Integration of the viscoelastic relations of behavior in the operator STAT_NON_LINE

Summary

This document describes the viscoelastic behaviors in the case of the ingredients necessary to the implementation of the non-linear algorithm STAT_NON_LINE described in [R5.03.01]. Data input of all the viscoelastic relations of behavior integrated in *Aster* have in a general way the same form. Only the way of introducing the principal data (the function speed of viscous deformation) varies: it is presented according to different the keyword which makes it possible to the user to choose the relation of behavior wished.

These quantities are calculated by method of an semi-implicit or implicit integration. From the initial state, or as from the moment of preceding calculation, one calculates the stress field resulting from an increment of deformation.

Contents

1 Introduction

One describes here the implementation of the non-linear model of viscoelasticity of Lemaître, which can be brought back for certain particular values of the parameters to a relation of viscoelastic behavior of Norton.

An alternative (depend on the fluence) of this model of Lemaître was added, for the modeling of the fuel assemblies (keyword `LEMAITRE_IRRA`). This model has as a characteristic to comprise an additional unelastic deformation: deformation of growth.

A viscoelastic model with threshold was added. It is about a material whose behavior is purely elastic until a threshold then once this exceeded threshold, the relation of behavior becomes a typical case of the relation of Lemaître (`LEMA_SEUIL`).

A model developed specifically to represent the nonlinear viscoelastic behavior of the pastilles of dioxide-to Uranium was more recently introduced. This model, heading `GATT_MONERIE`, the interest presents to be readjusted on a broad experimental basis (tests of compression on various products in a broad range of temperature, load and speed of request). The effects of porosities of manufacturing, of size of grain and temperature on the speed of creep stationary of the pastilles, in particular, could be identified on these tests.

Lastly, a viscoelastic model with creep in logarithm of the fluence was established, it is accessible by the keyword `VISC_IRRA_LOG`.

For each one of these models, one supposes that the material is isotropic (except for the deformation of growth, which, it, is uniaxial). They can be used in 3D, in plane deformations (`D_PLAN`) and into axisymmetric (`AXIS`).

One presents in this note the equations constitutive of the models and their establishment in *Code_Aster*.

2 Continuous relation

One places oneself on the assumption of the small disturbances and one divides the tensor of the deformations into an elastic part, a thermal part, an unelastic part (known) and a viscous part. The equations are then:

$$\boldsymbol{\varepsilon}_{tot}=\boldsymbol{\varepsilon}_e+\boldsymbol{\varepsilon}_{th}+\boldsymbol{\varepsilon}_a+\boldsymbol{\varepsilon}_v$$
$$\boldsymbol{\sigma}=\boldsymbol{A}(T)\boldsymbol{\varepsilon}_e$$
$$\dot{\boldsymbol{\varepsilon}}_v=g\left(\sigma_{eq},\lambda,T\right)\frac{3}{2}\frac{\tilde{\boldsymbol{\sigma}}}{\sigma_{eq}}$$

with:

λ : cumulated viscous deformation $\dot{\lambda}=\sqrt{\frac{2}{3}\dot{\varepsilon}_v:\dot{\varepsilon}_v}$

$\tilde{\sigma}$: diverter of the constraints $\tilde{\sigma}=\sigma-\frac{1}{3}Tr(\sigma)I$

σ_{eq} : equivalent constraint $\sigma_{eq}=\sqrt{\frac{3}{2}\tilde{\sigma}:\tilde{\sigma}}$

$A(T)$: tensor of elasticity

3 Nature of the function G for each relation of behavior

3.1 Relation LEMAITRE

In this case, g express yourself explicitly (σ is a scalar here):

$$g(\sigma, \lambda, T)=\left(\frac{1}{K}\frac{\sigma}{\lambda^{1/m}}\right)^n \text{ with } \frac{1}{K}\geq 0, \frac{1}{m}\geq 0, n>0$$

The data of the material characteristics are those provided under the keywords factors `LEMAITRE` or `LEMAITRE_FO` of the operator `DEFI_MATERIAU`.

`LEMAITRE= _F (N=n, UN_SUR_K=` $\frac{1}{K}$ `, UN_SUR_M =` $\frac{1}{m}$ `)`

The Young modulus E and the Poisson's ratio ν are those provided under the keywords factors `ELAS` or `ELAS_FO`.

3.2 Relation of LEMAITRE depending on the fluence (LEMAITRE_IRRA)

This paragraph describes the dependence with respect to the fluence (and its treatment) of the relation of behavior viscoplastic of J. Lemaître, introduced for the modeling of the fuel assemblies and applicable to the elements 2D and 3D solid masses and the elements `PIPE`, under the keyword `LEMAITRE_IRRA`..

3.2.1 Formulation of the model

The equations are the following ones:

$$\begin{cases} \dot{\varepsilon}_v=\frac{3}{2}\dot{p}\frac{\sigma^D}{\sigma_{eq}} \\ \dot{p}=\left[\frac{\sigma_{eq}}{p^{1/m}}\right]^n\left(\frac{1}{K}\frac{\phi}{\phi_0}+L\right)^{\beta} e^{-\frac{Q}{R(T+T_0)}} \\ \overbrace{(A^{-1}(T)\sigma)}^{\cdot}=\dot{\varepsilon}_{tot}-\dot{\varepsilon}_v-\dot{\varepsilon}_g-\dot{\varepsilon}_{th} \end{cases}$$

with:
$T_0=273{,}15\,°C$
$n>0$, $1/K\geq 0$, $1/m\geq 0$
$\phi_0>0$, $Q/R\geq 0$, $L\geq 0$, β unspecified reality

The coefficients are provided under the keywords `LEMAITRE_IRRA` and `ELAS` of `DEFI_MATERIAU` and ϕ is neutron flow (quotient of the increment of fluence, definite by the keyword `AFFE_VARC` of `AFFE_MATERIAU`, by the increment of time).

The law of growth is: $\varepsilon_g(t)=f(T,\Phi_t)\varepsilon_g^0$ with ε_g^0 uniaxial deformation unit in a reference mark R_1 given by the user using the keyword `SOLID MASS` (see [U4.42.01] and [U4.43.01]) and $f(T,\Phi_t)$ .est also a function defined by the user in `DEFI_MATERIAU` ([U4.43.01]).

