Rate of refund of energy in linear thermoelasticity

Summarized:

One presents the computation of the rate of refund of energy G by the method θ in 2D or 3D for a linear thermoelastic problem. It is explained how the field θ is introduced into *Code_Aster* and how rate of energy restitution is calculated with operator CALC_G.

Studies mechanic-reliability engineers of evaluating of probability of starting of the fracture require, moreover, its derivative compared to a variation of field controlled by another field. One details the establishment of this option in the code.

The computation of G is available as well for a crack with a grid (conventional finite elements) as for a crack nonwith a grid (finite elements nouveau riches: method X-FEM). The computation of its derivative is as for him available only in 2D, for a crack with a grid.

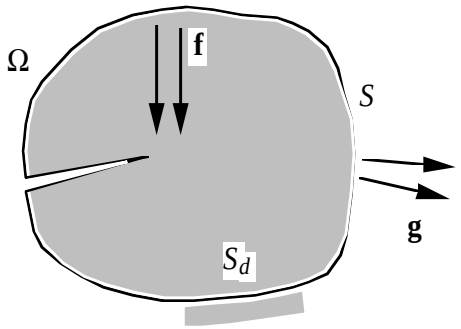
Contents

1 Computation of rate of energy restitution by the method θ in linear thermoelasticity

1.1 Behavior model

One considers a fissured elastic solid occupying the field Ω of space R^2 or R^3. That is to say:

- u the field of displacement,
- T the field of temperature,
- f the field of volume forces applied to Ω,
- g the field of surface forces applied to part S of $\partial\Omega$,
- U the field of displacements imposed on part S_d of $\partial\Omega$.



Appear 1.1-a: Elastic solid fissured

to simplify, one is placed in **linear elasticity and small strains**, but this approach spreads without sorrow with plasticity [R7.02.07], with the large deformations, the dynamics…
One indicates by:

- ε the tensor of the strains,
- ε^0 the tensor of predeformations,
- ε^{th} the tensor of the strains of thermal origin,
- σ the tensor of the stresses,
- σ^0 the tensor of the initial stresses,
- $\Psi(\varepsilon, \varepsilon^0, \sigma^0, T)$ density of free energy,
- Λ the elasticity tensor.

ε is connected to the field of displacement $\boldsymbol{u}$ by:

$$\varepsilon(\boldsymbol{u}) = \frac{1}{2}(u_{i,j} + u_{j,i})$$

The density of free energy $\Psi(\varepsilon, \varepsilon^0, \sigma^0, T)$ is identified by a traction test and of thermal expansion in small strains. $\Psi(\varepsilon, \varepsilon^0, \sigma^0, T)$ is a convex and differentiable function.

$$\Psi(\varepsilon, \varepsilon^0, \sigma^0, T) = \frac{1}{2}(\varepsilon - \varepsilon^{th} - \varepsilon^0 + \Lambda^{-1}\sigma^0)\,\Lambda\,(\varepsilon - \varepsilon^{th} - \varepsilon^0 + \Lambda^{-1}\sigma^0)$$

The constitutive law of an elastic material is written in the form:

$$\sigma=\frac{\partial \Psi}{\partial \varepsilon}(\varepsilon,\varepsilon^0,\sigma^0,T)=\Lambda(\varepsilon-\varepsilon^{th}-\varepsilon^0)+\sigma^0$$
$$\text{avec } \varepsilon^{th}_{ij}=\alpha(T-T_{ref})\delta_{ij}$$

If the initial strains ε^0 and the forced initial are null, the density of free energy is written:

$$\Psi(\varepsilon,T)=\frac{1}{2}\lambda(\varepsilon_{ii})^2+\mu\varepsilon_{ij}\varepsilon_{ij}-3K\alpha(T-T_{réf})\varepsilon_{kk}+\frac{9}{2}K\alpha^2(T-T_{réf})^2$$

The behavior model is written:

$$\sigma_{ij}=\lambda\varepsilon_{kk}\delta_{ij}+2\mu\varepsilon_{ij}-3K\alpha(T-T_{réf})\delta_{ij}$$

λ and μ are the coefficients of LAME.
α is the thermal coefficient of thermal expansion.
$T_{réf}$ is the reference temperature.
K, voluminal modulus of compressibility, is connected to the coefficients of LAME by: $3K=3\lambda+2\mu$.

The behavior model starting from the modulus of YOUNG E and the Poisson's ratio ν is:

$$\sigma_{ij}=\frac{E}{1+\nu}\left(\varepsilon_{ij}+\frac{\nu}{1-2\nu}(tr\,\varepsilon)\delta_{ij}\right)-\frac{\alpha E}{1-2\nu}(T-T_{réf})\delta_{ij}$$

$$\text{avec :}\quad \lambda=\frac{\nu E}{(1+\nu)(1-2\nu)}$$
$$\mu=\frac{E}{2(1+\nu)}$$
$$3K=\frac{E}{1-2\nu}$$

1.2 Potential energy and relations of equilibrium

One defines spaces of the fields kinematically admissible V and V_0.

$$V \quad =\{\boldsymbol{v}\text{ admissibles},\boldsymbol{v}=\boldsymbol{U}\text{ sur }S_d\}$$
$$V_0 \quad =\{\boldsymbol{v}\text{ admissibles},\boldsymbol{v}=0\text{ sur }S_d\}$$

With the assumptions of [§1.1] (and for $\sigma^0=\varepsilon^0=0$), **the relations of equilibrium in weak formulation** are:

$$\begin{cases}\boldsymbol{u}\in V\\ \int_\Omega \sigma_{ij}v_{i,j}\,d\Omega=\int_\Omega f_i v_i\,d\Omega+\int_S g_i v_i\,d\Gamma,\ \forall\,\boldsymbol{v}\in V_O\end{cases}$$

They are obtained by minimizing the total potential energy of the system:

$$W(\boldsymbol{v})=\int_\Omega \Psi(\varepsilon(\boldsymbol{v}),T)\,d\Omega-\int_\Omega f_i v_i\,d\Omega+\int_S g_i v_i\,d\Gamma$$

Indeed, if this functional calculus is minimal for the field of displacement $\boldsymbol{u}$, then:

$$\begin{aligned}\delta W &= \int_\Omega \frac{\partial \Psi}{\partial \varepsilon_{ij}} \delta \varepsilon_{ij} d\Omega - \int_\Omega f_i \delta v_i d\Omega - \int_S g_i \delta v_i d\Gamma \\ &= \int_\Omega \sigma_{ij} \frac{1}{2}(\delta v_{i,j} + \delta v_{j,i}) d\Omega - \int_\Omega f_i \delta v_i d\Omega - \int_S g_i \delta v_i d\Gamma \\ &= \int_\Omega \sigma_{ij} \delta v_{i,j} d\Omega - \int_\Omega f_i \delta v_i d\Omega - \int_S g_i \delta v_i d\Gamma \qquad = \ 0\end{aligned}$$

We thus find the balance equations and the behavior model while having posed: $\sigma_{ij} = \frac{\partial \Psi}{\partial \varepsilon_{ij}}$.

1.3 Lagrangian statement of rate of energy restitution

By definition [bib1] rate of energy restitution local G is defined by the opposite of derivative of potential energy compared to the field Ω :

$$G = -\frac{\partial W}{\partial \Omega}$$

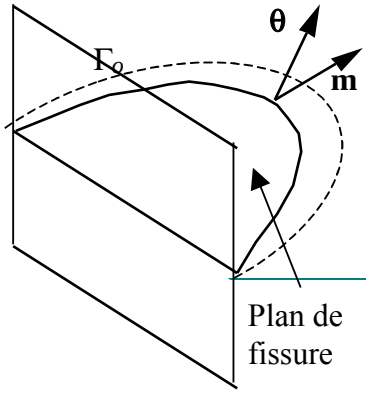
This rate of refund can be calculated in *Code_Aster* by the method θ , which is **a Lagrangian method of derivative of potential energy** [bib4] [bib2]. One considers transformations $F^\eta : \boldsymbol{M} \to \boldsymbol{M} + \eta\theta(\boldsymbol{M})$ of the area of reference Ω in a modelling Ω^η field of the propagations of the crack, which at a material point $\boldsymbol{P}$ make correspond a spatial point $\boldsymbol{M}$. These transformations should modify only the position of the crack tip Γ_0 . The fields θ must thus be tangent with $\partial\Omega$, i.e. by noting $\boldsymbol{n}$ the norm with $\partial\Omega$:

$$\theta \in \Theta = \{\mu \text{ tels que } \mu . \boldsymbol{n} = 0 \text{ sur } \partial\Omega\}$$

Notice

> *This family of functions of transformation must be sufficiently regular. In particular, it must be at least twice differentiable per pieces in $\boldsymbol{P}$ and in η (so that the partial derivatives seconds commutate) and carry out a diffeomorphism for each value of the parameter η (that ensures the reversibility of the process).*

That is to say $\boldsymbol{m}$ the unit norm with Γ_0 located in the tangent plane at $\partial\Omega$ (i.e. tangent with the plane of crack) and returning in Ω .



Appear 1.3-a: Crack tip in 3D

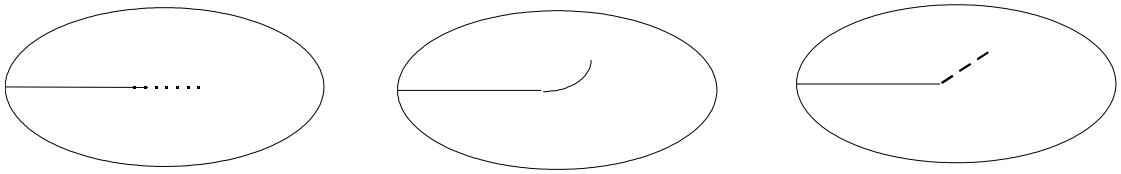
According to proposal 7 of [bib4], rate of energy restitution local G is solution of the variational equation:

$$\int_{\Gamma_0} G\theta.\boldsymbol{m} = G(\theta) \ , \ \forall \theta \in \Theta$$

where $G(\theta)$ is defined by the opposite of derivative of potential energy $W(\boldsymbol{u}(\eta))$ in the equilibrium compared to the initial evolution of the crack tip η :

$$G(\theta) = -\dot{W} = -\left. \frac{d\,W(\boldsymbol{u}(\eta))}{d\,\eta} \right|_{\eta=0}$$

The quantity $\theta.\boldsymbol{m}$ represents the normal velocity of the crack tip. In addition, $G(\theta)$ the same value has that it is about a right propagation [Figure1.3-b] (A) or of a propagation curves [Figure 1.3 - B] (b) insofar as that Ci with the same tangent at the beginning (then one can about it nothing say). On the other hand, one cannot say anything case of the propagation in a direction marking an angle [bib5] [Figure 1.3-b] (c).



Appear 1.3-b: Various geometries of propagations

Thereafter, when no confusion is possible, one will indicate par. the Lagrangian derivative in a virtual crack propagation velocity θ. That is to say $\phi(\eta, \boldsymbol{M})$ a field spatial (or eulerian) unspecified definite on $R^+ \times \Omega$, we will note his material description (or Lagrangian) $\bar{\varphi}(\eta, \boldsymbol{P}) = \varphi(\eta, F^{\eta}(\boldsymbol{P}))$ and her derivative particulate (or Lagrangian) compared to $\frac{\partial \varphi}{\partial \eta}$ this virtual propagation $\dot{\varphi} = \left(\frac{\partial \bar{\varphi}}{\partial \eta} \right)_{\eta=0}$.

