DE LA RECHERCHE À L'INDUSTRIE

Paris - Saclay

www.cea.fr

AMITEX_FFT training

-

Practice

-

V8.17.13

-

10/10/2023

Prerequisites for training

- Pre-requesites for amitex_fftp (gcc/openmpi/fftw)
- Octave
- Paraview
- Mfront
- Meld (if possible)
- (Solution to read .pptx and .pdf files)

Lionel Gélébart

OVERVIEW

Installation

Geometry description for AMITEX
-> reading vtk file *paraview* + generation (with *matlab/octave*)

amitex_fftp command line
-> First simple linear simulation

Xml files material, loading-output, algorithms
-> Linear simulations
-> First non linear simulation (ex : viscoelasticity)
-> Finite strain simulations (ex : rotation)

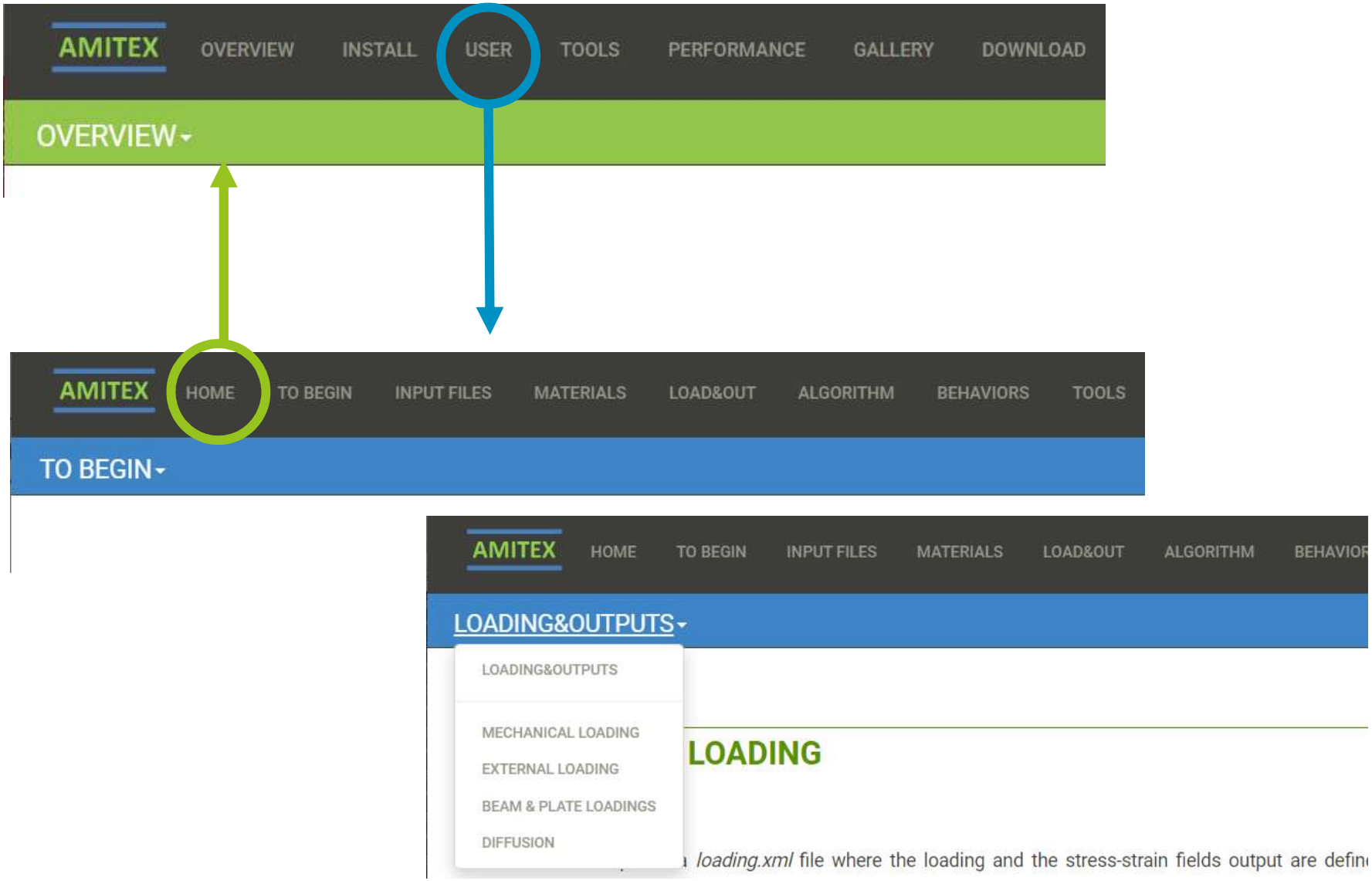
Behaviors
-> umat –user behaviors
-> MFRONT-user behaviors

Composite voxels

Practice : - proposed application
- free application

THE WEBSITE IS THE REFERENCE DOCUMENT!

http://www.maisondelasimulation.fr/projects/amitex/general/_build/html/index.html



FOR CEA - SRMA, INFO ON MARQUISES' WEBSITE

http://marquises/wiki/_build/html/usage.html#softwares

INSTALLATION

- Linux-based OS

- Pre-requisites

compiler : gfortran (>v5.0.0) OR ifort (and nothing else!)
MPI library : openMPI OR intelMPI
fftw3 : simple **AND** double precision, development version
Mfront (optionnal)

ifort+intelMPI > gfortran+openMPI

Installations :
If root or super user => 1. Prefer 'package installer' (apt-get, yum install etc…)
=> 2. Install by yourself (see amitex_ffp's website)
Else => Ask your administrator !
Or => Install by yourself on your home (see amitex_ffp's website)

- Installation

1 In file *install* :
Adjust FC, MPIFC, FFT, FFT_inc, FFT_lib

2 Launch *install*

```
$ ./install
```

-> Executable : (amitex)/libAmitex/bin/amitex_fftp

install

```
# Compiler : ifort or gfortran
FC=ifort
FC=gfortran

# MPI compiler
MPIFC=mpif90
#MPIFC=mpiifort
. . .
FFT=fftw3_f03
. . .
FFT_inc=<path_to_fftw_include>
FFT_lib=<path_to_fftw_lib>
```

INSTALLATION

- In *<my_home>/ :*

1 - Install amitex_fftp

Untar the archive

```
$ tar xvf amitex_fftp-vx.x.x.tar
```

In *amitex_fftp*: Adjust *install* -> FC, MPIFC, FFT, FFT_inc, FFT_lib

On linux ubuntu:
FC=gfortran
MPIFC=mpif90
FFT=fftw3_f03
FFT_inc=/usr/include
FFT_lib=/usr/lib64

Launch *install* :

```
$ ./install
$ ls /libAmitex/bin
```

2 – Launch validation tests

Can be long if the number of available cores is small (typically 20min for 6 cores).

Tip : add an « exit 0 » in script_tests.sh after a few tests.

In *amitex_fftp/validation :*

```
$ ./script_test.sh
```

On a standalone PC

or

```
$ llsubmit script_tests_poincare
```

or

```
$ qsub script_tests_marquises
```

On a cluster

or …

AMITEX_TRAINING DIRECTORY : OVERVIEW

❑ In *<my_home>/ :*

amitex_training/

➢ env_amitex_training.sh : define environment variables
- To be adjusted to your own configuration
- Before using amitex_fftp :

$ source env_amitex_training.sh

➢ 7 directories

- ❑ Scripts : script shell to launch simulation
- ❑ Microstructures : vtk images + matlab/octave files
- ❑ Materials : xml files for material properties
- ❑ Loadings_outputs : xml files for loading and output description
- ❑ Algorithms : xml files for algorithm parameters
- ❑ Behaviors : umat and MFRONT user behaviors
- ❑ Matlab_octave : tools (pre-post processing)

\+ solutions directories in each directory!

GEOMETRY : UNIT-CELL DESCRIPTION

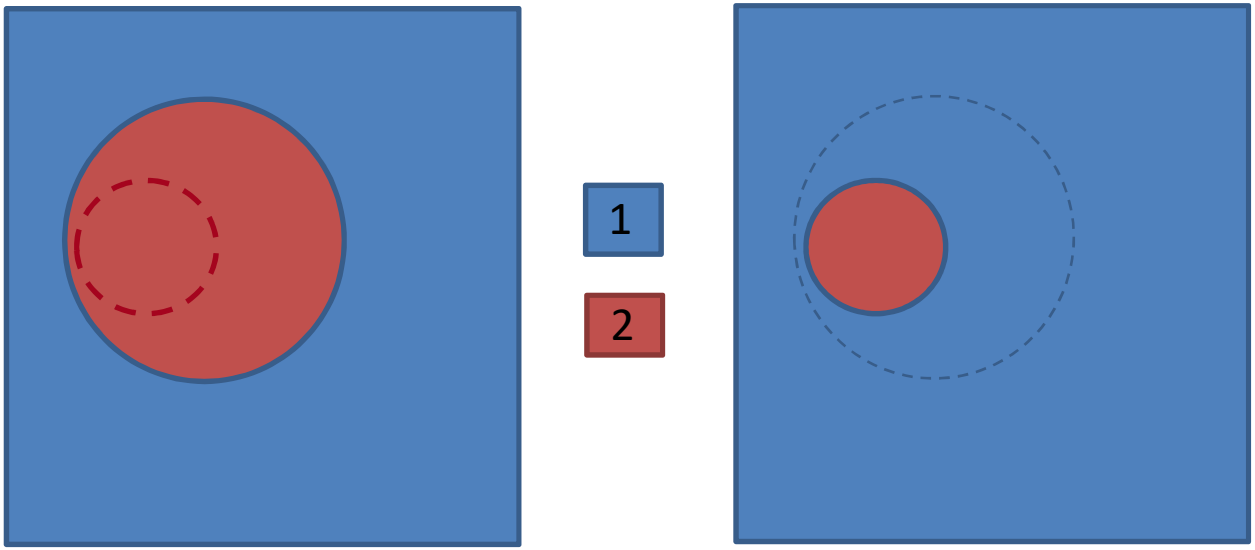
- **Material** = a set of voxels with same behavior law
  (isotropic elasticity, orthotropic elasticity, VonMises plasticity, crystal plasticity etc…)

- **Zone = within a material** a set of voxel with the same material coefficients

Example

a unit cell with :

2 materials (1 is plastic and 2 is elastic)
1 zone in material 1
2 zones in material 2 (with different Young moduli)



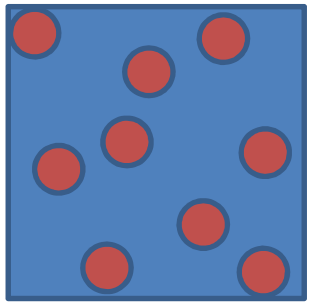
Material - field

Zone - field

GEOMETRY : UNIT-CELL DESCRIPTION

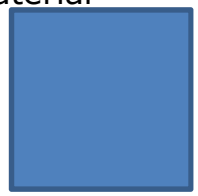
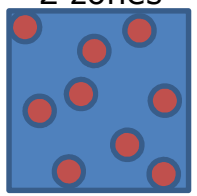
➢ **A non-unique description : an example**