Note:

> *Fluence, time and flow Φ_0 must be expressed into cubes units such as the report Φ/Φ_0 maybe without dimension. Q/R is in Kelvin. T is in $°C$.*

3.2.2 Treatment of the dependence with respect to the fluence

The model describes above corresponds in fact to a normal law of Lemaître, defined by the three coefficients n, $1/K'$ and $1/m$ with:

$$\frac{1}{K'}=\left(\frac{1}{K}\frac{\Phi}{\Phi_0}+L\right)^{\beta/n} e^{-\frac{Q}{nR(T+T_0)}}$$

It is thus enough to calculate $1/K'$ and to provide it like data to calculation instead of $1/K$.
In addition, in the calculation of the elastic constraint, one adds to the unelastic deformations (worthless by default) the deformation of growth expressed above, after having carried out the change of reference mark between the local reference mark and the reference mark R_1.

3.3 Relation `LEMA_SEUIL`

For this behavior, G is expressed also explicitly (since it is about a typical case of the relation of `LEMAITRE` presented Ci above):

If $D\leq 1$ then $g(\sigma,\lambda,T)=0$ (purely elastic behavior)

If $D>1$ then $g(\sigma,\lambda,T)=A\left(\frac{2}{\sqrt{3}}\sigma\right)\Phi$ with $A\geq 0$, $\Phi\geq 0$

With: $D=\frac{1}{S}\int_0^t \sigma_{eq}(u)du$

The data materials to be informed by the user must be provided under the keyword `LEMA_SEUIL` or `LEMA_SEUIL_FO` of the operator `DEFI_MATERIAU` :

```
LEMA_SEUIL = _F (A=A,   S=S)
```

As for the parameter Φ, it is the flow of neutron which bombards the material (quotient of the increment of fluence, defined by the keyword `AFFE_VARC` of `AFFE_MATERIAU`, by the increment of time).
The Young modulus E and the Poisson's ratio ν are those provided under the keywords factors `ELAS` or `ELAS_FO`.

3.4 Relation `VISC_IRRA_LOG`

For this relations, g do not express yourself explicitly. The behavior is represented by a unidimensional creep test, with constant constraint, which utilizes the time passed since the moment when the constraint is applied. The relation of behavior is defined here by the data of four functions f_1, g_1, f_2, g_2 describing the evolution of the viscous deformation in the course of time:

$$\varepsilon_v=\lambda=f_1(t)\,g_1(\sigma,T)+f_2(t)\,g_2(\sigma,T)$$ **éq 3.4-1**

The function g is calculated then numerically by eliminating time t in the following way:

1) for a given triplet (σ, λ, T), one solves in t the equation [éq 3.2-1] by the method of Newton (see [bib2]). An approximation of the solution is found $t(\sigma, \lambda, T)$,
2) the value of the function is obtained g in (σ, λ, T) by deriving compared to time the equation [éq 3.2-1] (see [bib1]):

$$\dot{\varepsilon}_v=\dot{\lambda}=g(\sigma, \lambda, T)=f_1'(t)g_1(\sigma, T)+f_2'(t)g_2(\sigma, T)$$

and in substituent in this new equation the value of $t(\sigma, \lambda, T)$ found previously. One finds the formulation uniaxial following:

$$\dot{\varepsilon}_v=\dot{\lambda}=g(\sigma, \lambda, T)=f_1'(t(\sigma, \lambda, T))g_1(\sigma, T)+f_2'(t(\sigma, \lambda, T))g_2(\sigma, T)$$

The form of the four functions f_1, g_1, f_2, g_2 is preset and the user introduces only some parameters into the command file.

For VISC_IRRA_LOG, one a:

$$f_1(t)=\ln(1+\omega.\Phi.t)$$
$$g_1(\sigma, T)=A.\sigma.e^{-\frac{Q}{T}}$$
$$f_2(t)=\Phi.t$$
$$g_2(\sigma, T)=B.\sigma.e^{-\frac{Q}{T}}$$

parameter Φ, is the flow of neutrons. It is indicated in DEFI_MATERIAU, is taken equal to 1 and must then be well informed under the keyword factor AFFE_VARC.

Parameters A, B, ω and Q are those provided under the keyword factor VISC_IRRA_LOG of the operator DEFI_MATERIAU.

It will be noted that, for all the functions:

t express yourself in hours
T express yourself in $°C$
σ express yourself in MPa

It is thus necessary to return of the coherent data with these units in the command file and the file of grid.

The Young modulus E and the Poisson's ratio ν are those provided under the keywords factors ELAS or ELAS_FO.

3.5 Relation GATT_MONERIE

Because of residual porosities of manufacturing affecting the pastilles fuel worked out by sintering, the speed of viscous deformation included a component of dilation, depend on shearing and average constraint according to:

$$\dot{\varepsilon}_v = g\left(\sigma_{eq}, \sigma_m, \lambda, f, T\right)\frac{3}{2}\frac{\tilde{\sigma}}{\sigma_{eq}} + g_d\left(\sigma_{eq}, \sigma_m, \lambda, f, T\right)\frac{1}{3}I$$

with:

f : voluminal fraction of porosity

σ_m : average constraint $\sigma_m = \frac{1}{3}Tr(\sigma)$

Functions (g, g_d) derive from a potential of dissipation $\Psi\left(\sigma_{eq}, \sigma_m, \lambda, f, T\right)$ according to:

$$g = \frac{\partial\Psi}{\partial\sigma_{eq}}, \; g_d = \frac{\partial\Psi}{\partial\sigma_m}.$$

This potential of dissipation does not depend on the cumulated plastic deformation (see [3]) and is written:

$$\Psi\left(\sigma_{eq}, \sigma_m, f, T\right) = \left(1 - \theta\left(\sigma_Y, T\right)\right)\Psi_1\left(\sigma_{eq}, \sigma_m, f, T\right) + \theta\left(\sigma_Y\right)\Psi_2\left(\sigma_{eq}, \sigma_m, f, T\right)$$

with:

$$\sigma_Y = \sqrt{\frac{B_1}{B_1 + \frac{A_1}{4}}\sigma_{eq}{}^2 + \frac{9A_1}{4B_1 + A_1}\sigma_m{}^2}$$

(Ψ_1, Ψ_2) correspondent with two distinct modes of viscous flow (low constraint and strong constraint) defined by:

$$\Psi_i(\sigma_{eq}, \sigma_m, f) = \frac{\dot{\varepsilon}_{0i}\sigma_{0i}}{n_i + 1}\left[A_i(f)\left(\frac{3\sigma_m}{2\sigma_{0i}}\right)^2 + B_i(f)\left(\frac{\sigma_{eq}}{\sigma_{0i}}\right)^2\right]^{\frac{n_i+1}{2}}$$

$$\dot{\varepsilon}_{0i} = \dot{\bar{\varepsilon}}_{0i}\chi_i(d)\, e^{-\frac{Q_i}{RT}}$$