Remarks [bib6]:

•The fact of adopting two visions different (eulerian and Lagrangian) introduced structurally from the notions of cross derivabilities. Thus, this particulate derivative of a spatial field called Lagrangian derivative consists in deriving $\phi(\eta, \boldsymbol{M})$ by fixing the material point $\boldsymbol{P} = \left(\boldsymbol{F}^{\boldsymbol{\eta}}\right)^{-1}(\boldsymbol{M})$. One transposes the field of Lagrangian representation, then one derives it compared to η before reconverting it of eulerian representation.

•It is pointed out that this Lagrangian derivative is related to eulerian derivative $\frac{\partial \varphi}{\partial \eta}$ by the relation $\dot{\varphi} = \frac{\partial \varphi}{\partial \eta} + \nabla \varphi . \theta$

Notices [bib4]:

The eulerian derivative $\frac{\partial \varphi}{\partial \eta}$ depends only on Ω restricted with $\delta\Omega$, i.e. trace of Ω on the crack tip.

With these notations, rate of energy restitution in this propagation θ is written (by means of **the Reynolds' transport theorem** cf [§4.2.1]):

$$-G(\theta)=\int_{\Omega}\overbrace{\psi-f_i u_i}^{\cdot}+(\psi-f_i u_i)\theta_{k,k}\,d\Omega-\int_{S}\overbrace{g_i u_i}^{\cdot}+g_i u_i\left(\theta_{k,k}-\frac{\partial\theta}{\partial n_k}n_k\right)d\Gamma$$

However

$$\dot{\Psi}(\varepsilon,\varepsilon^0,\sigma^0,T)=\frac{\partial\psi}{\partial\varepsilon_{ij}}\dot{\varepsilon}_{ij}+\frac{\partial\psi}{\partial\varepsilon^0_{ij}}\dot{\varepsilon}_{ij}^{\,0}+\frac{\partial\psi}{\partial\sigma^0_{ij}}\dot{\sigma}_{ij}^{\,0}+\frac{\partial\psi}{\partial T}\dot{T}$$

T, $\boldsymbol{f}$, $\boldsymbol{g}$, σ^0, ε^0 being supposed independent of η, i.e. being the restriction on Ω (or $\delta\Omega$) of fields defined on R^3, there are the following relations:

$$\begin{aligned}\dot{T} &= T_{,k}\theta_k\\ \dot{f}_i &= f_{i,k}\theta_k\\ \dot{g}_i &= g_{i,k}\theta_k\\ \dot{\varepsilon}_{ij}^{\,0} &= \varepsilon_{ij,k}^{\,0}\theta_k\\ \dot{\sigma}_{ij}^{\,0} &= \sigma_{ij,k}^{\,0}\theta_k\end{aligned}$$

Indeed, if one considers loadings and materials φ which are **the restriction on the geometry** Ω (or part of its border) of fields defined on R^3 entire:

$$\exists\Phi\,/\,\varphi=\Phi_{|\Omega}=0$$

The derivative compared to the parameter η commutating with this restriction, one has result

$$\frac{\partial\varphi}{\partial\eta}=\left(\frac{\partial\Phi}{\partial\eta}\right)_{|\Omega}=0_{|\Omega}=0$$

the Note:

- *This assumption is checked only for sufficiently regular fields (for example pertaining to spaces of Sobolev of Ω). Their definition should not be impacted by the variation of border.*
- *In the case of derivative of rate of energy restitution compared to a variation of field (cf [§4]) the eulerian derivative of the field of temperature could not be neglected any more.*

In addition, one as supposed as **the eulerian derivatives of the characteristic materials** φ are null, which is true only on the problem discretized with the current features of operator DEFI_MATERIAU. Their gradient on each element is also null by construction (they are discretized P_0 i.e. constant by finite elements), it results from this that the Lagrangian derivative is null:

$$\dot{\varphi}=\underbrace{\frac{\partial\varphi}{\partial\eta}}_{=0}+\underbrace{\nabla\varphi.\theta}_{=0}\ \text{pour}\ \varphi\in\{E,\nu,\alpha,T_{ref}\}$$

Caution:

With characteristic variable materials within finite elements of the contour θ of computation, this simplification is not licit any more.

Comme $\Psi(\varepsilon,\varepsilon^0,\sigma^0,T)=\frac{1}{2}(\varepsilon-\varepsilon^{th}-\varepsilon^0+\Lambda^{-1}\sigma^0)\Lambda(\varepsilon-\varepsilon^{th}-\varepsilon^0+\Lambda^{-1}\sigma^0)$

on a
$$\frac{\partial\Psi}{\partial\varepsilon_{ij}}=\Lambda_{ijkl}\left(\varepsilon_{kl}-\varepsilon^{th}_{kl}-\varepsilon^0_{kl}\right)+\sigma^0_{ij}=\sigma_{ij}$$
$$\frac{\partial\Psi}{\partial\varepsilon^0_{ij}}=-\Lambda_{ijkl}\left(\varepsilon_{kl}-\varepsilon^{th}_{kl}-\varepsilon^0_{kl}+\Lambda^{-1}_{klpq}\sigma^0_{pq}\right)=-\sigma_{ij}$$
$$\frac{\partial\Psi}{\partial\sigma^0_{ij}}=\left(\varepsilon_{ij}-\varepsilon^{th}_{ij}-\varepsilon^0_{ij}+\Lambda^{-1}\sigma^0\right)$$

d'où $$\dot{\Psi}=\sigma_{ij}\dot{\varepsilon}_{ij}-\sigma_{ij}\varepsilon^0_{ij,k}\theta_k+\Lambda^{-1}\sigma_{ij}\sigma^0_{ij,k}\theta_k+\frac{\partial\Psi}{\partial T}T_{,k}\theta_k$$

In addition, according to proposal 2 of [bib4]: $\left(\dot{\varphi}_{i,j}\right)=\dot{\varphi}_{i,j}-\varphi_{i,p}\theta_{p,j}$

$$\dot{\varepsilon}_{ij}=\frac{1}{2}\left(\dot{u}_{i,j}+\dot{u}_{j,i}\right)-\frac{1}{2}\left(u_{i,p}\theta_{p,j}+u_{j,p}\theta_{p,i}\right)$$

And one can eliminate $\dot{\boldsymbol{u}}$ from the statement from $G(\theta)$ by noticing that $\dot{\boldsymbol{u}}$ is kinematically admissible and by means of **the balance equation** :

$$\int_\Omega\sigma_{ij}\dot{u}_{i,j}d\Omega=\int_\Omega f_i\dot{u}_i d\Omega+\int_S g_i\dot{u}_i d\Gamma+\int_{S_d}\sigma_{ij}n_j U_{i,k}\theta_k d\Gamma$$

from where:

$$\begin{aligned}G(\theta) &= \int_\Omega\dot{\psi}-f_i\dot{u}_i-\dot{f}_i u_i+\left(\psi-f_i u_i\right)\theta_{k,k}d\Omega-\int_S\left(g_i\dot{u}_i+\dot{g}_i u_i\right)d\Gamma-\int_S g_i u_i\left(\theta_{k,k}-\frac{\partial\theta}{\partial\eta_k}\eta_k\right)d\Gamma\\ &= \int_\Omega\sigma_{ij}\dot{u}_{i,j}-f_i\dot{u}_i d\Omega-\int_S g_i\dot{u}_i d\Gamma-\int_\Omega\dot{f}_i u_i d\Omega-\int_\Omega\frac{1}{2}\sigma_{ij}\left(u_{i,j}\theta_{p,j}+u_{j,p}\theta_{p,i}\right)d\Omega\\ &\quad+\int_\Omega\frac{\partial\psi}{\partial T}\dot{T}+\left(\psi-f_i u_i\right)\theta_{k,k}d\Omega-\int_S\dot{g}_i u_i+g_i u_i\left(\theta_{k,k}-\frac{\partial\theta}{\partial\eta_k}\eta_k\right)d\Gamma\\ &\quad+\int_\Omega\sigma_{ij}\varepsilon^0_{ij,k}\theta_k-\Lambda^{-1}_{ijpq}\sigma_{pq}\sigma^0_{ij,k}\theta_k d\Omega\end{aligned}$$

and finally:

$$\begin{aligned}G(\theta) &= \int_\Omega\sigma_{ij}u_{i,p}\theta_{p,j}-\psi\theta_{k,k}-\frac{\partial\psi}{\partial T}T_{,k}\theta_k d\Omega\\ &\quad+\int_\Omega\sigma_{ij}\varepsilon^0_{ij,k}\theta_k-\Lambda^{-1}_{ijpq}\sigma_{pq}\sigma^0_{ij,k}\theta_k d\Omega\\ &\quad+\int_\Omega f_i u_i\theta_{k,k}+f_{i,k}\theta_k u_i d\Omega\\ &\quad+\int_S g_{i,k}\theta_k u_i+g_i u_i\left(\theta_{k,k}-\frac{\partial\theta}{\partial\eta_k}\eta_k\right)d\Gamma\\ &\quad-\int_{S_d}\sigma_{ij}\eta_j U_{i,k}\theta_k d\Gamma\end{aligned}$$

Note:

- *In strains of Eulerian-Lagrange the first intégrande becomes* $h_{i,p}\sigma_{ij}u_{i,p}\theta_{p,j}$ *with* $h_{i,j}=\delta_{i,j}+u_{i,j}$.
- *In axisymetry, there is the formal analogy* $(x,y)\Leftrightarrow(r,z)$ *and all the components of the gradients implying the component orthoradiale are null except* $\varphi_{\theta,\theta}=\frac{\varphi_r}{r}$. *Moreover the surface element is multiplied by* R *to take into account the computation of the integral for a unit of radian.*
- *The possibility of taking into account fields of imposed displacements was not developed. Those are not constrained besides by the crack propagation since they appear via the equilibrium condition.*
- *In the surface term there are normal derivatives on the surface which do not have a meaning for the elements of skin used in Code_Aster. One thus resorts to the differential geometry and the derivatives contravariantes for better apprehending this intégrande on the surface of computation (cf [Appendix 2]).*

2 Discretization of rate of energy restitution

2.1 Method θ in dimension 2

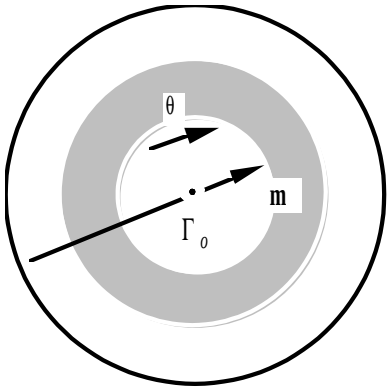
One recalls that rate of energy restitution G is solution of the variational equation:

$$\int_{\Gamma_0} G(S)\theta(s).\boldsymbol{m}(s)ds = G(\theta)\ ,\ \forall \theta \in \Theta$$

where:

- $\boldsymbol{m}$ is the unit norm with the crack tip Γ_0 located in the tangent plane at $\partial\Omega$ and returning in Ω
- $\Theta = \{\mu \text{ tels que } \mu.\boldsymbol{n} = 0 \text{ sur } \partial\Omega\}$.

