Modelizations second Summarized

gradient

One presents here the modelizations second gradient exit of works of Chambon et al. ([bib1], [bib2], [bib3]) and second gradient of thermal expansion resulting from works of Fernandes et al. ([bib4], [bib5]).

These modelizations fit in the frame of the mediums with microstructure and have like numerical purpose to give convergent results compared to the smoothness of the spatial discretization to avoid obtaining localised solutions. They must be used since the mechanical rheological models considered present a softening of the behavior translating the damage or the degradation of a material before cracking.

The modelization second gradient of thermal expansion is, in fact, a simplified approach of the second gradient restricted with the materials fixed with the phenomenon of dilatancy. The numerical purpose is to reduce to a significant degree the computing times. It lends itself particularly well to the géomatériaux one.

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1 The model second gradient

1.1 brief Presentation of the mediums with microstructure

In the beginning of this theory, one finds works of Mindlin ([bib6], [bib7]) in the frame of linear elasticity. These works were then resumed by Germain ([bib8], [bib9]) who gave of it a statement by application of the principle of the virtual wors, bases numerical methods for an application by finite elements.

This theory implies the definition of an enriched kinematics. Besides the classical field of displacements u_i , one considers the tensor of the second order, noted f_{ij} and called microscopic kinematical gradient, which models at the same time the strains and the rotations at the level of the grains of structure. One draws here attention to the fact that, in the frame of the mediums with microstructure, the microscopic deformation gradient does not have any raison d'être related to the gradient of any field depend on macroscopic displacement. It is not necessarily symmetric. The microscopic deformation gradient f_{ij} is a variable as well as macroscopic displacement u_i , contrary to the classical strain field (macroscopic), which is obtained to him by derivative

$$\varepsilon_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)$$

a fact essential with the base of the writing of this theory relates to the statement of the principle of objectivity or also of material indifference:

The virtual power of the internal forces to a system is null in any virtual motion rigidifying the system at time considered.

By neglecting the statement of the external forces of volume for reasons of simplification of writing, the consequence of the axiom of the virtual powers of the internal forces leads to the statement of the variational formulation, for any kinematically admissible field $\left(u_i^*, f_{ij}^*\right)$

$$\int_{\Omega}\left(\sigma_{ij}\frac{\partial u_i^*}{\partial x_j}+\tau_{ij}\left(f_{ij}^*-\frac{\partial u_i^*}{\partial x_j}\right)+\Sigma_{ijk}\frac{\partial f_{ij}^*}{\partial x_k}\right)dv=\int_{\partial\Omega}\left(t_i u_i^*+T_{ij}f_{ij}^*\right)ds \quad (1)$$

where t_i and T_{ij} are respectively the tensile forces and the double forces corresponding to the boundary conditions, on the border $\partial\Omega$, combined kinematical variables.

The variational formulation (1) is another layer to express the relations of equilibrium which are 2) expressed

$$\frac{\partial\left(\sigma_{ij}-\tau_{ij}\right)}{\partial x_j}=0 \quad (2$$

$$\frac{\partial\Sigma_{ijk}}{\partial x_k}-\tau_{ij}=0 \quad (3)$$

and one finds for the statement of the boundary conditions

$$t_i=\left(\sigma_{ij}-\tau_{ij}\right)n_j \quad (4)$$

$$T_{ij}=\Sigma_{ijk}n_k \quad (5)$$

where n_j the outgoing norm at the border indicates $\partial\Omega$.

To supplement the problem, it is necessary to define the constitutive laws which will bind the static variables σ_{ij} τ_{ij} , Σ_{ijk} respectively with the history of the kinematical variables of $\frac{\partial u_i}{\partial x_j}$, $\left(f_{ij}-\frac{\partial u_i}{\partial x_j}\right)$ and $\frac{\partial f_{ij}}{\partial x_k}$.

These models already proved that they were effective from the point of view of the regularization. However, they are complex in their use because of various constitutive laws to specify. Moreover, discretization by the finite element method in 3D induced the addition of 9 additional degrees of freedom per node corresponding to the components f_{ij} . The computing times are then relatively important and consequently NON-compatibles with the type of studies which we wish to carry out.

1.2 The model second gradient

On the basis of the preceding model, expressed by the relation (1), one can restrict the kinematics by forcing the microscopic gradient to be equal to the macroscopic gradient (see Chambon et al. [bib2] for a detailed analysis)

$$f_{ij}=\frac{\partial u_i}{\partial x_j} \quad (6)$$

the advantage of this assumption is to reduce the number of independent variables and to introduce simpler constitutive laws. The statement of the virtual powers altered after some algebraic handling is written then for any kinematically admissible field u_i^*

$$\int_{\Omega}\left(\sigma_{ij}\frac{\partial u_i^*}{\partial x_j}+\Sigma_{ijk}\frac{\partial^2 u_i^*}{\partial x_j\partial x_k}\right)dv=\int_{\partial\Omega}\left(p_i u_i^*+P_i Du_i^*\right)ds \quad (7)$$

where p_i and P_i are the boundary conditions defined by

$$p_i=\sigma_{ij}n_j-n_k n_j D\Sigma_{ijk}-\frac{D\Sigma_{ijk}}{Dx_k}n_j-\frac{D\Sigma_{ijk}}{Dx_j}n_k+\frac{Dn_l}{Dx_l}\Sigma_{ijk}n_j n_k-\frac{Dn_j}{Dx_k}\Sigma_{ijk} \quad (8)$$

$$P_i=\Sigma_{ijk}n_j n_k \quad (9)$$

with

Dq which indicates the normal derivative of the variable q : $Dq=\frac{\partial q}{\partial x_j}n_j$

$\frac{Dq}{Dx_j}$ which indicates tangential derivative of the variable q : $\frac{Dq}{Dx_j}=\frac{\partial q}{\partial x_j}-n_j Dq$

the assumption on the equality between strain field microscopic and macroscopic (6) a direct impact has on the statement of the boundary conditions because the variables u_i^* and f_{ij}^* are not independent any more.