Elastic composite (isotropic elasticity)
N inclusions (same elastic coeff.)
Matrix

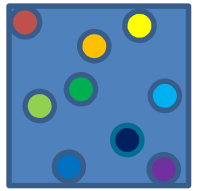


5 possible descriptions for AMITEX

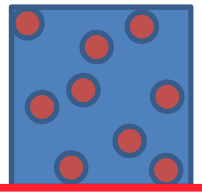
❑ 1 material – 2 zones

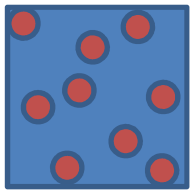
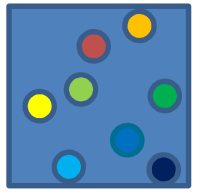
❑ 1 material – (N+1) zones

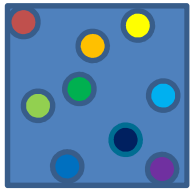
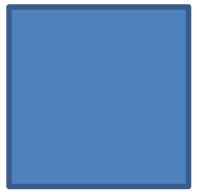
❑ 2 materials - 1 zone / material




❑ 2 materials - 1 zone / 'inclusion'

❑ N+1 materials - 1 zone / material

To choose :

➢ Think 'output'!
  -> Per material average (by default)
  -> Per zone average (on demand)

➢ Think 'intput' (*material.xml* file)!
  -> Avoid large number of materials

GEOMETRY : INPUT VTK FILES

➢ Exemple 2 materials with Nzones in material 'inclusions'

vtk header

```
# vtk DataFile Version 4.5
Materiau
BINARY
DATASET STRUCTURED_POINTS
DIMENSIONS    65    65    65
ORIGIN    0.000    0.000    0.000
SPACING    1.000000    1.000000    1.000000
CELL_DATA    262144
SCALARS MaterialId short
LOOKUP_TABLE default
```

❑ In *Microstructures/vtk :*

```
$ more zone_al2p5_64.vtk
```

WARNING

Values in vtk file

➢ Between 1 and N (or 0 and (N-1))

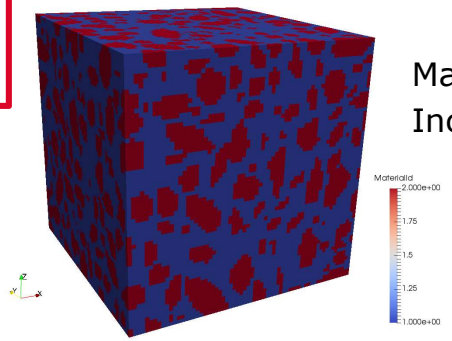
1 (or 0) associated to numM=1 in *material.xml*

2 (or 1) associated to numM=2 in *material.xml*

➢ No skipping values (ex ~~: 1,2,4,5~~)

```
$ paraview mat_al2p5_64.vtk &
```

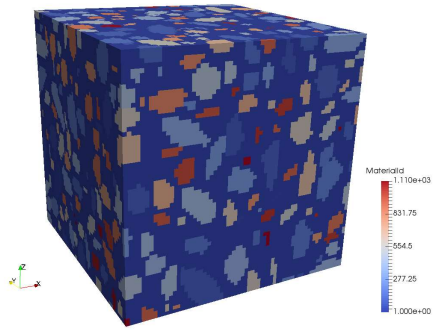
+ Apply
+ Representation menu : « surface »
+ Coloring menu : « MaterialID »



Matrice : 1
Inclusions : 2

File / open / zone_al2p5_64.vtk
+ Apply
+ Representation menu : « surface »
+ Coloring menu : « MaterialID »

Matrice : 1
Inclusion1 : 1
Inclusion2 : 2
Inclusion3 : 3
Etc…



GEOMETRY : INPUT VTK FILES GENERATION

➢ GENERATE .vtk files for amitex_fftp with matlab/octave script files

❑ In *Microstructures/*

$ «my_editor »
two_spheres.m

uses functions in Microstructures/matlab_octave :
gen_grid
savefieldvtk

OCTAVE

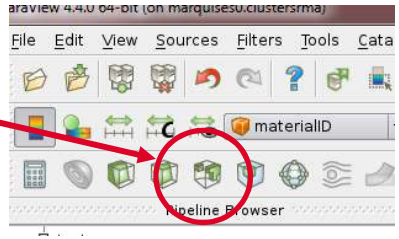
```
$ octave
> two_spheres
> exit
```

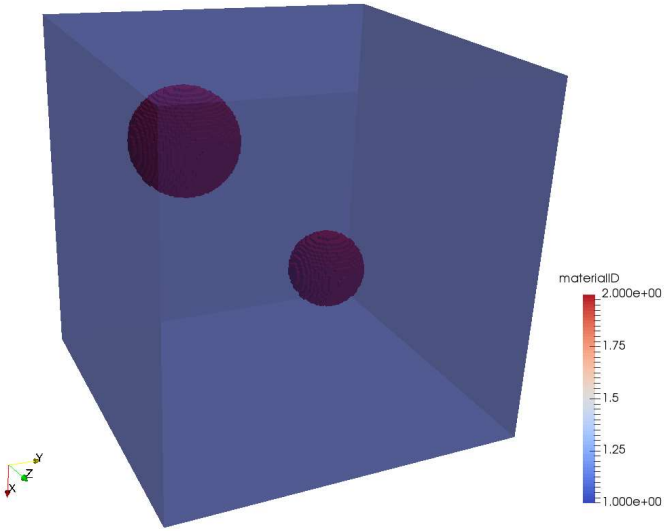
vtk/2spheres.vtk

PARAVIEW

File / Open / *vtk/2spheres.vtk*
+ Apply
+ Representation menu : « surface »
+ Coloring menu : « MaterialID »
+ Opacity menu : 0,5

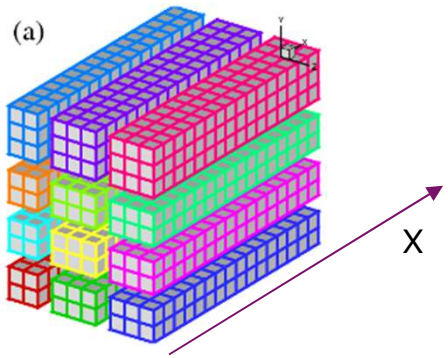
Filter « threshold »
+Minimum menu : 1,5
+ Apply





GEOMETRY : 2D INPUT VTK FILES GENERATION

➢ **WARNING** for 2D unit-cells (1 voxel thickness)



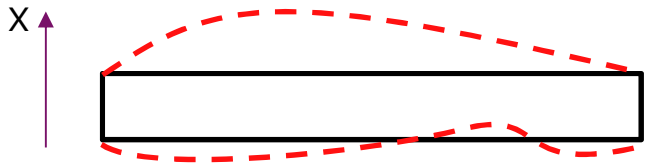
AMITEX uses a 2D MPI decomposition with X-pencils

2D unit-cell (1voxel thickness)

➢ MUST BE DEFINED IN THE (YZ) PLANE!

2D unit-cell (1voxel thickness) in AMITEX ⟺

PLANE STRAIN
or GENERALIZED PLANE STRAIN
or PLANE STRESS (if simulation with an additionnal void layer)



Exx non uniform -> violate Periodicity Condition

=> Exx uniform (idem Exy, Exz)

AMITEX_FFTP COMMAND LINE

$ amitex_fftp -help

0/ help (this message)
mpirun (-np n) amitex_fftp -help OR SIMPLY : amitex_fftp -help

1/ general case
mpirun (-np n) amitex_fftp -nm <num_mat.vtk> -nz <num_zone.vtk> -a <algo.xml> -c <load.xml> -m <mat.xml> -s <output

2/ one material (assumes num_mat.vtk full of 1)
mpirun (-np n) amitex_fftp -nz <num_zone.vtk> -a <algo.xml> -c <load.xml> -m <mat.xml> -s <output>

3/ one zone per material (assumes num_zone.vtk full of 1)
mpirun (-np n) amitex_fftp -nm <num_mat.vtk> -a <algo.xml> -c <load.xml> -m <mat.xml> -s <output>

4/ one material with one zone per voxel (assumes num_zone.vtk varying from 1 to the number of voxels)
assumes also dx=dy=dz=1.
mpirun (-np n) amitex_fftp -a <algo.xml> -c <load.xml> -m <mat.xml> -NX nx -NY ny -NZ nz -s <output>

5/ one material with one zone per voxel (assumes num_zone.vtk varying from 1 to the number of voxels)
mpirun (-np n) amitex_fftp -a <algo.xml> -c <load.xml> -m <mat.xml> -NX nx -NY ny -NZ nz -DX dx -DY dy -DZ dz -s <output>

FIRST SIMPLE LINEAR SIMULATION

- In *Scripts/*

$ «my_editor » *script_linear1.sh &*

```
#!/bin/bash

# Environment variables
source ../env_amitex_training.sh

MPIRUN="mpirun -np 12"
MPIRUN="mpirun"

# INPUT FILES
MATEVTK="../Microstructures/vtk/mat_al2p5_64.vtk"
MATEXML="../Materials/mat_lin.xml"
LOADXML="../Loadings_outputs/def_imp_mini.xml"
ALGOXML="../Algorithms/algo_default.xml"

# LAUNCH SIMU WITH 2 MATERIALS (ONE ZONE/MATERIAL)

mkdir res_linear1 #don't forget!

$MPIRUN amitex_fftp  -nm $MATEVTK  -a $ALGOXML -c $LOADXML -m $MATEXML  -s res_linear1/res
```

Same env. as used to compile amitex_fftp

Not always necessary

Crash if directory does not exist

Inputs

$ «my_editor »/open/ *mat_lin.xml, def_imp_mini.xml, algo_default.xml*

FIRST SIMPLE LINEAR SIMULATION

- In *Scripts/* Launch simulation `$ ./script_linear1.sh`

➡ Outputs

standard output on screen systematically :

Error, Warning messages

- .log file
- .std file
- .mstd file
- +copy of xml input files

on demand only :
- .vtk files
- .zstd files

→ Uncomment 'Output_vtkList' in *def_imp_mini.xml*

.log file
To check the number of process
To check the correct reading of vtk and xml files
Error/warning messages

.std file
Unit-cell averages and standard deviations

.mstd file
Per material averages and standard deviations

.zstd files
Per zone averages and standard deviations

.vtk files
Stress, strain, internal variables fields

FIRST SIMPLE LINEAR SIMULATION

- Plot macroscopic behavior
  - In *Scripts* :

```
$ gnuplot
gnuplot> load "plot1.gp"
```

→ plot "res_linear1/res.std" u 8:2 w l

- Apply simple modifications
  - In *Loadings_outputs/def_imp_mini.xml* : `$ cp def_imp_mini.xml  def_imp_vtk.xml`

Uncomment 'Output_vtkList'

