Material & Structure Analysis Suite

Multiscale Materials Modeling

Version 9.1

Z-set software is distributed by

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Chapter 1

Multiscale Modeling

Multiscale tools in Z-set

This section presents some tools about the non-linear multi-scale modeling of multi-phase materials and composites, developed in Z-set. The aim of these approaches is to describe the behavior of a structure from the local constitutive equations of the constituents.

Several Mean-Field homogenization approaches are available, to allow accurate prediction of the macroscopic stress-strain response of composite materials, which is related to the description of their complex microstructural behavior exemplified by the interaction between the constituents, such as Voigt, Reuss, Self consistent, etc... In the development of the homogenization procedures for non linear materials, we have to define both the homogenization step itself, which consists in averaging the local fields to obtain the overall ones and the often more complicated localization step, where a local problem for each sub-volume is solved in order to obtain approximations for the local field behavior. In this context, the microstructure of the material under consideration is basically taken into account by representative volume elements (RVE).

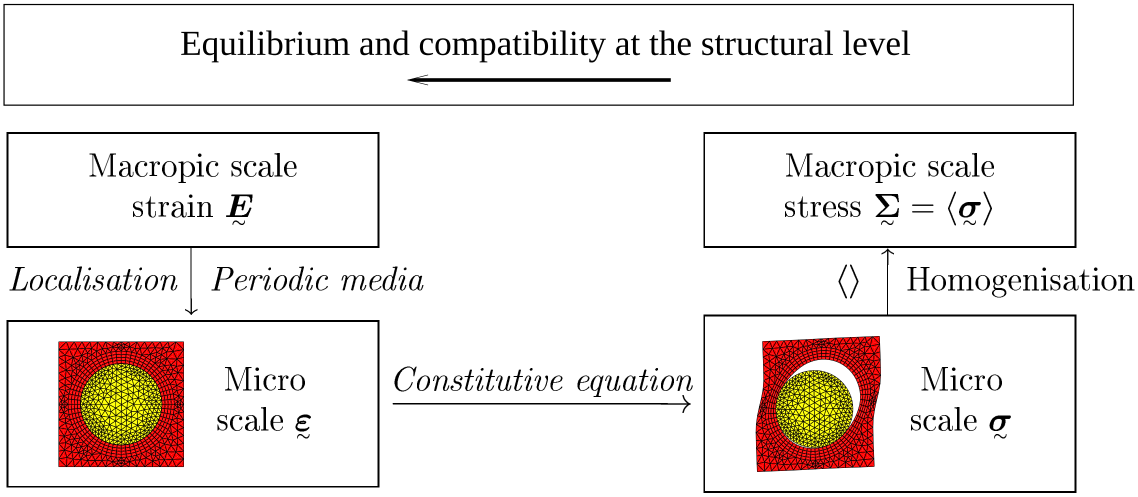
From a general point of view, the description of the macroscopic behavior of solid heterogeneous media with multi-materials is a very difficult task. In the multiscale tools in Z-set, one distinct set of constitutive equations is attributed to each sub-volume, which are treated independently. Each sub-volume then possesses its own stress/strain tensor. The macroscopic behaviour is obtained by averaging the corresponding non-uniform local behaviour law using the well-known homogenization schemes. Consequently, it is possible to mix different types of constitutive equations for each sub-volume. In principle, all mechanical Z-mat models can be used in the multi-mat model, including other multi-mat models themselves.

Multiscale tools in Z-set, are called “Multimat” for static interface and “Phase-field” for dynamic interface, with additional evolution equation related to the interface mobility.

Imbricated finite element method (FE^2 model)

This model has been developed during the past few years [Feyel] in order to directly replace the constitutive equations (at the structural scale). At each Gauss point of the structural scale, the constitutive equations are thus replaced by an other finite element computation at the composite scale. The figure bellow shows the schematic principle of the FE^2 approach :

- finite element computation at the structural scale which delivers the macroscopic strain $\boldsymbol{E}$,
- localization which determines the local strain field at the fiber/matrix scale $\boldsymbol{\epsilon}$,
- a finite element computation which delivers the local stress field $\boldsymbol{\sigma}$,
- homogenization of $\boldsymbol{\sigma}$ to compute the macroscopic stress $\boldsymbol{\Sigma}$.



Any localization/homogenization scheme can be used, but in the specific SiC/Ti case, the regular position of the fiber into the matrix allows to use the classical periodic homogenization.

Localization/homogenisation scheme:
Description:

Two files are necessary, the first one `periodic.mat` is defined in the `**material` section of the macroscopic problem and the second one `file_local` is defined in the `**local` section of the `periodic.mat` file.

Syntax:
This is the syntax of the `periodic.mat` file.

```
 ***behavior mmc_fe2
 **local periodic
 **file file_name ]
[**update_tg_matrix tg_matrix_option ]
[**import name name_dest ]
```

where `file_name` is the name of the file where the localization options are indicated. The `import` option specifies which macroscopic parameters must imported in the microscopic problem. *name* is the name of the parameter in the macroscopic problem and *name_dest* is its name in the microscopic problem.

Syntax:
This is the syntax of the `**file file_name` file.

```
**convergence ctype
**reinit itype
**maxiter maxiter
**ratio ratio
**local_problem local_name
**localization ltype
   *impose_elset_dof elset_name
   *macro_E_size Esize
*homogeneisation htype
   *macro_flux_size Fsize
```

***convergence* give the convergence type : `absolu`, `automatic`

***reinit* (see `***sequence`)

***maxiter* maximum number of iteration to solve the microproblem.

***ratio* specify the maximum global ratio for the convergence.

***localisation* method of localisation form the macroscopic scale to the microscopic scale. Two types : `to_periodic_plane_strain` or `to_general_periodic_plane_strain`.
`*macro_E_size` size of the macroscopic strain tensor (4 in 2D or 6 in 3D.

***homogeneisation* method of homogenisation. Two types : `classic_2d` or `classic_3d`
`*macro_flux_size` size of the macroscopic stress tensor.

Example of a FE^2 test:

Macroscopic problem:

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% This is the macroscopic problem          %%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

****calcul
***mesh **predefined rve2d
***resolution newton
**sequence 1
*time 0.5
*increment 10
*ratio .1
*algorithm p1p2p3
*iteration 100
***bc
**impose_element_dof  1 E11 1. time
***material    *file periodic.mat
***output
    **test
      *precision 5
      *small 1.e-8
      *gauss_var 1 1 eto11 eto22 eto33 eto12 sig11 sig22 sig33 sig12
****return

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% This is the periodic.mat file            %%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
***behavior mmc_fe2
  **local periodic
  **file file_local
  **update_tg_matrix  ask_localization
***return

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% This is the file_local file              %%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
**convergence absolu
**reinit p1p2p3
**maxiter 1000
**ratio .005
**local_problem micro
**localisation to_general_periodic_plane_strain
    *impose_elset_dof ALL_ELEMENT
    *macro_E_size 4
**homogeneisation classic_2d
    *macro_flux_size 4
***return
```

Microscopic problem:
Description:

This part is the description of the microscopic problem. No comment, see `****calcul`.

```
****calcul
  ***mesh
    **elset ALL_ELEMENT periodic_general_plane_strain
            periodic_info total_displacement_field
***linear_solver frontal
***resolution
  **sequence
    *ratio absolu 0.001
    *time  1.
    *increment 30
    *algorithm   eeeeee
  ***bc
    **impose_nodal_dof
      centre  U1 0.
      centre  U2 0.
      ALL_NODE U3 0.
  ***equation
    **mpc2 gauche U1 droite U1
    **mpc2 gauche U2 droite U2