It was already shown that this model compared to the corrects the dependence of the thickness of the tapes of localization discretization of the mesh (see Chambon et al. [bib1] or Matsushima et al. [bib3]). For that, the model can be used in taking into account two different constitutive laws, one to describe the part classical first gradient and the other for the second gradient. With regard to the latter, any relation can-being considered, but until today, it is in general of the linear elasticity which was selected.

1.3 Spatial discretization by finite elements

Written in its form of equation 7 , the discretization by the finite element method of the statement of the second gradient supposes that the fields u_i and u_i^* are twice differentiable. The numeric work implementation of such a condition implies the integration of C1-continuous finite elements (as that was proposed by Chambon et al. [bib1] in the frame of this unidimensional formulation second gradient or Zervos et al. [bib10] in a similar approach in deformation gradient).

One second approach consists in introducing a mixed formulation by the means of Lagrange multipliers. That consists in weakening the mathematical stress (6) in the writing of the variational formulation (7). One obtains then for any kinematically admissible field $\left(u_i^*, f_{ij}^*, \lambda_{ij}^*\right)$

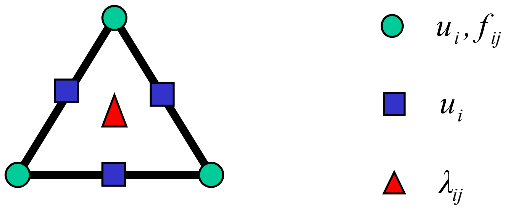
$$\int_\Omega \left(\sigma_{ij} \frac{\partial u_i^*}{\partial x_j} + \Sigma_{ijk} \frac{\partial f_{ij}^*}{\partial x_k} + \lambda_{ij} \left(f_{ij}^* - \frac{\partial u_i^*}{\partial x_j} \right) - \lambda_{ij}^* \left(f_{ij} - \frac{\partial u_i}{\partial x_j} \right) \right) dv = \int_{\partial \Omega} \left(t_i u_i^* + T_{ij} f_{ij}^* \right) ds \qquad (10)$$

where λ_{ij} are the Lagrange multipliers. The advantage of this new statement comes owing to the fact that the interpolations of the nodal unknowns, that are $\left(u_i, f_{ij}, \lambda_{ij}\right)$, require only conditions of C0-continuity. The disadvantage is due, on the other hand, with the addition of new degrees of freedom which does not make it possible to make decrease the number of unknowns of the problem.

The numeric work implementation suggested in Code_Aster is detailed in chapter 3 . One specifies here only spaces of approximation of the variables defining the kinematical field. The polynomial interpolations are the following ones:

1) shape functions of the second order for the variables of displacements u_i ,
2) of the first order shape functions for the microscopic tensor of the strains f_{ij}
3) of the constant functions by element for the Lagrange multipliers λ_{ij} .

One speaks about a formulation second gradient P2-P1-P0. The modelization is currently available in Code_Aster only under the assumption of the plane strains. One gives in figure 1.3-a a representation of the finite element associated with this combination of interpolations.



Appear **1.3-a** : Discretization finite element of the model second gradient for the plane strains

2 The model second gradient of thermal expansion

the principle of the mediums with microstructure is based on the taking into account of the microscopic strains to introduce into the form of the model an internal length. If the effectiveness of the regularization brought by the model second gradient is not any doubt, the computing times of simulations can become prohibitory. To decrease them in the particular frame of the dilating materials (for which the voluminal strain evolves according to the loading) one restricts the generality of the effect regularizing in the dilating mediums with microstructure.

2.1 The dilating mediums with microstructure

the kinematics of these mediums is defined by the field of usual displacement u_i , the noted microscopic voluminal variation χ and its gradients. By duality with this enriched kinematics, the static variables of the classical macroscopic stresses are introduced σ_{ij} , the microscopic stress of thermal expansion κ and the double vectorial stresses of thermal expansion S_j . The variable κ is the combined component of the relative voluminal strain (of the macroscopic field compared to microscopic) $\varepsilon_V-\chi$, while the components S_j define a vector which is combined gradient of microscopic thermal expansion $\frac{\partial \chi}{\partial x_j}$.

In a way similar to the statement of the virtual power of the mediums with microstructure of chapter 1.1 , and by again neglecting the statement of the external forces of volume for analytical simplification, one finds for the dilating mediums with microstructure, for any kinematically admissible field $\left(u_i^*, \chi^*\right)$

$$\int_\Omega \left(\sigma_{ij}\frac{\partial u_i^*}{\partial x_j}+\kappa\left(\varepsilon_V^*-\chi^*\right)+S_j\frac{\partial \chi^*}{\partial x_j}\right)dv=\int_{\partial\Omega}\left(t_i u_i^*+m\chi^*\right)ds \tag{11}$$

For which

$$t_i=\left(\sigma_{ij}+\kappa\delta_{ij}\right)n_j \tag{12}$$

$$m=S_j n_j \tag{13}$$

are the boundary conditions, expressed on the border $\partial\Omega$, combined by duality with the kinematical variables u_i and χ respectively.