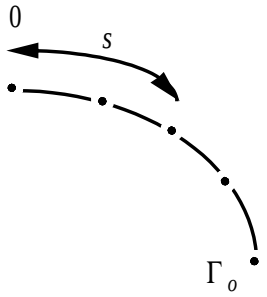
In dimension 2, **the crack tip Γ_0 is brought back to a point $\boldsymbol{M_0}$**, and one can choose a unit θ field in the vicinity of this point, so that: $G(\boldsymbol{M_0}) = G(\theta)$



Appear 2.1-a: Crack tip in 2D

2.2 Method θ in dimension 3

the dependence of $G(\theta)$ with respect to the field θ on the crack tip is more complex. The scalar field $G(s)$ can be discretized on a basis which we will note $(p_j(s))_{1 \leqslant j \leqslant N}$.



Appear 2.2-a: Discretization of the crack tip in 3D (curvilinear abscisse) P

Is G_j the components of $G(s)$ in this base:

$$G(s) = \sum_{j=1}^{N} G_j\, p_j(s)$$

One also gives oneself a base of functions tests for the fields θ, length P:

$$\tilde{\Theta}=\{\theta^i\in\Theta, i=1,\dots,P\}$$

$\tilde{\Theta}$ is a subset finite length of the group Θ.

$G(s)$ being solution of the variational equation $\int_{\Gamma_0} G(s)\theta(s).\boldsymbol{m}(s)ds=G(s), \forall\theta\in\Theta$, check G_j them then in particular:

$$\int_{\Gamma_0}\left(\sum_{j=1}^{N} G_j p_j(s)\right)\bar{\theta}^i.m(s)ds=G(\theta^i), \forall i\in[1,P]$$

that is to say:

$$\sum_{j=1}^{N}\left(\int_{\Gamma_0} p_j(s)\bar{\theta}^i.m(s)ds\right)G_j=G(\theta^i), \forall i\in[1,P]$$

G_j Can thus be given by solving the linear system with P equations and N unknowns:

$$\begin{aligned}\sum_{j=1}^{N} a_{ij}G_j &= b_i, i=1,P\\ \text{avec } a_{ij} &= \int_{\Gamma_0} p_j(s)\bar{\theta}^i(s).m(s)ds\\ b_i &= G(\theta^i)\end{aligned}$$

This system has a solution if one chooses P independent θ^i fields such as: $P\geqslant N$. It can comprise more equations than unknowns, in which case it is solved within the meaning of the least squares.

Note:

One gives oneself actually a base of functions tests for the trace of the fields θ on the crack tip Γ_0, noted $\bar{\theta}:\bar{\theta}(s)=\theta_{|\Gamma_0}(s)$. The data of the value of $\bar{\theta}^i$ on the crack tip Γ_0 is enough then to identify the field θ^i on all the field.

2.3 Choice in *Aster* of the discretization of G in dimension 3

2.3.1 Description of spaces of approximations

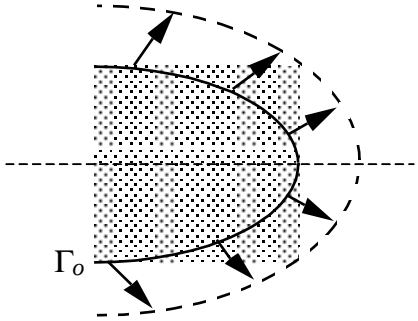
Note:

***In dimension 2**, there is no problem because by choosing a unit θ field in the vicinity of the crack tip, one obtains the relation $G=G(\theta)$. The rate of refund of energy is independent of the field θ.*

In dimension 3, the dependence of $G(\theta)$ with respect to the field θ on the crack tip is more complex. In *Code_Aster*, one can calculate:

- The value of $G(\theta)$ for a field θ given by the user (cf orders `CALC_G /OPTION= `CALC_G_GLOB'` [U4.82.03]). It is interesting to choose the unit θ field in the vicinity of the crack tip and such as:

$$\theta(s).\boldsymbol{m}(s)=1, \forall s \text{ abscisse curviligne de } \Gamma_0$$



Appear 2.3-a: Discretization of the crack tip in 3D (normal)

One obtains in this case a total rate of refund $\bar{G}$ corresponding to a uniform progression of crack such as:

$$\bar{G}\,l=\int_{\Gamma_0} G(s)\,ds=G(\theta)$$

where l is the length of the upper lip or lower of crack.

•Local rate of energy restitution $G(s)$ solution of the variational equation

$$\int_{\Gamma_0} G(s)\theta(s).\boldsymbol{m}(s)\,ds=G(\theta),\forall\,\theta\in\Theta$$

In this case, the user does not give a field θ, the fields θ^i necessary to the computation of $G(s)$ are calculated automatically (cf orders CALC_G/OPTION= `CALC_G' [U4.82.03]).

In *Code_Aster*, one chose **two families of bases** of functions tests for $\bar{\theta}$ and of decomposition for $G(s)$ (cf [§2.2]):

•**Polynomials of LEGENDRE** $\gamma_j(s)$ of degree j $(O\le j\le Deg_{max})$.

•**Shape functions** of the node k of Γ_0: $\phi_k(s)$ $(1\le k\le NNO=$nombre de noeuds de $\Gamma_0)$ (of degree 1 for the linear elements and of degree 2 for the quadratic elements).

Let us recall that the polynomials of LEGENDRE constitute a not normalized orthogonal family. They are obtained by the relation of recurrence:

$$(n+1)P_{n+1}(t)-(2n+1)\,t\,P_n(t)+n\,P_{n-1}(t)=0$$

In particular:

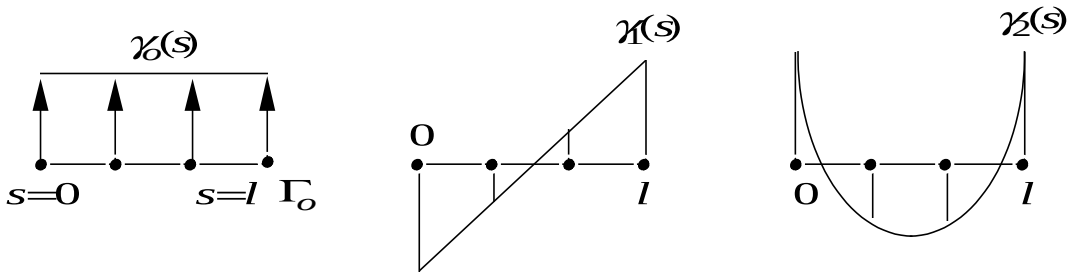
$$P_0(t)=1$$
$$P_1(t)=t$$
$$P_2(t)=\frac{(3t^2-1)}{2}$$
$$P_3(t)=\frac{(5t^3-3t)}{2}$$

In *Code_Aster*, one normalizes them in the form:

$$\gamma_j(s)=\sqrt{\frac{2j+1}{l}}\,P_j\left(\frac{2s}{l}-1\right)$$

where:

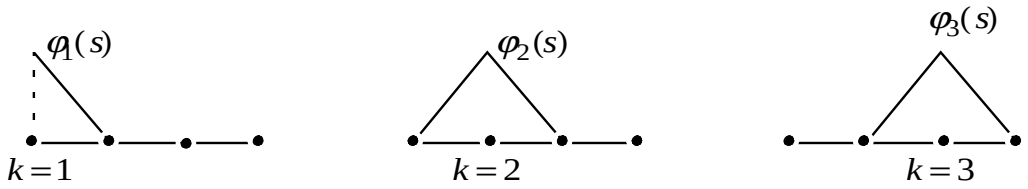
- s is the curvilinear abscisse of Γ_0,
- l the length of the crack tip Γ_0.



Appear 2.3-b: Polynomials of Legendre

In *Code_Aster*, one limits oneself to $Deg_{max}=7$ like maximum degree.

The shape functions $\varphi_k(s)$ are associated with the discretization of Γ_0.



Appear 2.3-c: Shape functions of the crack tip (linear elements)

Let us recall that one is brought to discretize $G(s)$ along the crack tip:

$$G(s)=\sum_{j=1}^{N} G_j p_j(s)$$

and to give a base of functions tests $\left(\bar{\theta}^i(s)\right)_{1\leq i\leq N}$ for the trace of the field θ on the crack tip Γ_0.

There thus exist several possible choices of discretizations, summarized in the table below:

	Polynomials of LEGENDRE	Shape functions
$G(s)$	$G(s)=\sum_{j=0}^{NDEG} G_j \gamma_j(s)$	$\sum_{j=1}^{NNO} G_j \varphi_j(s)$
$\bar{\theta}(s)$	$\left(\gamma_i(s)\right)_{1\leq i\leq NDEG}$	$\left(\varphi_i(s)\right)_{1\leq i\leq NNO}$

Table 2.3-1: Choice of the discretization

NNO : many nodes of the crack tip Γ_0

$NDEG$: maximum degree of the polynomials of LEGENDRE chosen by the user $NDEG\leq Deg_{max}=7$

In command CALC_G (cf [U4.82.03]) key words LISSAGE_THETA and LISSAGE_G make it possible to choose the discretization of $\bar{\theta}$ and of $G(s)$.

The options available in *Aster* are summarized in the following table:

	$\bar{\theta}(s)$	
	Polynomials of LEGENDRE	**Shape functions**

$G(s)$	**Polynomials of LEGENDRE**	LISSAGE_THETA = "LEGENDRE" LISSAGE_G = "LEGENDRE" (1st case)	LISSAGE_THETA = "LAGRANGE" LISSAGE_G = "LEGENDRE" (2nd case)
	Shape functions	Nonavailable	LISSAGE_THETA = "LAGRANGE" "LAGRANGE_REGU" LISSAGE_G = "LAGRANGE" "LAGRANGE_NO_NO" "LAGRANGE_REGU" (3rd case)

Table 2.3-2: Options of discretization of *Code_Aster*

2.3.2 First case (LEGENDRE-LEGENDRE)

$G(s)$ is broken up according to the polynomials of Legendre:

$$G(s)=\sum_{j=0}^{NDEG} G_j \gamma_j(s)$$

The base of the functions tests for $\theta(s)$ is defined starting from the polynomials of Legendre: $\theta(s)$

$$\tilde{\Theta}=\{\theta^i\in\Theta : \bar{\theta}^i(s).\boldsymbol{m}(s)=\varphi_i(s), i=1,\dots,NDEG\}$$

$NDEG$ The components G_j are given by solving the linear system with $NDEG$ equations:

$$\begin{cases} \sum_{j=0}^{NDEG} a_{ij} G_j = b_i, i=1, NDEG \\ \text{avec} \begin{cases} a_{ij}=\int_{\Gamma_0} \gamma_i(s)\gamma_j(s)\,ds \\ b_i = G(\theta^i) \end{cases} \end{cases}$$

The polynomials of Legendre forming an orthonormal base on Γ_0, one has $a_{ij}=\delta_{ij}$ and the linear system is thus summarized with:

$G_j = G(\theta^j)$ and thus $G(s)=\sum_{j=0}^{NDEG} G(\theta^j)\gamma_j(s)$.

