Nonlocal modeling with gradients of internal variables GRAD_VARI

Summary

One presents here nonlocal modeling to gradient of internal variables entitled GRAD_VARI in Code_Aster. This modeling is resulting from work of E. Lorentz [Feeding-bottle 1]. The algorithm making it possible to solve the regularization and equilibrium equations however was modified compared to the initial version of the model.

Nonlocal modelings of type GRAD_VARI are available in 3D (3D_GRAD_VARI), axisymmetric (AXIS_GRAD_VARI) and plane deformations (D_PLAN_GRAD_VARI).

Contrary to the old version, the use of GRAD_VARI is relatively simple, since it is enough to specify modeling X_GRAD_VARI in AFFE_MODELE, to specify a characteristic length under the keyword NON_LOCAL in DEFI_MATERIAU, and to check that the law of behavior which one wishes to use is quite available in nonlocal version.

One presents the writing and the digital processing of this model.

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1 Recall on the theory of the models with gradient

The models with gradient presented here were developed by E. Lorentz [bib1] in order to be able to describe the material behavior requested by strong gradients of the mechanical fields which appear in the damaged zones or in the vicinity of geometrical singularities. Indeed, in the case of strong gradients, the behavior of a material point is not independent any more of its entourage but depends on the behavior on its vicinity, from where the introduction of gradients into the models.

From a digital point of view, the calculation of a structure with a classical law of damage local shows that the damaged zone is always located on only one finite elements sleep and thus that the answer of the structure depends on the adopted grid: the models with gradient mitigate this problem.

In what follows, we make a short recall of this theory.

1.1 Construction of the models with gradient

This formulation is restricted with generalized standard materials [Feeding-bottle 2].

The models with gradient of internal variables consist in introducing the gradient of internal variables into a generalized standard formulation [Feeding-bottle 2].

That is to say a an internal variable and A its associated thermodynamic force, and is $\Delta(\dot{a})$ potential of dissipation. If it is considered that Δ also depends on the gradient on $\dot{a}$, $\Delta=\Delta(\dot{a},\nabla\dot{a})$, one cannot then write the principle of normality locally:
$A\in\partial\Delta(\dot{a},\nabla\dot{a})$

Indeed, such a writing would require the introduction of 2 variables locally independent a and a_∇, to which 2 thermodynamic forces would be associated $A=-\frac{\partial\Phi}{\partial a}$, $A_\nabla=-\frac{\partial\Phi}{\partial a_\nabla}$ such as:
$(A,A_\nabla)\in\partial\Delta(\dot{a},\dot{a}_\nabla)$

If one calls F the threshold of elasticity associated with the potential $\Delta(\dot{a},\dot{a}_\nabla)$, the preceding equation is equivalent to:

$$\Delta(\dot{a},\dot{a}_\nabla)=\underset{(A,A_\nabla)\ /\ F(A,A_\nabla)\leq 0}{Sup}\left[\dot{a}\ A+\dot{a}_\nabla A_\nabla\right]$$

And one a:
$\dot{a}=\dot{\lambda}\frac{\partial F}{\partial A}$, $\dot{a}_\nabla=\dot{\lambda}\frac{\partial F}{\partial A_\nabla}$

The problem here is that the variables are not independent and are bound by the nonlocal constraint $a_\nabla=\nabla a$ so that one is not sure to check:
$\dot{a}_\nabla=\dot{\lambda}\frac{\partial F}{\partial A_\nabla}=\nabla\dot{a}$

One then proposes to forget the assumption of normal flow in each point of the structure while preserving the formalism of generalized standard materials but at the level of the structure, where the variables of state are now it field of deformation $\boldsymbol{\varepsilon}$ and it field internal variables a. The total free energy and the total potential of dissipation are thus defined:

$$F_{\Phi}(\boldsymbol{\varepsilon}, a)=\int_{\Omega}\Phi(\boldsymbol{\varepsilon}(x), a(x), \nabla a(x))\,dx$$
$$D(\dot{a})=\int_{\Omega}\Delta(\dot{a}(x), \nabla \dot{a}(x))\,dx$$

Total potential of dissipation D is now a function of field $\dot{a}$, and the writing $A\in\partial D(\dot{a})$ a direction begins again.