The relations of equilibrium of this problem are written

$$\frac{\partial \sigma_{ij}}{\partial x_j}+\frac{\partial \kappa}{\partial x_i}=0 \tag{14}$$

$$\kappa+\frac{\partial S_j}{\partial x_j}=0 \tag{15}$$

the system of equations made up of [(12), (13), (14) and (15)] is obtained classically by application of the theorem of the divergence and an integration by part of (11).

2.2 The model second gradient of thermal expansion

According to a principle similar to that implemented for the model second gradient of chapter 1.2 , one introduces a mathematical stress to force the equality between the voluminal strains macroscopic ε_V and microscopic χ

$$\chi=\varepsilon_V \quad (16)$$

the statement of the virtual powers is then the following one, for any kinematically admissible field u_i^*

$$\int_\Omega \left(\sigma_{ij} \frac{\partial u_i^*}{\partial x_j} + S_j \frac{\partial^2 u_i^*}{\partial x_i \partial x_j} \right) dv = \int_{\partial\Omega} \left(p_i u_i^* + P n_i D u_i^* \right) ds \quad (17)$$

where p_i and P are the boundary conditions defined by

$$p_i=\sigma_{ij} n_j - n_i n_j DS_j - \frac{DS_j}{Dx_j} n_i - \frac{DS_j n_j}{Dx_i} + \frac{Dn_p}{Dx_p} S_j n_j n_i \quad (18)$$

$$P=S_j n_j \quad (19)$$

As for the model second gradient, the assumption on the equality between microscopic and macroscopic strain field voluminal (16) has a direct impact on the statement of the boundary conditions because the variables u_i^* and χ^* are not independent any more.

For reasons of simplicity, one supposes that $P=0$. The consequence of this assumption is that $S_j n_j=0$ on the border, which reduces the statement (18) to

$$p_i=\sigma_{ij} n_j - \frac{\partial S_j}{\partial x_j} n_i \quad (20)$$

a remarkable property of this simplification comes owing to the fact that it statement of the boundary conditions breaks up then into the classical part $\sigma_{ij} n_j$ and a second term which does not induce components of shears.

The balance equation is written

$$\frac{\partial \sigma_{\mathrm{ij}}}{\partial x_j} - \frac{\partial^2 S_j}{\partial x_i \partial x_j} = 0 \quad (21)$$

2.3 spatial Discretization by finite elements

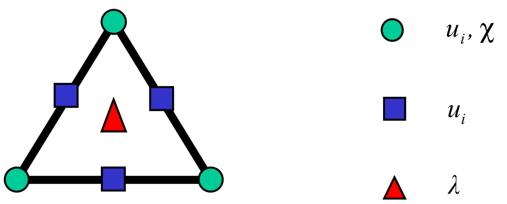
the goal of the approach of the second gradient of thermal expansion is to define a regularizing model, making it possible to ensure the independence of the results compared to the spatial discretizations, by introducing a minimum of nodal unknowns into her approach by finite elements. For that one limits oneself to the applications considering of the dilating materials. However, to discretize by the finite element method the statement (17) has as consequence to impose that the field of the unknowns of displacement as its divergence are continuous and differentiable. That returns has to take into account of the finite elements C1-continuous.

One then proposes to introduce the mathematical stress (16) into the statement of the mediums with microstructure dilating by means of a coupling of Lagrange multipliers and penalization. One obtains then for any kinematically admissible field $\left(u_i^*, \chi^*, \lambda^*\right)$

$$\int_{\Omega}\left(\sigma_{ij}\frac{\partial u_i^*}{\partial x_j}+S_j\frac{\partial \chi^*}{\partial x_j}-\lambda\left(\varepsilon_V^*-\chi^*\right)+\lambda^*\left(\varepsilon_V-\chi\right)+r\left(\varepsilon_V-\chi\right)\left(\varepsilon_V^*-\chi^*\right)\right)dv = \int_{\partial\Omega}\left(p_i u_i^*+P n_i D u_i^*\right)ds \quad (22)$$

the numeric work implementation suggested in Code_Aster is detailed in chapter 3 . One specifies here only spaces of approximation of the variables defining the kinematical field. The polynomial interpolations are the following ones:
A modelization P2-P1-P0 in plane strains

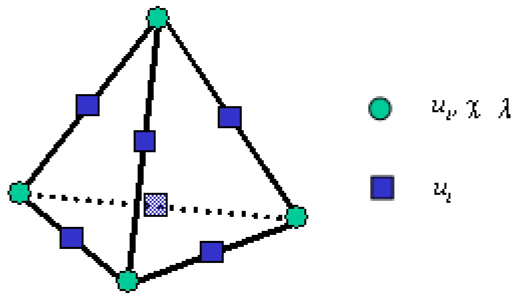
1) of the shape functions of the second order for the variables of displacements u_i
2) of the first order shape functions for the tensor of the voluminal strains microscopic χ
3) of the constant functions by element for the Lagrange multipliers λ .



Appear **2.3-a** : Discretization finite element of the model second gradient of thermal expansion for the plane strains

a modelization P2-P1-P1 in 3D

1) of the shape functions of the second order for the variables of displacements u_i
2) first order shape functions for the tensor of the voluminal strains microscopic χ and for the Lagrange multipliers λ .