χ_i functions of the size of grain such as: $\chi_1(d) = d^{-2}$, $\chi_2(d) = 2d_0^2\left(1 - \cos\left(\frac{d}{d_0}\right)\right)$

coefficients (A_i, B_i) are deduced from a micromechanical analysis:

$$A_i(f) = \left(n_i\left(f^{-\frac{1}{n_i}} - 1\right)\right)^{\frac{-2n_i}{n_i+1}}, \quad B_i(f) = \left(1 + \frac{2}{3}f\right)(1 - f)^{\frac{-2n_i}{n_i+1}},$$

θ function of coupling depend on the first invariant of the constraints and the temperature

the law of evolution of porosity is given by: $\dot{f} = (1 - f)\, Tr\left(\dot{\varepsilon}_v\right)$

The final expression of the function g is:

$$g(\sigma_{eq}, \sigma_m) = (1 - \theta)\frac{d\Psi_1}{d\sigma_{eq}} + \theta\frac{d\Psi_2}{d\sigma_{eq}} + \frac{d\theta}{d\sigma_{eq}}\left(\Psi_2 - \Psi_1\right)$$

$$\frac{d\Psi_i}{d\sigma_{eq}} = \dot{\varepsilon}_{0i}\, B_i(f)\left(\frac{\sigma_{eq}}{\sigma_{0i}}\right)\left[A_i(f)\left(\frac{3\sigma_m}{2\sigma_{0i}}\right)^2 + B_i(f)\left(\frac{\sigma_{eq}}{\sigma_{0i}}\right)^2\right]^{\frac{n_i-1}{2}}$$

$$\frac{d\theta}{d\sigma_{eq}}=\frac{1}{2}\left[1-\tanh^2\left(\phi\left(\sigma_I\right)\right)\right]\frac{d\phi}{d\sigma_{eq}}$$

$$\begin{cases}\Phi\left(\sigma_Y\right)=\dfrac{T-\tilde{T}\left(\sigma_Y\right)}{h}\\ \tilde{T}\left(\sigma_Y\right)=w\,\sigma_Y^q\end{cases}\Rightarrow\frac{d\Phi}{d}\sigma_{\text{eq}}=\frac{d\Phi}{d\sigma_Y}\frac{d\sigma_Y}{d\sigma_{\text{eq}}}=\frac{-B_1\text{qw}\,\sigma_{\text{eq}}\,\sigma_Y^{q-2}}{\left(B_1+\dfrac{A_1}{4}\right)h}$$

whereas that of the function g_d is:

$$g_d(\sigma_{eq},\sigma_m)=(1-\theta)\frac{d\phi_1}{d\sigma_m}+\theta\frac{d\Phi_2}{d\sigma_m}+\frac{d\theta}{d\sigma_m}\left(\phi_2-\Phi_1\right)$$

$$\frac{d\Psi_i}{d\sigma_m}=\dot{\varepsilon}_{0\text{i}}\,A_i(f)\left(\frac{9\sigma_m}{4\sigma_{0\text{i}}}\right)\left[A_i(f)\left(\frac{3\sigma_m}{2\sigma_{0\text{i}}}\right)^2+B_i(f)\left(\frac{\sigma_{eq}}{\sigma_{0\text{i}}}\right)^2\right]^{\frac{n_i-1}{2}}$$

$$\frac{d\theta}{d\sigma_m}=\frac{1}{2}\left[1-\tanh^2\left(\phi\left(\sigma_Y\right)\right)\right]\frac{d\phi}{d\sigma_m}$$

$$\begin{cases}\phi\left(\sigma_Y\right)=\dfrac{T-\tilde{T}(\sigma_Y)}{\text{h}}\\ \tilde{T}(\sigma_Y)=w\,\sigma_Y^q\end{cases}\Rightarrow\frac{d\Phi}{d\sigma_m}=\frac{d\Phi}{d\sigma_Y}\frac{d\sigma_Y}{d\sigma_m}=\frac{-9A_1\text{qw}\,\sigma_m\sigma_I^{q-2}}{\left(4B_1+A_1\right)h}$$

The values of the various constants of the model are:

$$n_1=1.0\ ,\ Q_1=377\ 10^3\ J/mol\ ,\ \tilde{\dot{\varepsilon}}_{0_1}=2,725\ 10^{-10}\ Pa/h$$
$$n_2=8.0\ ,\ Q_2=462\ 10^3\ J/mol\ ,\ \tilde{\dot{\varepsilon}}_{0_2}=9,14\ 10^{-41}\ Pa/h\ ,\ d_0=15\ microns$$
$$\sigma_{0_1}=\sigma_{0_2}=1\ Pa$$
$$h=600\ K\ ,\ q=-0.189\ ,\ w=47350.4$$

Positive parameters $\tilde{\dot{\varepsilon}}_{O_1},\tilde{\dot{\varepsilon}}_{O_2},d$ as well as the initial value of the voluminal fraction of pores are those provided under the keyword factor GATT_MONE of the operator DEFI_MATERIAU :

```
GATT_MONERIE = _F ( EPSI_01    = ε̇̃01  ,
                    EPSI_02    = ε̇̃02  ,
                    PORO_INIT = f(0)   ,
                    GRAIN_COMB= d   )
```

4 Integration of the relation of behavior

4.1 Establishment of the scalar equation for the implicit scheme and with constant elastic coefficients

One indicates by ε_{tot} total deflection at the moment $t+\Delta t$ and by $\Delta\varepsilon_{tot}$ variation of total deflection during the step of current time.

One calls ε_o deformation at the moment $t+\Delta t$ resulting from thermal dilation and unelastic deformations (among which possibly the deformations of growth appear, cf [§3.2]). One thus has:

$$\Delta\varepsilon_o=\left[\alpha(t+\Delta t)\left(T(t+\Delta t)-T_{ref}\right)-\alpha(t)\left(T(t)-T_{ref}\right)\right]I_3+\varepsilon_a(t+\Delta t)-\varepsilon_a(t)$$

where I_3 is the tensor identity of order 2 in dimension 3.