    **mpc2 haut U1 bas U1
    **mpc2 haut U2 bas U2

    **mpc2 bg U1 bd U1
    **mpc2 bg U2 bd U2
    **mpc2 bg U1 hg U1
    **mpc2 bg U2 hg U2
    **mpc2 bg U1 hd U1
    **mpc2 bg U2 hd U2
***material
  **elset fibre
    *file  fibre
  **elset matrice
    *file matrix
***output
    **test
      *precision 5
      *small 1.e-8
      *gauss_var 1 1 eto11 eto22 eto33 eto12 sig11 sig22 sig33 sig12
****return
```

General_TFA_Method

In this section, we recall the main line of the Transformation Field Analysis method introduced by Dvorak et al. [Dvorak, 1992]. This method is very similar to the FE^2 one (1. localization, 2.constitutive equations at the local scale, 3. homogenization), but it is technically very different. The TFA method is based on concentration and influence tensors and considers the plastic strain and thermal expansion as eigenstrains of the same nature. The composite scale is divided into a number of sub-volumes (N) inside which the mechanical fields are assumed to be uniform. A sub-volume r is thus a homogeneous part of the representative volume element. The TFA models link the local fields ($\boldsymbol{\sigma}_r$ and $\boldsymbol{\epsilon}_r$) to the macroscopic ones ($\boldsymbol{\Sigma}$ and $\boldsymbol{E}$) with the following relations :

$$\boldsymbol{\sigma}_r = \boldsymbol{B}_r : \boldsymbol{\Sigma} - \sum_{s=1}^{N} \boldsymbol{F}_{rs} : \boldsymbol{L}_s : \boldsymbol{\gamma}_s \tag{1}$$

$$\boldsymbol{\epsilon}_r = \boldsymbol{A}_r : \boldsymbol{E} + \sum_{s=1}^{N} \boldsymbol{D}_{rs} : \boldsymbol{\gamma}_s \tag{2}$$

with

$$\boldsymbol{\gamma}_r = \boldsymbol{\epsilon}_r - \boldsymbol{\epsilon}_r^e = \boldsymbol{\epsilon}_r^p + \epsilon_r^{th} \tag{3}$$

where $\boldsymbol{\gamma}_r$ is the formal eigenstrain. $\boldsymbol{A}_r$ and $\boldsymbol{B}_r$ are the elastic strain and stress concentration tensors respectively (fourth rank tensors) of the sub-volume V_r. $\boldsymbol{F}_{rs}$ and $\boldsymbol{D}_{rs}$ are the transformation influence tensors (fourth rank tensors); the subscript rs denotes the influence of the sub-volume s on the sub-volume r. These are determined by solving a set of linear problems (6 for the concentration tensors and 6*N for the influence tensors) by a finite element method. These tensors are function of the elastic behavior of each sub-volume and the shape of the VER. ϵ_s^{th} and ϵ_s^p denote the uniform thermal and plastic strain of the sub-volume s.

In the general case with varying local elastic behavior (temperature or damage induced), the formal eigenstrain $\boldsymbol{\gamma}_r$ is determined from the specification of the current state of the sub-volume, which can be generalized to take into account the thermal and damage effects on the elastic behavior. This generalized eigenstrain and the local behavior are obtained as follows,

$$\boldsymbol{\gamma}_r = \boldsymbol{\epsilon}_r - \boldsymbol{\epsilon}_r^e = \boldsymbol{\epsilon}_r^p + \boldsymbol{\epsilon}_r^{th} + \boldsymbol{\epsilon}_r^d \qquad \text{and} \qquad \boldsymbol{\sigma}_r = \widetilde{\boldsymbol{L}}(\boldsymbol{T})_r : (\boldsymbol{\epsilon}_r^e) = \boldsymbol{L}_r^0 : (\boldsymbol{\epsilon}_r - \boldsymbol{\gamma}_r) \tag{4}$$

where $\widetilde{\boldsymbol{L}}(\boldsymbol{T})_r$ is the thermally dependent and/or damaged elastic stiffness, which is related to the actual state of the sub-volume r and $\boldsymbol{L}_s^0$ is the initial undamaged matrix, which is independent of temperature.

$$\begin{cases} \boldsymbol{\gamma}_r = \boldsymbol{\epsilon}_r^p + \boldsymbol{\epsilon}_r^{th} & \text{if} \quad \widetilde{\boldsymbol{L}}(\boldsymbol{T})_r = \boldsymbol{L}_r \\ \boldsymbol{\gamma}_r = \boldsymbol{\epsilon}_r^p + \boldsymbol{\epsilon}_r^{th} + \boldsymbol{\epsilon}_r^d & \text{if} \quad \widetilde{\boldsymbol{L}}(\boldsymbol{T})_r \neq \boldsymbol{L}_r \end{cases}$$

and the eigenstrain related to the damage effect can be rewritten as follows :

$$\boldsymbol{\epsilon}_r^d = (\boldsymbol{I} - \widetilde{\boldsymbol{L}}(\boldsymbol{T})_r^{-1} : \boldsymbol{L}_r^0) : \epsilon_e = \boldsymbol{\epsilon}_r^g = (\widetilde{\boldsymbol{S}}_r - \boldsymbol{S}_r^0) : \boldsymbol{\sigma}_r \tag{5}$$

where $\tilde{\boldsymbol{S}}_r$ and $\boldsymbol{S}_r^0$ are respectively the actual and initial compliance of the sub-volume r.

It is important to note that damage or thermal change in the elastic modulus makes the eigenstrain not only a function of the plastic and thermal strain but also a function of the elastic strain. This dependence along with rate independent plasticity will make a two way coupling between all the local total strain rates and all the eigenstrains. In addition, various physical effects must be take into account, like the interaction between the interface on dislocation movement and the effects of the incoherent interface with the discontinuity of the displacements, in order to obtain a good local strain/stress redistributions, as well as a correct stress-strain behavior.

The TFA method is then considered in conjunction with the “Generalized Eigenstrain Model”, where corrected constitutive eigenstrain β_r is introduced and expressed in terms of the formal eigenstrain plus a correction:

$$\boldsymbol{\beta}_r = \boldsymbol{\gamma}_r + \boldsymbol{\xi}_r \tag{6}$$

Here the eigenstrain β_r is to be considered as an internal variable which must be assigned an evolution law, which can be tuned to fit the available data.

This evolution law is associated either with a stress localization or with a strain localization law but not both. In this case, the stress localization and the strain localization can be written as follows:

Strain localization :

$$\left\{\begin{array}{lcl} \boldsymbol{\epsilon}_r & = & \boldsymbol{A}_r : \boldsymbol{E} + \displaystyle\sum_{s=1}^{n} [\boldsymbol{D}_{sr} : \boldsymbol{\gamma}_s + \boldsymbol{E}_{sr} : \boldsymbol{\xi}_s] \quad \text{where} \quad \boldsymbol{E}_{sr} = \boldsymbol{D}_{sr} \\ \\ \boldsymbol{\sigma}_r & = & \boldsymbol{B}_r : \boldsymbol{\Sigma} - \displaystyle\sum_{s=1}^{n} \boldsymbol{F}_{sr} : \boldsymbol{L}_s : \boldsymbol{\beta}_s - \boldsymbol{L}_r : (\boldsymbol{\gamma}_r - \boldsymbol{\beta}_r) - \boldsymbol{B}_r : \displaystyle\sum_{s=1}^{n} c_s \boldsymbol{L}_s : (\boldsymbol{\gamma}_r - \boldsymbol{\beta}_r) \end{array}\right.$$

Stress Localization :

$$\left\{\begin{array}{lcl} \boldsymbol{\epsilon}_r & = & \boldsymbol{A}_r : \boldsymbol{E} + \displaystyle\sum_{s=1}^{n} [\boldsymbol{D}_{sr} : \boldsymbol{\gamma}_s + \boldsymbol{E}_{sr} : \boldsymbol{\xi}_s] \quad \text{where} \quad \boldsymbol{E}_{sr} = \boldsymbol{D}_{sr} - \delta_{sr} \boldsymbol{I} - c_r \boldsymbol{A}_s \\ \\ \boldsymbol{\sigma}_r & = & \boldsymbol{B}_r : \boldsymbol{\Sigma} - \displaystyle\sum_{s=1}^{n} \boldsymbol{F}_{sr} : \boldsymbol{L}_s : \boldsymbol{\beta}_s \end{array}\right.$$

where c_r is the volume fraction of the sub-volume r ($c_r = V_r/V$).

The macroscopic behavior (macroscopic strain $\boldsymbol{\Sigma}$ and stress $\boldsymbol{E}$) can be obtained by averaging the local stresses ($\boldsymbol{\sigma}_r$) and strain ($\boldsymbol{\epsilon}_r$) on the RVE :

$$\boldsymbol{\Sigma} = \Big\langle \boldsymbol{\sigma}(x) \Big\rangle_V = \sum_r c_r \boldsymbol{\sigma}_r \qquad , \qquad \boldsymbol{E} = \Big\langle \boldsymbol{\epsilon}(x) \Big\rangle_V = \sum_r c_r \boldsymbol{\epsilon}_r \tag{7}$$

Syntax:

```
***behavior general_tfa
 **material volume_fraction  name   |   **material_in_file <file>
  *file file_name
  [*integration method ]
  [*rotation <ROTATION> ]  |   [*rotation_list <file> ]
  [*volume_fraction_file <file> ]
 **material etc ...
 **localization <LOCALIZATION1>
 [**solver tfa_implicit1 ]
 [**reference_temperature double ]
 [**eigenstrain <EIGENSTRAIN> ]
***return
```

***material* specify the different sub-volumes and its volume fractions. The number of `**material` is equal to the number of sub-volumes.

***material_in_file* give the name of the external file where the different sub-volumes are defined. This file name is relative to the current working directory. Using `**material`, just one sub-volume can be specified whereas when `**material_in_file` is used, many sub-voumes can be defined.

***localization* specify the localization method for determining the strain and stress concentration tensors $(\boldsymbol{A}_r, \boldsymbol{B}_r)$ as well as the transformation influence tensors $(\boldsymbol{D}_{sr}, \boldsymbol{F}_{sr})$

***eigenstrain* define the evolution law for the eigenstrain variable, which is considered as an internal variable. It has the dimension of a strain.

***solver* A consistent tangent matrix is provided with this model if implicit integration is chosen, and the sub-materials have a consistent tangent.

The options `*rotation_list` or `**volume_fraction_file` only available when using `**material_in_file`.

Example:

```
***behavior general_tfa
  **solver tfa_implicit1
  **localization polycrystal
     C 50000.0
  **eigenstrain beta
     D 10000.0
  **material  0.2 grain1
   *file poly_trac_2.inp 2
   *rotation -149.676 15.61819 154.676
   *integration theta_method_a 1. 1.e-9 200
  **material 0.3 grain2
   *file poly_trac_2.inp 2
   *rotation -210.324 15.61819 205.324
   *integration theta_method_a 1. 1.e-9 200
  **material 0.5 grain3
   *file poly_trac_2.inp 2
   *rotation -94.2711 35.46958 171.271
   *integration theta_method_a 1. 1.e-9 200
***return
```

This is an example of the TFA behavior with three sub_volumes (`grain1`, `grain2` and `grain2`) with respective volume fractions `0.2`, `0.3` and `0.5`, using the polycrystal localization rule.

***behavior berveiller_zaoui

This behavior defines a model, proposed by Berveiller and Zaoui, as a general formulation of the self-consistent scheme [Berv78]. This model is specified for an isotropic elasto-plastic intergranular accommodation for plastically-flowing polycrystals.

$$\sigma_{ij} = \Sigma_{ij} + 2\alpha\mu(1-\beta)(E^p_{ij} - \varepsilon^p_{ij}) \qquad \text{where} \qquad \beta = \frac{2(4+5\nu)}{15(1-\nu)} \tag{8}$$

$$\alpha = \frac{1+6\mu h(1+\nu)/(7-5\nu)}{1+2\mu h(13-5\nu)/15(1-\nu)+8\mu^2h^2(1+\nu)/15(1-\nu)} \ \text{ and } \ h = \frac{3E^p}{2\Sigma} \tag{9}$$

where Σ_{ij} is the uniform applied stress, σ_{ij} is the uniform stress in one specified grain, E^p_{ij} is the equivalent macroscopic plastic strain and ε^p_{ij} is the uniform plastic strain in the same grain.

Syntax:

```
***behavior berveiller_zaoui
**mu   double
**nu   double
[**simplified ]
**material  volume_fraction    name     |   **material_in_file <file>
  *file  file_name
  [*integration  method ]
  [*rotation ROTATION ]  |   [*rotation_list <ROTATION> ]
  [*volume_fraction_file <file> ]
**material  etc ...
***return
```

**mu* is the Lame's coefficient μ.

**nu* is the Poisson's ratio ν.

**simplified* This option allows the use of an approximate expression of α, which is $\alpha = 1/(1+\mu h)$, instead of the equation given above Eq. (9).

Example:

```
***behavior
  **mu  75000.
  **nu  0.3
  **simplified
  **material  1.000000e+00  grain1
    *file trac_bz.inp 2
    *rotation   -1.496760e+02  1.561819e+01  1.546760e+02
  **material  1.000000e+00  grain2
    *file trac_bz.inp 2
    *rotation   -1.506460e+02  3.386400e+01  1.556460e+02
  **material  1.000000e+00  grain3
    *file trac_bz.inp 2
    *rotation   -1.371380e+02  4.159170e+01  1.421380e+02
***return
```

***behavior beta_multimat

This method considers piecewise constant eigenstrain in each material phase and proposes a localization rule for each material sub-volume [Cail92]. The total strain tensor in each phase is computed according to:

$$\dot{\underset{\sim}{\epsilon}}_i = \dot{\underset{\sim}{\epsilon}}^p_i + \dot{\underset{\sim}{\mathbf{E}}} - \dot{\underset{\sim}{\mathbf{E}}}^p + \left(\underset{\approx}{\mathbf{L}}_i\right)\left(\dot{\underset{\sim}{\mathbf{B}}} - \dot{\underset{\sim}{\beta}}_i\right)$$

where β_i is the eigenstrain in the sub-volume i and $\dot{\underset{\sim}{\mathbf{B}}}$ is deduced from the following equation:

$$\dot{\underset{\sim}{\mathbf{B}}} = \left\langle \underset{\approx}{\mathbf{L}}_i \right\rangle^{-1} \left\langle \left(\underset{\approx}{\mathbf{L}}\, c_i\right) : \dot{\underset{\sim}{\beta}}_i \right\rangle$$

and $< u >$ denotes the volume average of u.

Syntax:

```
     ***behavior beta_multimat
       **material  volume_fraction   name    |   **material_in_file <file>
       *file  file_name
       [*integration  method ]
       [*rotation ROTATION ]  |   [*rotation_list <ROTATION> ]
       [*volume_fraction_file <file> ]
      **material  etc ...
      **beta   name  <BETA_TFA>
      **localization   name  <LOCALIZATION2>
    ***return
```

***localization* specify localization rule for calculating the strain localisation tensor $\underset{\approx}{\mathbf{L}}$.

***beta* define the evolution law for the β internal variable in each sub-volume.

The localization rule and the evolution law must be defined for each volume. If the different sub-volumes have the same localization rule or the same evolution rule, it is possible to use ”all” instead of specifying the names of sub-volumes after `**beta` and `**localization`. In this case, `**beta` and `**localization` must be defined before behaviors.

Example:

```
***behavior beta_multimat
 **beta all delta D 300. delta 0.3
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
In this example, both phases austen and ferrit have the same evolution law for $\beta$
variable (**beta). Thus, the option "all" is used and the **beta is defined before
behaviors (**material).
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 **material .7 austen
  *file bugat1.austenite
  *rotation x3  -0.166667 0.649830 0.741582
            x1  -0.074915 0.741582 -0.666667
 **material .3 ferrit
  *file bugat1.ferrite
 **localization austen kroner poisson 0.3 ratio 1.
 **localization ferrit kroner poisson 0.3 ratio 1.
***return
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
beta_test1.mat
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

***behavior beta_multimat
 **localization all voigt mu 10100.
 **material .5 gr1
  *file beta_test1.mat 2
  *rotation -149.060000 18.010000 164.060000
 **beta      gr1 delta D 300.0 delta 0.3
**material .5 gr2
  *file beta_test1.mat 2
  *rotation -.060000 18.010000 164.060000
 **beta         gr2 delta D 300.0 delta 0.3
***return
```

***behavior voigt/voigt_fs

This behavior provides the Voigt/Taylor homogenization scheme, applied to multi-phase or multi-constituent heterogeneous materials. This model, which is also referred to as the uniform strain model, assumes a uniform total strain field among each sub-volume and the homogeneous macroscopic medium:

$$\begin{aligned} \boldsymbol{E} &= \boldsymbol{\epsilon}_1 = \boldsymbol{\epsilon}_2 = \ldots = \boldsymbol{\epsilon}_n \\ \boldsymbol{\Sigma} &= f_1\boldsymbol{\sigma}_1 + f_2\boldsymbol{\sigma}_2 + \ldots + f_n\boldsymbol{\sigma}_n \end{aligned} \tag{10}$$

where $\boldsymbol{E}$ and $\boldsymbol{\Sigma}$ are respectively the macroscopic strain and stress tensors. $\boldsymbol{\epsilon}_i$ and $\boldsymbol{\sigma}_i$ are respectively the local total strain and stress in the sub-volume i. The volume fraction of sub-volume i is denoted by f_i and n is the number of sub-volumes.

Syntax:

```
 ***behavior voigt
  **material volume_fraction  name   |  **material_in_file <file>
   *file file_name
  [*integration method ]
  [*rotation ROTATION ]  |  [*rotation_list <ROTATION> ]
  [*volume_fraction_file <file> ]
  **material etc ...
***return
```

Example:

```
***behavior voigt
%%%%%%%%%% Large deformation %%%%%%%%%%
%***behavior voigt_fs
%For the large deformation, the keyword "voigt\_fs" must be used instead of "voigt".
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 **material 0.5  m1
  *file voigt_elas2.inp 2
 **material 0.5 m2
  *file voigt_elas2.inp 3
***return

***behavior linear_elastic
 **elasticity young 200000. poisson 0.3
***return

***behavior linear_elastic
 **elasticity young 100000. poisson 0.3
***return
```

***behavior phasefield_phic

Description:

The present model belongs to the class of diffuse interface models, where the local state of an inhomogeneous microstructure is described by a conservative concentration field c and a non-conservative field ϕ [Amm10], the so-called order parameter. In the phase field approach, the free energy density for an inhomogeneous system can be approximated by the Ginzburg-Landau coarse-grained free energy functional, which contains a chemical free energy density $f_{ch}(c,\phi)$ and a gradient energy term:

$$f(c,\phi) = f_{ch}(c,\phi) + \frac{\alpha}{2}\nabla\phi.\nabla\phi$$

The usual specific quadratic contribution with respect to $\nabla\phi$ is related to the interfacial energy. The state laws and the complementary evolution laws for the phase field and chemical contributions are the following:

$$\mu = \frac{\partial f}{\partial c} = \frac{\partial f_{ch}}{\partial c} \qquad \underset{\sim}{\xi} = \frac{\partial f}{\partial \nabla\phi} = \alpha\ \nabla\phi$$

$$\underline{\mathbf{J}} = -L(\phi)\nabla\mu = -L(\phi)\nabla(\frac{\partial f}{\partial c}) \qquad \pi = -\beta\ \dot{\phi} - \frac{\partial f}{\partial \phi}$$

where μ is the chemical potential.

$L(\phi)$ is the Onsager coefficient, related to the chemical diffusivities D_1 and D_2 in both phases by means of the interpolation function $h(\phi)$ as:

$$L(\phi) = h(\phi)D_1/k_1 + (1-h(\phi))D_2/k_2$$

β material parameter, which is inversely proportional to the interface mobility.

α composition gradient energy coefficient.

The evolution equations for order parameter and concentration are respectively based on the time-dependent Ginzburg-Landau and usual diffusion equations, which are:

$$\nabla.\underset{\sim}{\xi} + \pi = -\beta\dot{\phi} + \nabla.(\alpha\nabla\phi) - \frac{\partial f_{\mathrm{ch}}}{\partial \phi} = 0$$

$$\dot{c} = -\nabla.(-L(\phi)\nabla\mu) = -\nabla.\left[-L(\phi)\left(\nabla\frac{\partial f_{\mathrm{ch}}}{\partial c}\right)\right]$$

Stored Variables:

prefix	size	description	default
dC	V	Concentration gradient	yes
J	V	Concentration flux	yes
dphi	V	Order parameter gradient	yes
xi	V	Microstress	yes
pi	S	Internal microforce	yes
C	S	the concentration	yes
phi	S	Order parameter	yes

Syntax:

```
    ***behavior phasefield_phic
     **energy  <ENERGY>
     ...
     **kinetics
      *mobility COEFFICIENT
     **chemical_interpolating_function val
```

`**energy` this option will be much more detailed in the `<ENERGY>` section.

`**kinetics` give the β coefficient.

`**chemical_interpolating_function` define the polynomial degree of interpolating function. Tree choices are availables.

CODE	DESCRIPTION
0	$h(\phi) = \phi$
1	$h(\phi) = \phi^2(3 - 2\phi)$
2	$h(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$

Example:

```
***behavior phasefield_phic
 **energy kim
  *phase1
   c1 0.7
   b1 0.0
   k1 1.
   D1 0.1
  *phase2
   c2 0.3
   b2 0.0
   k2 1.
   D2 0.1
  *interface
   energy 1.
   thickness 0.25
   zeta 0.05
   ENER 0.5
 **kinetics
  *mobility 1.
 **chemical_interpolating_function 1.
***return
```

***behavior elastic_phasefield

Description:
For `elastic_phasefield` behaviour displacement $\underline{\mathbf{u}}$, concentration c and order parameter ϕ are the degrees of freedom of the system. Finding $\phi(X,t), c(X,t), \vec{u}(X,t)), \forall(X, t>0)$ will be done by solving the system of equation.

$$c(X,0) = c_0(X)$$

$$\phi(X,0) = \phi_0(X)$$

$$\forall(t>0, \phi^*(X), c^*(X))$$

$$\begin{cases} \displaystyle\int_V (\pi\phi^* - \underline{\xi}.\nabla\phi^*)dv + \int_{\partial V} \zeta\phi^* ds = 0 & (1) \\ \displaystyle\int_V (\dot{c}c^* - \underline{\mathbf{J}}.\nabla c^*)dv + \int_{\partial V} jc^* ds = 0 & (2) \\ \displaystyle\int_V (-\underset{\sim}{\mathbf{\Sigma}} : \nabla\underline{\mathbf{u}}^* - \vec{f}.\underline{\mathbf{u}}^*)dv + \int_{\partial V} \vec{t}.\underline{\mathbf{u}}^* ds = 0 & (3) \end{cases}$$

The free energy density for the coupled phase field/diffusion/mechanical problem can be approximated by the Ginzburg-Landau coarse-grained free energy functional, which contains a chemical free energy density $f_{ch}(c,\phi)$, an elastic free energy density $f_e(\phi, c, \underset{\sim}{\epsilon})$ and a gradient term.

$$f(\phi, \nabla\phi, c, \underset{\sim}{\mathbf{E}}^e) = f_{ch}(\phi, c) + f_e(\phi, c, \underset{\sim}{\mathbf{E}}^e) + \frac{\alpha}{2}\nabla\phi.\nabla\phi$$

In addition to the chemical state laws, which is defined in the `phasefield_phic` behavior, the strain-stress relationship in the homogeneous effective medium obeys Hooke's law as follows

$$\underset{\sim}{\mathbf{\Sigma}} = \frac{\partial f}{\partial \underset{\sim}{\varepsilon}} = \underset{\approx}{\mathbf{C}}(\phi, c) : (\underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{E}}^\star(\phi, c))$$

where $\underset{\sim}{\mathbf{E}}$ and $\underset{\sim}{\mathbf{\Sigma}}$ are respectively the macroscopic strain and Cauchy stress quantities.

The effective elasticity tensor $\underset{\approx}{\mathbf{C}}$ and the effective eigenstrain $\underset{\sim}{\mathbf{E}}^\star$ due to phase transformation are presented in the `<HOMOGENIZATION>` section.

Stored Variables:

`prefix`	`size`	`description`	`default`
`sig`	T-2	Cauchy stress	yes
`eto`	T-2	Total (small deformation) strain	yes
`eel`	T-2	Elastic strain	yes
`defo_tr`	T-2	Effective eigenstsrain	no
`dC`	V	Concentration gradient	yes
`J`	V	Concentration flux	yes
`dphi`	V	Order parameter gradient	yes
`xi`	V	Microstress	yes
`pi`	S	Internal microforce	yes
`C`	S	the concentration	yes
`phi`	S	Order parameter	yes

Syntax:

```
***behavior elastic_phasefield
 **energy  <ENERGY>
  ...
 **kinetics
  *mobility COEFFICIENT
 **chemical_interpolating_function val
 **mechanical_interpolating_function  val
 **homogenization <HOMOGENIZATION>
 **phase1
  *elasticity1   <ELASTICITY>
   ...
  *eigen_coeff1 double
  [*delta1 double ]
  [*c_ref1 double ]
 **phase2
  *elasticity2   <ELASTICITY>
   ...
  *eigen_coeff2 double
  [*delta2  double ]
  [*c_ref2  double ]
```

`**mechanical_interpolating_function` Defines the polynomial degree of interpolating function. Tree choices are availables.

CODE	DESCRIPTION
0	$h_u(\phi) = \phi$
1	$h_u(\phi) = \phi^2(3 - 2\phi)$
2	$h_u(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$

`**homogenization` This option will be detailed in the `<HOMOGENIZATION>` section.

`**phase1` Definition of the material elastic parameters and eigenstrain induced by variation of concentration.

`**phase2` Identical as `**phase1`

The eigenstrain in the phase i is defined as follow

$$\underset{\sim}{\epsilon}_i^* = (\texttt{eigen\_coeff}_\texttt{i} + \texttt{delta}_\texttt{i}(c - \texttt{c\_ref}_\texttt{i}))\underset{\sim}{\mathbf{1}}, \qquad \text{where} \qquad i = \{1,2\}$$

Example:

```
***behavior elastic_phasefield
 **energy kim
  *phase1
   c1 0.7
   b1 0.0
   k1 1.
   D1 0.1
  *phase2
   c2 0.3
   b2 0.0
```

