Nonlocal modelization with gradients of Summarized `local variables`

GRAD_VARI

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

The nonlocal modelizations of type `GRAD_VARI` are available in 3D (`3D_GRAD_VARI`), axisymmetric (`AXIS_GRAD_VARI`) and plane strains (`D_PLAN_GRAD_VARI`).

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

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

Contents

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 behavior of materials 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 numerical point of view, the computation of a structure with a classical local damage model shows that the damaged zone is always located on only one layer of finite elements and thus that the response of structure depends on the adopted mesh: 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 the generalized standard materials [Feeding-bottle 2].

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

Either a a local variable and A its associated thermodynamic force, and or $\Delta(\dot{a})$ 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_{∇} , with which one would associate 2 thermodynamic forces $A=-\frac{\partial\Phi}{\partial a}$, $A_{\nabla}=-\frac{\partial\Phi}{\partial a_{\nabla}}$ 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 stress $a_{\nabla}=\nabla a$ 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 normal flow assumption in each point of structure while preserving the formalism of the generalized standard materials but at the level of structure, where the variables of state are now the strain field $\boldsymbol{\varepsilon}$ and the field of local variables a . The total free energy and the total potential of dissipation are thus defined:

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

The total potential of dissipation D is now a function of the field $\dot{a}$, and the writing $A\in\partial D(\dot{a})$ takes again a meaning.

The generalized behavior model is written now:

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

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 local 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.

The total free energy $F_{\Phi}(\boldsymbol{\varepsilon}, a)$ utilizes the gradient of the field of local variable a . However, it is known that the processing of the local variables by the finite element method in Code_Aster is carried out with Gauss points, 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 S "free from the stress $\alpha=a$, 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 compatibility condition 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, puisqu" it must tend towards 0 with convergence, but makes it possible to help with convergence.

While leaning on the assumption of convexity compared to a potentials F_{Φ} and D while adopting an implicit diagram of Eulerian, 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 of the fields of local 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^{-} the field of local variables at previous time represents. This minimization constitutes the constitutive law.

In the same way, while leaning on the assumption of convexity compared to (u, α) potential F_{Φ} and while adopting an implicit diagram of Eulerian, the resolution of the balance 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} the work of the external mechanical forces represents.

1.3 Spatial discretization by finite elements

to solve the problem of search for extrema, one carries out a spatial discretization by finite elements of the following quantities:

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

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

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

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

where N_{k^α} (resp. N_{k^λ}) are the shape functions associated with the node k for the field α (resp. λ), B_{k^u} are the shape functions of the calculated strains starting from derivatives of the shape functions associated with the node k for displacements.

One differentiates the shape functions according to the field insofar as the degree of interpolation used can be different according to the quantity considered.

In the model finite elements with integration with Gauss points, the integral on the volume of structure is evaluated by summation on Gauss points. 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 Gauss points, and the index g indicates that the field is evaluated with Gauss points starting from the values with the nodes:

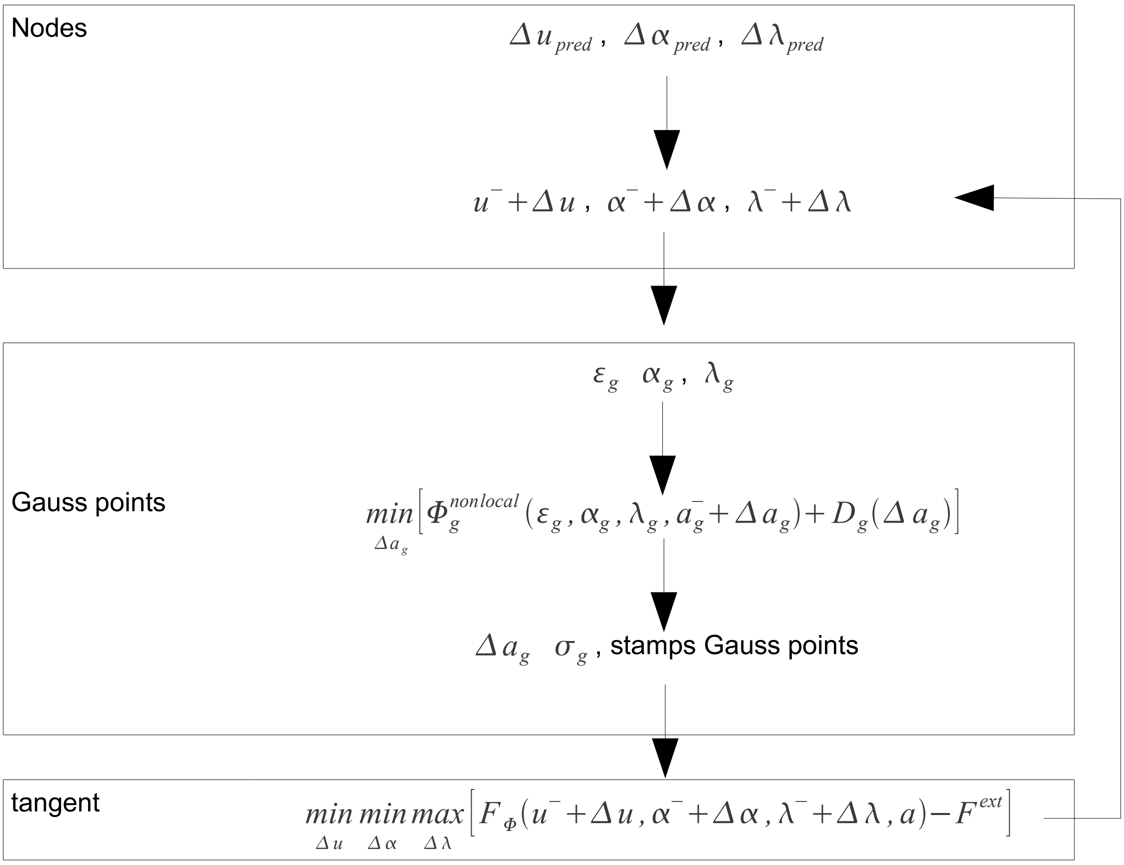
$$\varepsilon_g = \sum_{\text{k noeuds}} B_k^u(x_g) u_k$$