2.3.3 Second case (LEGENDRE-LAGRANGE)

$G(s)$ is broken up according to the polynomials of Legendre:

$$G(s)=\sum_{j=0}^{NDEG} G_j \gamma_j(s)$$

The base of the functions tests for $\theta(s)$ is defined starting from the shape functions of NNO the nodes of the crack tip:

$$\tilde{\Theta}=\{\theta^i\in\Theta : \bar{\theta}^i(s).\boldsymbol{m}(s)=\varphi_i(s), i=1,\dots,NNO\}$$

where $\varphi_i(s)$ is the shape function of the node i of the crack tip.

There are then NNO equations with $NDEG$ unknowns:

$$\begin{cases} \sum_{j=0}^{NNO} a_{ij} G_j = b_i, i = 1, NNO \\ \text{avec} \begin{cases} a_{ij} = \int_{\Gamma_0} \gamma_j(s)\, \varphi_i(s)\, ds \\ b_i = G(\theta^i) \end{cases} \end{cases}$$

In this case, one must have $NDEG \leq NNO$, that is to say $NDEG < min(7, NNO)$ where NNO is the number of nodes of the crack tip.

2.3.4 Third case (LAGRANGE-LAGRANGE)

$G(s)$ is defined by the shape functions of NNO the nodes of the crack tip:

$$G(s) = \sum_{j=0}^{NNO} G_j \varphi_j(s)$$

The base of the functions tests for $\theta(s)$ is defined starting from the shape functions of NNO the nodes of the crack tip:

$$\tilde{\Theta} = \{\theta^i \in \Theta : \bar{\theta}^i(s).\boldsymbol{m}(s) = \varphi_i(s), i = 1, \ldots, NNO\}$$

where $\varphi_i(s)$ is the shape function of the nœuddu i crack tip.

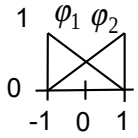
The system to be solved is the following:

$$\begin{cases} \sum_{j=0}^{NNO} a_{ij} G_j = G(\theta_i) \quad (i = 1, \ldots, NNO) \\ \text{avec } a_{ij} = \int_{\Gamma_0} \varphi_i(s)\, \varphi_j(s)\, ds \end{cases}$$

Linear elements:

If there are linear elements:

$$\varphi_1(x) = \frac{1}{2}(1-x)$$
$$\varphi_2(x) = \frac{1}{2}(1+x)$$



Elément de référence

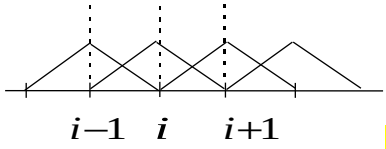
$$a_{i(i-j)} = a_{i,(i+j)} = 0, \text{ si } j \geq 2$$

$$a_{i(i-1)} = \int_{\Gamma_0} \varphi_i(s)\varphi_{i-1}(s)\, ds = \int_{s_{i-1}}^{s_i} \varphi_i(s)\varphi_{i-1}(s)\, ds$$

$$= \frac{s_i - s_{i-1}}{2} \int_{-1}^{+1} \varphi_i(x)\varphi_{i-1}(x)\, dx = \frac{s_i - s_{i-1}}{2} \int_{-1}^{+1} \frac{1}{4}(1-x^2)\, dx = \frac{1}{6}(s_i - s_{i-1})$$

$$a_{ii} = \frac{s_i - s_{i-1}}{2} \int_{-1}^{+1} \varphi_2^2(x)\, dx + \frac{s_{i+1} - s_i}{2} \int_{-1}^{+1} \varphi_1^2(x)\, dx$$

$$= \frac{s_i - s_{i-1}}{2} \int_{-1}^{+1} \frac{1}{4}(1+x)^2\, dx + \frac{s_{i+1} - s_i}{2} \int_{-1}^{+1} \frac{1}{4}(1-x)^2\, dx = \frac{1}{3}\left[(s_{i+1} - s_i) + (s_i - s_{i-1})\right]$$



Appear 2.3-d: Linear shape functions

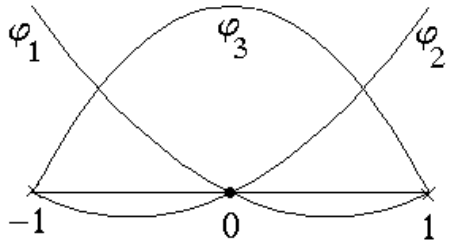
the matrix A_{ij} *is thus written:*

$$\frac{1}{6}\begin{pmatrix} 2(s_2-s_1) & (s_2-s_1) & 0 & 0 & \dots & 0 & 0 \\ (s_2-s_1) & 2(s_3-s_1) & (s_3-s_2) & 0 & \dots & 0 & 0 \\ 0 & (s_3-s_2) & 2(s_4-s_2) & (s_4-s_3) & \dots & 0 & 0 \\ 0 & 0 & (s_4-s_3) & 2(s_5-s_3) & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & 2(s_n-s_{n-2}) & (s_n-s_{n-1}) \\ 0 & 0 & 0 & 0 & \dots & (s_n-s_{n-1}) & 2(s_n-s_{n-1}) \end{pmatrix}$$

Quadratic elements:

If there are quadratic elements:

$$\varphi_1(x)=\frac{1}{2}x(x-1)$$
$$\varphi_2(x)=\frac{1}{2}x(x+1)$$
$$\varphi_3(x)=(1-x)(1+x)$$



Appear 2.3-e: Quadratic shape functions (Element of reference)

It is necessary to distinguish top node and medium node

- i = top node:

$$a_{i(i-j)} = a_{i,(i+j)} = 0 \text{, si } j \geq 3$$

$$a_{i(i-2)} = \int_{\Gamma_0} \varphi_i(s)\varphi_{i-2}(s)\,ds = \int_{s_{i-2}}^{s_i} \varphi_i(s)\varphi_{i-2}(s)\,ds$$

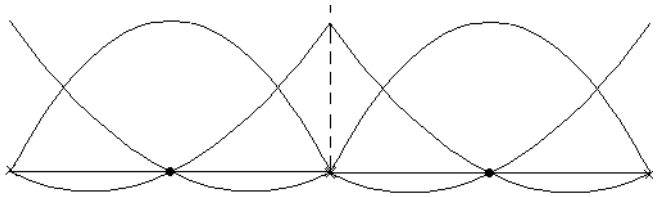
$$= \frac{(s_i - s_{i-2})}{2} \int_{-1}^{+1} \varphi_1(x)\varphi_2(x)\,dx = \frac{(s_i - s_{i-2})}{2} \int_{-1}^{+1} \frac{1}{4} x^2(x^2-1)\,dx$$

$$= -\frac{(s_i - s_{i-2})}{30}$$

$$a_{i(i-1)} = \int_{\Gamma_0} \varphi_i(s)\varphi_{i-1}(s)\,ds = \int_{s_{i-2}}^{s_i} \varphi_i(s)\varphi_{i-1}(s)\,ds = \frac{(s_i - s_{i-2})}{2} \int_{-1}^{+1} \varphi_2(x)\varphi_3(x)\,dx$$

$$= \frac{(s_i - s_{i-2})}{2} \int_{-1}^{+1} \frac{1}{2} x(x+1)^2(1-x)\,dx = \frac{(s_i - s_{i-2})}{15}$$

$$a_{ii} = \frac{s_i - s_{i-2}}{2} \int_{-1}^{+1} \varphi_2^2(x)\,dx + \frac{s_{i+2} - s_i}{2} \int_{-1}^{+1} \varphi_1^2(x)\,dx = \frac{2}{15}(s_{i+2} - s_{i-2})$$



Appear 2.3-f: Top node

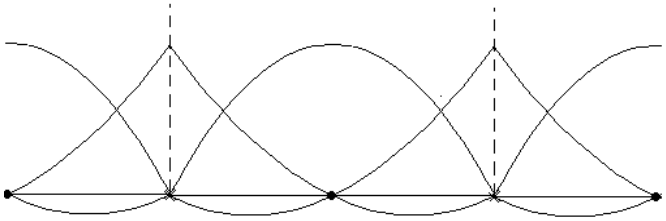
• i = medium node :

$$a_{i(i-j)} = a_{i,(i+j)} = 0 \text{, si } j \geq 2$$

$$a_{i(i-1)} = \int_{-1}^{+1} \frac{(s_{i+1} - s_{i-1})}{2} \varphi_3(x)\varphi_1(x)\,dx = \frac{(s_{i+1} - s_{i-1})}{2} \int_{-1}^{+1} \frac{1}{2} x(x-1)(1-x)(1+x)\,dx$$

$$= \frac{(s_{i+1} - s_{i-1})}{15}$$

$$a_{ii} = \int_{s_{i-1}}^{s_{i+1}} \varphi_i^2(s)\,ds = \frac{(s_{i+1} - s_i)}{2} \int_{-1}^{+1} (1-x)^2(1+x)^2\,dx = \frac{8}{15}(s_{i+1} - s_{i-1})$$

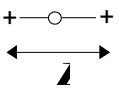


Appear 2.3-g: Medium node

the matrix A_{ij} is written:

$$\frac{1}{30}\begin{vmatrix} 4(s_3-s_1) & 2(s_3-s_1) & -(s_3-s_1) & 0 & 0 & \dots & 0 \\ 2(s_3-s_1) & 16(s_3-s_1) & 2(s_3-s_1) & 0 & 0 & \dots & 0 \\ -(s_3-s_1) & 2(s_3-s_1) & 4(s_5-s_1) & 2(s_5-s_3) & -(s_5-s_3) & \dots & 0 \\ 0 & 0 & 2(s_5-s_3) & 16(s_5-s_3) & 2(s_5-s_3) & \dots & 0 \\ 0 & 0 & -(s_5-s_3) & 2(s_5-s_3) & 4(s_7-s_3) & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & \dots & -(s_n-s_{n-2}) \\ 0 & 0 & 0 & 0 & 0 & \dots & 2(s_n-s_{n-2}) \\ 0 & 0 & 0 & 0 & 0 & \dots & 4(s_n-s_{n-2}) \end{vmatrix}$$

Typical case: $s_{i+2}-s_i=cste=l=$longueur d'un élément



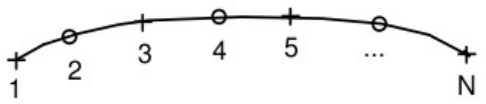
$$\frac{l}{30}\begin{vmatrix} 4 & 2 & -1 & 0 & 0 & \dots \\ 2 & 16 & 2 & 0 & 0 & \dots \\ -1 & 2 & 8 & 2 & -1 & \dots \\ 0 & 0 & 2 & 16 & 2 & \dots \\ 0 & 0 & -1 & 2 & 8 & \dots \\ . & . & & & & \\ . & . & & & & \\ . & . & & & & \end{vmatrix}$$