Appear **2.3-b** : Discretization finite element of the model second gradient of thermal expansion for 3D.

3 Numerical integration of the models second gradient

3.1 the modelizations second gradients in Code_Aster: "patchs regularizing"

the modelizations finite elements put in work in the frame of chapters 1 (second gradient) and 2 (second gradient of thermal expansion) follow an atypical protocol compared to the existing procedures in Code_Aster. The goal is to define the models second gradients like "patchs regularizing" to simplify at the same time the data-processing development and to generalize the validity of the method to all of the existing constitutive laws in Code_Aster. One interprets these two points in the continuation of this chapter.

The principle - identical for the two modelizations - thus consists with partition numerically the respective variational formulations (second gradient and second gradient of thermal expansion) of classical a part known as “local” and a “regularizing” part in the following way (in the case of the second gradient of thermal expansion)

$$\int_{\Omega}\left(\sigma_{ij}\frac{\partial u_i^*}{\partial x_j}\right)dv+\int_{\Omega}\left(S_j\frac{\partial \chi^*}{\partial x_j}-\lambda\left(\varepsilon_V^*-\chi^*\right)+\lambda^*\left(\varepsilon_V-\chi\right)+r\left(\varepsilon_V-\chi\right)\left(\varepsilon_V^*-\chi^*\right)\right)dv = \int_{\partial\Omega}\left(p_i u_i^*+Pn_i Du_i^*\right)ds \quad (23)$$

The computation regularizing term is independent of the local part under condition that the constitutive laws introduced to define the first order static variables σ_{ij} and of the second order S_j are independent. This restrictive assumption is thus currently compulsory and is the principal disadvantage of this strategy of design.

On the other hand, the interest comes owing to the fact that the “patch regularizing” to introduce is independent of the local part. It is thus enough to apply it to any type of modelization (mechanical, coupled hydro-mechanical, thermo-hydro-mechanics…). Moreover, numerically there is no data-processing impact on the part regularizing following integration of new constitutive laws first gradient.

3.2 The modelization second gradient

While thus following the stated principle to chapter 3.1 , the “patch regularizing” representative of the finite element second gradient describes in chapter 1.3 results in the numerical integration of the following formulation

$$\int_{\Omega}\left(\Sigma_{ijk}\frac{\partial f_{ij}^*}{\partial x_k}-\lambda_{ij}\left(\frac{\partial u_i^*}{\partial x_j}-f_{ij}^*\right)+\lambda_{ij}^*\left(\frac{\partial u_i}{\partial x_j}-f_{ij}\right)\right)dv \quad (24)$$

One details below the strain fields, of stresses associated and the tangent matrix. There is no local variable in the description of this finite element. For recall the nodal variables defining the degrees of freedom are the following ones: $\left(u_i, f_{ij}, \lambda_{ij}\right)$.

3.2.1 The strain field

$$E=\begin{pmatrix}\left(\frac{\partial u_i}{\partial x_j}-f_{ij}\right)\\ \frac{\partial f_{ij}}{\partial x_k}\\ \lambda_{ij}\end{pmatrix}$$

3.2.2 the field of the stresses

$$\Sigma=\begin{pmatrix}\lambda_{ij}\\ \Sigma_{ijk}\\ -\left(\frac{\partial u_i}{\partial x_j}-f_{ij}\right)\end{pmatrix}$$

3.2.3 the tangent matrix

the elementary tangent matrix of the modelization second gradient is composed, inter alia, of the tangent matrix of elementary stiffness $T^{\mathbf{2g}}$ associated with the constitutive law second gradient which binds the double stresses Σ_{ijk} to the gradients of the microscopic strains $\frac{\partial f_{ij}}{\partial x_k}$.

$$K^{\mathbf{el}}=\begin{pmatrix}0 & 0 & (\mathbf{Id})_{\dim(ij)}\\ 0 & \left(T^{\mathbf{2g}}\right)_{\dim(ijk)} & 0\\ (-\mathbf{Id})_{\dim(ij)} & 0 & 0\end{pmatrix}$$

3.3 The modelization second gradient of thermal expansion

While again following the stated principle to chapter 3.1 , the “patch regularizing” representative of the finite element second gradient of thermal expansion describes in chapter 2.3 results in the numerical integration of the formulation

$$\int_{\Omega}\left(S_j\frac{\partial\chi^*}{\partial x_j}-\lambda\left(\varepsilon_V^*-\chi^*\right)+\lambda^*\left(\varepsilon_V-\chi\right)+r\left(\varepsilon_V-\chi\right)\left(\varepsilon_V^*-\chi^*\right)\right)dv \quad (25)$$

One details below the strain fields, of stresses associated and the tangent matrix. There is no local variable in the description of this finite element. For recall the nodal variables defining the degrees of freedom are the following ones: (u_i,χ,λ) .