⇨ vizualize stress/strain fields

  - In *Loading_outputs/* `$ cp def_imp_mini.xml  traction.xml`

In *traction.xml* : except for xx component
replace *"Strain"* by *"Stress"*
assign *Value="0"*

In *script_linear1.sh* and launch simulation ⇨ Check results

FIRST SIMPLE LINEAR SIMULATION

- Apply simple modifications
  - In *Materials/*

```
$ cp mat_lin.xml  mat_pores.xml
```

In *mat_pores.xml* : assign nul elastic properties
do not touch reference material

⇨ Effect on the number of iterations
Visualize axial stress field (component 1) -> null stress in inclusions

```
$ cp mat_lin.xml  mat_poresb.xml
```

In *mat_poresb.xml* : adjust the reference material properties
Lambda0="2.e10" Mu0="1.35e10"

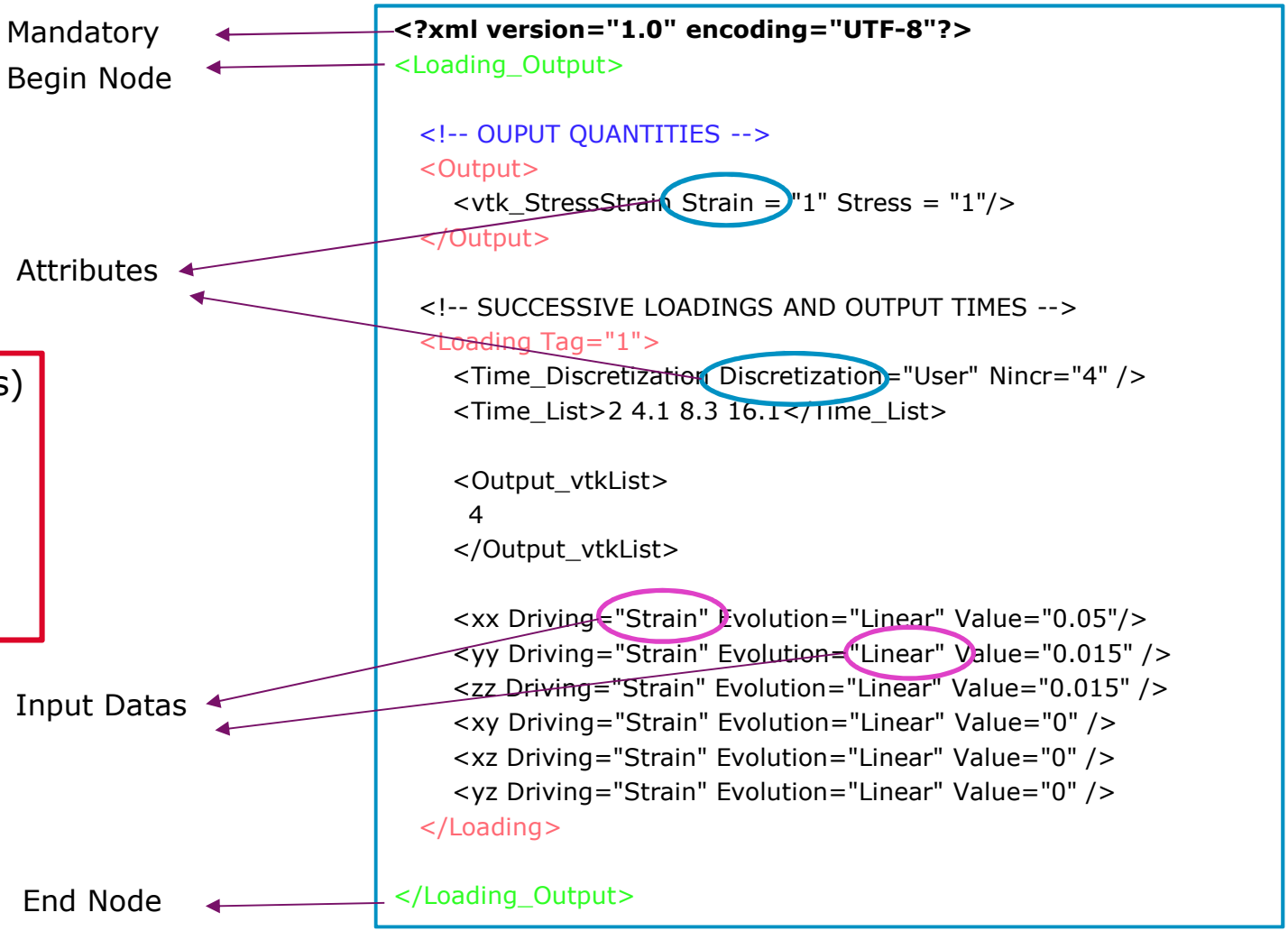
⇨ Effect on the number of iterations

Number of iterations
def_imp_mini 23
traction 25
def_imp_mini + pores ~200
def_imp_mini + poresb ~150

XML FILES

- PARSER : FoX library http://homepages.see.leeds.ac.uk/~earawa/FoX/

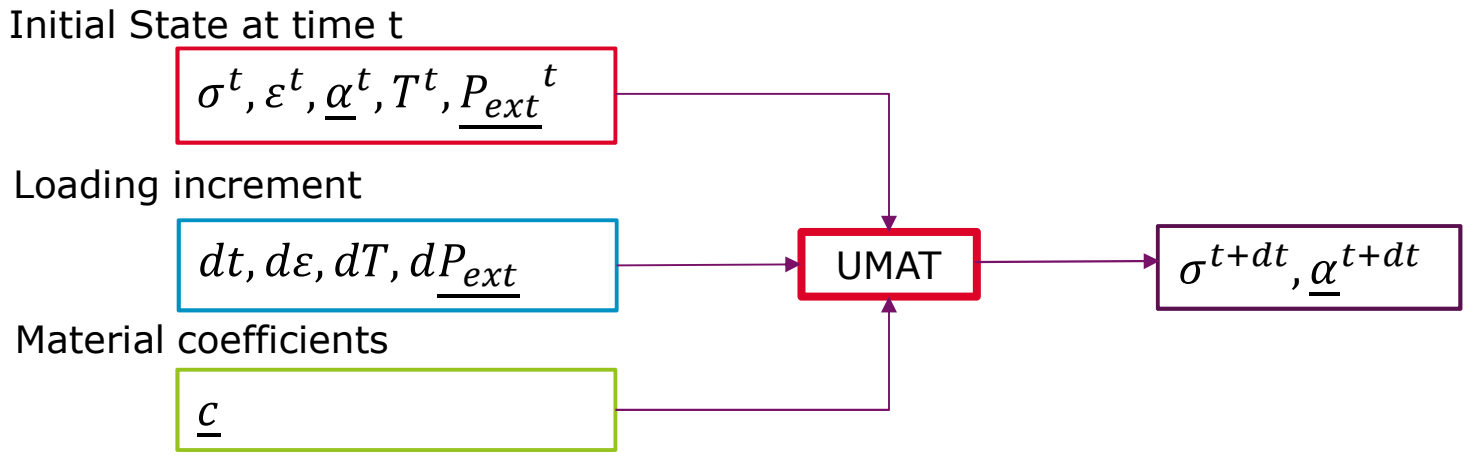
- SYNTAX :



- XML (nodes, attributes) is case sensitive
- Input datas are case insensitive, **except** 'path' names

XML FILES : MATERIAL PROPERTIES

- Behavior evaluation : UMAT procedure called on **every voxel**, at **every iteration**



UMAT format ➡ compatibility with CAST3M/ABAQUS and MFRONT

```
SUBROUTINE my_behavior( STRESS, STATEV, DDSDDE, SSE, SPD, SCD,&
                        RPL, DDSDDT, DRPLDE, DRPLDT,&
                        STRAN, DSTRAN, TIME, DTIME,&
                        TEMP, DTEMP, PREDEF, DPRED,&
                        CMNAME, NDI, NSHR, NTENS, NSTATV,&
                        PROPS, NPROPS, COORDS,&
                        DROT, PNEWDT, CELENT, DFGRD0, DFGRD1,&
                        NOEL, NPT, LAYER, KSPT, KSTEP, KINC )
```

loading.xml

Initialized by *material.xml*

XML FILES : MATERIAL PROPERTIES

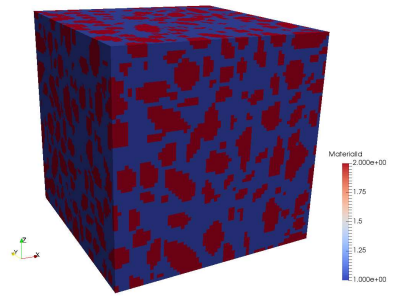
- See website

http://www.maisondelasimulation.fr/projects/amitex/general/_build/html/index.html

WARNING : the numM values are going from 1 to N associated
respectively to values 1 to N / or 0 to (N-1) in *mate.vtk*

➡ Prefer defining *mate.vtk* from 1 to N.

XML FILES : MATERIAL PROPERTIES



15’ then correction

- In *Materials/*

```
$ cp mat_lin.xml  mat_lin_2.xml
```

In *mat_lin_2.xml* : define 1 material with 2 zones, same material properties as mat_lin.xml
values defined in the xml file

```
$ cp mat_lin_2.xml  mat_lin_2b.xml
```

In *mat_lin_2b.xml* : idem
values defined in a ascii files (create Lambda.txt and Mu.txt in *Microstructures*)

```
$ cp mat_lin_2.xml  mat_lin_2c.xml
```

In *mat_lin_2c.xml* : idem
values defined in binary files (use lambda_mu_bin.m in *Microstructures*)

- In *Scripts/ : script_linear2.sh* launch simulations

- To compare results (should be identical) :

```
$ meld res_linear1/res.std res_linear2/res.std
```

XML FILES : LOADING-OUTPUT

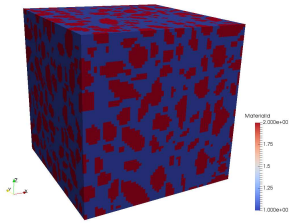
- See website
http://www.maisondelasimulation.fr/projects/amitex/general/_build/html/index.html

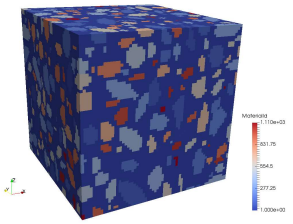
XML FILES : LOADING-OUTPUT

Exercise

15’ then correction

Microstructures*/vtk/mat_al2p5_64.vtk* and *zone_al2p5_64.vtk*





Behavior :

Matrix : elasiso

Inclusions : thermoelasiso, S=C:(E-a(T-To))

a=PROPS(3)=$10^{-5}K^{-1}$ and To=PROPS(4)=0K

Additionnal outputs :

stress field (.vtk)

per inclusion average (.zstd)

In Scripts : use *script_thermoelas.sh*

In Materials : $ cp mat_lin.xml mat_thermoelas.xml

In Loadings_Outputs : $ cp traction.xml char_thermoelas.xml

Adjust *mat_thermoelas.xml* and *char_thermoelas.xml*

Loading & output :

Initial temperature 0K

Time 0 to 1000s :

Uniaxial (xx) tensile test : 0->1% (Linear evolution)

Temperature 0K ->1000K (Linear evolution)

100 steps (useless in linear problem, used for exercise!)