← noeud sommet de bord
← noeud milieu
← noeud sommet

2.3.5 Third case (LAGRANGE_NO_NO-LAGRANGE)

This method is resulting from the Lagrange-Lagrange method but it is simplified: one replaces the resolution of the linear system by multiplying the values $G(\theta^i)$ by a weight coefficient.

$$G_i=\alpha_i G(\theta^i)$$

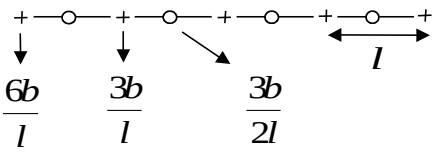


Appear 2.3-h: Method "node by node"

Moreover if $G(\theta^i)=cste=b, \forall i$ and that one considers G constant by element (this method does not have vectorial meaning), one a:

- top node of edge: $\frac{l}{30}(4+2-1)G=b$ that is to say $G=\frac{6}{l}b$
- top node: $\frac{l}{30}(-1+2+2+8-1)G=b$ that is to say $G=\frac{3}{l}b$

•medium node: $\frac{l}{30}(2+16+2)G=b$ that is to say $G=\frac{3}{2l}b$



What gives if the elements do not have constant lengths:

•edge top node: $\alpha_i=\frac{6}{(s_3-s_1)}$ or $\alpha_N=\frac{6}{(s_N-s_{N-2})}$

•top node: for example $\alpha_3=\frac{6}{(s_3-s_1)+(s_5-s_3)}=\frac{6}{(s_5-s_1)}$

is: $\alpha_i=\frac{6}{(s_{i+2}-s_{i-2})}$

or: $\alpha_i^{'}=\frac{3}{(s_{i+1}-s_i)}\approx\alpha_i$

•medium node: $\alpha_i=\frac{3}{2(s_{i+1}-s_i)}$

To activate this method it is necessary to specify in CALC_G: show

```
LISSAGE_G = "LAGRANGE_NO_NO"
LISSAGE_THETA = "LAGRANGE"
```

2.3.6 Third case (LAGRANGE_REGU-LAGRANGE_REGU)

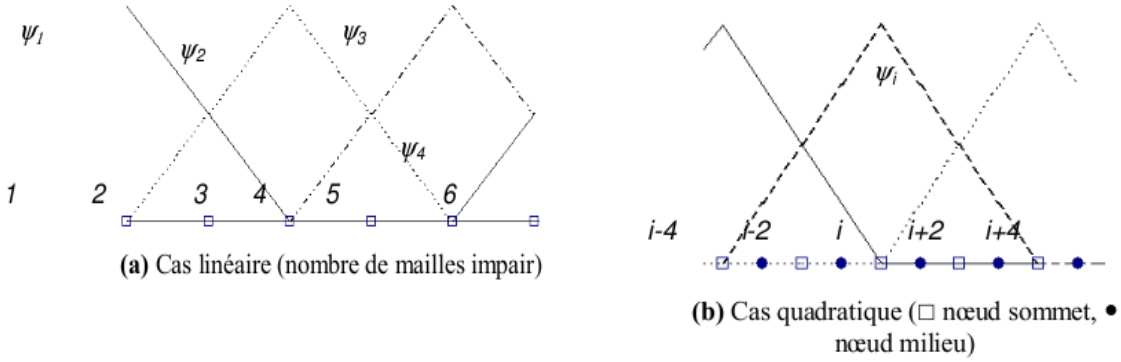
This régulasirée method is of exit of the Lagrange-Lagrange method, but it is modified in order to improve the robustness of it (reduction in the oscillations of G or of K along the crack tip for the quadratic meshes and the very irregular meshes).

The fields $\bar{\theta}^i$ and rate of energy restitution $G(s)$ are broken up on the same basis of noted functions ψ_k. The method "Lagrange regularized" consists in taking for ψ_k linear "shape functions" (whatever the basic mesh) whose support along the crack tip is wide on 4 meshes consecutive (against two for the method Lagrange classic), cf Appears 2.3-i.
That is to say N^{ma} the number of meshes in crack tip. Whatever the type of elements (linear or quadratic), the number N_θ of elements in the base $(\psi_k)_{k=1,N_\theta}$ equal to the number of fields θ^i to be built, is the following:

$N_\theta=\frac{N^{ma}}{2}+1$ if N^{ma} is even.

$N_\theta=\frac{(N^{ma}+1)}{2}+1$ if N^{ma} is odd.

In the case of an odd number of meshes, the last field θ is a simple linear interpolation on the last element enters 0 and 0.5, the preceding θ field being truncated.



(a) Cas linéaire (nombre de mailles impair)

(b) Cas quadratique (□ nœud sommet, • nœud milieu)

Appear 2.3-i: Lagrange method regularized

the system to solve is the following:

$$\sum_{j=0}^{N_\theta} a_{ij} G_j = G(\theta^i) \qquad (i=1, N_\theta)$$

$$\text{avec} \quad a_{ij} = \int_{\Gamma_0} \psi_i(s)\psi_j(s)\,ds$$

The base $(\psi_k)_{k=1,N_\theta}$ being identical for linear meshes and quadratic meshes, one will indicate in both cases by s_i the curvilinear abscisse of i - ème top node of the crack tip.

$a_{i(i-j)}=a_{i(i+j)}=0$ if $j\geq 2$

$$a_{i(i-1)} = \int_{\Gamma_0} \psi_i(s)\psi_{i-1}(s)ds = \int_{s_{k-2}}^{s_k} \psi_i(s)\psi_{i-1}(s)\,ds \qquad \text{avec} \quad k=2(i-1)+1$$

$$= \int_0^{s_k-s_{k-2}} \left(1-\frac{s}{s_k-s_{k-2}}\right)\frac{s}{s_k-s_{k-2}}\,ds = \frac{1}{6}(s_k-s_{k-2})$$

$$a_{ii} = \int_{\Gamma_0} \psi_i^2(s)ds = \frac{1}{3}(s_k-s_{k-2})$$

the matrix $A=[a_{ij}]$ is thus written:

$$\frac{1}{6}\begin{pmatrix} 2(s_3-s_1) & (s_3-s_1) & 0 & 0 & \dots \\ (s_3-s_1) & 2(s_5-s_1) & (s_5-s_3) & 0 & \dots \\ 0 & (s_5-s_3) & 2(s_7-s_3) & (s_7-s_5) & \dots \\ 0 & 0 & (s_7-s_5) & 2(s_9-s_5) & \dots \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \end{pmatrix}$$

Typical case amongst meshes odd: one names N_f the number of the last node

$$a_{N_\theta(N_\theta-1)} = \frac{1}{6}(s_{N_f}-s_{N_f-1})$$
$$a_{(N_\theta-1)(N_\theta-1)} = \frac{1}{3}(s_{N_f-1}-s_{N_f-3})+\frac{7}{12}(s_{N_f}-s_{N_f-1})$$
$$a_{N_\theta N_\theta} = \frac{1}{12}(s_{N_f}-s_{N_f-1})$$

Typical case of the closed crack tips: for reasons of conveniences of programming, the number of fields θ is calculated starting from the number of meshes as for the classical crack tips, even if one could have taken one of less of them. One is thus satisfied to add the following terms in the matrix:

$$a_{1(N_\theta-1)}=\frac{1}{6}(s_{N_f}-s_{N_f-2}) \quad a_{N_\theta 2}=\frac{1}{6}(s_3-s_1)$$

To activate this method it is necessary to specify in CALC_G:

```
LISSAGE_G = "LAGRANGE_REGU"
LISSAGE_THETA = "LAGRANGE_REGU"
```

2.3.7 Correction of the values at the ends of the crack tip

When the crack tip emerges, a particular additional processing is carried out.
It was observed for the lissages of the Lagrange type (and its alternatives) that the numerical values of $G(\theta^i)$ for $i=1$ and $i=n$ are particular "false". That is probably due to the order of the singularity which is not any more into -1/2 near free surfaces. Indeed, the order of the singularity to edges depends on ν (and of the angle between the crack tip and free surface and of the angle between the norm on the surface of crack and the norm on free surface). Even for a crack in an orthogonal plane at free surface and emerging of way orthogonal, the singularity is not -1/2 if $\nu\neq 0$.

In order to improve the results at the points of edge, one carries out a modification of $G(\theta^i)$ for $i=1$ and $i=n$ the lissage of LAGRANGE-LAGRANGE and with a modification directly of $G(s_i)$ for $i=1$ and $i=n$ the LAGRANGE_NO_NO-LAGRANGE, only for the option CALC_K_G. They are also modified $K_j(\theta^i)$ $j=I, II, III$. This processing is made even if conditions of symmetry are applied to edges of the bottom (whereas in this case, the order of the singularity is well into -1/2 and no processing would be necessary).

Linear lissage LAGRANGE-LAGRANGE and meshes

the assumption is made that $G(s_1)=G(s_2)=G(s_3)=G_a$ and that $G(s_n)=G(s_{n-1})=G(s_{n-2})=G_b$.
Then by multiplying the matrix A by the vector $G(s)$ one obtains:

$$G(\theta^1)=\frac{1}{2}(s_2-s_1)G_a$$
$$G(\theta^2)=\frac{1}{2}(s_3-s_1)G_a$$
...
$$G(\theta^{n-1})=\frac{1}{2}(s_n-s_{n-2})G_b$$
$$G(\theta^n)=\frac{1}{2}(s_n-s_{n-1})G_b$$

Is $G(\theta^1)=G(\theta^2)\frac{(s_2-s_1)}{(s_3-s_1)}$ and $G(\theta^n)=G(\theta^{n-1})\frac{(s_n-s_{n-1})}{(s_n-s_{n-2})}$

quadratic Lissage LAGRANGE-LAGRANGE and meshes

the assumption is made that $G(s_1)=G(s_2)=G(s_3)=G_a$ and that $G(s_n)=G(s_{n-1})=G(s_{n-2})=G_b$. Then by multiplying the matrix A by the vector $G(s)$ one obtains:

$$G(\theta^1)=\frac{1}{6}(s_3-s_1)G_a$$

$$G(\theta^2)=\frac{4}{6}(s_3-s_1)G_a$$

…

$$G(\theta^{n-1})=\frac{4}{6}(s_n-s_{n-2})G_b$$

$$G(\theta^n)=\frac{4}{6}(s_n-s_{n-2})G_b$$

Is $G(\theta^1)=\frac{1}{4}G(\theta^2)$ and $G(\theta^n)=\frac{1}{4}G(\theta^{n-1})$

Lissage LAGRANGE_NO_NO-LAGRANGE

One makes a linear extrapolation between 2nd and 3rd points of the bottom (resp. between the 2 penultimate points of the bottom). That is to say:

$G(s_1)=G(s_2)+\frac{(s_1-s_2)}{(s_3-s_2)}\left(G(s_3)-G(s_2)\right)$ and $G(s_n)=G(s_{n-1})\frac{(s_n-s_{n-1})}{(s_{n-2}-s_{n-1})}\left(G(s_{n-2})-G(s_{n-1})\right)$

2.4 Establishment of G in linear thermoelasticity in *Aster*

2.4.1 Element types and of loadings

In *Code_Aster*, it is possible to calculate in **linear thermoelasticity** rate of energy restitution in 2D $(G(\theta))$ and 3D (local value $G(s)$ or total value $(G(\theta))$ using command CALC_G [U4.82.03].