The relation of behavior generalized is written now:

$$\sigma=\frac{\partial F_{\Phi}}{\partial \varepsilon},\ A=-\frac{\partial F_{\Phi}}{\partial a},\ A\in\partial D(\dot{a})$$

1.2 Dualisation and discretization in time

It will be supposed subsequently that the energy of the model regularized is the sum of the energy of the local model and an additional term depending only on the gradient of the internal variable which one regularizes:

$$F_{\Phi}(\boldsymbol{\varepsilon}, a)=\int_{\Omega}\Phi^{loc}(\boldsymbol{\varepsilon}(x), a(x))+\Phi^{grad}(\nabla a(x))\,dx$$

This separation corresponds to the cases which we treat in Code_Aster, but it is possible to build models with gradient which do not correspond to this case.

Total free energy $F_{\Phi}(\boldsymbol{\varepsilon}, a)$ fact of intervening the gradient of the internal field of variable a. However, it is known that the treatment of the internal variables by the finite element method in Code_Aster is carried out at the points of Gauss, where one does not have information on the gradients. An additional field is thus introduced α, which will be defined in the nodes, on which will carry the additional term depend on the gradient and to which one will force to be equal to the field has in any point. The total free energy is written then:

$$F_{\Phi}(\boldsymbol{\varepsilon}, a, \alpha)=\int_{\Omega}\Phi^{loc}(\boldsymbol{\varepsilon}(x), a(x))+\Phi^{grad}(\nabla \alpha(x))\,dx$$

with the condition $\alpha = a$.

In order to free itself from the constraint $\alpha = a$, one dualise the latter by introducing a multiplier of Lagrange. The function is introduced:

$$F_{\Phi}(\boldsymbol{\varepsilon}, a, \alpha, \lambda)=\int_{\Omega}\Phi^{loc}(\boldsymbol{\varepsilon}(x), a(x))+\Phi^{grad}(\nabla \alpha(x))+\lambda(a-\alpha)\,dx$$

where λ is a multiplier of Lagrange and one has $F_{\Phi}(\boldsymbol{\varepsilon}, a, \alpha)=\max_{\lambda} F_{\Phi}(\boldsymbol{\varepsilon}, a, \alpha, \lambda)$

Lastly, one adds a quadratic term of penalization on the condition of compatibility between the fields a and α :

$$F_{\Phi}(\boldsymbol{\varepsilon}, a, \alpha, \lambda)=\int_{\Omega}\Phi^{loc}(\boldsymbol{\varepsilon}(x), a(x))+\Phi^{grad}(\nabla \alpha(x))+\lambda(\alpha-a)+\frac{r}{2}(\alpha-a)^2\,dx$$

where r is a coefficient of penalization. This additional term of penalization does not modify our problem, since it must tend towards 0 with convergence, but makes it possible to help with convergence.

While being based on the assumption of convexity compared to a potentials F_Φ and D and while adopting a diagram of implicit Euler, the temporal discretization of the preceding problem [éq 1.1-8] is reduced to the resolution of a problem of minimization relating to the increment Δa internal fields of variables. This problem is written for behaviors independent of time:

$$\min_{\Delta a}\left(\max_{\lambda} F_\Phi(\boldsymbol{\varepsilon},\alpha,\lambda,a^-+\Delta a)+D(\Delta a)\right)$$

where a^- represent the field of internal variables at the previous moment. This minimization constitutes the law of behavior.

In the same way, while being based on the assumption of convexity compared to (u,α) potential F_Φ and while adopting a diagram of implicit Euler, the resolution of the equilibrium equations is brought back to a problem of minimization relating to the increments $(\Delta u,\Delta\alpha)$. The discretized problem is written then:

$$\max_{\Delta\lambda}\min_{\Delta u}\min_{\Delta\alpha}\min_{\Delta a}\left(F_\Phi(\boldsymbol{\varepsilon}^-+\Delta\boldsymbol{\varepsilon},\alpha^-+\Delta\alpha,\lambda^-+\Delta\lambda,a^-+\Delta a)+D(\Delta a)-W^{ext}\right)$$

where W^{ext} represent the work of the external mechanical forces.

1.3 Space discretization by finite elements

To solve the problem of search for extrema, one carries out a space discretization by finite elements of the following sizes:

Displacement: $\boldsymbol{\varepsilon}(x)=\sum_{k\ noeuds} B_{k^u}(x)\ u_k$

"Regularized" internal variable: $\alpha(x)=\sum_{k\ noeuds} N_{k^\alpha}(x)\ \alpha_k$.