Output : vtk stress field at 500s and 1000s

per inclusion average : 3 steps /100

per unit-cell and per material average : 10 steps / 100

Time 1000s to 2000s :

Uniaxial (xx) tensile test : fix 1%

Temperature 1000K -> 500K (Linear evolution)

100 steps (useless in linear problem, used for exercise!)

Output : vtk stress field at 1500s and 2000s

per inclusion average (10 steps / 100)

per unit-cell and per material average : 15 steps / 100

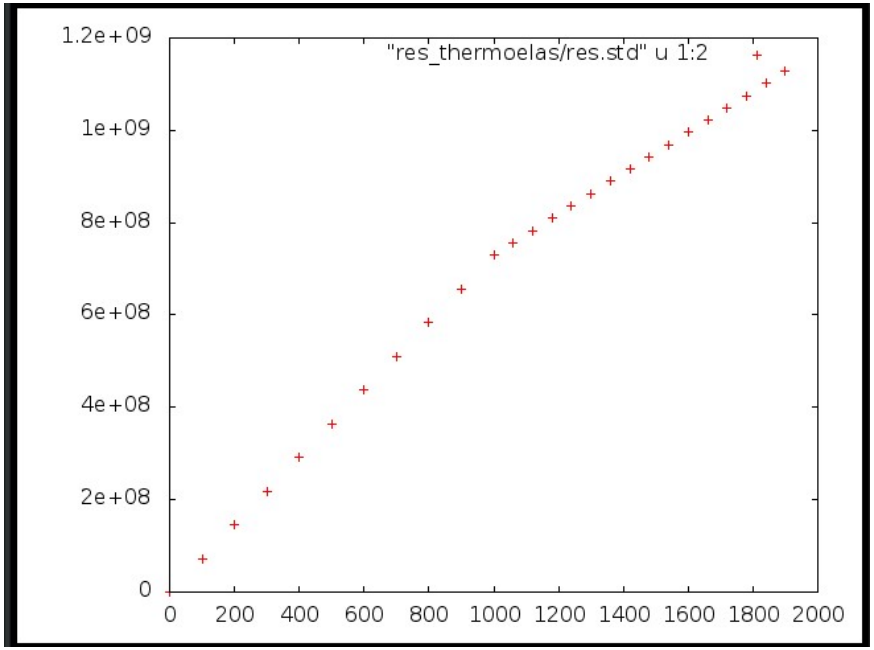
XML FILES : LOADING-OUTPUT

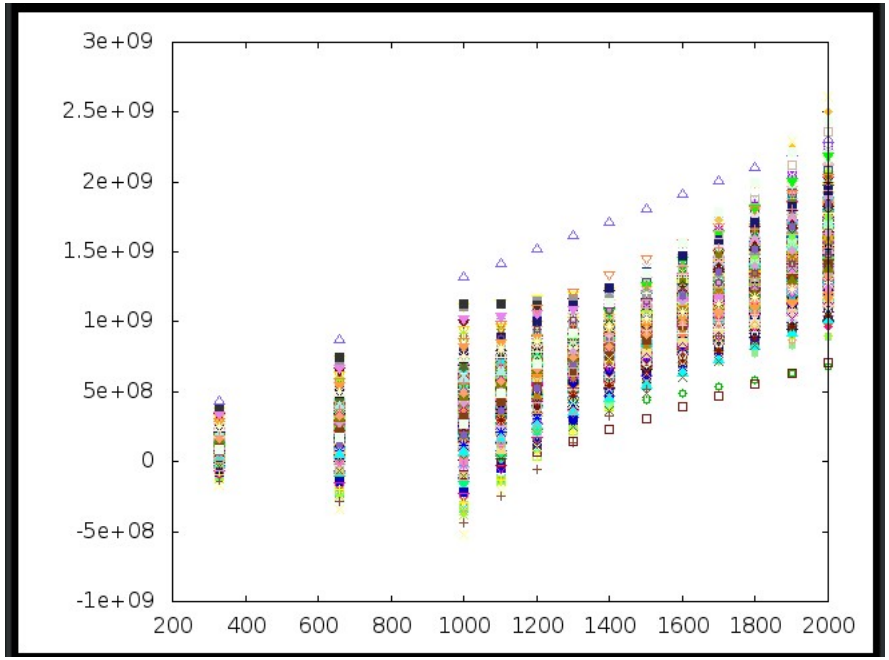
Exercise

15’ then correction

- In *Scripts/* use gnuplot (plot_thermoelas.gp)

#Macroscopic behavior (s11=f(t))
plot "res_thermoelas/res.std" u 1:2





#Per inclusion behavior (s11=f(t))
plot for [j=1:1110] "res_thermoelas/res_2.zstd" every 1110::j-1 u 1:2 notitle

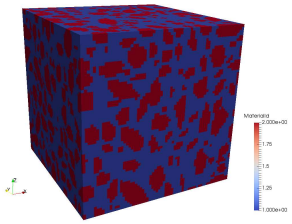
XML FILES : ALGORITHM

- See website
http://www.maisondelasimulation.fr/projects/amitex/general/_build/html/index.html

XML FILES : ALGORITHM

Exercise

- In *Scripts/* use *script_algo.sh*



Inclusions poreuses (contraste infini!)

- In *Algorithm/*

```
$ cp algo_default.xml  algo_nofilter.xml
```

Use the classical Green operator (~5200 iterations vs 157)

```
$ cp algo_default.xml  algo_noacv.xml
```

Remove convergence acceleration (~7800 iterations vs 157)

```
$ cp algo_default.xml  algo_nofilter_noacv.xml
```

Use the classical Green Operator
&
Remove convergence acceleration

(>10000 iterations!)

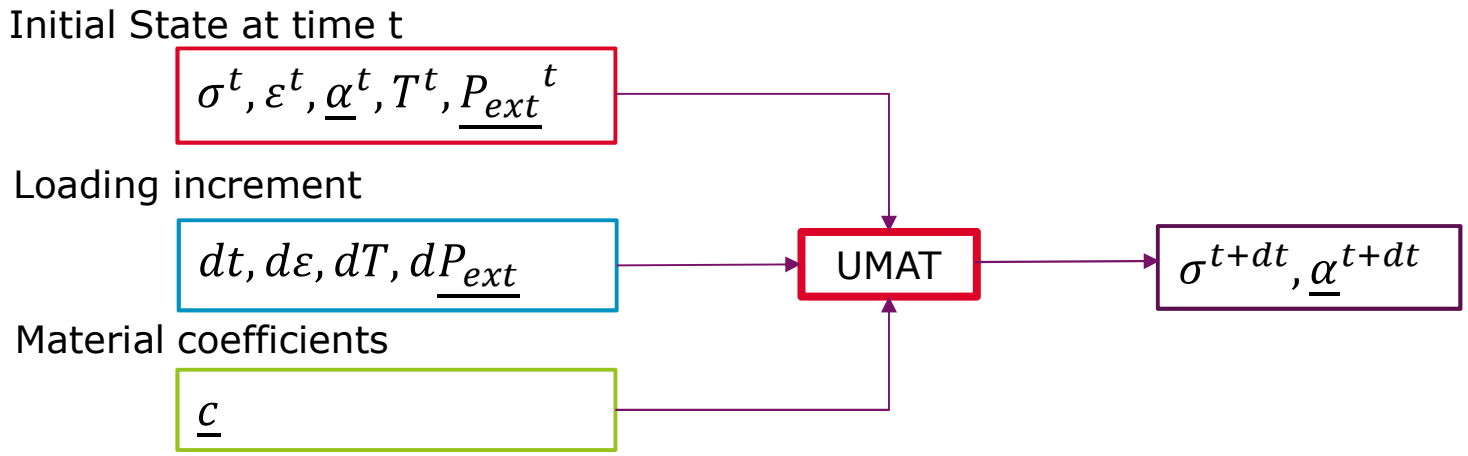
BEHAVIORS

- See website

http://www.maisondelasimulation.fr/projects/amitex/general/_build/html/index.html

BEHAVIORS : UMAT USER DEFINED

- Behavior evaluation : a UMAT-type procedure called on every voxel, at every iteration



UMAT format ➡ compatibility with CAST3M/ABAQUS and MFRONT

```
SUBROUTINE my_behavior( STRESS, STATEV, DDSDDE, SSE, SPD, SCD,&
                        RPL, DDSDDT, DRPLDE, DRPLDT,&
                        STRAN, DSTRAN, TIME, DTIME,&
                        TEMP, DTEMP, PREDEF, DPRED,&
                        CMNAME, NDI, NSHR, NTENS, NSTATV,&
                        PROPS, NPROPS, COORDS,&
                        DROT, PNEWDT, CELENT, DFGRD0, DFGRD1,&
                        NOEL, NPT, LAYER, KSPT, KSTEP, KINC )
```

loading.xml

Initialized by *material.xml*

BEHAVIORS : UMAT USER DEFINED

- Behavior evaluation : a UMAT-type procedure is called by each voxel, at each iteration

σ^t =**STRESS**
$\underline{\alpha^t}$ =**STATEV**
ε^t =**STRAN**
T^t =**TEMP**
$\underline{P_{ext}}^t$ = **PREDEF**

dt =**DTIME**
$d\varepsilon$ =**DSTRAN**
dT =**DTEMP**
$\underline{dP_{ext}}$ =**DPRED**

$\underline{c}$ =**PROPS**

```
SUBROUTINE my_behavior( STRESS, STATEV, DDSDDE, SSE, SPD, SCD,&
                        RPL, DDSDDT, DRPLDE, DRPLDT,&
                        STRAN, DSTRAN, TIME, DTIME,&
                        TEMP, DTEMP, PREDEF, DPRED,&
                        CMNAME, NDI, NSHR, NTENS, NSTATV,&
                        PROPS, NPROPS, COORDS,&
                        DROT, PNEWDT, CELENT, DFGRD0, DFGRD1,&
                        NOEL, NPT, LAYER, KSPT, KSTEP, KINC )
```

σ^{t+dt}=**STRESS**
$\underline{\alpha^{t+dt}}$=**STATEV**

WARNING : for Finite Strain behavior, the mechanical Load increment is given by DFGRD0 and DFGRD1
Instead of STRAN and DSTRAN

BEHAVIORS : AMITEX_FFTP NATIVE

- **Very few 'native' behaviors in AMITEX_FFTP**

  Why ?