The virtual field of propagation of crack θ is calculated automatically in command CALC_G starting from the information provided by the user. In 2D and 3D-total, it can also be calculated prior to the assistance of commands CALC_THETA [U4.82.02] or CREA_CHAMP [U4.44.11]).

These computations are valid for **the following modelizations** :

- D_PLAN (crack with a grid or not with a grid)
- C_PLAN (crack with a grid or not with a grid)
- AXIS (crack with a grid only)
- 3D (crack with a grid or not with a grid)

and for **the following** thermomechanical loadings:

- f, field of volume forces applied to Ω (mechanical loads of type PESANTEUR, ROTATION, FORCE_INTERNE)
- g, field of surface forces applied to part S of $\delta\Omega$ (including on the lips of crack: PRES_REP, FORCE_FACE)
- T, field of temperature (transmitted via the field material: AFFE_MATERIAU/AFFE_VARC)
- ε^0, field the preone (PRE_EPSI).

These **loadings** can depend on time and space. One does not take account of the term due to the displacements imposed on S_d, one thus should not impose conditions of Dirichlet on the lips of crack.

The characteristics of the material (E,ν,α) can depend on the temperature T and space while remaining constant by elements.

Moreover, a stress field **initial** σ^0 can be taken into account.

2.4.2 Environment necessary

Fissures with a grid:

For the computation of the rate of refund (options CALC_G and CALC_G_GLOB), it is necessary to characterize beforehand crack via the concept of the fond_fiss type (in 3D: list ordered nodes of the bottom, meshes of the upper lip and the lower lip; in 2D: basic node of crack and norm to crack), with command DEFI_FOND_FISS [U4.82.01].

When that the crack is laid out along an axis of symmetry, one can be satisfied not to represent that half of the model, and to specify by the key word the symmetry of loading SYME in DEFI_FOND_FISS. By default, one supposes that there is no symmetry. However the model presents a symmetry, CALC_G automatically detects it via the concept fond_fiss.

Fissure nonwith a grid (method X-FEM):

In 2D as in 3D, the crack must be defined, for mechanical computation and postprocessing, using command DEFI_FISS_XFEM. The key word CRACK must be indicated in CALC_G.

If the crack is not with a grid, it is not possible to take into account possible symmetries of the model compared to the lips of crack.

The computation of G is done in postprocessing, only starting from the field of solution displacement of computation on the model considered. In particular, the density of free energy and the forced are calculated starting from the field of displacement and the characteristics of the material.

2.4.3 Computations of the various terms of rate of energy restitution

the complete statement of $G(\theta)$ is given to [§1.3]. We will detail each term. The field θ is null apart from a disc of radius $R_{\text{sup}}(s)$ defined in chapter 3 [Figure 3.3-a]. Let us notice that as all the terms utilize θ or its gradient, the elementary terms are null apart from this disc of radius $R_{\text{sup}}(s)$. In command CALC_G, it is thus not necessary to specify the loadings which do not apply in this zone.

2.4.3.1 Elementary classical term

$$TCLA=\sigma_{ij}u_{i,p}\theta_{p,j}-\psi(\varepsilon(u),T)\theta_{k,k}$$

the density of elastic strain energy $\Psi(\varepsilon(u),T)$ is written in linear thermoelasticity:

•in 3D and AXIS :

$$\Psi(\varepsilon(\boldsymbol{u}),T)=\frac{1}{2}\lambda(\varepsilon_{ii})^2+\mu\,\varepsilon_{ij}\varepsilon_{ij}-\psi_{th}$$

•in plane strains:

$$\Psi(\varepsilon(\boldsymbol{u}),T)=\frac{(1-\nu)E}{2(1+\nu)(1-2\nu)}(\varepsilon_{xx}^2+\varepsilon_{yy}^2)+\frac{\nu E}{(1+\nu)(1-2\nu)}\varepsilon_{xx}\varepsilon_{yy}+\frac{E}{(1+\nu)}\varepsilon_{xy}^2-\psi_{th}$$

•in plane stresses:

$$\Psi(\varepsilon(\boldsymbol{u}),T)=\frac{E}{2(1-\nu^2)}(\varepsilon_{xx}^2+\varepsilon_{yy}^2)+\frac{\nu E}{(1-\nu^2)}\varepsilon_{xx}\varepsilon_{yy}+\frac{E}{(1+\nu)}\varepsilon_{xy}^2-\psi_{th}$$

with $\Psi_{th}=3K\alpha(T-T_{réf})\varepsilon_{ii}-\frac{9}{2}K\alpha^2(T-T_{réf})^2$

where:

$$3K=\frac{E}{1-2\nu} \quad ;\lambda=\frac{\nu E}{(1+\nu)(1-2\nu)} \quad ;2\mu=\frac{E}{1+\nu}$$

E : modulate YOUNG
ν : Poisson's ratio
λ , μ : coefficients of LAME
α : thermal thermal expansion

the density of elastic strain energy $\psi(\varepsilon(u),T)$ can be written in a general way in the form:

$$\Psi(\varepsilon(u),T)=\frac{1}{2}K(\varepsilon_{kk}-3\alpha(T-T_{réf}))^2+\frac{2\mu}{3}\varepsilon_{eq}^2$$

avec $\varepsilon_{eq}^2=\frac{3}{2}\varepsilon_{ij}^D\varepsilon_{ij}^D$ et $\varepsilon_{ij}^D=\varepsilon_{ij}-\frac{1}{3}\varepsilon_{kk}\delta_{ij}$

soit $\varepsilon_{eq}^2=\frac{1}{2}(3\varepsilon_{ij}\varepsilon_{ij}-\varepsilon_{kk}^2)$

et $$\begin{aligned}\Psi(\varepsilon(u),T) &= \frac{1}{2}K\varepsilon_{kk}^2-3K\alpha(T-T_{réf})\varepsilon_{kk}+\frac{9}{2}K\alpha^2(T-T_{réf})^2+\mu\varepsilon_{ij}\varepsilon_{ij}-\frac{\mu}{3}\varepsilon_{kk}^2\\ &= \frac{\lambda}{2}\varepsilon_{kk}^2+\mu\varepsilon_{ij}\varepsilon_{ij}-3K\alpha(T-T_{réf})\varepsilon_{kk}+\frac{9}{2}K\alpha^2(T-T_{réf})^2\end{aligned}$$

2.4.3.2 Term volume force

$$TFOR=f_i u_i \theta_{k,k}+f_{i,k}\theta_k u_i$$

2.4.3.3 Term forces surface

$$TSUR=g_{i,k}\theta_k u_i+g_i u_i\left(\theta_{k,k}-\frac{\partial\theta}{\partial n_k}n_k\right)$$

Note::

In this surface term there are normal derivatives on the surface which do not have a meaning for the elements of skin used in Code_Aster. One thus resorts to the differential geometry and the derivatives contravariantes for better apprehending this intégrande on the surface of computation (cf [Appendix 2]).

2.4.3.4 Thermal term

$$THER=-\frac{\partial\Psi}{\partial T}T_{,k}\theta_k$$

with:

$$\frac{\partial\Psi}{\partial T}(\varepsilon(u),T)=\left[\frac{1}{2}\frac{dK(T)}{dT}(\varepsilon_{kk}-3\alpha(T-T_{réf}))-3K\left(\alpha+\frac{d\alpha(T)}{dT}(T-T_{réf})\right)\right](\varepsilon_{kk}-3\alpha(T-T_{réf}))$$

2.4.3.5 Term of predeformations and initial stresses

$$TINI=\left[\sigma_{ij}\varepsilon_{ij,k}^0-\Lambda^{-1}_{ijpq}\sigma_{pq}\sigma_{ij,k}^0\right]\theta_k$$

One can notice that so $\sigma=0$ then $TINI=0$

Remark 1:

As the rest of this documentation, the presence of initial stresses is valid only in the case of elasticity, and here even isotropic linear. To be activated, it is thus necessary to be in an incremental behavior model (COMP_INCR) to a relation ELAS. It is not possible to provide a stress field initial in any another case.

Notice 2:

Taking into account the difficulty of validation, it is not for time not possible to cumulate predeformations (loading under key word `PRE-EPSI` *) and forced initial (key word* `SIGM_INIT` *of* `CALC_G` *).*

Notice 3:

In all the cases, this stress field initial must be ***AUTO-EQUILIBRE*** *, in absence of crack, with the only limiting conditions. The user will be able (would have…) to check that its stress field initial is licit by applying it in key word* `ETAT_INIT` *of operator* `STAT_NON_LINE` *, with an incremental elastic behavior (* `COMP_INCR, RELATION = "ELAS"` *), with the only limiting conditions; the result mechanical one must be the same stress field without additional strains.*

Notice 4:

The stress field initial must be used beforehand in thermomechanical computation. The approach of computation of rate of energy restitution in the presence of initial stresses is presented Figure 2.1 . One will also refer to the case dedicated test.