The gradient is expressed then thanks to the gradient of the functions of form: $\nabla\alpha(x)=\sum_{k\ noeuds}\nabla N_{k^\alpha}(x)\alpha_k$

Multiplier of Lagrange: $\lambda(x)=\sum_{k\ noeuds} N_{k^\lambda}(x)\lambda_k$

where N_{k^α} (resp. N_{k^λ}) are the functions of forms associated with the node k for the field α (resp. λ), B_{k^u} are the functions of form of the deformations calculated starting from the derivative of the functions of form associated with the node k for displacements.
One differentiates the functions from form according to the field insofar as the degree of interpolation used can be different according to the size considered.

In the model finite elements with integration at the points of Gauss, the integral on the volume of the structure is evaluated by summation on the points of Gauss. Energy F_Φ is thus written for the problem spatially discretized:

$$F_\Phi(\boldsymbol{\varepsilon},a,\alpha,\lambda)=\sum_g \omega_g \underbrace{\left[\Phi^{loc}(\boldsymbol{\varepsilon_g},a_g)+\Phi^{grad}((\nabla\alpha)_g)+\lambda_g(\alpha_g-a_g)+\frac{r}{2}(\alpha_g-a_g)^2\right]}_{\Phi_{g\ nonlocal}(\boldsymbol{\varepsilon_g},\alpha_g,\lambda_g,a_g)}$$

where ω_g corresponds to the weight of the points of Gauss, and the index g indicate that the field is evaluated at the points of Gauss starting from the values with the nodes:

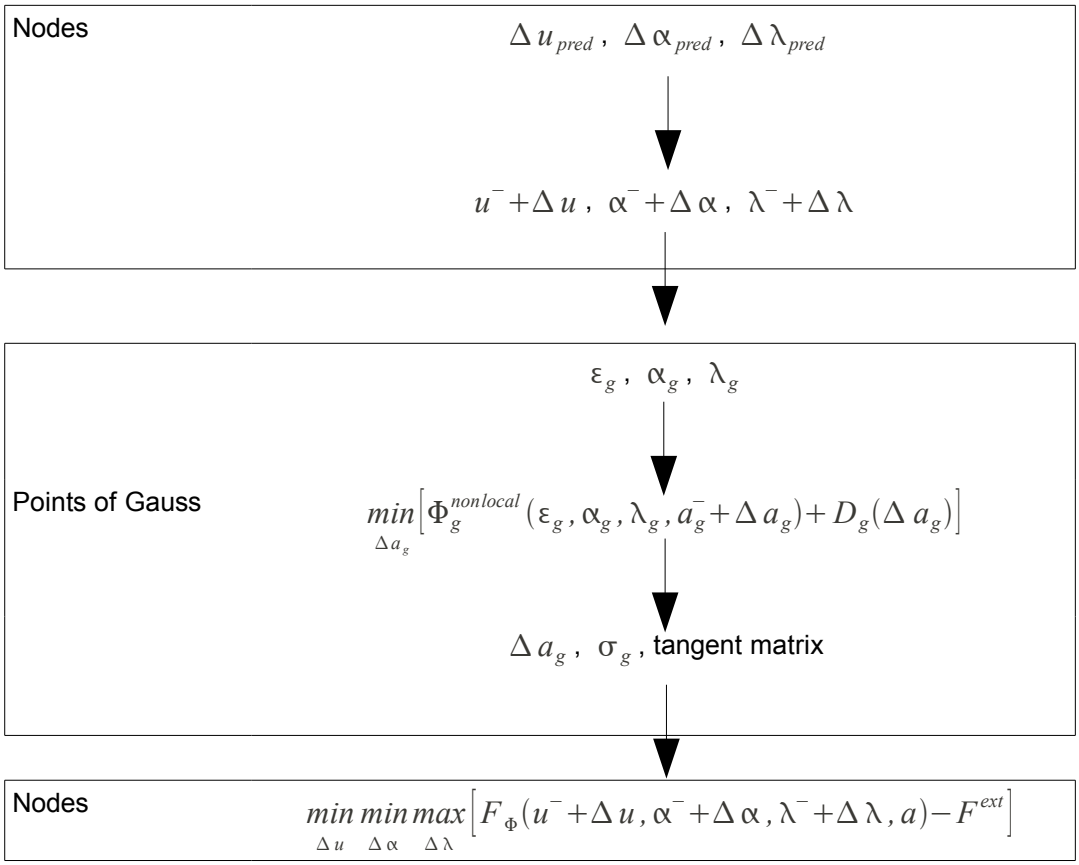
$$\varepsilon_g = \sum_{\text{k noeuds}} B_k^u(x_g) u_k$$

$$\alpha_g = \sum_{k\ noeuds} N_{k\alpha}(x_g)\ \alpha_k$$

$$(\nabla\alpha)_g = \sum_{k\ noeuds} \nabla N_{k\alpha}(x_g)\ \alpha_k$$

$$\lambda_g = \sum_{k\ noeuds} N_{k\lambda}(x_g)\ \lambda_k$$

The resolution of the discretized incremental problem thus corresponds with the following algorithm:



1.4 Integration of the law of behavior at the points of Gauss

The law of behavior is calculated at the point of Gauss. Evolution of the internal variable a at the point of Gauss is solution of following minimization:

$$\min_{\Delta a_g} \left[\Phi_{g\,nonlocal}(\boldsymbol{\varepsilon_g}, \alpha_g, \lambda_g, a_{g\_} + \Delta a_g) + D_g(\Delta a_g)\right]$$

The dualisation of the variable interns enables us to find a normal law of flow on the level of each point of Gauss, as for local modeling:

$$-\frac{\partial \Phi_{g\,nonlocal}}{\partial a_g} \in \partial(D_g)$$

When one calculates the thermodynamic force associated with the internal variable *has* by deriving "nonlocal" energy, one sees that simply amounts adding to the thermodynamic force of local modeling a term resulting from the energy of regularization:

$$-\frac{\partial \Phi_{g\,nonlocal}}{\partial a_g} = -\frac{\partial \Phi_{g\,loc}}{\partial a_g} + \left[\lambda_g + r(\alpha_g - a_g)\right]$$

This additional term, depend on the gradient of variable interns as it thereafter will be seen, causes to shift the value of the threshold compared to local modeling in the presence of gradient.

In practice, insofar as one applies this nonlocal modeling to laws of behavior standards generalized, it "is enough" to modify the expression of the thermodynamic force in the criterion, and to adapt the resolution of the nonlinear system to this new criterion.

Once the evolution of the calculated internal variable, one calculates the constraint by deriving energy compared to the field from deformation:

$$\sigma_g = \frac{\partial \Phi_{g\,nonlocal}}{\partial \boldsymbol{\varepsilon}_g} = \frac{\partial \Phi_{g\,loc}}{\partial \boldsymbol{\varepsilon}_g}$$

It is noticed immediately that the expression of the constraint is unchanged compared to local modeling.

In addition to the evolution of the internal variable and the constraint, we must also calculate the following, useful terms for the matrix of tangent correction (cf section 1.5):

$$\frac{\partial \sigma_g}{\partial \varepsilon_g}, \frac{\partial a_g}{\partial \varepsilon_g}, \frac{\partial a_g}{\partial \alpha_g}, \frac{\partial a_g}{\partial \lambda_g}$$

It should be noted that $\frac{\partial a_g}{\partial \alpha_g} = r\frac{\partial a_g}{\partial \lambda_g}$. It is thus enough to leave $\frac{\partial a_g}{\partial \lambda_g}$

1.5 Calculation of the internal forces

The mechanical equilibrium equation as well as the equation of regularization are solved with the local nodes by search for extremum:

$$\max_{\Delta\lambda}\min_{\Delta u}\min_{\Delta\alpha}\left(F_\Phi(\varepsilon^- + \Delta\varepsilon, \alpha^- + \Delta\alpha, \lambda^- + \Delta\lambda, a) - W^{ext}\right)$$

In the continuation, we leave side the external mechanical forces which are treated except for in Code_Aster. Internal forces associated with the nodal variables of the node n $(u_n\,,\ \alpha_n\,,\ \lambda_n)$ have as an expression:

$$F^u|_n = \frac{\partial F_\Phi}{\partial u_n} = \sum_g \omega_g \frac{\partial \Phi^{loc}}{\partial u_n} = \sum_g \omega_g \frac{\partial \Phi^{loc}}{\partial \varepsilon_g} : \frac{\partial \varepsilon_g}{\partial u_n} = \underbrace{\sum_g \omega_g \sigma_g : B_n^u}_{\int_\Omega B^T \sigma\, d\Omega}$$

$$F^\alpha|_n = \frac{\partial F_\Phi}{\partial \alpha_n} = \sum_g \omega_g \left[\frac{\partial \Phi^{grad}}{\partial(\nabla\alpha)_g}(\nabla N)_n^\alpha + \left[\lambda_g + r\left(\alpha_g - a_g\right)\right] N_n^\alpha\right]$$

$$F^{\lambda}|_n=\frac{\partial F_{\Phi}}{\partial \lambda_n}=\sum_g \omega_g\left(\alpha_g-a_g\right)N_n^{\lambda}$$