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

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

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

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



1.4 Nodes Integration of the constitutive law to

the constitutive law is calculated at the Gauss point. Evolution of the local variable a at the Gauss point east 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 local variable enables us to find a normal flow model on the level of each Gauss point, as for the local modelization:

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

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

$$-\frac{\partial \boldsymbol{\Phi}_g^{nonlocal}}{\partial a_g}=-\frac{\partial \boldsymbol{\Phi}_g^{loc}}{\partial a_g}+\left[\lambda_g+r(\alpha_g-a_g)\right]$$

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

In practice, insofar as one applies this nonlocal modelization to constitutive laws standards generalized, it "is enough" to modify the statement 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 local variable, one calculates the stress by deriving energy compared to the strain field:

$$\sigma_g=\frac{\partial \boldsymbol{\Phi}_g^{nonlocal}}{\partial \boldsymbol{\varepsilon}_g}=\frac{\partial \boldsymbol{\Phi}_g^{loc}}{\partial \boldsymbol{\varepsilon}_g}$$

It is noticed immediately that the statement of the stress is unchanged compared to the local modelization.

In addition to the evolution of the local variable and the stress, 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 Computation the internal forces

the mechanical balance 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. The internal forces associated with the nodal variables with the node n $(u_n , \alpha_n , \lambda_n)$ have as a statement:

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

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

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

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 frame of the generalized standard materials in which our modelization with gradient of local variable fits ensures the symmetry of the tangent matrix. It is thus enough to calculate the lower triangular matrix:

$$\frac{\partial F^u\big|_n}{\partial u_m}=\sum_g \omega_g B_m^u:\frac{\partial \sigma_g}{\partial \varepsilon_g}:B_n^u$$

$$\frac{\partial F^{\alpha}\big|_n}{\partial u_m}=-\sum_g \omega_g r\ B_m^u\frac{\partial a_g}{\partial \varepsilon_g}N_n^{\alpha}$$

$$\frac{\partial F^{\alpha}\big|_n}{\partial \alpha_m}=\sum_g \omega_g\left[(\nabla N)_m^{\alpha}\frac{\partial^2 \Phi^{grad}}{\partial^2(\nabla \alpha)_g}(\nabla N)_n^{\alpha}+rN_m^{\alpha}\left(1-\frac{\partial a_g}{\partial \alpha_g}\right)N_n^{\alpha}\right]$$

$$\frac{\partial F^{\lambda}\big|_n}{\partial u_m}=-\sum_g \omega_g B_m^u\frac{\partial a_g}{\partial \varepsilon_g}N_n^{\lambda}$$

$$\frac{\partial F^{\lambda}\big|_n}{\partial \alpha_m}=\sum_g \omega_g N_m^{\alpha}\left[1-\frac{\partial a_g}{\partial \alpha_g}\right]N_n^{\lambda}$$

$$\frac{\partial F^{\lambda}\big|_n}{\partial \lambda_m}=-\sum_g \omega_g N_m^{\lambda}\frac{\partial a_g}{\partial \lambda_g}N_n^{\lambda}$$