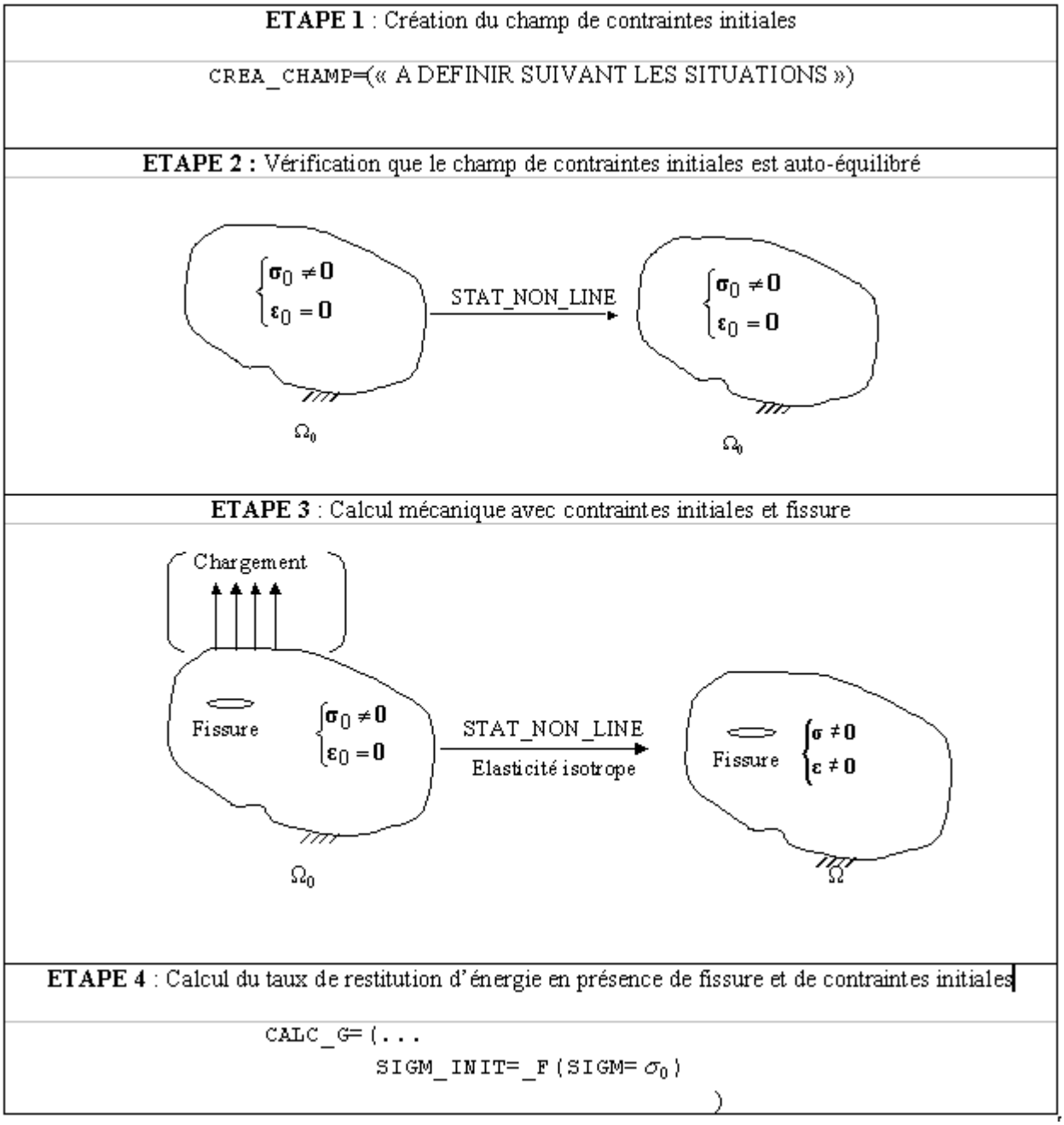
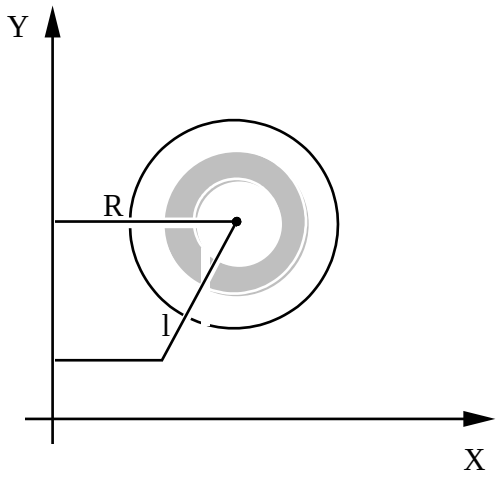


Figure 2.1 : Approach of computation in the presence of initial stresses.

2.4.4 Standardization of rate of energy restitution in *Aster*

2.4.4.1 Axisymetry

$G(\theta)$ such as it is established here, calculates the restitution of energy in the definite kinematics par. θ It can be necessary to standardize **it** (**with the hand! it is not done automatically in the code**) to be able to compare with an intrinsic value with the material, in particular into axisymmetric. Let us consider the case of an inclined crack, whose crack tip is at a distance R from the axis of symmetry:



Appear 2.4.4.1 - has: Crack tip in axisymetry

In *Aster*, the axis OY is the axis of symmetry in modelization "AXIS" and the rate of refund of energy calculated is:

$$G(\theta)=-\frac{dW}{dl}$$

where W is potential energy per unit of radian.

However the intrinsic value of rate of energy restitution is:

$$G=-\frac{dW_{totale}}{dA}$$

where:

- W_{totale} is total potential energy,
- dA is the variation of surface of crack.

with: $W_{totale}=2\pi W$
$dA=2\pi R\,dl$

from where: $\frac{dW_{totale}}{dA}=2\pi\frac{dW}{dl}\frac{dl}{dA}=\frac{1}{R}\frac{dW}{dl}$

and thus $G=\frac{1}{R}G(\theta)$ in axisymetry.

2.4.4.2 Other cases

In dimension 3, the value of $G(\theta)$ for a field θ given by the user are such as:

$$G(\theta)=\int_{\Gamma_0} G(s)\theta(s).\boldsymbol{m}(s)ds$$

By default, the direction of the field θ is normal with the crack tip in the plane of the lips. By choosing a unit θ field in the vicinity of the crack tip, one a:

$$\theta(s).\boldsymbol{m}(s)=1 \quad , \quad \forall s \text{ abscisse curviligne de } \Gamma_0$$

and:

$$G(\theta)=\int_{\Gamma_0} G(s)d\Gamma$$

That is to say G the total rate of refund of energy. To have its value per unit of length, it is necessary to divide the value obtained by the length of crack l :

$$G=\frac{G(\theta)}{l} \text{ en 3D}$$

In dimension 2 (C_PLAN and D_PLAN), the crack tip is tiny room to a point and the value of $G(\theta)$ is independent of the choice of the field θ (with $\theta\in\Theta$ and θ unit in the vicinity of the crack tip).

$$G=G(\theta) \quad , \quad \forall \theta\in\Theta$$

3 Introduction of the field θ into *Aster*

3.1 Conditions to fill

the field θ is a field of vectors, definite on the fissured solid, which represents the transformation of the field during a crack propagation within the meaning of [§1]. The transformation should modify only the position of the crack tip and not edge of the field $\delta\Omega$, i.e.: $\theta.\boldsymbol{n}=0$ on (n norm with $\delta\Omega$). Moreover, **the field θ must be regular** on Ω [bib4].

Because of the singularity of the field of displacement, it is interesting from the numerical point of view to use constant θ fields in a vicinity of Γ_0 , thus cancelling in this vicinity the singular terms $\psi\theta_{k,k}-\sigma_{ij}u_{i,p}\theta_{p,k}$ in $G(\theta)$.

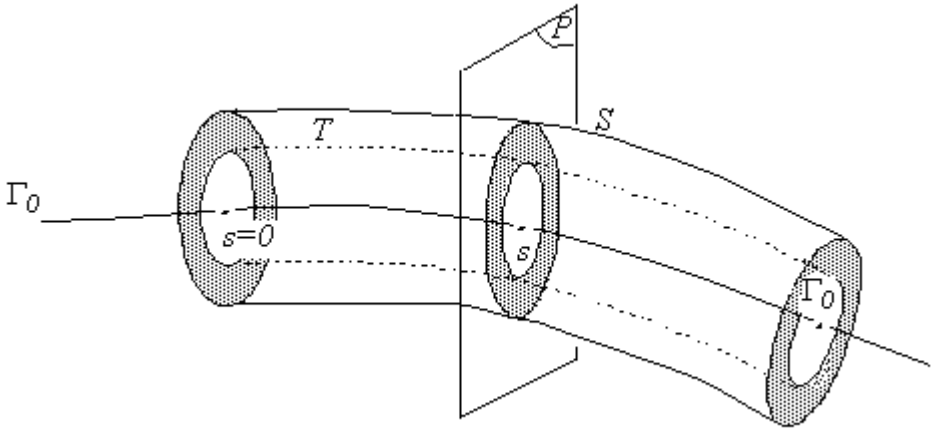
3.2 Choice of the field θ in dimension 3

3.2.1 Method of construction

One must build a checking θ field:

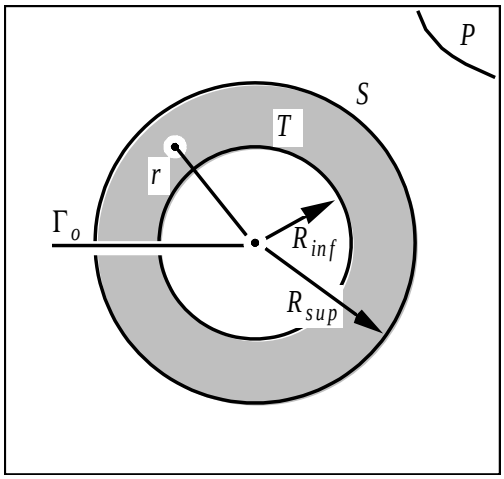
$$\begin{cases}\theta_n=\theta.\boldsymbol{n}=0 & \text{sur le bord du domaine } \delta\Omega \text{ (}\boldsymbol{n}\text{ est la normale à } \delta\Omega\text{)}\\ \bar{\theta}=\bar{\theta}_0 & \text{donné sur le fond de fissure } \Gamma_0\end{cases}$$

where $\bar{\theta}$ represents the trace of θ on Γ_0 .
One gives oneself two surfaces toric T and S (deformed cylinders) surrounding the crack tip Γ_0. to check the first condition above, it should in particular be taken care that contour S is strictly included in Ω .



Appear 3.2.1-a: Construction of the field θ in 3D (overall picture)

One notes $R_{inf}(s)$ the variable radius of T and $R_{sup}(s)$ that of S .



Appear 3.2.1-b: Construction of the field θ in 3D (plane of cut)

In any point of Γ_0, located by its curvilinear abscisse s, one can define a normal plane P into which the field θ is introduced in the following way:

- $\theta_n(r(s))=\bar{\theta}_0(s)$ pour $0\leq r(s)\leq R_{inf}(s)$
- $\theta_n(r(s))=0$ pour $r(s)\geq R_{sup}(s)$
- θ_n vary linearly compared to the radius $r(s)$ in contour $S(R_{sup}(s))\setminus T(R_{inf}(s))$
- θ_n is continuous in $S(R_{sup}(s))$.

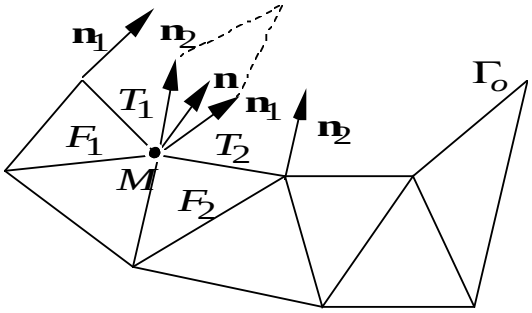
This way introduce θ is geometrical. It amounts giving itself two radius $R_{inf}(s)$ and $R_{sup}(s)$, and carrying out computations of distance from a point running to the crack tip to determine the value of θ in this point.

3.2.2 Calculation algorithms

the modulus $|\theta|$ of the field θ being given on all the crack tip Γ_0 (by the user or the method θ, to see [§2.3]), the problem is to determine the field θ (norm and direction) in any point of the field Ω.

One notes $|\theta|_i$, $R_{inf\,i}$ and $R_{sup\,i}$ respectively Γ_0 the modulus of the field θ, radius R_{inf} and R_{sup} for i - ème node of the crack tip.
The procedure of computation of the field θ in any point of Ω is the following one:

- **Computation of the field θ in each point of Γ_0 :** the modulus $|\theta|_i$ being given, the problem is to determine the direction of θ. θ must be locally in the tangent with the lips of crack and normal plane to the edge to which it belongs. θ being calculated with the nodes, in the general case (nonplane crack tip) the direction of θ will be realized on the 2 edges of Γ_0 having the joint node.



Appear 3.2.2-a: Construction of the field θ in 3D (normal)

Are F_1 and F_2 two sides belonging to the lips of crack and including the successive edges T_1 and T_2 of Γ_0. One calculates initially the norm $\boldsymbol{n_1}$ with the edge T_1 in the plane of the face F_1 then the norm $\boldsymbol{n_2}$ with the edge T_2 in the plane of the face F_2.