One poses $\Delta\varepsilon=\Delta\varepsilon_{tot}-\Delta\varepsilon_o$

As it is supposed here that μ is constant, one has the following relation between the diverters of $\Delta\sigma$ and $\Delta\varepsilon$:

$$\Delta\tilde{\sigma}=2\mu\left(\Delta\tilde{\varepsilon}-\Delta\varepsilon_v\right) \qquad \text{éq 4.1-1}$$

However, the law of flow is written, an implicit way:

$$\frac{\Delta\varepsilon_v}{\Delta t}=\frac{3}{2}g\left(\sigma_{eq},\lambda^-+\left(\Delta\varepsilon_v\right)_{eq},T\right)\frac{\tilde{\sigma}}{\sigma_{eq}} \qquad \text{éq 4.1-2}$$

One thus has, while eliminating $\Delta\varepsilon_v$ between [éq 4.1-1] and [éq 4.1-2]:

$$2\mu\Delta\tilde{\varepsilon}=\Delta\tilde{\sigma}+3\mu\Delta t\,.\,g\left(\sigma_{eq},\lambda^-+\left(\Delta\varepsilon_v\right)_{eq},T\right)\frac{\tilde{\sigma}}{\sigma_{eq}}$$

$$\left(\tilde{\sigma}^-+2\mu\Delta\tilde{\varepsilon}\right)=\left(1+3\mu\Delta t\frac{g\left(\sigma_{eq},\lambda^-+\left(\Delta\varepsilon_v\right)_{eq},T\right)}{\sigma_{eq}}\right)\tilde{\sigma} \qquad \text{éq 4.1-3}$$

While posing $\tilde{\sigma}^e = \tilde{\sigma}^- + 2\mu\,\Delta\,\tilde{\varepsilon}$, one thus has:

$$\sigma_{eq}^e = 3\mu\,\Delta t\,.\,g\left(\sigma_{eq},\lambda^- + \left(\Delta\,\varepsilon_v\right)_{eq},T\right) + \sigma_{eq} \qquad \textbf{éq 4.1-4}$$

However, one has according to [éq 4.1-2]:

$$\left(\Delta\,\varepsilon_v\right)_{eq} = \Delta t\,.\,g\left(\sigma_{eq},\lambda^- + \left(\Delta\,\varepsilon_v\right)_{eq},T\right)$$

From where:

$$\sigma_{eq}^e = 3\mu\left(\Delta\,\varepsilon_v\right)_{eq} + \sigma_{eq}$$

$$\left(\Delta\,\varepsilon_v\right)_{eq} = \frac{1}{3\mu}\left(\sigma_{eq}^e - \sigma_{eq}\right)$$

In substituent this last expression in [éq 4.1-4], one a:

$$\sigma_{eq}^e = 3\mu\,\Delta t\,.\,g\left(\sigma_{eq},\lambda^- + \frac{1}{3\mu}\left(\sigma_{eq}^e - \sigma_{eq}\right),T\right) + \sigma_{eq}$$

If one poses, $\sigma_{eq}^e,\lambda^-,T$ and Δt being known:

$$f(x) = 3\mu\,\Delta t\,.\,g\left(x,\lambda^- + \frac{1}{3\mu}\left(\sigma_{eq}^e - x\right),T\right) + x - \sigma_{eq}^e$$

one can then calculate the quantity $\sigma_{eq} = \left(\sigma^- + \Delta\,\sigma\right)_{eq}$ as being the solution of the scalar equation: $f(x)=0$ where $x=\sigma_{eq}$, convention adopted for the following paragraphs.
In the case of a law of Lemaître with threshold, `LEMA_IRRA_SEUIL`, the preceding equations are useful only once the crossed threshold. Indeed in-on this side threshold the behavior is elastic.

One discretizes the threshold implicitly:

$$D(\sigma^- + \Delta\,\sigma) = \frac{1}{S}\int_0^t \left(\sigma^- + \Delta\,\sigma\right)_{eq}(u)\,du$$

In the same way that for the integration of the laws of elastoplastic behavior of Von-Put, one distinguishes two cases then.

$D(\sigma^- + \Delta\,\sigma) \le 1$ then $g\left(\sigma^- + \Delta\,\sigma,\lambda,T\right) = 0$

$D(\sigma^- + \Delta\,\sigma) > 1$ then $g\left(\sigma^- + \Delta\,\sigma,\lambda,T\right) = A\,.\left(\frac{2}{\sqrt{3}}\sigma_{eq}\right)\varphi$

It results from it starting from the equation above:

$g\left(\sigma^- + \Delta\,\sigma,\lambda,T\right) \ne A\,.\left(\frac{2}{\sqrt{3}}\sigma_{eq}\right)\varphi$ imply $D(\sigma^- + \Delta\,\sigma) \le 1$

However g can take only the value 0 or $A.\left(\frac{2}{\sqrt{3}}\sigma_{eq}\right)\varphi$ thus

$g\left(\sigma^{-}+\Delta\sigma,\lambda,T\right)\neq A.\left(\frac{2}{\sqrt{3}}\sigma_{eq}\right)\varphi$ imply $D(\sigma^{-}+\Delta\sigma)\leq 1$ and $\Delta\sigma=A.\Delta\varepsilon$

that is to say $g\left(\sigma^{-}+\Delta\sigma,\lambda,T\right)=A.\left(\frac{2}{\sqrt{3}}\sigma_{eq}\right)\varphi$ then $D(\sigma^{-}+A.\Delta\varepsilon)>1$

The criterion of crossing of the threshold can thus be written $D(\sigma^{-}+A.\Delta\varepsilon)>1$

However $D(\sigma^{-}+A.\Delta\varepsilon)=\frac{1}{S}\int_{0}^{t}\left(\sigma^{-}+A.\Delta\varepsilon\right)_{eq}(u)du$

By discretizing time, one has then:

$$D(\sigma^{-}+A.\Delta\varepsilon)=\frac{1}{S}\int_{0}^{t^{-}}\left(\sigma^{-}+A.\Delta\varepsilon\right)_{eq}(u)du+\frac{1}{S}\int_{t^{-}}^{t}\left(\sigma^{-}+A.\Delta\varepsilon\right)_{eq}(u)du$$

$$D(\sigma^{-}+A.\Delta\varepsilon)=\frac{1}{S}\left(D^{-}S+\frac{\sigma_{eq}^{-}+\left(\sigma^{-}+A.\Delta\varepsilon\right)_{eq}}{2}\left(t-t^{-}\right)\right)$$