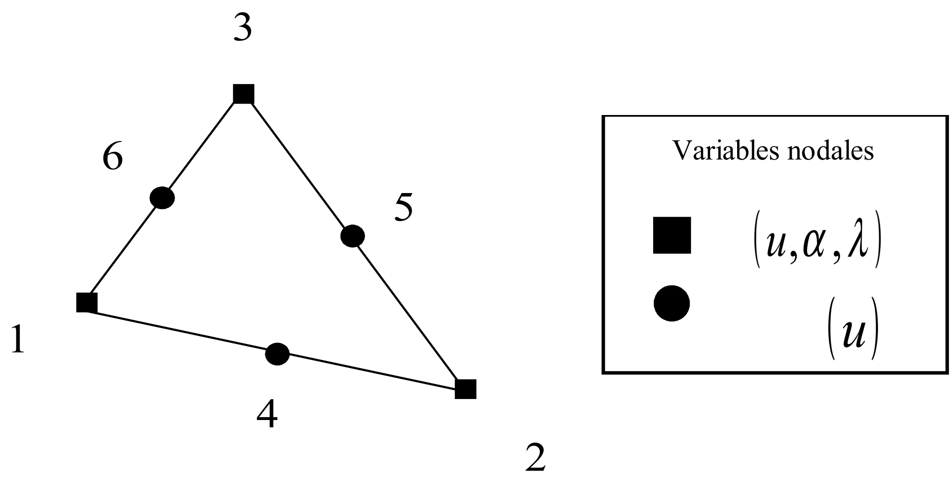
2 Choice of the finite elements

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

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

One thus considers shape functions P^2 for u , P^1 for α and P^1 for λ
the quadratic elements, TRIA6 and QUAD8 for 2D, TETRA10, PENTA15 and HEXA20 for 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 Gauss points corresponding elements linear, which results in an under-integration on displacements. The use of the families of Gauss points of the quadratic elements would imply an on-integration for α and λ, causing inopportune oscillations.

3 Modelizations available

These various elements are used in three types of modelizations:

Computation 2D in plane strains:	D_PLAN_GRAD_VARI (cf [U3.13.06])
Computation 2D into axisymmetric:	AXIS_GRAD_VARI (cf [U3.13.06])
Computation 3D:	3D_GRAD_VARI (cf [U3.14.11])

the plane stresses mode is not available yet.

4 Constitutive laws available with modelizations GRAD_VARI

the constitutive laws available in their nonlocal version to gradient of local variables are following

the ENDO_SCALAIRE	isotropic brittle elastic Constitutive law regularized (cf [R5.03.25])
ENDO_ISOT_BETON	isotropic and unilateral brittle Constitutive law elastic for the concrete (cf [R5.07.04])
VMIS_ISOT_LINE	elastoplastic Constitutive law with linear isotropic hardening (cf [R5.03.02])
VMIS_ISOT_TRAC	elastoplastic Constitutive law with nonlinear isotropic hardening with curve of tension (cf [R5.03.02])

5 the Councils/Procedure for the implementation of a new constitutive law with gradients of local variables

As one saw in section 1.4, the establishment of a new constitutive law with gradient of local variables, from a local law, is relatively simple, for little that the local law respects the frame of the generalized standard materials, and more particularly, that the criterion of evolution of the local variables utilizes a function convex threshold compared to the thermodynamic forces associated with the local variables (the thermodynamic force associated with the variable α is defined as follows: $F^a=-\dfrac{\partial W}{\partial a}$ where W is the free energy of the structure) and which one adopts a normal flow model to compute: the evolution of the local variables.

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

Type	Models local	nonlocal Model
Forces thermodynamic	$F^{a\,local}$	$F^{a\,non\ local}=F^{a\,local}+\lambda+r\alpha-ra$
Function threshold/criterion	$f\left[F^a{}_{local}\right]\ \le\ 0$	$f\left[F^{a\,non\ local}\right]\ \le\ 0$ It acts of the same function threshold but dependant on a modified thermodynamic force
Evolution (normal flow) (η multiplying of Lagrange)	$\Delta a=\Delta\eta\ \dfrac{\partial f}{\partial F^{a\,local}}$	$\Delta a=\Delta\eta\ \dfrac{\partial f}{\partial F^{a\,non\ local}}$ In the facts, it is enough to adapt the resolution of the criterion to the new Forced thermodynamic
force	$\sigma(\varepsilon, a)$	$\sigma(\varepsilon, a)$ the statement of the stress is unchanged
tangent Matrix	$\dfrac{\partial\sigma}{\partial\varepsilon}$	$\dfrac{\partial\sigma}{\partial\varepsilon}$ unchanged $\dfrac{\partial a}{\partial\varepsilon}$, $\dfrac{\partial a}{\partial\lambda}$ (additional terms)

the developer of a new nonlocal constitutive law will have to be based on the sources of the models 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 internal force and 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 models.

6 LORENTZ

1) bibliography E.: “Constitutive laws with gradients of local variables: construction, variational formulation and numeric work”, Doctorate implementation of the university Paris 6, April 27th, 1999.

2) HALPHEN B., NGUYEN Q.S.: “On the generalized standard materials”, Newspaper of Mechanics, vol. 14, No 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