$\boldsymbol{n_1}$ and $\boldsymbol{n_2}$ being unit norms, one from of deduced $\boldsymbol{n}=\frac{\boldsymbol{n_1}+\boldsymbol{n_2}}{2}$ then $\theta(M)=|\theta(M)|\boldsymbol{n}$ for $M\in\Gamma_0$.

It is considered that the sides F_i are right:

- If F_i is a triangle, the plane of the face F_i is defined.
- If F_i is a quadrangle, one cuts out F_i in 2 triangles F_{i1} and F_{i2}. One must then calculate the equations of the two planes containing the sides F_{i1} and F_{i2} do two calculations of norm per edge T_i.

This computation requires to know the sides belonging to the lips of crack and including an edge of Γ_0. In *Code_Aster*, the user returns all the surface elements belonging to the lips of crack. These sides appear in one or more mesh groups and are described in connectivities of the surface elements. The algorithm sorts these sides to preserve only those having 2 tops on Γ_0. The stages of the algorithm are the following ones:

- For each node of Γ_0, one extracts the meshes pertaining one to the lips from crack,
- Of these meshes, one tri those having two nodes on Γ_0,
- One recovers the type of the face (SORTED or QUAD) and one calculates the equation of the plane (S) tangent (S),
- For each edge of Γ_0 tops N_i, N_{i+1} computation of the norms $\boldsymbol{n_{i,1}}$ $\boldsymbol{n_{i+1,1}}$, $\boldsymbol{n_{i,2}}$ and $\boldsymbol{n_{i+1,2}}$.

Lastly, θ is calculated according to the following algorithm:

Buckle on the tops N_i of Γ_0 :

$$\boldsymbol{n_i}=\frac{1}{2}(\boldsymbol{n_{i,1}}+\boldsymbol{n_{i,2}})$$
$$\theta(N_i)=|\theta|_i\,\boldsymbol{n_i}$$

End of the loop on the tops N_i of Γ_0

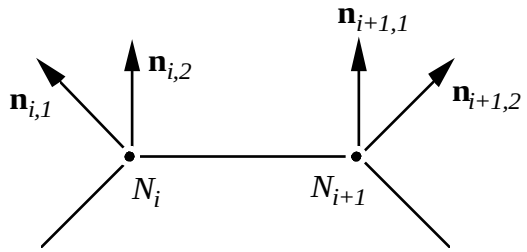
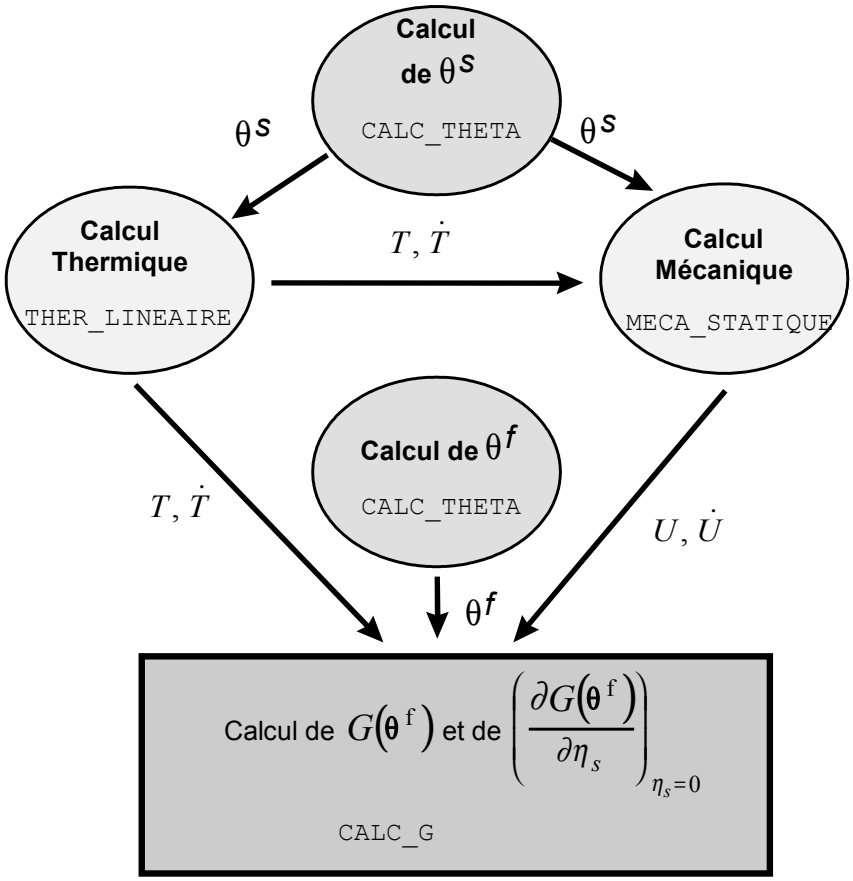


Figure 3.2.2-b: Notations of the norms to the crack tip

•**Computation of the projection Γ_0 of each point of Ω :**

For each the node is outside the field of definition with a right profile of the EXCLU type node: M

•Recovery of the coordinates of M



•

•Loop on the nodes N_k of Γ_0 $k=1, NNO-1$

Recovery of the coordinates of N_k and N_{k+1}

Computation of $s_k = \frac{N_k N_{k+1} . N_k M}{\| N_k N_{k+1} \|}$

$/ s_k < 0 : s_k = 0$

$/ s_k > 1 : s_k = 1$

Computation of the coordinates of $\bar{M}_k : \boldsymbol{O\bar{M}_k} = \boldsymbol{O\bar{N}_k} + s_k \boldsymbol{N_k N_{k+1}}$

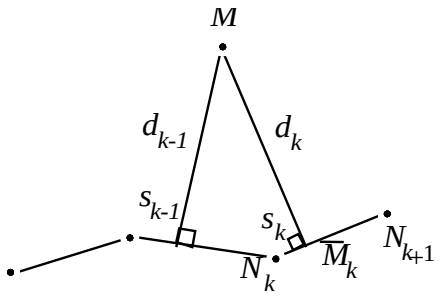
Computation of $d_k = d(M, \bar{M}_k)$

Fine buckles

•Recovery of i such as $d_i = \min_k (d_k)$

•Knowing i, one recovers N_i, N_{i+1}, s_i and the projection $\bar{M}$ of M on Γ_0 such as:

$$\boldsymbol{N_i \bar{M} = s_i N_i N_{i+1}}$$



•**Computation of the field θ in each point of Ω**:

Buckle on the nodes M

•Computation of the projection $\bar{M}$ of M on Γ_0 (cf above: give N_i, N_{i+1}, s_i)

•Computation of $d = d(M, \bar{M})$

•Computation from $\theta(\bar{M})$ linear interpolation:

$$\theta(\bar{M}) = (1 - s_i)\theta(N_i) + s_i \theta(N_{i+1})$$

•Linear computation $R_{inf}(s_i)$ $R_{sup}(s_i)$ deetpar interpolation:

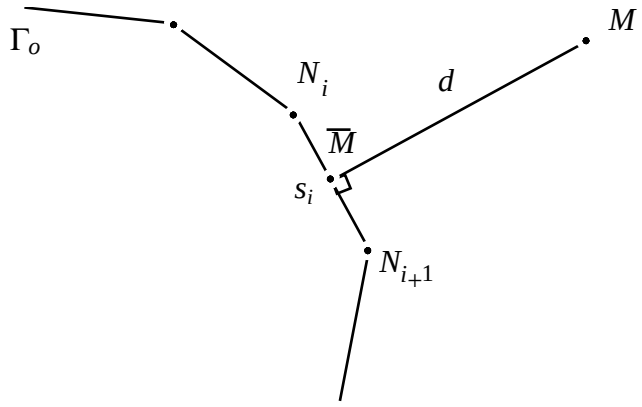
$$R_{inf}(s_i) = (1 - s_i) R_{inf\,i} + s_i R_{inf\,i+1}$$
$$R_{¿}(s_i) = (1 - s_i) R_{sup\,i} + s_i R_{sup\,i+1}$$

/ Si $d > R_{sup}(s_i)$, $\theta(M) = 0$

/ Si $d < R_{inf}(s_i)$, $\theta(M) = \theta(\bar{M})$

/ Si $R_{inf}(s_i) \le d \le R_{sup}(s_i)$, $\alpha = \dfrac{d - R_{inf}(s_i)}{R_{sup}(s_i) - R_{inf}(s_i)}$ et $\theta(M) = (1 - \alpha)\theta(\bar{M})$

Fine Figure



3.2.2-d buckles: Computation of the champen θ 3D

3.3 Choice of the field θ in dimension 2

It acts of a cas particulier of dimension 3. Γ_0 is limited to a point, the user chooses radius R_{inf} and R_{sup}, the modulus θ in crack tip $|\theta_0|$ and the field θ are built so that:

$$\theta(r)=0 \quad \text{si} \quad r \geq R_{sup}$$
$$\theta(r)=|\theta_0|\boldsymbol{n} \quad \text{si} \quad r \leq R_{inf}$$
$$\theta(r)=\frac{R_{sup}-r}{R_{sup}-R_{inf}}|\theta_0|\boldsymbol{n} \quad \text{si} \quad R_{inf} \leq r \leq R_{sup}$$

To check the condition $\theta . \boldsymbol{n}=0$ on $\delta\Omega$, it should in particular be taken care that the contour of radius R_{sup} is strictly included in Ω.

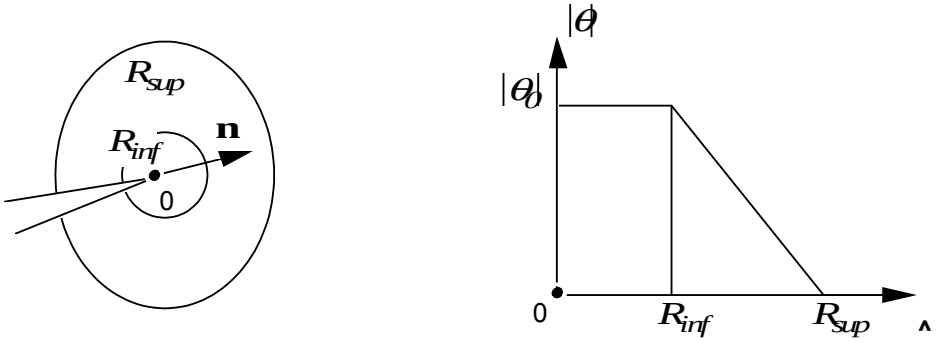


Figure 3.3-a: Computation of the field θ in 2D

3.4 Another method

the user can enter itself the field θ, by means of command CREA_CHAMP [U4.72.04] of *Code_Aster* which makes it possible to affect θ node by node or nodes group.

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Description of the versions of the document

Index document	Version Aster	Author (S) Organization (S)	Description of the modifications
D	7.4		Introduction of computation of the derivative
E	8.4	E. Crystal, EDF-R&D/AMA	Introduction of the method “Lagrange regularized”
F	9.4	E. Crystal, EDF-R&D/AMA	Modification of the way present the discretization of G and deen θ 3D