4.2 Resolution of the scalar equation: principle of the routine `ZEROF2`

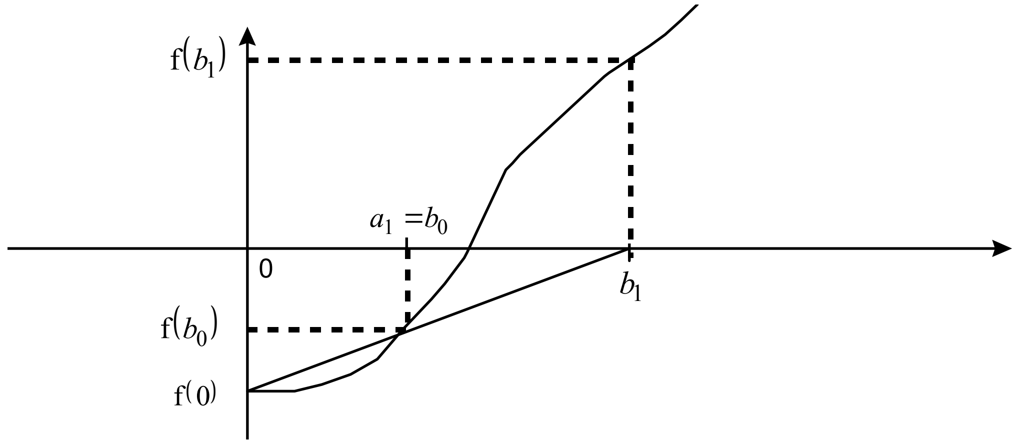
It is shown easily that, if the requirements in the paragraph [§3] on the characteristics of materials are checked, the function f is strictly increasing and the equation $f\left(x\right)=0$ admits a single solution.

If $\sigma_{eq}^{e}=0$, then the solution is $x=0$. If not, one a: $f\left(0\right)=-\sigma_{eq}^{e}<0$

The problem thus consists in finding for a function f unspecified the solution of the equation $f\left(x\right)=0$ knowing that this solution exists, that $f\left(0\right)<0$ and that f is strictly increasing.

The algorithm adopted in `ZEROF2` is the following:

- one leaves $a_0=0$ and $b_0=x_{ap}$ where x_{ap} is an approximation of the solution. If it is necessary (i.e. if $f\left(b_0\right)<0$), one brings back oneself by the method of the secants ($z_n=\frac{a_n f\left(b_n\right)-b_n f\left(a_n\right)}{f\left(b_n\right)-f\left(a_n\right)}$ then $a_{n+1}=b_n$ and $b_{n+1}=z_n$) in one or more iterations if $f(a)<0$ and $f(b)>0$:



(In the case of the figure above, this first sentence was done in an iteration: $a_1 = b_0$ and $f(b_1) > 0$).

- one calculates N_d = whole part $\left(\sqrt{N_{\max}}\right)$ where $N_{\max}$ is the maximum number of iterations which one gave oneself. One then solves the equation by the method of the secants by using however the method of dichotomy with each time n is multiple of N_d :

1)
If N_d divided n
$$z_n = \frac{a_n + b_n}{2}$$
if not
$$z_n = \frac{a_n f(b_n) - b_n f(a_n)}{f(b_n) - f(a_n)}$$
finsi
$n = n+1$
if $|f(z)| > \varepsilon$
if $f(z) < 0$
$a_{n+1} = z_n \qquad b_{n+1} = b_n$
if not
$a_{n+1} = a_n \qquad b_{n+1} = z_n$
finsi
to go in 1)
if not
The solution is: $x = z_n \rightarrow FIN$
finsi

This second part of the algorithm allows to treat in a reasonable iteration count the cases where f is very strongly non-linear, whereas the method of the secants would have converged too slowly. These cases of strong non-linearity meet in particular with the law of LEMAITRE, for values of $\frac{n}{m}$ large.

4.3 Calculation of the constraint at the end of the step of current time

According to [éq 4.1-3], if x is the solution of the scalar equation, while posing:

$$b\left(x,\sigma_{eq}^{e}\right)=\frac{1}{1+3\mu\,\Delta t\,\dfrac{g\left(x,\lambda^{-}+\dfrac{1}{3\mu}\left(\sigma_{eq}^{e}-x\right),T\right)}{x}}=\frac{x}{\sigma_{eq}^{e}}$$

one a:

$$\tilde{\sigma}=b\left(x,\sigma_{eq}^{e}\right)\tilde{\sigma}^{e} \qquad \textbf{éq 4.3-1}$$

If $\sigma_{eq}^{e}=0$, which is equivalent according to the scalar equation to $x=0$, one prolongs b by continuity. For that, one poses $y(x)=\lambda^{-}+\dfrac{1}{3\mu}\left(\sigma_{eq}^{e}-x\right)$ and $G(x)=g\left(x,y(x),T\right)$. The derivative of G express yourself according to the derivative partial of g at the point $\left(x,y(x),T\right)$:

$$G'(x)=\frac{\partial g}{\partial x}\left(x,y(x),T\right)-\frac{1}{3\mu}\frac{\partial g}{\partial y}\left(x,y(x),T\right)$$

Prolongation of b by continuity gives then:

$$b(0,0)=\frac{1}{1+3\mu\,\Delta t\,G'(0)}$$

and one has, always if $\sigma_{eq}^{e}=0$, $\tilde{\sigma}=0$.

Once one calculated $\tilde{\sigma}$, one obtains σ by the relation (K is supposed to be constant here):

$$\sigma=\sigma^{-}+\Delta\sigma=\tilde{\sigma}+\left(\frac{1}{3}Tr\left(\sigma^{-}\right)+K\,Tr\left(\Delta\varepsilon\right)\right)I_{3} \qquad \textbf{éq 4.3-2}$$

4.4 Semi-implicit diagram

With an implicit digital diagram [éq 4.1-2], in the case, for example, where g does not depend on λ, only intervenes by the calculation of $\Delta\varepsilon_v$ the value of the constraint at the end of the step of time. It can result from it from the important digital errors if the constraint strongly varies in the course of time (see [bib2]).