  Compatibility with the umat interface (ABAQUS, CAST3M compatible)

  -> user-defined behaviors

  -> MFRONT defined behaviors

  -> A very large collection of standard behaviors (CAST3M compatible)

- **Native behaviors as simple examples and tests : in libAmitex/src/materiaux**

  Linear behaviors

elasiso.f90	linear isotropic elasticity (small strains – linearized strain)
elasaniso.f90	linear orthotropic elasticity
elasiso_GD.f90	linear isotropic elasticity (finite strains – Green-Lagrange strain)
elasiso_eigs.f90	linear elasticity with eigenstrain
paramextelasiso.f90	linear elasticity + dependance with external parameters
thermoelasiso.f90	linear elasticity + dependance with temperature

  Applied stress 'behavior' (for porosity, pressured porosity etc…)

contrainte_imposee.f90	applied stress (6 components)

  Non-linear behavior

viscoelas_maxwell.f90	Maxwell visco-elasticity

BEHAVIORS : UMAT USER DEFINED

Exercise : I - **building** your own behavior (fortran)

- In *Behaviors/*

1

```
$ cp ../../amitex_fftp-vX.Y.Z/libAmitex/src/materiaux/Makefile ./
```

Adjust **Makefile** (if necessary):

FC=gfortran or ifort

ldecomp=path_to_2decomp

2

```
$ cp ../../amitex_fftp-vX.Y.Z/libAmitex/src/materiaux/elasiso.f90 ./elasiso2.f90
```

Adjust **elasiso2.f90** :

rename function : elasiso-> elasiso2

3

```
$ make clean
$ make
```

Generate : *libUmatAmitex.so*

Verify that subroutine elasiso2 is contained in *libUmatBehavior.so*

```
$ nm –D libUmatAmitex.so
```

BEHAVIORS : UMAT USER DEFINED

Exercise : II - **testing** your own behavior (fortran) on a single voxel

- In *Scripts/*  *script_testelasiso2.sh*  A single voxel submitted to uniaxial tensile test

- In *Materials/*

1

```
$ cp mat_lin.xml mat_test_elasiso2.xml
```

Adjust *mat_test_elasiso2.xml*

Lib=''path_to_libUmatAmitex.so''
Law=''elasiso2''
remove material numM=2

- In *Scripts/*

```
$ ./script_test_elasiso2.sh
```

2

Check results

Young modulus : $E = \mu(3\lambda + 2\mu)/(\lambda + \mu)$= 2,7.$10^{10}$ (3*4+2*2,7)/(4+2,7)=7,011940.10^{10} Pa
=> Uniaxial stress at 0,05 strain : E*0,05=0,35059701.10^{10} Pa

BEHAVIORS : MFRONT USER DEFINED

Exercise 1 : I - **building** your own behavior (mfront)

- In *Behaviors/*

http://tfel.sourceforge.net/StandardElastoViscoPlasticityBrick.html

Example : Standard Elasto-Plastic behavior : *SEVP.mfront*

$$\underline{\sigma} = \underline{\mathbf{D}} : \underline{\epsilon}^{\mathrm{el}}$$

$$\underline{\epsilon}^{\mathrm{to}} = \underline{\epsilon}^{\mathrm{el}} + \sum_{i_p=0}^{n_p} \underline{\epsilon}^{\mathrm{p}}_{i_p} + \sum_{i_{vp}=0}^{n_{vp}} \underline{\epsilon}^{\mathrm{vp}}_{i_{vp}}$$

$$\underline{\dot{\epsilon}}^{\mathrm{p}} = \dot{\lambda} \frac{\partial g}{\partial \underline{\sigma}}$$

```
@Brick "StandardElastoViscoPlasticity" {
  stress_potential : "Hooke" {young_modulus : 200e3, poisson_ratio : 0.3},
  inelastic_flow : "Plastic" {
    criterion : "Mises",
    isotropic_hardening : "Voce" {R0 : 300, Rinf : 900, b : 1},
    isotropic_hardening : "Voce" {R0 : 0, Rinf : 300, b : 10},
    kinematic_hardening : "Armstrong-Frederick" {C : 1.5e3, D : 5}
  }
};
```

Plasticity criterion : Von Mises

$$g(\underline{\sigma}, p) = \phi\left(\underline{\sigma} - \sum_i \underline{X}_i\right) - \sum_i R_i(p)$$

Isotropic Hardening (Voce)

$$R(p) = R_\infty + (R_0 - R_\infty)\, exp(-b\,p)$$

Kinematic Hardening (Armstrong-Frederick)

$$\begin{cases} \underline{X} = \frac{2}{3} C\, \underline{a} \\ \underline{\dot{a}} = \dot{p}\, \underline{n} - D \dot{p}\, \underline{a} \end{cases}$$

The von Mises stress is defined by:

$$\sigma_{\mathrm{eq}} = \sqrt{\frac{3}{2}\, \underline{s} : \underline{s}} = \sqrt{3\, J_2}$$

where: - $\underline{s}$ is the deviatoric stress defined as follows:

$$\underline{s} = \underline{\sigma} - \frac{1}{3} \mathrm{tr}(\underline{\sigma})\, \underline{I}$$

BEHAVIORS : MFRONT USER DEFINED

Exercise 1 : I - **building** your own behavior (mfront)

- In *Behaviors/*

1 Compile the behavior and store it in a dynamic library (.so)

```
$ mfront --obuild --interface=umat SEVP.mfront
```

Generate :
src/libUmatBehaviour.so
castem/SEVP.dgibi
include/…

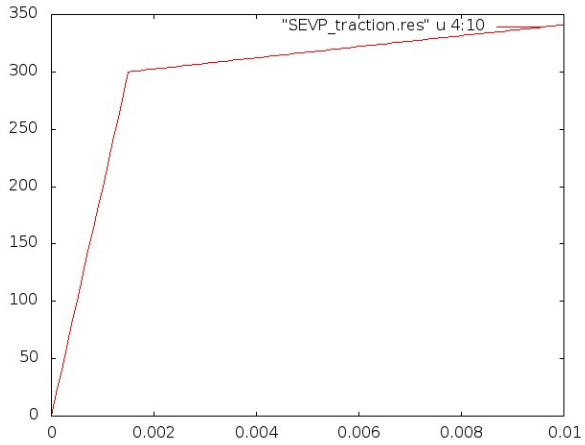
2 Test your implementation with « mtest »

```
$ mtest SEVP_traction.mtest
```

Generate : *SEVP_traction.res*

In gnuplot :

```
plot "SEVP_traction.res" u 2:8 w l
```



BEHAVIORS : MFRONT USER DEFINED

Exercise 1 : II - **testing** your own behavior (mfront) on a single voxel

- In *Scripts/* — *script_testsevp.sh* → A single voxel submitted to uniaxial tensile test

- In *Materials/*

1 `$ cp mat_test_elasiso2.xml mat_test_sevp.xml`

Adjust *mat_test_sevp.xml*

Lib=''path_to_libUmatAmitex.so''
Law=''umatsevp''
Coeff
IntVar
Ref. Material
(lambda=115384,mu=76923)

- In *Behaviors/*

`$ more castem/SEVP.dgibi`

```
** Tridimensional example
** 'OPTION' 'DIMENSION' 3 'MODELISER' 'TRID' ;

coel = 'MOTS' 'YOUN' 'NU' 'RHO' 'ALPH';

statev = 'MOTS' 'EEXX' 'EEYY' 'EEZZ' 'EEXY' 'EEXZ' 'EEYZ' 'KHXX'
'KHYY' 'KHZZ' 'KHXY' 'KHXZ' 'KHYZ' 'P';
```

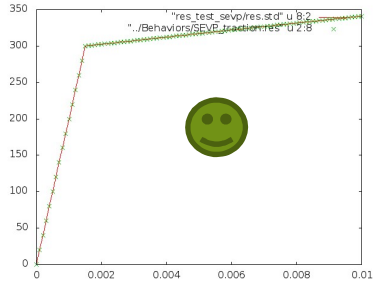
WARNING : The first 4 coefficients are usefull for CAST3M, not used by AMITEX

- In *Loadings_Outputs/* `$ cp traction.xml traction_sevp.xml`

2 Adjust *traction_sevp.xml*

- In *Scripts/* `$ ./script_testsevp.sh`

3 Gnuplot `plot "res_test_sevp/res.std" u 8:2 w l, "../Behaviors/SEVP_traction.res" u 2:8`



BEHAVIORS : MFRONT USER DEFINED

Exercise 2 : idem with *Behaviors/SEVP_matcoeff.mfront*

Material coeff. can be modified in .xml files

- In *Behaviors/*

  1

   *SEVP_matcoeff.mfront* and *SEVP_matcoeff_traction.mtest*

  Compile *SEVP_matcoeff.mfront*
  Test *SEVP_matcoeff_traction.mtest*

- In *Materials/*

  2

  ```
  $ cp mat_test_sevp.xml mat_test_sevp2.xml
  ```

  Adjust *mat_test_sevp2.xml* 

- In *Scripts/*

  3

  ```
  $ ./script_testsevp.sh
  ```

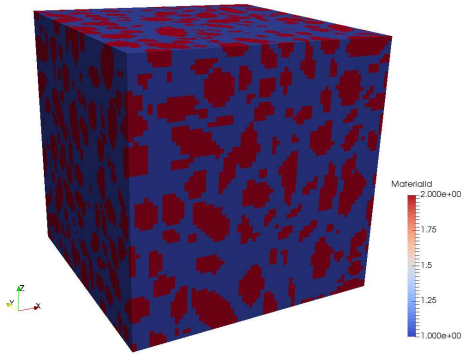
  Gnuplot

  ```
  plot "res_test_sevp2/res.std" u 8:2 w l, "../Behaviors/SEVP_traction.res" u 2:8
  ```

BEHAVIORS : MFRONT USER DEFINED

Exercise 3 : Application – elasto-plastic matrix with elastic inclusions

(=matrix elasticity)



- In *Scripts/* *script_sevp2_incl.sh*

1

- In *Materials/*

2

```
$ cp mat_test_sevp2.xml mat_sevp2_incl.xml
```

Adjust *mat_sevp2_incl.xml*

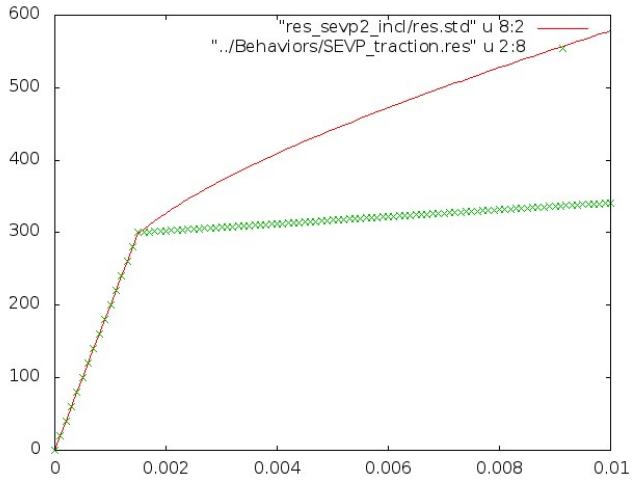
- In *Scripts/*

```
$ ./script_sevp2_incl.sh
```