3.3.1 The strain field

$$E=\begin{pmatrix}(\varepsilon_V-\chi)\\ \frac{\partial\chi}{\partial x_j}\\ \lambda\end{pmatrix}$$

3.3.2 the field of the stresses

$$\Sigma=\begin{pmatrix}r(\varepsilon_V-\chi)+\lambda\\ S_j\\ -(\varepsilon_V-\chi)\end{pmatrix}$$

3.3.3 the tangent matrix

the elementary tangent matrix of the modelization second gradient is composed, inter alia, of the tangent matrix of elementary stiffness S^{2d} associated with the constitutive law second gradient of thermal expansion which binds the double stresses S_j to the gradients of the microscopic voluminal strains $\frac{\partial \chi}{\partial x_j}$.

$$K^{el} = \begin{pmatrix} r & 0 & 1 \\ 0 & \left(S^{2d}\right)_{\dim(j)} & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

4 The Councils/Procedure for the use of the models second gradient

Some handling simple are to be defined in the command file Code_Aster to use the modelizations second gradients. The approach is on the other hand same whatever the local modelization. Examples are available in the base of the benchmarks of validation of Code_Aster. One can quote, inter alia, the biaxial tests in linear elasticity in compression referred ssll117, the construction of a column of soil into nonlinear (Hujeux constitutive law in hydraulic coupled porous environment) referred wtnv132 or the triaxial compression test in linear elasticity referred sslv117.

4.1 Linear elasticity second gradient

to use the modelizations second gradients it is necessary to define two constitutive laws respectively to describe the macroscopic relations between stresses σ_{ij} and microscopic ε_{ij} strains and the relations between double stresses (Σ_{ijk} for the second gradient or S_j the second gradient of thermal expansion) and deformation gradient $\frac{\partial f_{ij}}{\partial x_k}$ for the second gradient or voluminal deformation gradient $\frac{\partial \chi}{\partial x_j}$ for the second gradient of thermal expansion.

For the choice of the behavior of the type first gradient – that which intervenes in the local modelization described in section 3.1 – it has no restriction there: all the constitutive laws are possible. On the other hand, one currently lays out of only one behavior model of the type second gradient. It is the linear elasticity suggested by Mindlin ([bib6], [bib7]) of which here the writing in 2D

$$\begin{bmatrix} \Sigma_{111} \\ \Sigma_{112} \\ \Sigma_{121} \\ \Sigma_{122} \\ \Sigma_{211} \\ \Sigma_{212} \\ \Sigma_{221} \\ \Sigma_{222} \end{bmatrix} = \begin{bmatrix} a^{12345} & 0 & 0 & a^{23} & 0 & a^{12} & a^{12} & 0 \\ 0 & a^{145} & a^{145} & 0 & a^{25} & 0 & 0 & a^{12} \\ 0 & a^{145} & a^{145} & 0 & a^{25} & 0 & 0 & a^{12} \\ a^{23} & 0 & 0 & a^{34} & 0 & a^{25} & a^{25} & 0 \\ 0 & a^{25} & a^{24} & 0 & a^{34} & 0 & 0 & a^{23} \\ a^{12} & 0 & 0 & a^{25} & 0 & a^{145} & a^{145} & 0 \\ a^{12} & 0 & 0 & a^{25} & 0 & a^{145} & a^{145} & 0 \\ 0 & a^{12} & a^{12} & 0 & a^{23} & 0 & 0 & a^{12345} \end{bmatrix} . \begin{bmatrix} \chi_{111} \\ \chi_{112} \\ \chi_{121} \\ \chi_{122} \\ \chi_{211} \\ \chi_{212} \\ \chi_{221} \\ \chi_{222} \end{bmatrix} \quad (26)$$

where $\chi_{ijk}=\frac{\partial f_{ij}}{\partial x_k}$ and all the terms of the matrix depend on five constants according to the following relation

$$\begin{cases} a^{12345}=2\left(a^1+a^2+a^3+a^4+a^5\right) \\ a^{23}=a^2+2a^3 \\ a^{12}=a^1+\frac{a^2}{2} \\ a^{145}=\frac{a^1}{2}+a^4+\frac{a^5}{2} \\ a^{25}=\frac{a^2}{2}+a^5 \\ a^{34}=2\left(a^3+a^4\right) \end{cases}$$

Fernandes and al [bib5] applied this model for the second gradient of thermal expansion by simplifying the statement (26)) in 2D by

$$\begin{bmatrix} S_1 \\ S_2 \end{bmatrix}=\begin{bmatrix} 3a^1 & 0 \\ 0 & 3a^1 \end{bmatrix}\cdot\begin{bmatrix} \frac{\partial \chi}{\partial x_1} \\ \frac{\partial \chi}{\partial x_2} \end{bmatrix} \quad (27)$$

4.2 the names of the modelizations in Code_Aster

the assumption of the plane strains is currently possible for the modelizations second gradients in Code_Aster. For the second gradient the name of the modelization is D_PLAN_2DG while for the second gradient of thermal expansion the name of the modelization is D_PLAN_DIL.

Meshes accepted are QUAD9 and TRIA7 for two modelizations P2-P1-P0 second gradients. For the second gradient of thermal expansion it is also possible to use meshes QUAD8 and TRIA6 in which case the modelization is then defined without Lagrange multipliers and the mathematical stress (16)) is only ensured by the penalization.

For the applications 3D, the name of the modelization is 3D_DIL for the second gradient of thermal expansion. Meshes accepted are TETRA10, PENTA15 or HEXA20 for interpolations P2-P1-P1.