To cure that and to improve the resolution, one discretizes the law of flow in way semi - implicit:

$$\frac{\Delta\varepsilon_v}{\Delta t}=\frac{3}{2}g\left(\left(\sigma^-+\frac{\Delta\sigma}{2}\right)_{eq},\lambda^-+\frac{(\Delta\varepsilon_v)_{eq}}{2},T^-+\frac{\Delta T}{2}\right)\frac{\left(\tilde{\sigma}^-+\frac{\Delta\tilde{\sigma}}{2}\right)}{\left(\sigma^-+\frac{\Delta\sigma}{2}\right)_{eq}} \quad \textbf{éq 4.4-1}$$

To transform in the most economic way what was programmed previously (while following the implicit formulation [éq 4.1-2]), it is enough to divide each member of the equation [éq 4.4-1] by 2:

$$\frac{(\Delta\varepsilon_v/2)}{\Delta t}=\frac{3}{2}\frac{g\left(\left(\sigma^-+\frac{\Delta\sigma}{2}\right)_{eq},\lambda^-+\frac{(\Delta\varepsilon_v)_{eq}}{2},T^-+\frac{\Delta T}{2}\right)}{2}\frac{\left(\tilde{\sigma}^-+\frac{\Delta\tilde{\sigma}}{2}\right)}{\left(\sigma^-+\frac{\Delta\sigma}{2}\right)_{eq}}$$

and to make the same thing with the relation [éq 4.1-1]:

$$\frac{\Delta\tilde{\sigma}}{2}=2\mu\left(\frac{\Delta\tilde{\varepsilon}}{2}-\frac{\Delta\varepsilon_v}{2}\right)$$

It is noted that this system is same form as that consisted the equations [éq 4.1-1] and [éq 4.1-2], the data being $\frac{\Delta\varepsilon}{2}$ instead of $\Delta\varepsilon$, unknown factors being respectively $\frac{\Delta\sigma}{2}$ and $\frac{\Delta\varepsilon_v}{2}$ instead of $\Delta\sigma$ and $\Delta\varepsilon_v$ and the function $\frac{g}{2}$ replacing the function g.

One can thus use the resolution of the paragraphs [§4.1] with [§4.3] as well as the algorithm corresponding while introducing $\frac{\Delta\varepsilon}{2}$ and by dividing the function g by 2. It then remains to multiply the results $\frac{\Delta\sigma}{2}$ and $\frac{\Delta\varepsilon_v}{2}$ by 2 to obtain the increments of constraint and viscous deformation calculated by the semi-implicit diagram (it $\Delta\sigma$ and it $\Delta\varepsilon_v$ equation [éq 4.4-1]).

It will be noticed that the calculation of the tangent operator is not affected by this modification of the digital diagram. Indeed, one has obviously:

$$\frac{\partial \Delta \sigma}{\partial \Delta \varepsilon}=\frac{\partial\left(\frac{\Delta \sigma}{2}\right)}{\partial\left(\frac{\Delta \varepsilon}{2}\right)}$$

4.5 Typical case of the law GATT_MONERIE

If the reasoning of the §4.2 is taken again, the equation is obtained:

$$\sigma_{eq}^{e}=3\mu\,.\Delta t\,.\,g\left(\sigma_{eq},\sigma_{m},f,T\right)+\sigma_{eq} \qquad \text{éq 4.5-1}$$

The fact that this law does not depend on the cumulated plastic deformation thus simplifies this equation. On the other hand, an additional unknown factor is introduced: voluminal fraction of porosity. Another equation is thus necessary. To find it, it is enough to write the law of Hooke binding the spherical parts of the increments of constraint and elastic strain according to:

$$Tr\left(\Delta \sigma\right)=3\mathrm{K}\left(Tr\left(\Delta \varepsilon\right)-Tr\left(\Delta \varepsilon_{v}\right)\right)$$

Knowing in addition that:

$$Tr\left(\Delta \varepsilon_{v}\right)=\frac{\Delta f}{1-f},$$

one can express the average constraint according to the voluminal fraction of porosity, i.e.:

$$\Delta \sigma_{m}=K\left(Tr\left(\Delta \varepsilon\right)-\frac{\Delta f}{1-f}\right),$$

what leads us to the second scalar equation:

$$\Delta f-(1-f)\,g_{d}\left(\sigma_{eq},\sigma_{m}^{-}+3\mathrm{K}\left(Tr(\Delta \varepsilon)-\frac{\Delta f}{1-f}\right),f,T\right)=0 \qquad \text{éq 4.5-2}$$

We thus obtain two coupled scalar equations whose unknown factors are the equivalent constraint and the voluminal fraction of porosity:

$$\begin{cases} 3\mu\Delta t\,.\,g\left(\sigma_{eq},\sigma_{m}^{-}+3\mathrm{K}\left(Tr\left(\Delta \varepsilon\right)-\frac{\Delta f}{1-f}\right),f,T\right)+\sigma_{eq}-\sigma_{eq}^{e}=0 \\ \Delta f-\left(1-f\right)\,g_{d}\left(\sigma_{eq},\sigma_{m}^{-}+3\mathrm{K}\left(Tr\left(\Delta \varepsilon\right)-\frac{\Delta f}{1-f}\right),f,T\right)=0 \end{cases}$$

Let us note f_{d} the scalar function defined by:

$$f_{d}(x)=x-f^{-}-\left(1-x\right)\,g_{d}\left(\sigma_{eq},\sigma_{m}^{-}+3\mathrm{K}\left(Tr\left(\Delta \varepsilon\right)-\frac{x-f^{-}}{1-x}\right),x,T\right),$$

expression in which the equivalent constraint is regarded as a given parameter.

It is noticed that:

$$f_{d}\left(0\right)=-f^{-}\leq 0\ .$$

In addition, the sign of the trace the speed of deformation viscoplastic is determined by the sign of the average constraint and this function of porosity:

$$\sigma_m(x)=\sigma_m^-+3K\left(Tr(\Delta\varepsilon)-\frac{x-f^-}{1-x}\right)$$

is monotonous decreasing on the interval $[0\,;\,1-f^-[$ and presents a vertical asymptote on the upper limit of this interval.

Taking into account these elements, two cases arise:

$\sigma_m^-+3KTr(\Delta\varepsilon)<0\Rightarrow\sigma_m(x)<0\ \ \nabla x\in[0\,;\,1-f^-[$: in this case $f_d(f^-)>0$.

$\sigma_m^-+3KTr(\Delta\varepsilon)>0\Rightarrow\sigma_m(f_{rig})=0$ with $f_{rig}=(1-f^-)\dfrac{\sigma_m^-+3KTr(\Delta\varepsilon)}{1+\sigma_m^-+3KTr(\Delta\varepsilon)}$: in this case, $f_d(f^-)<0$ and $f_d(f_{rig})>0$.