```
    k2 1.
    D2 0.1
   *interface
    energy 1.
    thickness 0.25
    zeta 0.05
    ENER 0.5
  **kinetics
   *mobility 1.
  **chemical_interpolating_function 1.
  **mechanical_interpolating_function 1.
  **homogenization Khachaturyan
  **phase1
   *elasticity1
    young 70000.
    poisson 0.3
   *eigen_coeff1 0.000
   *delta1 0.0015
   *c_ref1 0.
  **phase2
   *elasticity2
    young 70000.
    poisson 0.3
   *eigen_coeff2  0.000
   *delta2 0.0015
   *c_ref2 0.
 ***return
```

***behavior plastic_phasefield

Description:

In the proposed model, the total free energy is postulated to have the form of a Ginzburg-Landau free energy functional accounting for interfaces through the square of the order parameter gradient. The total free energy F of the body is then defined by the integral over the volume V of a free energy density f, which can be split into a chemical free energy density f_{ch}, a coherent mechanical energy density f_u, and the square of the order parameter gradient:

$$\begin{aligned} F(\phi, \nabla\phi, c, \underset{\sim}{\mathbf{E}}^e, V_k) &= \int_V f(\phi, \nabla\phi, c, \underset{\sim}{\mathbf{E}}^e, V_k)\, dv \\ &= \int_V \left[f_{\mathrm{ch}}(\phi, c) + f_u(\phi, c, \underset{\sim}{\mathbf{E}}^e, V_k) + \frac{\alpha}{2}|\nabla\phi|^2 \right] dv \end{aligned} \tag{11}$$

V_k is the set of internal variables for the phase k in order to describe the hardening state in each phase and $\underset{\sim}{\mathbf{E}}^e$ is the effective elastic strain tensor.

The irreversible behaviour is described by the introduction of a dissipation potential, which can be split into three parts, which are the phase field part $\Omega_\phi(\phi, c)$, the chemical part $\Omega_c(\phi, c)$ and the mechanical dissipation potential $\Omega_u(\phi, c, \underset{\sim}{\mathbf{\Sigma}}, A_k)$:

$$\Omega(\phi, c, \underset{\sim}{\mathbf{\Sigma}}, A_k) = \Omega_\phi(\phi) + \Omega_c(c) + \Omega_u(\phi, c, \underset{\sim}{\mathbf{\Sigma}}, A_k)$$

A_k is the set of thermodynamic forces associated with the internal variables V_k and $\underset{\sim}{\mathbf{\Sigma}}$ is the effective macroscopic strain for the phase k.

The chemical free energy density f_{ch} of the binary alloy is a function of the order parameter ϕ and of the concentration field c, which is much more described in the <ENERGY> section. The second contribution to the free energy density is due to mechanical effects. Assuming that elastic behaviour and hardening are uncoupled, the mechanical part of the free energy density f_u is decomposed into a coherent elastic energy density f_e and a plastic part f_p as:

$$f_u(\phi, c, \underset{\sim}{\mathbf{E}}^e, V_k) = f_e(\phi, c, \underset{\sim}{\mathbf{E}}^e) + f_p(\phi, c, V_k)$$

In the proposed model, we consider that the system consists of a two-phase elastoplastic binary alloy 1 and 2, which are separated by a plane diffuse interface, with one non-linear isotropic hardening and one non-linear kinematic hardening in each phase. The specific free energy taken as the state potential of the material is chosen as a function of all state variables. Assuming again that there is no coupling between elasticity and hardening, the free energy is split into three terms, corresponding to the elastic energy, the kinematic hardening part and the isotropic part. To satisfy the condition of thermodynamic stability, it is sufficient to choose a positive definite quadratic function in the components of elastic strain tensor and all internal state variables as follows:

$$f_k = \frac{1}{2}\left(\underset{\sim}{\varepsilon}_k - \underset{\sim}{\varepsilon}_k^\star\right) : \underset{\approx}{\mathbf{C}}_k : \left(\underset{\sim}{\varepsilon}_k - \underset{\sim}{\varepsilon}_k^\star\right) + \frac{1}{3} C_k \underset{\sim}{\alpha}_k : \underset{\sim}{\alpha}_k + \frac{1}{2} b_k Q_k r_k^2$$

b_k, Q_k and C_k are the material parameters for isotropic and kinematic hardening states and $k = \{1, 2\}$ corresponding to the two phases. Consequently, the Cauchy stress tensor and the associated thermodynamic force variables $\underset{\sim}{\mathbf{X}}$ and R for the phase k are deduced as follows:

$$\underset{\sim}{\sigma}_k = \frac{\partial f_{ek}}{\partial \underset{\sim}{\varepsilon}_k} = \underset{\approx}{\mathbf{C}}_k : \underset{\sim}{\varepsilon}^e \quad , \quad R_k = \frac{\partial f_{pk}}{\partial r_k} = b_k Q_k r_k \quad , \quad \underset{\sim}{\mathbf{X}}_k = \frac{\partial f_{pk}}{\partial \underset{\sim}{\alpha}_k} = \frac{2}{3} C_k \underset{\sim}{\alpha}_k$$

The partition hypothesis requires a decomposition of the total strain in each phase into elastic, eigen and plastic parts:

$$\underset{\sim}{\varepsilon}_1 = \underset{\sim}{\varepsilon}_1^e + \underset{\sim}{\varepsilon}_1^\star + \underset{\sim}{\varepsilon}_1^p \quad \text{and} \quad \underset{\sim}{\varepsilon}_2 = \underset{\sim}{\varepsilon}_2^e + \underset{\sim}{\varepsilon}_2^\star + \underset{\sim}{\varepsilon}_2^p$$

where the local parameter for each phase may depend on the local concentration c, but not on order parameter ϕ.

Furthermore, the mechanical dissipation is assumed to be due to three mechanisms: the inelastic strain, the kinematic hardening and the isotropic hardening. Thus, the dissipation potential can be split into a plastic contribution, which is called the yield function, a nonlinear kinematic hardening term and a nonlinear isotropic hardening term and can be expressed as a convex scalar valued function as follows :

$$\Omega_{uk}(\sigma_k, \underset{\sim}{\mathbf{X}}_k, R_k) = g_k(\underset{\sim}{\sigma}_k, \underset{\sim}{\mathbf{X}}_k, R_k) + \frac{3D_k}{4C_k}\underset{\sim}{\mathbf{X}}_k : \underset{\sim}{\mathbf{X}}_k + \frac{R_k^2}{2Q_k}$$

Assuming that the elastoplastic phase field behaviour of each phase is treated independently, we define a yield function for each phase as:

$$g_k(\sigma_k, \underset{\sim}{\mathbf{X}}_k, R_k) = \sigma_k^{\text{eq}} - R_k - \sigma_k^0 \quad \text{where} \quad \sigma_{\text{eq}} = \sqrt{\frac{3}{2}(\underset{\sim}{\mathbf{s}}_k - \underset{\sim}{\mathbf{X}}_k) : (\underset{\sim}{\mathbf{s}}_k - \underset{\sim}{\mathbf{X}}_k)} \quad \text{and} \quad \underset{\sim}{\mathbf{s}}_k = \underset{\sim}{\sigma}_k - \frac{1}{3}\,\text{Trace}\,\underset{\sim}{\sigma}_k \underset{\sim}{\mathbf{1}}$$

with σ_k^0 is the initial yield stress, σ_k^{eq} is the von Mises equivalent stress and $\underset{\sim}{\mathbf{s}}_k$ is the deviatoric stress tensor.

According to the normality rule for standard materials, the evolution laws of the internal variables are derived from the dissipation potential. For phenomena which do not depend explicitly on time, such as rate independent plasticity, the potential is not differentiable. Then, the partial derivative of Ω_k with respect to g is simply replaced by a plastic multiplier $\dot{\lambda}$ to write a rate independent plastic model. Consequently, the evolution laws can be expressed as:

$$\dot{\underset{\sim}{\varepsilon}}{}_k^p = \frac{\partial \Omega_{uk}}{\partial \underset{\sim}{\sigma}_k} = \dot{\lambda}_k \underset{\sim}{\mathbf{n}}_k, \quad \dot{r}_k = \frac{\partial \Omega_{uk}}{\partial R_k} = \dot{\lambda}_k \left(1 - \frac{R_k}{Q_k}\right), \quad \dot{\underset{\sim}{\alpha}}_k = \frac{\partial \Omega_{uk}}{\partial X_k} = \dot{\lambda}_k \left(\underset{\sim}{\mathbf{n}}_k - \frac{3D_k}{2C_k}\underset{\sim}{\mathbf{X}}_k\right)$$

where $\underset{\sim}{\mathbf{n}}_k = \partial g_k / \partial \underset{\sim}{\sigma}_k$ is the normal to the yield surface and defines the flow direction and the plastic multiplier $\dot{\lambda}$ is determined from the consistency condition $dg_k/dt = 0$ [1].

The elastoplastic and phase field behaviours of each phase are treated independently and the effective behaviour is obtained using homogenization relation. In the proposed model, the Voigt's scheme is used, where the basic assumptions are that the strain field is uniform among the phases at each material point. Using Voigt's model, we assume a uniform total strain at any point in the diffuse interface between elastoplastically inhomogeneous phases. The effective stress is expressed in terms of the local stress average with respect to both phases weighted by the volume fractions:

$$\underset{\sim}{\mathbf{\Sigma}} = \phi\, \underset{\sim}{\sigma}_1 + (1-\phi)\, \underset{\sim}{\sigma}_2 \qquad , \qquad \underset{\sim}{\mathbf{E}} = \underset{\sim}{\varepsilon}_1 = \underset{\sim}{\varepsilon}_2$$

The stresses of both phases $\underset{\sim}{\sigma}_1$ and $\underset{\sim}{\sigma}_2$ are given by Hooke's law for each phase:

$$\underset{\sim}{\sigma}_1 = \underset{\approx}{\mathbf{C}}_1 : (\underset{\sim}{\varepsilon}_1 - \underset{\sim}{\varepsilon}_1^\star - \underset{\sim}{\varepsilon}_1^p) \quad , \quad \underset{\sim}{\sigma}_2 = \underset{\approx}{\mathbf{C}}_2 : (\underset{\sim}{\varepsilon}_2 - \underset{\sim}{\varepsilon}_2^\star - \underset{\sim}{\varepsilon}_2^p)$$

where $\underset{\approx}{\mathbf{C}}_1$ and $\underset{\approx}{\mathbf{C}}_2$ are respectively the tensor of elasticity moduli in 1 and 2 phases.

The stress at any point in the interface is computed from the average of the above local stresses as follows:

$$\underset{\sim}{\mathbf{\Sigma}} = \phi\, \underset{\approx}{\mathbf{C}}_1 : (\underset{\sim}{\varepsilon}_1 - \underset{\sim}{\varepsilon}_1^\star - \underset{\sim}{\varepsilon}_1^p) + (1-\phi) \underset{\approx}{\mathbf{C}}_2 : (\underset{\sim}{\varepsilon}_2 - \underset{\sim}{\varepsilon}_2^\star - \underset{\sim}{\varepsilon}_2^p)$$

From the above relation, it follows that the strain-stress relationship in the homogeneous effective medium obeys Hooke's law with the following equation:

$$\underset{\sim}{\mathbf{\Sigma}} = \underset{\approx}{\mathbf{C}}_{\text{eff}} : (\underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{E}}^p - \underset{\sim}{\mathbf{E}}^\star)$$

---

[1] The first consistency condition, $g_k = 0$, means that the state of stress is on the actual yield surface, the second $\dot{g}_k = 0$, means that an increase of the state of stress stays on the yield surface. Elastic unloading occurs when $g_k < 0$ or $\dot{g}_k < 0$, the internal variables then keeping a constant value.

where the effective elasticity tensor $\underset{\approx}{\mathbf{C}}_{\text{eff}}$ is obtained from the mixture rule of the elasticity matrix for both phases:

$$\underset{\approx}{\mathbf{C}}_{\text{eff}} = \phi\, \underset{\approx}{\mathbf{C}}_1 + (1-\phi)\underset{\approx}{\mathbf{C}}_2$$

and the effective eigenstrain $\underset{\sim}{\mathbf{E}}^{\star}$ and plastic strain $\underset{\sim}{\mathbf{E}}^{p}$ vary continuously between their respective values in the bulk phases as follows:

$$\underset{\sim}{\mathbf{E}}^{\star} = \underset{\approx}{\mathbf{C}}_{\text{eff}}^{-1} : (\phi\, \underset{\approx}{\mathbf{C}}_1 : \underset{\sim}{\varepsilon}_1^{\star} + (1-\phi)\underset{\approx}{\mathbf{C}}_2 : \underset{\sim}{\varepsilon}_2^{\star})$$

$$\underset{\sim}{\mathbf{E}}^{p} = \underset{\approx}{\mathbf{C}}_{\text{eff}}^{-1} : (\phi\, \underset{\approx}{\mathbf{C}}_1 : \underset{\sim}{\varepsilon}_1^{p} + (1-\phi)\underset{\approx}{\mathbf{C}}_2 : \underset{\sim}{\varepsilon}_2^{p})$$

In the case of nonhomogeneous elasticity, it must be noted that $\underset{\sim}{\mathbf{E}}^{\star}$ and $\underset{\sim}{\mathbf{E}}^{p}$ are not the average of their respective values for each phase.

According to the Voigt homogenization theory, the local energy stored in the effective homogeneous elastic material is expressed in terms of the average value of the local elastic energy with respect to both phases weighted by their volume fractions:

$$f_e(\phi, c, \underset{\sim}{\mathbf{E}}) = \phi\, f_{e1}(c, \underset{\sim}{\varepsilon}_1^{e}) + (1-\phi) f_{e2}(c, \underset{\sim}{\varepsilon}_2^{e}) = \frac{1}{2}\,(\underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{E}}^{\star} - \underset{\sim}{\mathbf{E}}^{p}) : \underset{\approx}{\mathbf{C}}_{\text{eff}} : (\underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{E}}^{\star} - \underset{\sim}{\mathbf{E}}^{p})$$

and

$$f_p(\phi, c, V_k) = \phi\, f_{p1}(c, \underset{\sim}{\alpha}_{\alpha}) + (1-\phi) f_{p2}(c, \underset{\sim}{\alpha}_{\beta})$$

Similary, the irreversible part of the mechanical behaviour for effective material is defined with respect to the mechanical dissipation potentials $\Omega_{u1}(c, \underset{\sim}{\sigma}_1, A_1)$ and $\Omega_{u2}(c, \underset{\sim}{\sigma}_2, A_2)$ for 1 and 2 phases respectively by means of the shape function ϕ as:

$$\Omega_u(\phi, c, \underset{\sim}{\mathbf{\Sigma}}, A_k) = \phi\, \Omega_{u1}(c, \underset{\sim}{\sigma}_1, A_1) + (1-\phi)\, \Omega_{u1}(c, \underset{\sim}{\sigma}_2, A_1)$$

Stored Variables:

`prefix`	`size`	`description`	`default`
`C`	S	the concentration	yes
`phi`	S	Order parameter	yes
`dC`	V	Concentration gradient	yes
`dphi`	V	Order parameter gradient	yes
`J`	V	Concentration flux	yes
`xi`	V	Microstress	yes
`pi`	S	Internal microforce	yes
`sig`	T-2	Cauchy stress	yes
`eto`	T-2	Total (small deformation) strain	yes
`eel`	T-2	Elastic strain	yes
`ep`	T-2	Effective inelastic strain	yes
`sig1`	T-2	Cauchy stress	yes
`ep1`	T-2	Inelastic strain for the first phase	yes
`eel1`	T-2	Elastic strain for the first phase	yes
`alpha1`	T-2	kinematic hardening internal variable for the first phase	yes
`epcum1`	V	cumulated plasticity equivalent for the first phase	yes
`sig2`	T-2	Cauchy stress	yes
`ep2`	T-2	Inelastic strain for the second phase	yes
`eel2`	T-2	Elastic strain for the second phase	yes
`alpha2`	T-2	kinematic hardening internal variable for the second phase	yes
`epcum2`	V	cumulated plasticity equivalent for the second phase	yes

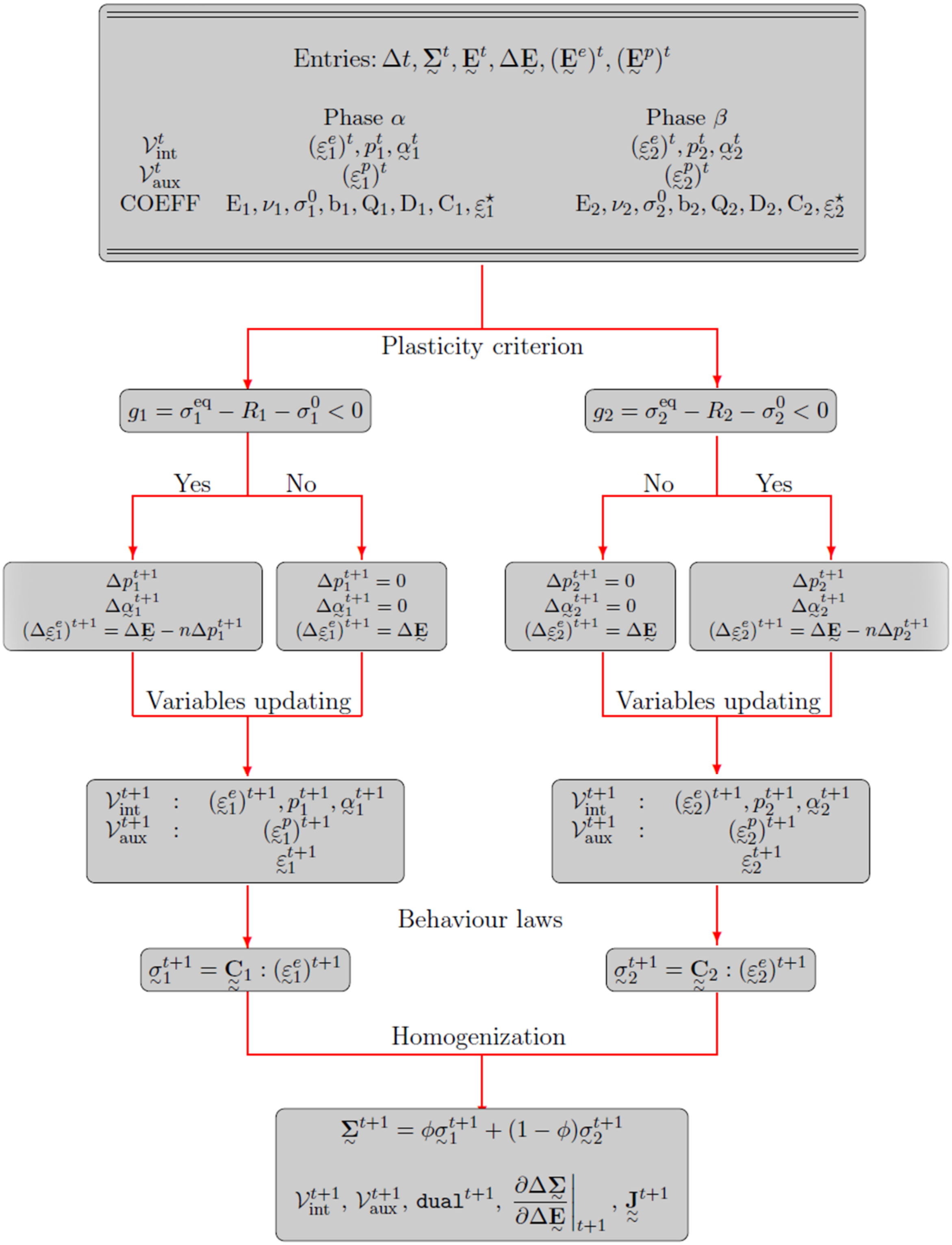


Figure 1: Integration of constitutive equations for Voigt/Taylor scheme. p_1 and p_2 are respectively the accumulated plastic strain in 1 and 2 phases

Syntax:

```
    ***behavior plastic_phasefield
     **energy  <ENERGY>
     **kinetics
      *mobility COEFFICIENT
     **chemical_interpolating_function val
     **mechanical_interpolating_function  val
     **homogenization [name]
     **phase1
       *elasticity1   <ELASTICITY>
       *eigen_coeff1 COEFFICIENT
         *delta1 COEFFICIENT
         *c_ref1 COEFFICIENT
     *plastic
      R01  COEFFICIENT.
      B1  COEFFICIENT
      Q1  COEFFICIENT
      C1  COEFFICIENT
      D1  COEFFICIENT
     **phase2
       *elasticity2   <ELASTICITY>
       *eigen_coeff2 COEFFICIENT
         *delta2  COEFFICIENT
         *c_ref2  COEFFICIENT
    *plastic
      R02 COEFFICIENT
      B2  COEFFICIENT
      Q2  COEFFICIENT
      C2  COEFFICIENT
      D2  COEFFICIENT
```

`**phase1` Definition of the material elastic parameters and eigenstrains induced by variation of concentration. The eigenstrains are defined as follow $\underset{\sim}{\varepsilon}^* = (\texttt{eigen\_coeff1}+\texttt{delta1}(c-\texttt{c\_ref1}))\underset{\sim}{\mathbf{1}}$

`**phase2` Identical as `**phase1`

Example:

```
***behavior plastic_phasefield
 **energy kim
  *phase1
    c1 0.7
    b1 0.0
    k1 1.
    D1 0.1
  *phase2
    c2 0.3
    b2 0.0
    k2 1.
    D2 0.1
  *interface
    energy 1.
```

```
    thickness 0.25
    zeta 0.05
    ENER 0.5
 **kinetics
  *mobility 1.
 **chemical_interpolating_function 1.
**mechanical_interpolating_function 1.
**phase1
  *elasticity1
    young 70000.
    poisson 0.3
  *eigen_coeff1 0.001
  *delta1 0.0015
  *c_ref1 0.
  *plastic
   R01 15.
   B1 0.
   Q1 0.
   C1 0.
   D1 0.
 **phase2
  *elasticity2
    young 70000.
    poisson 0.3
  *eigen_coeff2  0.000
  *delta2 0.0015
  *c_ref2 0.
 *plastic
   R02 70000000.
   B2 0.
   Q2 0.
   C2 0.
   D2 0.
***return
```

Chapter 2

Material Components

<BETA_TFA>

Description:

This object class is used for specifying the evolution laws of $\underset{\sim}{\beta}$ variable. This variable has the dimension of a strain and is to be considered as an internal variable in each sub-volume.

The following types of evolution laws of $\underset{\sim}{\beta}$ variable may be chosen:

CODE	DESCRIPTION
beta_d	$\dot{\boldsymbol{\beta}}_{\boldsymbol{s}} = \dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}} - D_s \dot{p}_s \boldsymbol{\beta}_{\boldsymbol{s}} - \dfrac{\texttt{det}(\dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}})\ \boldsymbol{P}}{\dot{p}_s^2}\boldsymbol{I}$
beta_matrix	$\dot{\boldsymbol{\beta}}_{\boldsymbol{s}} = \dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}} - D_s \dot{p}_s \boldsymbol{S}_s : \boldsymbol{\beta}_{\boldsymbol{s}}$
kroner	$\dot{\boldsymbol{\beta}}_{\boldsymbol{s}} = \dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}}$
delta	$\dot{\boldsymbol{\beta}}_{\boldsymbol{s}} = \dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}} - D \dot{p}_s (\boldsymbol{\beta}_{\boldsymbol{s}} - \delta \boldsymbol{\epsilon}^{\boldsymbol{p}}_{\boldsymbol{s}}) - \dfrac{\texttt{det}(\dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}})\ \boldsymbol{P}}{\dot{p}_s^2}\boldsymbol{I}$
free	$\dot{\boldsymbol{\beta}}_{\boldsymbol{s}} = \dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}} - C_b \dot{p}_s \boldsymbol{\beta}_{\boldsymbol{s}} + \dfrac{\texttt{det}(\dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}}) C_{e3}}{\dot{p}_s^2}\boldsymbol{I}$

where $\texttt{det}(A)$ represents the determinant of a matrix A. $\boldsymbol{P}$ is the extreme pressure and $\dot{p}_s$ is the rate of accumulated plastic strain $\dot{p}_s = \sqrt{\frac{2}{3}(\dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}} : \dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}}_{\boldsymbol{s}})}$.

Syntax:

The syntax for a BETA_TFA object requires that a name of the sub-volume must be given, followed by the type and whatever coefficients are allowed for the corresponding model.

`beta_d`

```
**beta   name  beta_d
  D <double>
  [pressure <double>]
```

`beta_matrix`

```
**beta   name  beta_matrix   double
  poisson  <double>
  ratio <double>
```

`kroner`

```
**beta   name  kroner
```

`delta`

```
**beta   name  delta
  D  <double>
  delta <double>
  [pressure <double>]
```

free

```
**beta   name  free
  Ce3  <double>
  Cb   <double>
```

<EIGENSTRAIN> beta

Description:
This object class provides the eigenstrain models in general TFA framework. It is used to define the evolution law of the "eigenstrain" which is the strain measure of mismatch between phase locations:

$$\dot{\boldsymbol{\beta}}_r = \dot{\boldsymbol{\epsilon}}^p_r - D(\boldsymbol{\beta}_r - \omega \boldsymbol{\epsilon}^p_r)||\dot{\boldsymbol{\epsilon}}^p_r||$$

$$\dot{\boldsymbol{\xi}}_r = -D(\boldsymbol{\xi}_r + (1-\omega)\boldsymbol{\epsilon}^p_r)||\dot{\boldsymbol{\epsilon}}^p_r||$$

Syntax:

```
**eigenstrain  beta
  D  double
  [omega  double ]
```

<ENERGY>

Description:

This class is used for specifying the chemical free energy density in phase field model $f_{\mathrm{ch}}(c,\phi)$ and to calculate its partial derivatives $\dfrac{\partial f_{\mathrm{ch}}}{\partial c}, \dfrac{\partial f_{\mathrm{ch}}}{\partial \phi}, \dfrac{\partial^2 f_{\mathrm{ch}}}{\partial \phi^2}, \dfrac{\partial^2 f_{\mathrm{ch}}}{\partial c^2}, \dfrac{\partial^2 f_{\mathrm{ch}}}{\partial c \partial \phi}...$

The chemical free energy density of binary alloy is a function of the order parameter ϕ and of the concentration field c. In order to ensure the coexistence of both phases α and β discriminated by ϕ, f_{ch} must be non-convex with respect to ϕ. Consequently, f_{ch} is split into a local homogeneous free energy $f_0(c,\phi)$, which is built with the free energy densities of the two phases f_1 and f_2 and a double well potential accounting for the free energy penalty of the interface [Amm10]:

$$f_{\mathrm{ch}}(\phi,c) = f_0(c,\phi) + W g(\phi) \qquad \text{where} \qquad g(\phi) = \phi^2(1-\phi)^2$$

where W is the height of the double-well barrier. Both material parameters W and α are calculated in function of the interfacial energy σ and the interfacial thickness δ as

$$W = 6\Lambda\frac{\sigma}{\delta} \qquad \text{and} \qquad \alpha = 3\frac{\sigma\lambda}{\Lambda} \qquad \text{where} \qquad \Lambda = \ln[(1-\zeta)/\zeta]$$

The material parameter ζ specifies the way that the interface width δ has been defined, Assuming that the interface region ranges from ζ to $1-\zeta$.

Syntax:

The basic input syntax here is:

```
**energy  <ENERGY>
 *phase1
   c1 COEFFICIENT
   b1 COEFFICIENT
   k1 COEFFICIENT
   D1 COEFFICIENT
 *phase2
   c2 COEFFICIENT
   b2 COEFFICIENT
   k2 COEFFICIENT
   D2 COEFFICIENT
 *interface
   energy COEFFICIENT
   thickness COEFFICIENT
   zeta COEFFICIENT
   ENER COEFFICIENT
```

**interface* specify the material parameters related to the phase field interface, which are the interfacial energy σ, the interfacial thickness δ and ζ

The following coefficients are available:

`k1,k2` are respectively the curvatures of the local free energies f_1 and f_2 with respect to concentration.

`b1,b2` are the heights of the free energies f_1 and f_2.

`c1,c2` are the coherent equilibrium concentrations.

`D1,D2` are the chemical diffusivities in both phases 1 and 2.

CODE	DESCRIPTION
`kim`	Polynomial formulation of homogeneous free energy
`afa`	Interpolating free energy densities

`kim` The chemical free energy density is a quadratic function of the concentration, where the chemical free energies of the two phases are interpolated for intermediate values of ϕ with a polynomial $h(\phi)$ varying in a monotonic way between both phases:

$$f_0(\phi, c) = h(\phi) f_1(c) + [1 - h(\phi)] f_2(c)$$

where f_1 and f_2 are the chemical free energy densities of both phases, which have been described by simple quadratic functions of the concentration c:

$$f_i(c) = \frac{1}{2} k_i (c - a_i)^2 + b_i$$

where $i = \{1, 2\}$ denotes phase 1 or 2.

`afa` This energy is obtained by a linear interpolation of the free energy parameters $a(\phi), b(\phi)$ and $k(\phi)$. It is summarised as:

$$f_0(\phi, c) = \frac{1}{2} k(\phi)(c - a(\phi))^2 + b(\phi)$$

where

$$a(\phi) = a_2 + \Delta a h(\phi), \quad k(\phi) = \frac{k_1 k_2}{k_1 + h(\phi)\Delta k} \quad \text{and} \quad b(\phi) = b_2 + \mu_{\text{eq}} \left(\Delta a + \frac{(\mu_{\text{eq}})^2 \Delta k}{2\bar{k}} \right) h(\phi)$$

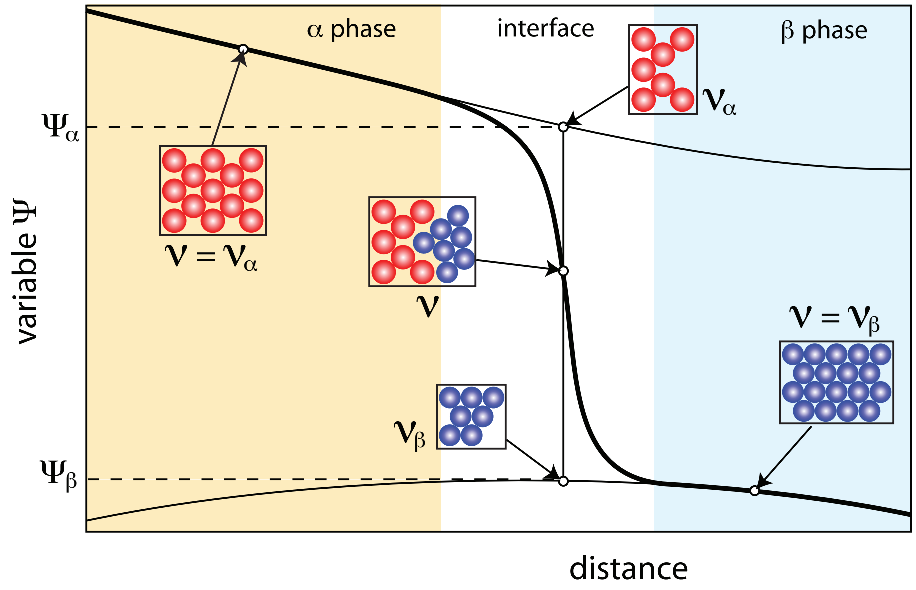
<HOMOGENIZATION>

Description:

This object class provides the way of introducing linear and nonlinear mechanical constitutive equations into the standard phase field approach. In the region where both phases coexist, the local behaviour in both phases is interpolated in order to replace an heterogeneous medium by an equivalent homogeneous one [Amm10].

`CODE`	DESCRIPTION
Voigt	uniform strain field among the phases
Khachaturyan	interpolation scheme

`Voigt` It is a Voigt model, which is also referred to as the uniform strain model. Its basic assumptions are that the strain field is uniform among the phases. One distinct set of constitutive equations is attributed to each individual phase k at any material point. Each phase at a material point then possesses its own stress/strain tensor $(\underset{\sim}{\sigma}_1, \underset{\sim}{\varepsilon}_1)$ and $(\underset{\sim}{\sigma}_2, \underset{\sim}{\varepsilon}_2)$. The overall strain and stress quantities $\underset{\sim}{\mathbf{\Sigma}}, \underset{\sim}{\mathbf{E}}$ at this material point must then be averaged or interpolated from the values attributed to each phase, using the well-known results of homogenization theory. Following a naive representation depicted in the figure below, each material point, i.e. $\mathcal{V}$, within a diffuse interface can be seen as a local mixture of the two abutting phases 1 and 2 with proportions fixing $\mathcal{V}_1$ and $\mathcal{V}_2$ given by complementary functions of ϕ. It must be emphasized that this representation involves the presence of fields Ψ_1 and Ψ_2 in phases 2 and 1 respectively, which has no incidence on the bulk of those phases.



Schematic illustration of the underlying material representative volume element $\mathcal{V} = \{\mathcal{V}_1 \cup \mathcal{V}_2,\ \mathcal{V}_1 \cap \mathcal{V}_2 = \emptyset\}$ at each material point of a diffuse interface.

The local energy stored in the effective homogeneous elastic material is expressed in terms of the average value of the local elastic energy with respect to both phases weighted by their volume fractions:

$$f_e(\phi, c, \underset{\sim}{\epsilon}) = \frac{1}{2}\,(\underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{E}}^\star) : \underset{\approx}{\mathbf{C}} : (\underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{E}}^\star) = h_u(\phi)\, f_{e1} + (1 - h_u(\phi)) f_{e2}$$

where the elastic energy densities of 1 and 2 phases can be expressed as:

$$\begin{cases} f_{e1} = \dfrac{1}{2}\,(\underset{\sim}{\mathbf{E}} - \underset{\sim}{\varepsilon}_1^\star) : \underset{\approx}{\mathbf{C}}_1 : (\underset{\sim}{\mathbf{E}} - \underset{\sim}{\varepsilon}_1^\star) \\[2ex] f_{e2} = \dfrac{1}{2}\,(\underset{\sim}{\mathbf{E}} - \underset{\sim}{\varepsilon}_2^\star) : \underset{\approx}{\mathbf{C}}_2 : (\underset{\sim}{\mathbf{E}} - \underset{\sim}{\varepsilon}_2^\star) \end{cases}$$

Using Voigt's model, we assume a uniform total strain at any point in the diffuse interface between elastoplastically inhomogeneous phases. The effective stress is expressed in terms of the local stress average with respect to both phases weighted by the volume fractions:

$$\underset{\sim}{\mathbf{\Sigma}} = h_u(\phi)\, \underset{\sim}{\sigma}_1 + (1 - h_u(\phi))\, \underset{\sim}{\sigma}_2 = \underset{\approx}{\mathbf{C}} : (\underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{E}}^\star) \qquad \text{and} \qquad \underset{\sim}{\mathbf{E}} = \underset{\sim}{\varepsilon}_1 = \underset{\sim}{\varepsilon}_2$$

where the effective elasticity tensor $\underset{\approx}{\mathbf{C}}$ is obtained from the mixture rule of the elasticity matrix for both phases and the effective Eigenstrain $\underset{\sim}{\mathbf{E}}^\star$ vary continuously between their respective values in the bulk phases as follows:

$$\underset{\approx}{\mathbf{C}} = h_u(\phi)\, \underset{\approx}{\mathbf{C}}_1 + (1 - h_u(\phi)) \underset{\approx}{\mathbf{C}}_2$$

$$\underset{\sim}{\mathbf{E}}^\star = \underset{\approx}{\mathbf{C}}^{-1} : (h_u(\phi)\, \underset{\approx}{\mathbf{C}}_1 : \underset{\sim}{\varepsilon}_1^\star(c) + (1 - h_u(\phi)) \underset{\approx}{\mathbf{C}}_2 : \underset{\sim}{\varepsilon}_2^\star(c))$$

`Khachaturyan` It is an interpolation scheme, where the material behaviour is described by a unified set of constitutive equations that explicitly depend on the concentration or the phase variable. Each material parameter is usually interpolated between the limit values known for each phase. Linear mixture interpolations are adopted respectively for eigenstrain and elasticity moduli tensor:

$$\underset{\sim}{\mathbf{E}}^\star = h_u(\phi)\, \underset{\sim}{\varepsilon}_1^\star + (1 - h_u(\phi))\, \underset{\sim}{\varepsilon}_2^\star \quad , \quad \underset{\approx}{\mathbf{C}} = h_u(\phi)\, \underset{\approx}{\mathbf{C}}_1 + (1 - h_u(\phi))\, \underset{\approx}{\mathbf{C}}_2$$

Hooke's law relates the strain tensor to the stress tensor by the following expression:

$$\begin{aligned} \underset{\sim}{\mathbf{\Sigma}} &= \underset{\approx}{\mathbf{C}} : (\underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{E}}^\star) \\ &= (h_u(\phi)\, \underset{\approx}{\mathbf{C}}_1(c) + (1 - h_u(\phi))\, \underset{\approx}{\mathbf{C}}_2(c)) : (\underset{\sim}{\mathbf{E}} - h_u(\phi)\, \underset{\sim}{\varepsilon}_1^\star - (1 - h_u(\phi))\, \underset{\sim}{\varepsilon}_2^\star) \end{aligned} \tag{1}$$

Contrary to the previous Voigt homogenization scheme, the elastic energy of the effective homogeneous material is no longer the average of energy densities of both phases. It is indeed not possible to distinguish an explicit form for the elastic energy densities in each phase. The elastic energy is then postulated as:

$$f_e(\phi, c, \underset{\sim}{\epsilon}) = (\underset{\sim}{\mathbf{E}} - h_u(\phi)\, \underset{\sim}{\varepsilon}_1^\star(c) - (1 - h_u(\phi))\, \underset{\sim}{\varepsilon}_2^\star(c)) : \underset{\approx}{\mathbf{C}} : (\underset{\sim}{\mathbf{E}} - h_u(\phi)\, \underset{\sim}{\varepsilon}_1^\star(c) - (1 - h_u(\phi))\, \underset{\sim}{\varepsilon}_2^\star(c))$$

<LOCALIZATION1>

The localisation object is used to evaluate the strain and stress concentration tensors $(\boldsymbol{A}_r, \boldsymbol{B}_r)$ as well as the transformation influence tensors $(\boldsymbol{D}_{sr}, \boldsymbol{F}_{sr})$. Several localization rules are available, such as `Voigt`, `Reuss`, `Mori_Tanaka` etc ...

Syntax:
The syntax depends on the type of localization:

```
**localization name
[*consistency <value>]
  ...
```

**consistency* give the precision, for the TFA consistency checks. In fact, some relations on the TFA method could be checked using the given ratio, which is especially useful for the **localization numeric which allows the user to give his own tensors. It is also useful for debugging. The relations that will be verified are

$$\sum_r \boldsymbol{D}_{sr} - \boldsymbol{I} + \boldsymbol{A}_s = 0$$

$$\sum_r \boldsymbol{D}_{sr} \boldsymbol{L}_r^{-1} = 0$$

$$\sum_r c_r \boldsymbol{D}_{rs} = 0$$

$$c_s \boldsymbol{L}_s \boldsymbol{D}_{sr} - c_r \boldsymbol{D}_{rs}^T \boldsymbol{L}_r = 0$$

Theses relations are verified for each sub-volume s and the checks are passed when the residual (absolute or relative) is smaller than a preset threshold, which is set in the input-file. The default value of consistency depends on the localization type.

`mori_tanaka` This method is used only for 2 sub-volumes, where the matrix is supposed to be the sub-volume 1 and the direction of fibers is 3. The matrix is isotropic.