4.3 An example with accompanying notes

Here an example of command file to the format Code_Aster. The comments introduced by the character *$* are specific to the “regularizing patchs” introduced by the modelizations second gradients.

reading of the mesh (quadratic)

```
MY = LIRE_MAILLAGE ()
```

$ Duplication of the mesh (quadratic). Only meshes are duplicated, the nodes remain common. The goal is to associate with each one of these meshes a different modelization only on the structure part. As regards the application of the boundary conditions one does not duplicate meshes, it is directly the statement (20) which will be applied.

```
MAIL=CRÉA_MAILLAGE (MAILLAGE=MA,
```

```
                    CREA_GROUP_MA= (_F (NOM=' ROCHE_REG',
                                        GROUP_MA=' ROCHE')))
```

$ Introduction of central nodes to the finite elements of the new mesh for an interpolation P2-P1-P0. Procedure necessary to take into account the interpolations of the Lagrange multipliers.

```
MAILLAGE=CRÉA_MAILLAGE (MAILLAGE=MAIL,
                       MODI_MAILLE= (_F (GROUP_MA = “ROCHE_REG”,
                                        OPTION = “QUAD8_9”),
                                     _F (GROUP_MA = “ROCHE_REG”,
                                        OPTION = “TRIA6_7”)))
```

$ Assignment of a modelization to each mesh.

```
MODELE=AFFE_MODELE (MAILLAGE = MAILLAGE,
                   AFFE = (_F (GROUP_MA = “ROCK”,
                              PHENOMENE = “MECHANICAL”,
                              MODELISATION = “D_PLAN”),
                           _F (GROUP_MA = “ROCHE_REG”,
                              PHENOMENE = “MECHANICAL”,
                              MODELISATION = “D_PLAN_DIL”)))
```

<u>Taking into account of the boundary conditions:</u>
<u>*$* Attention the statement of the boundary conditions with taking into account of the modelizations second gradients differs from that of the local modelizations (see chapter 1).</u>

```
CHCI=AFFE_CHAR_MECA (MODELE=MODELE,
                    DDL_IMPO= (...),…)
```

<u>Definition of materials parameters for the constitutive law first gradient</u>

```
SOL1 = DEFI_MATERIAU (…)
```

<u>*$* Definition of materials parameters for the constitutive law second gradient. Currently was introduced only the linear elasticity second gradient suggested by Mindlin.</u>

```
SOL2 = DEFI_MATERIAU (ELAS_2NDG =_F (A1=10, A2=0, A3=0, A4=0, A5=0),…)
```

$ Assignment of materials parameters according to the same procedure as for the definition of the modelizations.

```
= AFFE_MATERIAU SUBDUE (MAILLAGE = MAILLAGE,
                     AFFE = (_F (TOUT = “ROCK”,
                     MATER =  SOL1,),
                     _F (GROUP_MA = “ROCHE_REG”,
                        MATER = SOL2)))
```

$ Definition of nonlinear static computation with a constitutive law associated with each one of the modelization: behavior of the Drucker-Prager type for the first gradient, and linear elasticity for the second U1

```
gradient = STAT_NON_LINE (MODELS = MODELS,
                   CHAM_MATER = SUBDUE,
                   EXCIT = (_F (CHARGE = CHCI),…),
                   SOLVER = (_F (METHODE=' MUMPS',)),
                   COMP_INCR = (_F (GROUP_MA=' ROCHE',
                                   RELATION=' DRUCK_PRAGER',),
                                _F (GROUP_MA=' ROCHE_REG',
                                   RELATION=' ELAS',),),
                   NEWTON = _F (MATRICE   = “TANGENT”, REAC_ITER = 1),
```

```
INCREMENT = _F (LIST_INST = TEMPS))
```

4.4 Estimate of the parameter of regularization `A1 (2nd gradient of thermal expansion)`

With an aim of characterizing the value as well as possible to be assigned to the parameter of regularization, `A1`, of the 2nd gradient of thermal expansion, it is possible to determine a limit higher than this parameter according to the tangent matrix of velocity of very model of lenitive behavior.
In this way, the user will be able to determine according to the size of meshes with problem which he deals the value of the parameter `A1` best adapted has his problem.

This computation is based on an analytical problem $2D$ of a tape of shears [bib2 and bib11].

The fracture in the géomatériaux ones is often characterized by the training of zones to located strains, reporting a transition of zones of homogeneous strains towards modes of nonhomogeneous strains. The appearance of this phenomenon can be seen on the theoretical level like the spontaneous change of the mode of strain, compared to a bifurcation of a branch of the equilibrium, i.e. the intersection of two branches of solutions functions of the parameters of control. In the frame of the continuums, it is possible to release under restricted conditions of the criteria of bifurcation making it possible to identify the parameter of control causing the appearance of the tape of shears, as well as the potential directional senses of this one. On the other hand, for the classical continuums, the mode of “post-localization”, in particular the bandwidth of shears, cannot be characterized. The experimental results show nevertheless that this width is an intrinsic element with the properties of the material, related to its microstructure (form and size of the grains, Desrues and Viggiani [bib12]) and its initial state (index of the vacuums and stress state). The use of the theory of the second local gradient of thermal expansion makes it possible to enrich the kinematics by the medium thus translating the effects of the microstructure on a total scale. In this section, we will extract from a two-dimensional analytical problem the elements allowing to characterize the bandwidth of shears lasting the mode of “post-localization”.