In all the cases, we thus have a framing of the solution. On the other hand, the strict monotony of the function f_d to cancel is not guaranteed.

In order to use the routine ZEROF2, we proceed to a chained solution of these two scalar equations. One carries out two imbricated calls indeed to ZEROF2 : the first call solves equation 4.5.2.

With each iteration of this resolution, the current increment of porosity Δf^i allows to calculate $Tr(\Delta\sigma^i)$ according to:

$$Tr(\Delta\sigma^i)=3K\left(Tr(\Delta\varepsilon)-\frac{\Delta f^i}{1-f^-+\Delta f^i}\right),$$

then σ_{eq}^i by resolution of equation 4.5.1 (second call to ZEROF2) :

$$3\mu\Delta t.g\left(\sigma_{eq(i)},\sigma_m^-+3K\left(Tr(\Delta\varepsilon)-\frac{\Delta f_i}{1-f^--\Delta f_i}\right),\Delta f_i,T\right)+\sigma_{eq(i)}-\sigma_{eq}^e=0\ .$$

A good approximation for porosity (x_{ap}) adopted at the beginning of these iterations is obtained according to:

$$\sigma_m^-+3KTr(\Delta\varepsilon)<0\Rightarrow x_{ap}=f^-\ ,$$
$$\sigma_m^-+3KTr(\Delta\varepsilon)>0\Rightarrow x_{ap}=f_{rig}=(1-f^-)\frac{\sigma_m^-+3KTr(\Delta\varepsilon)}{1+\sigma_m^-+3KTr(\Delta\varepsilon)}\ .$$

Once convergence reached, the calculation of the constraints must take account of the variation of volume induced by the variations of voluminal fraction of porosity. Equation 4.3-2 must thus be modified according to:

$$\sigma=\sigma^-+\Delta\sigma=\tilde{\sigma}+\left(\frac{1}{3}Tr(\sigma^-)+K\left(Tr(\Delta\varepsilon)-\frac{\Delta f}{1-f}\right)\right)I_3$$

Lastly, the variations of porosity are neglected during the calculation of the tangent operator so that only the derivative of the function g compared to the equivalent constraint is necessary:

$$
\begin{cases}
\frac{dG(\sigma_{eq})}{d\sigma_{eq}}=(1-\theta)\frac{d^2\psi_1}{d\sigma_{eq}^2}+\theta\frac{d^2\psi_2}{d\sigma_{eq}^2}+\frac{d^2\theta}{d\sigma_{eq}^2}(\psi_2-\psi_1)+2\frac{d\theta}{d\sigma_{eq}}\frac{d(\psi_2-\psi_1)}{d\sigma_{eq}}\\
\frac{d^2\psi_i}{d\sigma_{eq}^2}=\frac{1}{\sigma_{eq}}\frac{d\psi_i}{d\sigma_{eq}}+\frac{n_i-1}{\sigma_{0i}}\dot{\varepsilon}_{0i}\left(B_i(f)\left(\frac{\sigma_{eq}}{\sigma_{0i}}\right)\right)^2\left[A_i(f)\left(\frac{3\sigma_m}{2\sigma_{0i}}\right)^2+B_i(f)\left(\frac{\sigma_{eq}}{\sigma_{0i}}\right)^2\right]^{\frac{n_i-3}{2}}\\
\frac{d^2\theta}{d\sigma_{eq^2}}=\frac{1}{2}\frac{d^2\phi}{d\sigma_{eq^2}}\left[1-th^2(\phi(\sigma_I))\right]-\left(\frac{d\phi}{d\sigma_{eq}}\right)^2 th(\phi(\sigma_I))\left[1-th^2(\phi(\sigma_I))\right]\\
\Rightarrow\frac{d^2\theta}{d\sigma_{eq^2}}=\frac{d\theta}{d\sigma_{eq}}\left[\frac{1}{\sigma_{eq}}+\frac{9B_1(q-2)\sigma_{eq}}{(4B_1+A_1)\sigma_{I^2}}-2\frac{d\phi}{d\sigma_{eq}}th(\phi(\sigma_I))\right]
\end{cases}
$$

As explained to the §4.4, the adaptation to the semi-implicit case is brought back to a simple division by two of the two functions of flow (g, g^d).

Note: for the calculation of the coefficients $A1$ and $A2$ according to porosity, the following expression was used:

$$A_i(f)=f^{\frac{2}{n_i+1}}\left(n_i\left(1-f^{\frac{1}{n_i}}\right)\right)^{\frac{-2n_i}{n_i+1}}.$$

This second expression indeed has the advantage of being defined for a worthless porosity.

4.6 Taking into account of the variation of the elastic coefficients according to the temperature

One has, if A is the tensor of elasticity:

$$\Delta\varepsilon=\Delta\varepsilon_v+\Delta(A^{-1}\sigma)$$

with:

$$\Delta(A^{-1}\sigma)=A^{-1}(T^-+\Delta T)(\sigma^-+\Delta\sigma)-A^{-1}(T^-)\sigma^-$$

This is translated in the equations of [§4.4] by:

$$2\mu\left(\frac{\Delta\tilde{\varepsilon}}{2}\right)-\left(\tilde{\sigma}^-+\frac{\Delta\tilde{\sigma}}{2}\right)=3\mu\Delta t\frac{g\left(\left(\sigma^-+\frac{\Delta\sigma}{2}\right)_{eq},\lambda^-+\frac{(\Delta\varepsilon_v)_{eq}}{2},T^-+\frac{\Delta T}{2}\right)}{2}\frac{\left(\tilde{\sigma}^-+\frac{\Delta\sigma}{2}\right)}{\left(\sigma^-+\frac{\Delta\sigma}{2}\right)_{eq}}-\tilde{\sigma}^-\left(\frac{2\mu^-+2\mu}{4\mu^-}\right)$$

While posing:

$$\tilde{\sigma}^e=\left(\frac{2\mu^-+2\mu}{4\mu^-}\right)\tilde{\sigma}^-+2\mu\left(\frac{\Delta\tilde{\varepsilon}}{2}\right)$$

and

$$Tr(\sigma^e)=\left(\frac{3K^-+3K}{6K^-}\right)Tr(\sigma^-)+3K\,Tr\left(\frac{\Delta\varepsilon}{2}\right)$$

one is reduced exactly to the preceding case [§4.4].

5 Calculation of the tangent operator

If $\sigma^e_{eq}=0$ and $x=0$, one takes the tensor of elasticity as tangent operator.