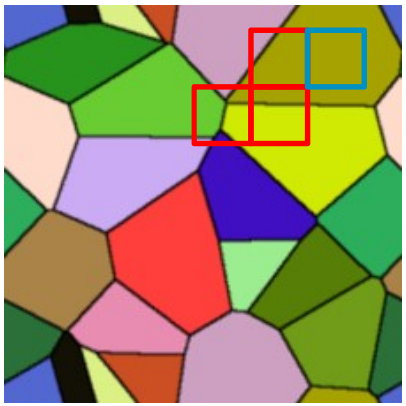
3

Gnuplot

```
plot "res_sevp2_incl/res.std" u 8:2 w l,"../Behaviors/SEVP_traction.res" u 2:8
```



COMPOSITE VOXELS



Homogeneous Voxel

Composite Voxels with N 'phases' (here 2, 2 and 6)

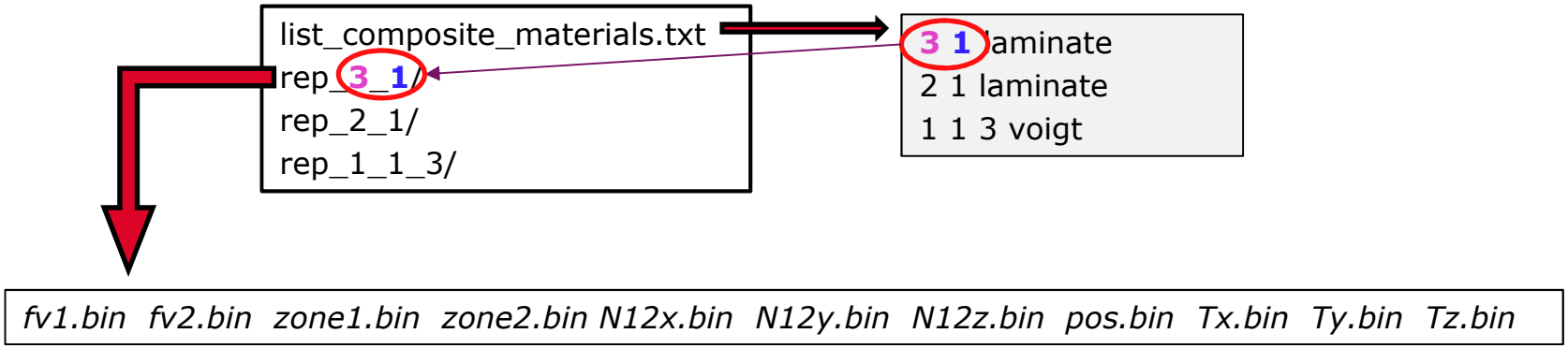
Composite voxel = mixture of different 'phases', characterized by :

- Its position in the grid (linear indice in the 3D grid)
- The number of phases
- The volume fraction of phases
- The properties (coeff and initial int. Variables) of the phases
- If 'laminate' homogenization rule : the « normal » and « tangent » vectors

Each phase is associated to a « material » and a « zone » (in the sense of AMITEX)

COMPOSITE VOXELS

For amitex, the complete definition is given in a folder containing in the example below :



Each binary file collects (one value per composite voxel)

- The volume fraction of phases 1 and 2 (1 for **material *i***, 2 for **material *j*** in *rep_i_j*)
- The **zone number** for material *i* and *j* , for respectively phases 1 and 2
- The normal and tangent vector (for 'laminate' homogenization)
- The position (linear index in the 3D grid)

In general, « material » and « zone » numbers correspond to the materialID.vtk and zoneID.vtk used for simulation without composite voxels

Possibility to add « interphase » material or zone (which are too thin to appear in materialID.vtk or zoneID.vtk)

COMPOSITE VOXELS

Example : No « interphase » material or zone

1 material with 27 zones + composite voxels NO « INTERPHASE » MATERIAL OR ZONE

```
<?xml version="1.0" encoding="UTF-8"?>
<Materials>

<!-- REFERENCE MATERIAL -->
<Reference_Material Lambda0="5.76923076923077e8" Mu0="3.84615384615385e8"/>

<!-- MATERIAL 1  -->
<Material numM="1" Lib="/home/gelebart/amitex_fftp/libAmitex/src/materiaux/libUmatAmitex.so" Law="elasiso" >

        <Coeff Index="1" Type="Constant_Zone" File="materiaux/coefficients/Lambda1_polyx27G_R21.bin" Format="binary"/>
        <Coeff Index="2" Type="Constant_Zone" File="materiaux/coefficients/Mu1_polyx27G_R21.bin" Format="binary"/>

        <Coeff_composite Index="1" Type="Constant_Zone" File="materiaux/coefficients/Lambda1_polyx27G_R21.bin" Format="binary" />
        <Coeff_composite Index="2" Type="Constant_Zone" File="materiaux/coefficients/Mu1_polyx27G_R21.bin" Format="binary"/>

</Material>

<!-- DIRECTORY FOR THE DEFINITION OF COMPOSITE VOXELS -->
<Material_composite>
            <Coeff_composite directory="microstructures/voxcomp/polyX_27G_R21_reuss"/>
</Material_composite>

</Materials>
```

Isotropic behavior for modified Newton-Raphson algorithm
~ initial elastic behavior

Removing this section -> Simulation without any composite voxels

COMPOSITE VOXELS

Example 2 : « interphase » material and/or zone

See website

COMPOSITE VOXELS

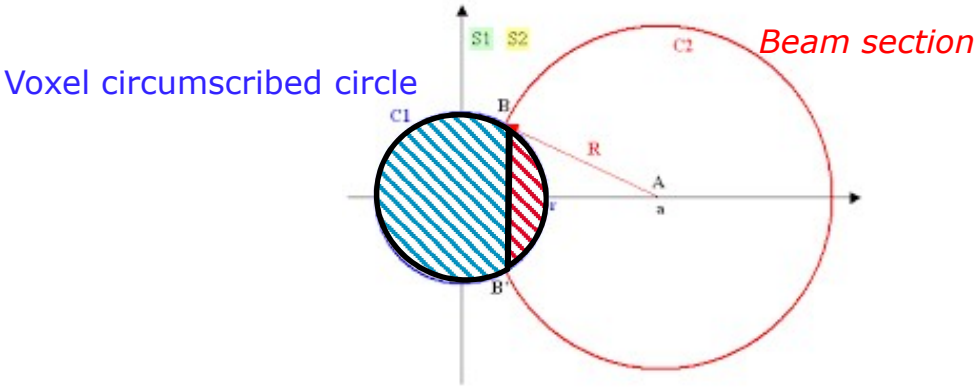
- See website
  http://www.maisondelasimulation.fr/projects/amitex/user_guide/_build/html/materials.html

COMPOSITE VOXELS

Exercise : Generate composite voxels for AMITEX

- In *Microstructures/* *cube_cylinder_composite.m*

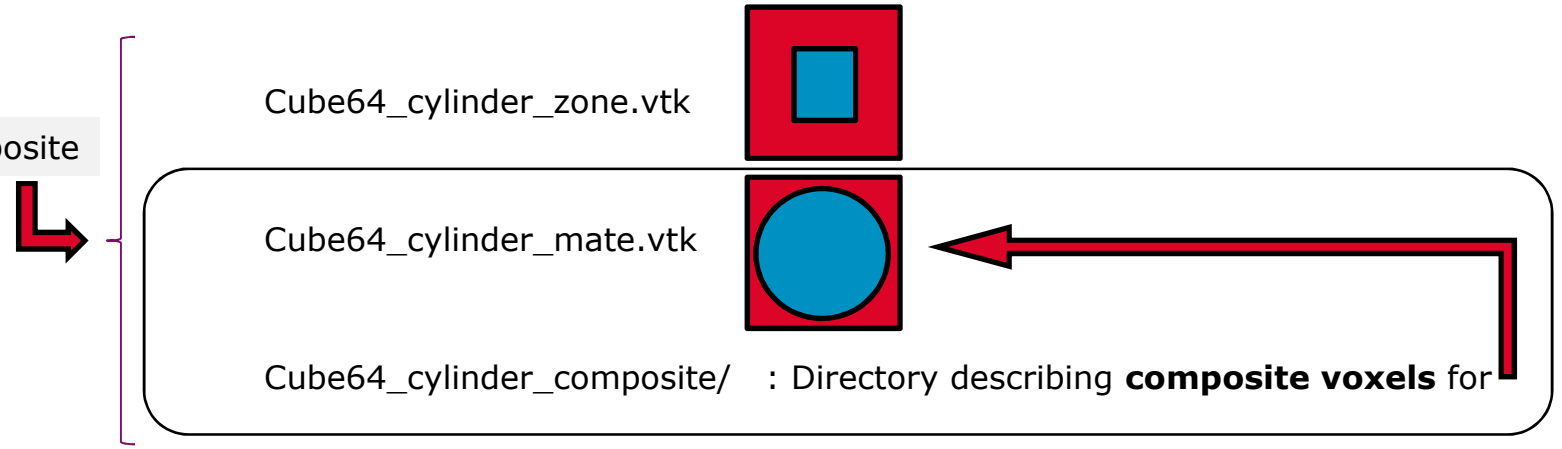
Volume fraction approximation : intersection disk (around a composite voxel) / disk (beam cross-section)
analytical solution



- In *Microstructures/*

octave

cube_cylinder_composite



COMPOSITE VOXELS

Exercise : use composite voxels in AMITEX

- In *Scripts/*  *script_voxcomp.sh*

- In *Materials/*

```
$ cp mat_lin.xml mat_voxcomp.xml
```

Adjust *mat_voxcomp.xml*

Add <Coeff_composite Index=…/>

Add <Material_composite>…<Material_composite/>

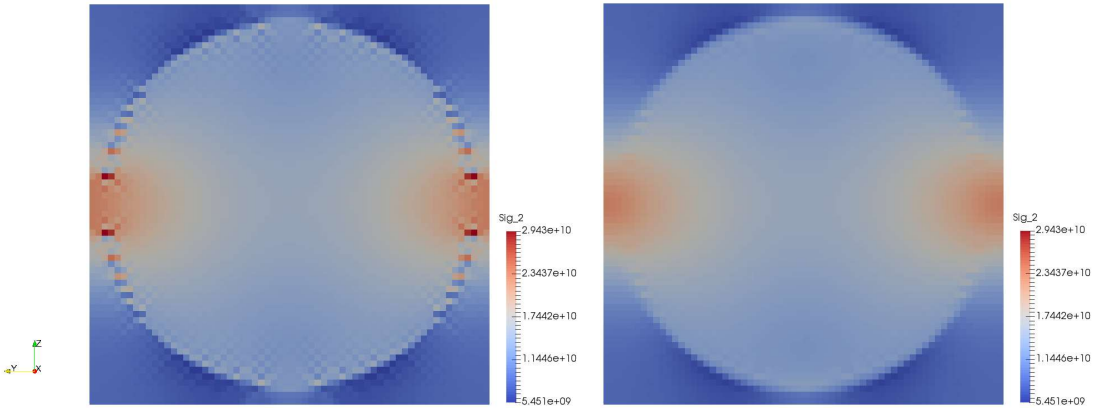
```
$ cp mat_lin.xml mat_voxcomp0.xml
```