The formulation of the problem of velocity is written then in the following form, by considering the constant body forces:

$$\int_{\Omega} \dot{\sigma}_{ij}\dot{\epsilon}_{ij}(u^*)+\dot{S}_j\eta_j(u^*)dv=\int_{\partial\Omega} \dot{F}_i u_i^* ds \quad \forall u^* \in \mathcal{V}_0 \qquad (28)$$

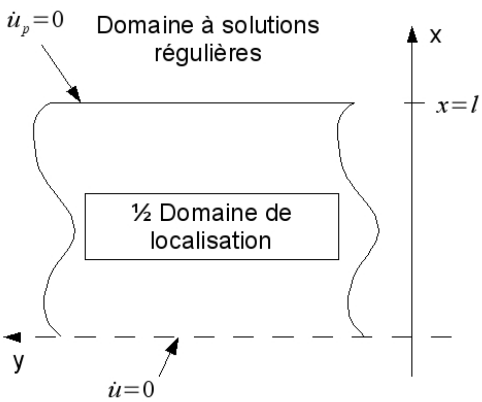
$\dot{\sigma}_{ij}$, $\dot{S}_j$ and $\dot{F}_i$ are the temporal derivatives of the terms introduced into equation 17 .

4.4.1 Analytical resolution

the two-dimensional analytical problem tackled below was solved by [bib2] for a model of second complete gradient with the model local elastoplastic of Mohr-Coulomb described by [bib13]. The example consists in applying the model of second gradient of thermal expansion in a sheared layer and determining the solutions of the problem of velocity.

considers a layer defined in the planavecl' (x, y) z axis perpendicular to the plane. Chambon and al. [bib2] consider an infinite layer ranging between two definite planes paret $x=0$ $x=l$ (Figure 4.4-a). The fields of displacement are notésdans u the directionetdans x v the direction.etsont y $\dot{u}$ $\dot{v}$ supposed not to depend that deet x their derivatives compared will àseront x noted. ′

The initial state of the material is definite homogeneous . The evolutions of the boundary conditions applied to the field are the following ones: for



Appear 4.4-a : ÉtudiéOn field

- , $x=0$ for $\dot{u}=0$ $\dot{v}=0$
- , are $x=l$ $\dot{F}_i$ known.

The body forces are supposed to be constant.
The conditions of symmetry applied to frontièreindiquent $x=0$ that the field studied with a total width of. $2l$ This
problem can be seen as analysis of the behavior of a tape of localization, where the directional sense of the tape is supposed and the stress state is left free of any restriction. The border of the endéfinit field $x=l$ the zone of transition between the zone from localization (studied field) and the field from an unspecified solid where the solutions are supposed to be regular and stable.

The gradient of the field of displacement in the field takes the following shape : (29

$$\dot{u}_{i,j}=\begin{bmatrix}\dot{u}' & 0\\ \dot{v}' & 0\end{bmatrix}$$)29

the macroscopic strain field is written explicitly: (30

$$\dot{\epsilon}_{ij}=\frac{1}{2}\left(\dot{u}_{i,j}+\dot{u}_{j,i}\right)=\begin{bmatrix}\dot{u}' & \frac{1}{2}\cdot\dot{v}'\\ \frac{1}{2}\cdot\dot{v}' & 0\end{bmatrix}$$)30

the only non-zero term of the gradient of the voluminal strains is : (31

$$\frac{\partial\dot{\epsilon}_v}{\partial x_1}=\dot{u}''$$)31

the application of the principle of the virtual wors to the field of displacement imposed after 2 integrations by parts gives the following balance equations for the problem of velocity: (32

$$\frac{\partial\dot{\sigma}_{ij}}{\partial x_j}-\frac{\partial^2\dot{S}_j}{\partial x_i\partial x_j}=0\ \Rightarrow\ \begin{cases}\dot{\sigma}'_{11}-\dot{S}''_1 & = & 0\\ \dot{\sigma}'_{12} & = & 0\end{cases}$$)32

the boundary conditions provide in: $x=l$ (33

$$\begin{cases}\dot{\sigma}_{11}-\dot{S}'_1 & = & \dot{F}_1\\ \dot{\sigma}_{12} & = & \dot{F}_2\\ 3a^1\dot{u}''' & = & 0\end{cases}$$)33

spatial integration of the balance equations by taking account of the boundary conditions for a homogeneous problem, the solutions of the problem respect the following equations: (34

$$\begin{cases}\dot{\sigma}_{11}-\dot{S}'_1 & = & \dot{F}_1\\ \dot{\sigma}_{12} & = & \dot{F}_2\end{cases}$$)34

the constitutive laws of the first and second gradients, the equations become : (35

$$\begin{cases}H_{1111}\dot{u}'+H_{1112}\dot{v}'-3a^1\dot{u}''' & = & \dot{F}_1\\ H_{1211}\dot{u}'+H_{1212}\dot{v}' & = & \dot{F}_2\end{cases}$$)35

the system of equations coupled differentials can be reduced to an equation, the second equation expressing a linear relation between the first gradients of vertical and horizontal displacements in the tape. (36

$$\begin{cases} H_{1111}\dot{u}' + H_{1112}\dfrac{\dot{F}_2 - H_{1211}\dot{u}'}{H_{1212}} - 3a^1\dot{u}''' = \dot{F}_1 \\ \dfrac{\dot{F}_2 - H_{1211}\dot{u}'}{H_{1212}} = \dot{v}' \end{cases} \quad)36$$