The tangent matrix is written in the following way:

$$K=\begin{pmatrix}\frac{\partial F^u}{\partial u} & \frac{\partial F^u}{\partial \alpha} & \frac{\partial F^u}{\partial \lambda}\\ \frac{\partial F^{\alpha}}{\partial u} & \frac{\partial F^{\alpha}}{\partial \alpha} & \frac{\partial F^{\alpha}}{\partial \lambda}\\ \frac{\partial F^{\lambda}}{\partial u} & \frac{\partial F^{\lambda}}{\partial \alpha} & \frac{\partial F^{\lambda}}{\partial \lambda}\end{pmatrix}$$

The framework of generalized standard materials in which our modeling with gradient of internal variable fits ensures the symmetry of the tangent matrix. It is thus enough to calculate the lower triangular matrix:

$$\frac{\partial F^u|_n}{\partial u_m}=\sum_g \omega_g B_m^u:\frac{\partial \sigma_g}{\partial \varepsilon_g}:B_n^u$$
$$\frac{\partial F^{\alpha}|_n}{\partial u_m}=-\sum_g \omega_g r\ B_m^u\frac{\partial a_g}{\partial \varepsilon_g}N_n^{\alpha}$$
$$\frac{\partial F^{\alpha}|_n}{\partial \alpha_m}=\sum_g \omega_g\left[(\nabla N)_m^{\alpha}\frac{\partial^2\Phi^{grad}}{\partial^2(\nabla\alpha)_g}(\nabla N)_n^{\alpha}+rN_m^{\alpha}\left(1-\frac{\partial a_g}{\partial \alpha_g}\right)N_n^{\alpha}\right]$$
$$\frac{\partial F^{\lambda}|_n}{\partial u_m}=-\sum_g \omega_g B_m^u\frac{\partial a_g}{\partial \varepsilon_g}N_n^{\lambda}$$
$$\frac{\partial F^{\lambda}|_n}{\partial \alpha_m}=\sum_g \omega_g N_m^{\alpha}\left[1-\frac{\partial a_g}{\partial \alpha_g}\right]N_n^{\lambda}$$
$$\frac{\partial F^{\lambda}|_n}{\partial \lambda_m}=-\sum_g \omega_g N_m^{\lambda}\frac{\partial a_g}{\partial \lambda_g}N_n^{\lambda}$$

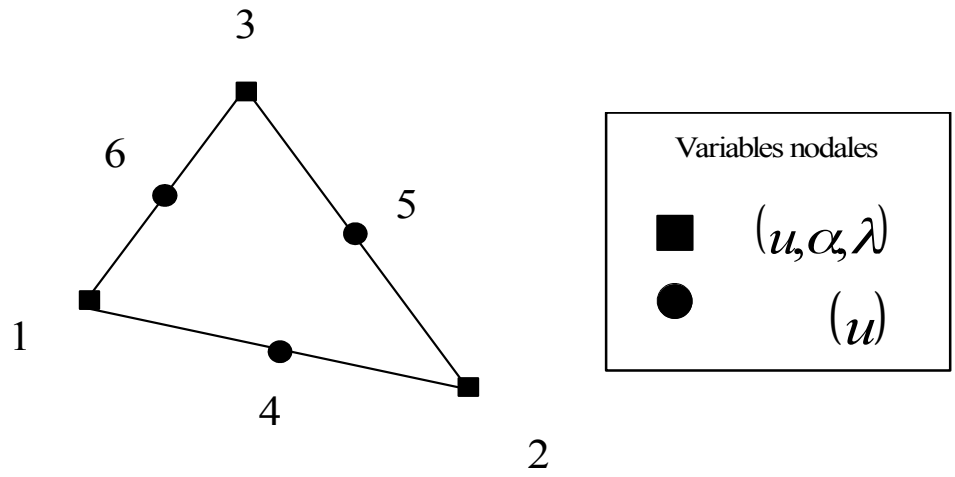
2 Choice of the finite elements

The introduction of new nodal variables forces to use elements compatible with the new formulation. One is in the presence of three nodal unknown factors: displacements u, the regularized variable α and the multiplier of Lagrange λ.