```
**localization mori_tanaka
 *geometry cylinder <double> <double> |  **geometry sphere <double>
[*consistency <double>]
[*correction stiffness <double>]
```

**geometry* geom is sphere or cylinder. r1 and r2 define the geometry of cylinder and sphere.

**consistency* some relations between localisation and influence tensors could be checked using the given ratio.

**correction* a correction for the asymptotic tangent stiffness is done using corrected values for the eigenstrains, instead of using the current tangent stiffness, that needs the evaluation of the instantaneous strain and stress concentration tensors [chab01].

The elastic concentration and influence tensors are evaluated using the Mori-Tanaka method, by the following relations:

$$\boldsymbol{A}_s = \boldsymbol{T}_s \left(\sum_{s=1}^{r} c_r \boldsymbol{T}_r \right)^{-1} \quad \text{where} \quad \boldsymbol{T}_r = \left[\boldsymbol{I} + \boldsymbol{S} \boldsymbol{L}_1^{-1} \left(\boldsymbol{L}_r - \boldsymbol{L}_1 \right) \right]^{-1}$$

$$\boldsymbol{D}_{rr} = \left(\boldsymbol{I} - \boldsymbol{A}_r \right) \left(\boldsymbol{L}_r - \boldsymbol{L}_s \right)^{-1} \boldsymbol{L}_r \quad \text{and} \quad \boldsymbol{D}_{rs} = \left(\boldsymbol{I} - \boldsymbol{A}_r \right) \left(\boldsymbol{L}_s - \boldsymbol{L}_r \right)^{-1} \boldsymbol{L}_s$$

In the matrix, $\boldsymbol{T}_1 = \boldsymbol{I}$ and $\boldsymbol{S}$ is the effective Eshelby tensor. The localisation tensor is obtained as follows

$$\boldsymbol{L} = \sum_r c_r \boldsymbol{L}_r \boldsymbol{A}_r$$

`voigt` This scheme assumes a uniform total strain field among each sub-volume as well as the macroscopic effective material.

```
**localization  voigt
[*consistency <double>]
```

Under the dual assumption of $\boldsymbol{\epsilon}_r = \boldsymbol{E}$, the localisation and influence tensors, using the voigt method, are:

$$\boldsymbol{A}_s = \boldsymbol{I}, \quad \boldsymbol{D}_{rs} = 0, \quad \boldsymbol{F}_{sr} = \delta_{rs}\boldsymbol{I} - c_r \boldsymbol{L}_s \boldsymbol{L}^{-1} \qquad \forall r, s$$

$$\text{and} \quad \boldsymbol{L} = \sum_r c_r \boldsymbol{L}_r \boldsymbol{A}_r = \sum_r c_r \boldsymbol{L}_r$$

`reuss` The Reuss scheme assumes homogeneity of stress among each sub-volume and the macroscopic effective medium.

```
**localization  reuss
[*consistency <double>]
```

The localisation and influence tensors, using the Reuss assumption $\boldsymbol{\sigma}_r = \boldsymbol{\Sigma}$, are:

$$\boldsymbol{A}_s = \boldsymbol{L}_s^{-1}\boldsymbol{L}, \qquad \boldsymbol{F}_{sr} = 0, \qquad \boldsymbol{D}_{sr} = \boldsymbol{I} - c_r \boldsymbol{A}_s = \boldsymbol{I} - c_r \boldsymbol{L}_s^{-1}\boldsymbol{L} \qquad \forall r, s$$

$$\boldsymbol{B}_s = \boldsymbol{I} \qquad \text{and} \qquad \boldsymbol{L}^{-1} = \sum_r c_r \boldsymbol{L}_r^{-1}$$

`numeric` The localisation and influence tensors A_s and D_{rs} can be directly read from a file, which are given explicitly by the user.

```
**localization numeric
   *number_of_subvolumes <integer>
   *A <tensor list> | *localization_tensors_ar_file <file>
   *D <tensor list> | *localization_tensors_drs_file <file>
   [*consistency <double>]
```

The default value of consistency is $1.e^{-2}$. The tensors A and D are given in a 6x6 representation, with 6 doubles per line and no empty lines between the tensors. The number of sub-volumes should be specified before reading any tensor. Both tensors A_r and D_{rs} should be given in the following form:

$$\begin{array}{cccc} D(0,0) & D(0,1) & \ldots & D(0,n-1) \\ D(1,0) & D(1,1) & \ldots & D(1,n-1) \\ \vdots & \vdots & \vdots & \vdots \\ D(n-1,0) & D(n-1,1) & \ldots & D(n-1,n-1) \end{array}$$

where n denotes the number of sub-volumes.

`polycrystal` This is particularly useful for the approximation of the macroscopic behaviour of the polycrystal for which each grain has a different elastic stiffness or stiffness orientation tensor

```
**localization polycrystal
   C <double>
```

The elastic concentration and influence tensors are :

$$\boldsymbol{D}_{sr} = (\delta_{sr} - c_r)(\boldsymbol{I} - C\boldsymbol{L}^{-1}) \quad \text{and} \quad \boldsymbol{E}_{sr} = \boldsymbol{I} + \boldsymbol{D}_{sr} - c_r\boldsymbol{A}_s$$

$$\boldsymbol{L}^{-1} = \sum_r c_r \boldsymbol{L}_r^{-1} \quad \text{and} \quad \boldsymbol{A}_s = \boldsymbol{L}_s^{-1}\boldsymbol{L}$$

`tfa_selfconsistent_sphere` The selfconsistent TFA localization is used for N spherical inclusions and anisotropic elasticity. Each sphere can have its own rotation and elasticity.

```
**localization tfa_selfconsistent_sphere
[*consistency <double>]
[*p_integration <integer>]
[*lhom_max_iterations <integer>]
```

**p_integration* The number of points for the numerical integration on the surface of the unit sphere, the default value is 25.

**max* Maximum number of iterations to find the homogeneised medium, where the default value is 10.

**consistency* The default value is $1.0e^{-10}$.

Using the selfconsistent method, the elastic concentration and influence tensors are given by the following relations:

$$\boldsymbol{D}_{sr} = (\boldsymbol{I} - \boldsymbol{A}_s)(\boldsymbol{L}_s - \boldsymbol{L})^{-1}(\delta_{sr}\boldsymbol{I} - c_r\boldsymbol{A}_r^T)\boldsymbol{L}_r, \quad \boldsymbol{A}_r = (\boldsymbol{L}^* + \boldsymbol{L}_s)^{-1}(\boldsymbol{L}^* + \boldsymbol{L})$$

$$\boldsymbol{F}_{sr} = (\boldsymbol{I} - \boldsymbol{B}_s)(\boldsymbol{L}_s^{-1} - \boldsymbol{L}^{-1})^{-1}(\delta_{sr}\boldsymbol{I} - c_r\boldsymbol{B}_r^T)\boldsymbol{L}_s^{-1}, \quad \boldsymbol{L} = \left(\sum_r c_r(\boldsymbol{L}^* + \boldsymbol{L}_s)^{-1}\right) - \boldsymbol{L}^*$$

where $\boldsymbol{L}^* = \boldsymbol{P} - \sum_r c_r\boldsymbol{L_s}$ is the Hill's constaint tensor and $\boldsymbol{P}$ is the Hill polarization tensor [Hers54, Suvo02, kron58] .

The steps to evaluate the localization tensor $\boldsymbol{L}$ are:

- First estimate : $L^0 = \sum_r c_r\boldsymbol{L_s}$
- Estimate $\boldsymbol{L}(\boldsymbol{P})$
- Calculate $(max|Ln - Ln + 1| < consistency)$
- Main loop until the $|Pn - Pn + 1| < consistency$ or until nmax is reached.

`multilayer` Multilayer localization only valid for 3D problems and tensor size 6. The geometry of the layer is given by : $(1, 2)$ plane of the layers and 3 direction perpendicular to the layers.

```
**localization  mutlilayer
[*consistency <double>]
```

Numerical calculations of localisation and influence tensor:
It is possible to calculate the influence and localisation tensors using a numerical method. Numerical approximation of localization and eigenstrain influence tensors in the literature are given by Dvorak and Teply[dvor93] as well as Paley and Aboudi [Pale92]. The theoretical developments are not presented here.
Usage : `Zrun -micmac` *name.inp*.
These tensors can be read in Multimat using `**localization numeric`

Syntax:

```
****micmac
***no_sqrt2
***local local
***compute_A
***compute_B
***grad options
***compute_D
***check_consistency
```

****no_sqrt2* do keep the sqrt2 in the non diagonal terms. Please use this option.

****local* specify the name of the localisation problem (see FE^2) method

****compute_A* to compute the strain localisation tensor.

****compute_B* to compute the stress localisation tensor.

****grad* specify the strain apply to the local problem to calculate (see example).

****compute_D* to compute the strain influence tensors.

****check_consistency* to verify the relations between A and D.

Example:
A 2D generalized plane strain example.

```
****micmac
  ***no_sqrt2
  ***local local
  ***compute_A
  ***compute_B
  ***grad 4 1. 0. 0. 0.
  ***grad 4 0. 1. 0. 0.
  ***grad 4 0. 0. 1. 0.
  ***grad 4 0. 0. 0. 1.
% if 3D problem, use :
% ***grad 6 1. 0. 0. 0. 0. 0.
% ***grad 6 0. 1. 0. 0. 0. 0.
% ***grad 6 0. 0. 1. 0. 0. 0.
% ***grad 6 0. 0. 0. 1. 0. 0.
% ***grad 6 0. 0. 0. 0. 1. 0.
% ***grad 6 0. 0. 0. 0. 0. 1.
  ***compute_D
  ***check_consistency
****return
```

<LOCALIZATION2>

This localisation object evaluates the overall elastic stiffness $\boldsymbol{L}$.

Syntax:
The syntax depends on the localization rule.

```
**localization name
   ...
```

`voigt` Using the Voigt scheme, the elastic stiffness is $\boldsymbol{L} = 2\mu\boldsymbol{I}$

```
**localization  voigt
  mu <double>
```

`matrix` The elastic stiffness is the Fourth-order compliance tensor $\boldsymbol{L} = \boldsymbol{S}$

```
**localization  matrix
  young double
  poisson doule
```

`kroner` The overall elastic stiffness is $\boldsymbol{L} = \alpha(\boldsymbol{L_r}(\boldsymbol{I} - \boldsymbol{S}))$ where S is the effective Eshelby tensor and $\boldsymbol{L_r}$ is the elasticity matrix of the sub-volume r.

```
**localization  kroner
  alpha double
  poisson doule
  ratio doule
```

`tangente` The elastic stiffness is $\boldsymbol{L} = A\boldsymbol{I}$:

$$\text{where} \qquad A = \frac{2\mu\mu_p(7 - 5\nu_p)}{\mu_p(7 - 5\nu_p) + 2\mu(4 - 5\nu_p)}$$

$$\text{and} \quad f = \frac{\sqrt{\underset{\sim}{\dot{\mathbf{E}}}^p : \underset{\sim}{\dot{\mathbf{E}}}^p}}{\sqrt{\underset{\sim}{\dot{\sigma}} : \underset{\sim}{\dot{\sigma}}}}, \qquad \mu_p = \frac{\mu}{1 + 2\mu f} \qquad \text{and} \qquad \nu_p = \frac{\nu + 2\mu(1+\nu)f/3}{1 + 4\mu(1+\nu)f/3}$$

```
**localization  tangente
  mu double
  poisson doule
```

Chapter 3

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