If not, one obtains this operator by deriving the equation [éq 4.3-1] compared to $\Delta\varepsilon$:

$$\frac{\partial\tilde{\sigma}}{\partial\Delta\varepsilon}=\frac{\partial\Delta\tilde{\sigma}}{\partial\Delta\varepsilon}=\frac{\partial b(x,\sigma^e_{eq})}{\partial\Delta\varepsilon}\tilde{\sigma}^e+b(x,\sigma^e_{eq})\frac{\partial\tilde{\sigma}^e}{\partial\Delta\varepsilon}$$

then while also deriving [éq 4.3-2] compared to $\Delta\varepsilon$:

$$\frac{\partial\Delta\sigma}{\partial\Delta\varepsilon}=\frac{\partial\Delta\tilde{\sigma}}{\partial\Delta\varepsilon}+KI_3\frac{\partial Tr(\Delta\varepsilon)}{\partial\Delta\varepsilon}=\frac{\partial\Delta\tilde{\sigma}}{\partial\Delta\varepsilon}+KI_3^t I_3$$

It will be noted that, in these equations, the tensors of order 2 and order 4 are respectively compared to vectors and matrices. I_3 is here a tensor of a nature 2, compared to a vector:

$$^tI_3=(1,1,1,0,0,0)$$

One has moreover:

$$\frac{\partial b(x,\boldsymbol{\sigma}^e_{eq})}{\partial\Delta\boldsymbol{\varepsilon}}=\frac{\partial b}{\partial x}(x,\boldsymbol{\sigma}^e_{eq})\frac{\partial x}{\partial\Delta\boldsymbol{\varepsilon}}+\frac{\partial b}{\partial\boldsymbol{\sigma}^e_{eq}}(x,\boldsymbol{\sigma}^e_{eq})\frac{\partial\boldsymbol{\sigma}^e_{\mathrm{eq}}}{\partial\Delta\boldsymbol{\varepsilon}}$$

It is thus necessary to calculate $\frac{\partial x}{\partial\Delta\boldsymbol{\varepsilon}}$. For that, one derives the scalar equation implicitly compared to $\Delta\boldsymbol{\varepsilon}$.

To simplify, one will omit thereafter in the writing of g and of its derivative the parameter T .

One has then:

$$[3\mu\Delta t G'(x)+1]\frac{\partial x}{\partial\Delta\boldsymbol{\varepsilon}}+\Delta t\frac{\partial g}{\partial y}(x,y)\frac{\partial\boldsymbol{\sigma}^{\mathbf{e}}_{\mathbf{eq}}}{\partial\Delta\boldsymbol{\varepsilon}}=\frac{\partial\boldsymbol{\sigma}^{\mathbf{e}}_{\mathbf{eq}}}{\partial\Delta\boldsymbol{\varepsilon}}$$

From where:

$$\frac{\partial x}{\partial\Delta\boldsymbol{\varepsilon}}=\frac{1-\Delta t\frac{\partial g}{\partial y}(x,y)}{1+3\mu\Delta t G'(x)}\frac{\partial\boldsymbol{\sigma}^{\mathbf{e}}_{eq}}{\partial\Delta\boldsymbol{\varepsilon}}$$

$$\frac{\partial x}{\partial\Delta\boldsymbol{\varepsilon}}=\frac{1-\Delta t\frac{\partial g}{\partial y}(x,y)}{1+3\mu\Delta t G'(x)}\frac{3\mu}{\boldsymbol{\sigma}^{\mathbf{e}}_{\mathbf{eq}}}\tilde{\boldsymbol{\sigma}}^e$$

with the expression of $G'(x)$ obtained with [§4.3].

One obtains finally the following expression of the tangent operator:

$$\frac{\partial\Delta\boldsymbol{\sigma}}{\partial\Delta\boldsymbol{\varepsilon}}=K\,\mathbf{I}_3^t\,\mathbf{I}_3+2\,\mu\left[\gamma\,\tilde{\boldsymbol{\sigma}}^{et}\,\tilde{\boldsymbol{\sigma}}^{e}+b\left(x,\boldsymbol{\sigma}_{eq}^{e}\right)\mathbf{A}\right]$$

with

$$A=\frac{\partial\Delta\tilde{\boldsymbol{\varepsilon}}}{\partial\Delta\boldsymbol{\varepsilon}}=\mathbf{J}_6-\frac{1}{3}\mathbf{I}_3{}^t\,\mathbf{I}_3$$ where $\mathbf{J}_6$ is the matrix identity of row 6.

$$\gamma=\frac{3}{2\left(\boldsymbol{\sigma}_{\mathbf{eq}}^{\mathbf{e}}\right)^3}\left[\boldsymbol{\sigma}_{\mathbf{eq}}^{\mathbf{e}}\frac{1-\Delta t\dfrac{\partial g}{\partial y}(x,y)}{1+3\,\mu\,\Delta t\,G'(x)}-x\right]$$

Note:

In the case of the law `VISC_IRRA_LOG`, it is checked easily that:

$$G'(x)=\frac{1}{f'_1 g_1+f'_2 g_2}\left[g_1 g'_1\left(f'^2_1-f_1 f''_1\right)+g_2 g'_2\left(f'^2_2-f_2 f''_2\right)+g_1 g'_2\left(f'_1 f'_2-f''_1 f_2\right)\right.$$
$$\left.+g_2 g'_1\left(f'_1 f'_2-f_1 f''_2\right)-\frac{1}{3\mathrm{m}}\left(f''_1 g_1+f''_2 g_2\right)\right]$$
$$\frac{\partial g}{\partial\lambda}(x,y,T)=\frac{f''_1 g_1+f''_2 g_2}{f'_1 g_1+f'_2 g_2}$$

where $f_1, f'_1, f''_1, f_2, f'_2, f''_2$ *the values indicate of* f_1 *and* f_2 *and their derivative at the point* $t(x,y,T)$ *and where* g_1, g'_1, g_2, g'_2 *the values indicate of* g_1 *and* g_2 *and of their derivative compared to* σ *at the point* (x,T) *(see [bib1]).*

6 Bibliography

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7 Description of the versions of the document

Version Aster	Author (S) Organization (S)	Description of the modifications
7.4	P. of BONNIERES	Initial text
8.4	S. LECLERCQ, R.MASSON	Laws GATT-MONERIE and LEMA_SEUIL
9.3	P. of BONNIERES	Suppression ZIRC_CYRA2, ZIRC_EPRI.