possibility to refine locally the mesh.
- Possibility to add pre-placed rectangular inclusions (for rebars, notches, etc).
- Possibility to limit the location of the boundary conditions to a certain part of an edge, or a certain point.
- Possibility for the logarithmic creep behaviour to affect the damage parameters.