the solutions of this system of equations linear differentials of order 2 are expressed as the sum of a particular solution answering the imposed boundary conditions and of a partial solution established starting from the roots of the characteristic polynomial of this system: One $\dot{u}' = \dot{u}'_0 + \dot{u}'_p$ supposes for $\dot{u}'_p$ a solution of the typequi $\dot{u}'_p = e^{\eta x}$ allows to establish the following characteristic equation: (37

$$H_{1111} - H_{1112}\frac{H_{1211}}{H_{1212}} - 3a^1\eta^2 = 0 \quad)37$$

can then give the statement of the solution partial according to the material parameters of the first and second gradient: that is to say

$$(38 \quad \eta^2 = \frac{H_{1111}H_{1212} - H_{1112}H_{1211}}{3a^1 H_{1212}} \quad)38$$

the constitutive law of first gradient being elastoplastic, the solutions will be different depending on the state from the region considered. In a region with elastic behavior, the constitutive law écritet $\dot{\sigma} = A\,\dot{\epsilon}$ in a region with plastic behavior. $\dot{\sigma} = H^{ep}\dot{\epsilon}$ Finally

the solutions of the problem take the following shapes according to the sign of (39

$$\eta^2 = \Delta = \frac{H_{1111}H_{1212} - H_{1112}H_{1211}}{3a^1 H_{1212}} \quad)39$$

- , then $\Delta > 0$ (40

$$\dot{u}' = \dot{u}'_0 + \left(C_{11}\exp(\eta_1 x) + C_{12}\exp(\eta_2 x)\right) \quad)40$$

$\eta_i = \pm\sqrt{\Delta}$ $\dot{u}'_0$ from the equation of the particular solution: and

$$\dot{u}'_0 = \frac{H_{1212}\dot{F}_1 - H_{1112}\dot{F}_2}{H_{1111}H_{1212} - H_{1112}H_{1211}} \quad (41 \quad \dot{v}'_0 = \frac{H_{1111}\dot{F}_2 - H_{1211}\dot{F}_1}{H_{1111}H_{1212} - H_{1112}H_{1211}} \quad)41$$

, the solutions partiellesvérifient $\dot{u}'_p$ the following equations: (42

$$\frac{H_{1111}H_{1212} - H_{1112}H_{1211}}{3a^1 H_{1212}}\dot{u}'_p - \dot{u}'''_p = 0 \quad)42$$

the conditions of symmetry of the studied field and, one $\dot{u}'_p(l) = 0$ from of deduced that null C_{11} C_{12} coefficientsetsont. If

- , then $\Delta < 0$ (43

$$\dot{u}' = \dot{u}'_0 + (C_{21}\cos(\omega x) + C_{22}\sin(\omega x)) \quad)43$$

. Just $\omega=\sqrt{\frac{H_{1211}H_{1112}-H_{1212}H_{1111}}{3a^{1}H_{1212}}}$ as for the solutions previously established for the zones where, $\Delta>0$ the solution partiellevérifie $\dot{u}_p^{'}$ equation 42 42
The statement of the solution in the zone where reveals $\Delta<0$ goniometrical functions. It is thus clear that a zone of localization can appear in structure. One can then admit that the structure privileges a length interns, $l_c=2\pi/\omega$ expressing oneself according to the first mode of lower energy. It
is also noted that the dependence internal length is l_c in. $\sqrt{a^1}$ It is interesting to also notice that the condition of appearance of the solutions of bifurcations is controlled only by the terms of the model of first gradient. In other words, the taking into account of a kinematics enriched restricted in the mediums by second gradient does not modify the value of the parameter of control causing the appearance of a solution forked as tapes of shears. Numerical

4.4.2 resolution

elementary computation option PDIL_ELGA , determines, for a given initial state of the stresses and local variables, the value of A1 _LC2 established according to the following formula: (44

$$\text{A1\_LC2}=\frac{a^1}{l_c^2}=\frac{\left[H_{1211}H_{1112}-H_{1111}H_{1212}\right]}{3H_{1212}(2\pi)^2} \quad)44$$

various directional senses of the tape of shears. The writing of the components clarifies tensor of stiffness of the classical local model is obtained via the routines of computation of the tangent matrixes of velocity.
A rotation of the tape of shears of angleimplic θ a local rotation applied to the components of the tensor of the stresses. It makes it possible to estimate the new components of the local tensor constitutive of the model of classical behavior, bearing on the first gradient of displacements.
The angular discretization used is first of all. $5°$ Around the first raised maximum, one carries out a discretization with then $1°$. $0.2°$ In this way, one ensures oneself to obtain A1 a precise value of parameter _LC2.

The user can then define the value of A1 adapted to the spatial discretization of studied structure, knowing that a minimum of 6 elements on LC appears necessary to guarantee independence with the meshes of the results.

The numerical validation of computation option PDIL_ELGA is carried in benchmarks SSNV208A, SSNP125A and WTNV132C. Functionality

5 and checks

the list of the tests of validation for the second gradient: Benchmark

description	SSL
117 (modelizations a->e) Test	of D_PLAN_DIL (see V3.01.117) for modelization P2-P1-P0 (see §4.212
117f Test	of D_PLAN_2DG (see V3.01.117) for modelization P2-P1-P1 SSL
117g Test	of D_PLAN_DIL (see V3.01.117) for modelization P2-P1-P1 sslv
117a Test	of 3D_DIL (see V3.04.117) for modelization P2-P1-P1 Bibliography

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7 of the versions of the document Index

document Version	Aster Author	(S) Organization (S) Description	of the modifications A
9.3	R.	FERNANDES initial	Text