The internal field of variable being related to the deformations via the criterion, it is preferable to take the same degree of interpolation for the internal field of regularized variable α that for the deformation, i.e. a degree less than displacements from which the deformations are derived. One chooses the same degree of interpolation for the multiplier of Lagrange λ that for the regularized variable α.

Functions of forms are thus considered P^2 for u, P^1 for α and P^1 for λ
The quadratic elements, TRIA6 and QUAD8 for the 2D, TETRA10, PENTA15 and HEXA20 for the 3D, were developed. The components of displacement are assigned to all the nodes of the element

whereas the components of the two other nodal variables are affected only with the nodes tops. For more clearness, element TRIA6 is represented below:



One uses the families of points of Gauss of the corresponding elements linear, which results in an under-integration on displacements. The use of the families of points of Gauss of the quadratic elements would imply an on-integration for α and λ, causing inopportune oscillations.

3 Modelings available

These various elements are used in three types of modelings:

Calculation 2D in plane deformations:	D_PLAN_GRAD_VARI
Calculation 2D into axisymmetric:	AXIS_GRAD_VARI
Calculation 3D:	3D_GRAD_VARI

The mode forced plane is not yet available.

4 Laws of behavior available with modelings GRAD_VARI

The laws of behavior available in their nonlocal version to gradient of internal variables are the following ones

ENDO_SCALAIRE	Law of fragile elastic behavior isotropic regularized (cf [R5.03.25])
ENDO_ISOT_BETON	Law of isotropic and unilateral fragile behavior elastic for the concrete (cf [R5.07.04])
VMIS_ISOT_LINE	Elastoplastic law of behaviour to linear isotropic work hardening (cf [R5.03.02])
VMIS_ISOT_TRAC	Elastoplastic law of behaviour to nonlinear isotropic work hardening with traction diagram (cf [R5.03.02])

5 The Councils/Procedure for the implementation of a new law of behavior to gradients of internal variables

As one saw in the section 1.4, the establishment of a new law of behavior to gradient of internal variables, starting from a local law, is relatively simple, for little that the local law respects the framework of generalized standard materials, and more particularly, than the criterion of evolution of

the internal variables utilizes a convex function threshold compared to the thermodynamic forces associated with the internal variables (the thermodynamic force associated with the variable α is defined as follows: $F^a=-\frac{\partial W}{\partial a}$ where W is the free energy of the structure) and which one adopts a normal law of flow to calculate the evolution of the internal variables.

The table below summarizes the stages to pass from a local law of behavior to a nonlocal law of behavior:

Type	Local model	Nonlocal model
Thermodynamic force	$F^{a\,local}$	$F^{a\,non\ local}=F^{a\,local}+\lambda+r\alpha-ra$
Function threshold/criterion	$f\left[F^{a}{}_{local}\right] \leq 0$	$f\left[F^{a\,non\ local}\right] \leq 0$ It is the same function threshold but dependent on a modified thermodynamic force
Evolution (normal flow) (η multiplier of Lagrange)	$\Delta a=\Delta\eta\ \frac{\partial f}{\partial F^{a\,local}}$	$\Delta a=\Delta\eta\ \frac{\partial f}{\partial F^{a\,non\ local}}$ In the facts, it is enough to adapt resolution of the criterion to the new thermodynamic force
Constraint	$\sigma(\varepsilon, a)$	$\sigma(\varepsilon, a)$ The expression of the constraint is unchanged
Tangent matrix	$\frac{\partial\sigma}{\partial\varepsilon}$	$\frac{\partial\sigma}{\partial\varepsilon}$ unchanged $\frac{\partial a}{\partial\varepsilon}$, $\frac{\partial a}{\partial\lambda}$ (additional terms)

The developer of a new nonlocal law of behavior will have to be based on the sources of the laws established right now to see how the additional terms (regularizing terms and additional terms of the tangent matrix) must be last in the various routines. All the part concerning construction of the vector forces intern and of the matrix of correction at the total level does not have to be modified by the developer, it is indeed enough to comply with the rules of programming in force for the already established laws.

6 Bibliography

1) LORENTZ E.: “Laws of behavior to gradients of internal variables: construction, variational formulation and numeric work”, Doctorate implementation of the university Paris 6, April 27th, 1999.

2) HALPHEN B., NGUYEN Q.S.: “On generalized standard materials”, Newspaper of Mechanics, vol. 14, NR^{O} 1.1975.

7 Description of the versions of the document

Version Aster	Author (S) Organization (S)	Description of the modifications
9.2	V.GODARD	Initial text