Adjust *mat_voxcomp0.xml*

Comment <Material_composite>…<Material_composite/>

- In *Scripts/*

```
$ ./script_voxcomp.sh
```



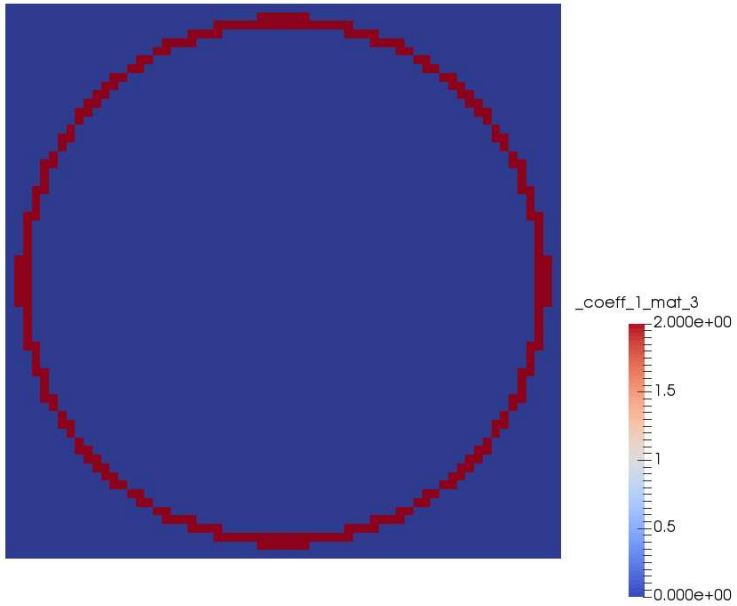
COMPOSITE VOXELS

Exercise : use composite voxels in AMITEX

- In *Scripts/* *script_voxcomp.sh*

*mpirun amitex_fftp -nm $MATEVTK ….. **-coeff2print i***

One vtk file per material with coefficient i



Pour un matériau composite à quoi correspond le coefficient (ou variable interne) i ?
Ici : coeff 1 = nombre de phases

DE LA RECHERCHE À L'INDUSTRIE

COMPOSITE VOXELS

```
!=====================================================================
!>          FONCTION UMAT_VOIGT
!!-------------------------------------------------------------------
!! integration d'un modele composite de Voigt à N phases (déformation homogène)
!! formalisme HPP
!!
!!-------------------------------------------------------------------
!!
!!   \param[in]   umatTab Tableau du type dérivé Umatptr
!!              - contient les pointeurs de fonction vers le comportement de chaque phase
!!
!!   ================================================================
!!     COEFFICIENTS
!!     -----------------
!!
!!     Coeff(ncoeff) tableau de coefficients, ordre defini ci-dessous
!!                  avec ncoeff = 2N+sum(ncoeffi)
!!
!!     1  - nPhase     nombre de phases dans le matériau composite
!!     2  - ncoeff1    nombre de coeff de chaque loi
!!     3  - ncoeff2
!!          .......
!!     1+N - ncoeffN
!!
!!     2+N - FV 1      fractions volumiques de chaque phase
!!     3+N - FV 2
!!           ....
!!     2N  - FV N-1
!!
!!     1+2N,2N+ncoeff1
!!               Coeff1           coefficients pour le materiau 1
!!     1+2N+ncoeff1, 2N+ncoeff1+ncoeff2
!!               Coeff2           coefficients pour le materiau 2
!!           ....
!!           ....
!!     1+2N+ncoeff1+...+ncoeffn-1, 2N+ncoeff1+.....+ncoeffN
!!                CoeffN          coefficients pour le materiau n
!!
!!   ================================================================
!!   ================================================================
!!     VARIABLES INTERNES
!!     ----------------------
!!
!!     Varint(nvarint) tableau de variables internes, ordre defini ci-dessous
!!                  avec nvarint= 7N + sum(nVari)
!!
!!          1  - nvar1           nombre de var. internes de chaque loi
!!          2  - nvar2
!!          .....
!!          N  - nvarN
!!
!!          1+N,6+N
!!             Sig1            Contraintes dans la phase 1 (notation Voigt)
!!          7+N,6+N+nVar1
!!             VarInt1         Variables internes de la phase 1
!!             ........
!!             ........
!!          1+6*(i-1)+N+nVar1+...+nVari-1,6*i+N+nVar1+....+nVari-1
!!             Sigi            Contraintes dans la phase i (notation Voigt)
!!          1+6*i+N+nVar1+...+nVari-1,6*i+N+nvar1+...+nVari
!!             VarintI         Variables internes de la phase i
!!             ........
!!             ........
!!          1+6*(N-1)+N+nVar1+...+nVarn-1,6*N+N+nVar1+.....+nVarn-1
!!             SigN        contraintes dans la phase N
!!
!!          1+6*N+N+nVar1+.....+nVarn-1,6*N+N+sum(nVari)
!!             VarintN     Variables internes dans la phase N
!!
!!   ================================================================
!!
!!
!! \param[out] Sig, Varint
!!
!!-------------------------------------------------------------------
!! ATTENTION - ATTENTION - ATTENTION : notation de Voigt,
!!           pour la deformation : x2 sur les termes de cisaillement
!!                     soit ici NT0,NT1 et T0T1
!!           pour la contrainte  : pas de facteur 2
!!-------------------------------------------------------------------
!!
!! Notation CAST3M (Voigt, ordre 11 22 33 12 13 23)
!=====================================================================
```

COMPOSITE VOXELS

```
!=====================================================================
!>          FONCTION UMATREUSS
!!-------------------------------------------------------------------
!! integration d'un modele composite de REUSS a N phases
!!
!! formalisme HPP
!!
!!-------------------------------------------------------------------
!!
!! \param[in]   dt         Vecteur des pas de temps nouveau et ancien (dt_new,dt_old)
!! \param[in]   umatTab Tableau du type dérivé Umatptr contenant les pointeurs
!!                  de fonction vers le comportement de chaque phase
!!
!!   ================================================================================
!!     COEFFICIENTS
!!     ----------------------
!!
!!     Coeff(ncoeff) tableau de coefficients, ordre defini ci-dessous
!!                 avec ncoeff = 4*N+ncoeff1+.............+ncoeffn
!!
!!
!!     1    - nPhase                       nombre de phases dans le matériau composite
!!     2    - ncoeff1                      nombre de coeff de chaque loi
!!     3    - ncoeff2
!!           .......
!!     1+N  - ncoeffN
!!
!!     2+N  - FV 1                 fractions volumiques de chaque phase (n-1 données la nieme vérifiant FV N = 1 - sum(FV I)
!!     3+N  - FV 2
!!           ....
!!     2N   - FV N-1
!!
!!     2N+1,2N+2
!!           (/ Lambdaeq, Mueq /)            coefficients de Lamé équivalents au comportement élastique initial du matériau 1
!!     2N+3,2N+2+ncoeff1
!!           Coeff1                      coefficients pour le materiau 1
!!     2N+3+ncoeff1,2N+4+ncoeff1
!!           (/ Lambdaeq, Mueq /)            coefficients de Lamé équivalents au comportement élastique initial du matériau 2
!!     2N+5+ncoeff1, 2N+4+ncoeff1+ncoeff2
!!           Coeff2                      coefficients pour le materiau 2
!!          ....
!!          ....
!!     2N+2*(N-1)+ncoeff1+.....+ncoeffn-1+1,4*N+ncoeff1+.............+ncoeffn-1
!!           (/ Lambdaeq, Mueq /)            coefficients de Lamé équivalents au comportement élastique initial du matériau N
!!     4*N+ncoeff1+.............+ncoeffn-1+1,4*N+ncoeff1+.............+ncoeffn
!!           CoeffN                      coefficients pour le materiau n
!!   ================================================================================
!!   ================================================================
!!     VARIABLES INTERNES
!!     ----------------------
!!
!!     Varint(nvarint) tableau de variables internes, ordre defini ci-dessous
!!                 avec nvarint= 13N + sum(nVari)
!!
!!     1  - nvar1           nombre de var. internes de chaque loi
!!     2  - nvar2
!!          .....
!!     N  - nvarN
!!
!!     1+N,6+N
!!          Def1                    composantes de la defomation, phase 1
!!
!!     7+N,12+N
!!          Def1_old                 composantes de la deformation pas precedent, phase 1
!!
!!     13+N,12+N+nvar1
!!          VarInt1                  variables internes, phase 1
!!
!!     13+N+nvar1,18+N+nvar1
!!          Def2                    composantes de la defomation, phase 2
!!
!!     19+N+nvar1,24+N+nvar1
!!          Def2_old                 composantes de la deformation pas precedent, phase 2
!!
!!     25+N+nvar1,24+N+nvar1+nvar2
!!          VarInt2                  variables internes, phase2
!!          .........
!!
!!     N+12*(N-1)+1+nvar1+...+nvarn-1,N+12*(N-1)+6+nvar1+...+nvarn-1
!!          Defn                    composantes de la defomation, phase N
!!
!!     N+12*(N-1)+7+nvar1+...+nvarn-1, N+12*(N-1)+12+nvar1+...+nvarn-1
!!          Defn_old                 composantes de la deformation pas precedent, phase N
!!
!!     13*N+nvar1+...+nvarn-1+1,13*N+nvar1+...+nvarn
!!          Varintn                  variables internes, phaseN
!!
!!   ================================================================
!!
!!   autres paramètres d'entrée : voir formalisme UMAT
!!
!! \param[out] Sig, Varint
!!
!!-------------------------------------------------------------------
!! ATTENTION - ATTENTION - ATTENTION : notation de Voigt,
!!           pour la deformation : x2 sur les termes de cisaillement
!!           pour la contrainte  : pas de facteur 2
!!-------------------------------------------------------------------
!!
!! Notation CAST3M (Voigt, ordre 11 22 33 12 13 23)
!=====================================================================
```

COMPOSITE VOXELS

```
!=====================================================================
!>          FONCTION UMATLAMINATE
!!-------------------------------------------------------------------
!! integration d'un modele composite LAMINATE a N phases
!!
!! formalisme HPP
!!
!!-------------------------------------------------------------------
!!
!! \param[in]   dt         Vecteur des pas de temps nouveau et ancien (dt_new,dt_old)
!! \param[in]   umatTab Tableau du type dérivé Umatptr contenant les pointeurs
!!                  de fonction vers le comportement de chaque phase
!!
!!   ================================================================================
!!     COEFFICIENTS
!!     ----------------------
!!
!!      Coeff(ncoeff) tableau de coefficients, ordre defini ci-dessous
!!                avec ncoeff = 4*N+6+ncoeff1+.............+ncoeffn
!!
!!
!!     1    - nPhase                      nombre de phases dans le matériau composite
!!     2    - ncoeff1                     nombre de coeff de chaque loi
!!     3    - ncoeff2
!!           .......
!!     1+N  - ncoeffN
!!
!!     2+N  - FV 1                fractions volumiques de chaque phase (n-1 données la nieme vérifiant FV N = 1 - sum(FV I)
!!     3+N  - FV 2
!!           ....
!!     2N   - FV N-1
!!
!!     2N+1 - Nx                        Composantes du vecteur normal à l'interface
!!     2N+2 - Ny
!!     2N+3 - Nz
!!     2N+4 - Tx                        Composantes d'une direction tangeant à l'interface
!!     2N+5 - Ty
!!     2N+6 - Tz
!!
!!     2N+7,2N+8
!!           (/ Lambdaeq, Mueq /)            coefficients de Lamé équivalents au comportement élastique initial du matériau 1
!!     2N+9,2N+8+ncoeff1
!!           Coeff1                     coefficients pour le materiau 1
!!     2N+9+ncoeff1,2N+10+ncoeff1
!!           (/ Lambdaeq, Mueq /)            coefficients de Lamé équivalents au comportement élastique initial du matériau 2
!!     2N+11+ncoeff1, 2N+10+ncoeff1+ncoeff2
!!           Coeff2                     coefficients pour le materiau 2
!!          ....
!!          ....
!!     2N+6+2*(N-1)+ncoeff1+.....+ncoeffn-1+1,4*N+6+ncoeff1+.............+ncoeffn-1
!!           (/ Lambdaeq, Mueq /)            coefficients de Lamé équivalents au comportement élastique initial du matériau N
!!     4*N+6+ncoeff1+.............+ncoeffn-1+1,4*N+6+ncoeff1+.............+ncoeffn
!!           CoeffN                     coefficients pour le materiau n
!!   ================================================================================
!!   ====================================================
!!    VARIABLES INTERNES
!!    ----------------------
!!
!!    Varint(nvarint) tableau de variables internes, ordre defini ci-dessous
!!                avec nvarint= 10N + sum(nVari)
!!
!!    1  - nvar1          nombre de var. internes de chaque loi
!!    2  - nvar2
!!         .....
!!    N  - nvarN
!!
!!    1+N,3+N
!!         DefA1                composantes de la defomation Anti-Plane
!!                           dans la phase 1 (ordre NN,NT0,NT1, notation Voigt)
!!    4+N,6+N
!!         SigP1                composantes de la contrainte Plane
!!                           dans la phase 1 (ordre T0T0,T1T1,T0T1, notation Voigt)
!!    7+N,9+N
!!         DefA1_old              composantes de la deformation Anti-Plane
!!                           du pas de temps précédent
!!    10+N,9+N+nvar1
!!         VarInt1                variables internes phase 1
!!
!!    10+N+nvar1,12+N+nvar1
!!         DefA2                composantes de la defomation Anti-Plane
!!                           dans la phase 2 (ordre NN,NT0,NT1, notation Voigt)
!!    13+N+nvar1,15+N+nvar1
!!         SigP2                composantes de la contrainte Plane
!!                           dans la phase 2 (ordre T0T0,T1T1,T0T1, notation Voigt)
!!    16+N+nvar1,18+N+nvar1
!!         DefA2_old              composantes de la deformation Anti-Plane
!!                           du pas de temps précédent
!!    19+N+nvar1,18+N+nvar1+nvar2
!!         VarInt2                variables internes phase2
!!
!!     .........
!!     .........
!!     .........
!!
!!    N+9*(N-1)+1+nvar1+...+nvarn-1,N+9*(N-1)+3+nvar1+...+nvarn-1
!!         DefAn                composantes de la defomation Anti-Plane
!!                           dans la phase N (ordre NN,NT0,NT1, notation Voigt)
!!    N+9*(N-1)+4+nvar1+...+nvarn-1,N+9*(N-1)+6+nvar1+...+nvarn-1
!!         SigPn                composantes de la contrainte Plane
!!                           dans la phase N (ordre T0T0,T1T1,T0T1, notation Voigt)
!!    N+9*(N-1)+7+nvar1+...+nvarn-1, N+9*(N-1)+9+nvar1+...+nvarn-1
!!         DefAn_old              composantes de la deformation Anti-Plane
!!                           du pas de temps précédent
!!    10*N+nvar1+...+nvarn-1+1,10*N+nvar1+...+nvarn
!!
!! ============================================================
!! ATTENTION – ATTENTION – ATTENTION => voir Voigt, Reuss
!============================================================
```

COMPOSITE VOXELS

Exercise : use composite voxels in AMITEX

- In *Scripts/*  *script_voxcomp.sh*

BEAM / PLATE APPLICATION

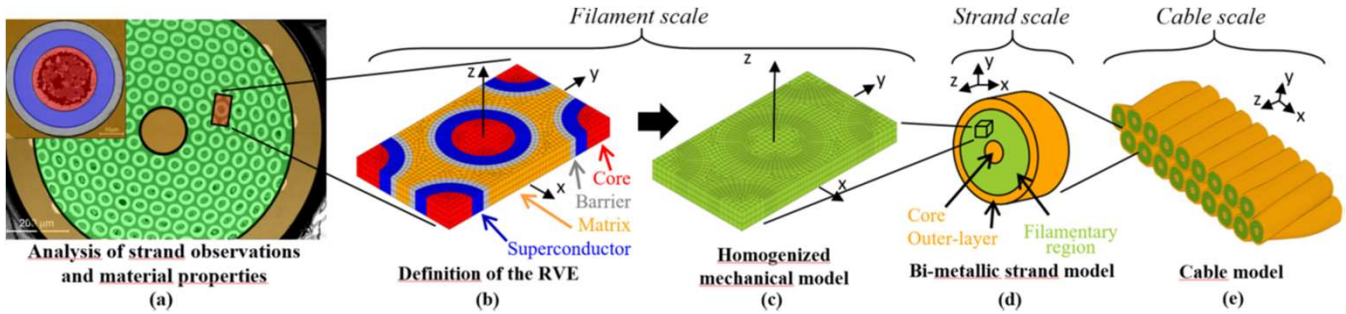
Homogeneous beam with circular cross-section

DEFORMEDSHAPE

Homogeneous beam with circular cross-section

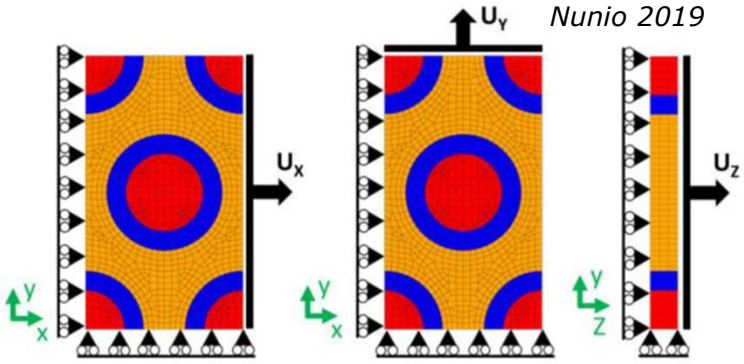
TP – SUPERCONDUCTING CABLES

- Context : superconducting cables (for magnets)



Nunio 2019

- Filament scale

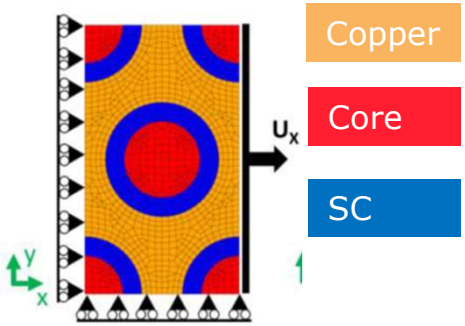


Nunio 2019

FEM Boundary conditions ⟺ Periodicity

1 - Create the microstructure
2 - Perform elastic simulation with arbitrary properties
- uniaxial tensile test in X
- applied axial strain 0,01
3- Perform elasto-plastic simulations

TP – SUPERCONDUCTING CABLES



COMPONENTS	E(GPa)	σ_y(MPa)	C(MPa)	γ
Copper	129	39	35960	310
Filament Core	3	-	-	-
SC region (Nb_3Sn SG)	171	-	-	-

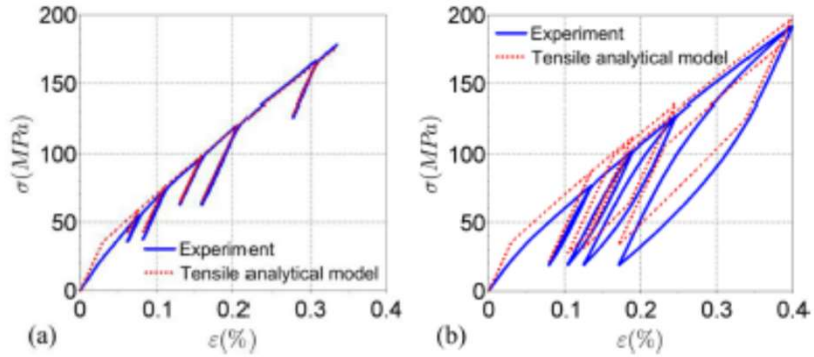
Kinematic Hardening

$$\dot{X} = C\dot{\varepsilon}_p - \gamma X\dot{p}$$

Lenoir 2019

1 – Introduce non-linear behavior with the given properties

2 – Simulate loading-unloading



Lenoir 2019

DE LA RECHERCHE À L'INDUSTRIE

cea

TP – PARALLEL COMPUTING

TP –

Pour ces 3 exercices : utiliser elasiso.f90 comme point de départ (pour chaque comportement : renommer le fichier et le nom de la fonction)

Dégradation du module élastique avec le temps = E = E0.exp(-t/tau)+E1

Gonflement d'une phase avec un paramètre extérieur Pext (ex : fluence ~qté d'irradiation reçue par le matériau)

Sig = c(esp-eps_g)
Eps_g = Pext.Eps0.Id
Appliquer un chargement Pext (0->1) + plateau + rampe (1 -> 0)

Même simulation avec la Température :

Sig = c(esp-eps_g)
Eps_g = Pext.Eps0.Id
Appliquer un chargement Pext (0->1) + plateau + rampe (1 -> 0)

Changement de trajet de chargement (avec comportement cinématique 'induit') :
application traction/pression interne tube

loi MFRONT : plasticité avec faible écrouissage isotrope
chargement 1 : pression interne avec effet de fond : pilotage eps_yy 0%->1%
+ maintien sig_zz=0,5*sig_yy (autres composantes : contrainte = 0)

chargement 2 : traction uniaxiale : eps_zz 0->1% (autres composantes : contrainte = 0)
traction uniaxiale : eps_zz 1% -> 0% (autres composantes : contrainte = 0)
pression interne avec effet de fond : pilotage eps_yy 0%->1%
+ maintien sig_zz=0,5*sig_yy (autres composantes : contrainte = 0)

TP –

Tube sollicité en pression interne : effet des voxels composites

Composite à N inclusions avec proprietes variables de chaque inclusion

Propriétés (coeff. Ou var. internes) continuement variables

coeff. Continuement variable (cas 1 matériau / cas 2 matériaux)

cas 2 matériaux variable (cas 1 matériau / cas 2 matériaux)

Grandes transformations : rotation pure

Mise en évidence écrouissage cinématique induit par des inclusions élastiques