Calculation of the stress intensity factors in linear thermoelasticity

Summary:

One presents the method of calculating of the stress intensity factors K_I, K_{II} and K_{III} in linear thermoelasticity. The formulation regards the rate of refund of energy as the symmetrical bilinear shape of the field of displacement $\boldsymbol{u}$ and uses the explicit expressions of the fields of singular displacements known in plane linear elasticity.

This method is usable using the option `CALC_K_G` of the order `CALC_G`, as well for a crack with a grid (classical finite elements) as for a crack nonwith a grid (finite elements nouveau riches: method X-FEM).

This method is also usable to calculate the factors of intensity of the constraints associated with the clean modes with vibration with a structure.

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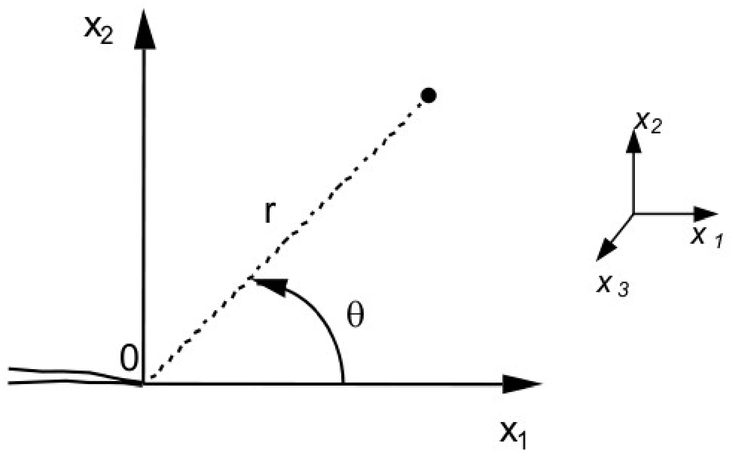
1.1 Presentation in plane linear thermoelasticity



Are the axes of Cartesian coordinates $O x_1$ in the prolongation of the crack and $O x_2$ perpendicular with the crack. The problem is plan. We will express the Cartesian components of displacements and the constraints according to the polar coordinates r and θ.

In linear elasticity, the system of the equilibrium equations, without voluminal force, and the boundary conditions homogeneous on the crack, the worthless constraints ad infinitum, admit a noncommonplace solution of the form $\boldsymbol{u_i}=\sqrt{(r)}\,g_i(\theta)$. The constraints are infinite at the bottom of the crack like $r^{-1/2}$ [bib3].

For an unspecified problem in plane linear elasticity (plane strains or plane stresses), the field of displacement $\boldsymbol{u}$ can break up into a singular part and a regular part. The singular part, also called singularity, is that clarified above Ci -. It is associated with the factors of intensity of the constraints K. In linear elasticity, modes of rupture I (opening) and II (slip plan) are separate:

$$\boldsymbol{u}=\boldsymbol{u_R}+K_I\boldsymbol{u_S^I}+K_{II}\boldsymbol{u_S^{II}}$$

with:

$$\begin{cases} u_{S1}^I=\dfrac{1+\nu}{E}\left(\dfrac{r}{2\pi}\right)^{1/2}\cos\left(\dfrac{\theta}{2}\right)(k-\cos\theta) \\ u_{S2}^I=\dfrac{1+\nu}{E}\left(\dfrac{r}{2\pi}\right)^{1/2}\sin\left(\dfrac{\theta}{2}\right)(k-\cos\theta) \end{cases}$$

$$\begin{cases} u_{S1}^{II} = \frac{1+\nu}{E} \left(\frac{r}{2\pi}\right)^{1/2} \sin\left(\frac{\theta}{2}\right)\left(k+\cos\theta-2\right) \\ u_{S2}^{II} = -\frac{1+\nu}{E} \left(\frac{r}{2\pi}\right)^{1/2} \cos\left(\frac{\theta}{2}\right)\left(k+\cos\theta-2\right) \end{cases}$$

where:

$k=3-4\nu$ in plane deformations D_PLAN
$k=(3-\nu)/(1+\nu)$ in plane constraints C_PLAN

and:

E YOUNG modulus
ν Poisson's ratio

The distribution of the singular constraints in the vicinity of the crack is given by the formulas:

$$\begin{cases} \sigma_{11}^S = K_I \sigma_{11}^I + K_{II} \sigma_{11}^{II} \\ \sigma_{12}^S = K_I \sigma_{12}^I + K_{II} \sigma_{12}^{II} \\ \sigma_{22}^S = K_I \sigma_{22}^I + K_{II} \sigma_{22}^{II} \end{cases}$$

with:

$$\begin{cases} \sigma_{11}^I = \frac{1}{(2\pi r)^{1/2}} \cos(\frac{\theta}{2})(1-\sin(\frac{\theta}{2})\sin(\frac{3\theta}{2})) \\ \sigma_{12}^I = \frac{1}{(2\pi r)^{1/2}} \cos(\frac{\theta}{2})\sin(\frac{\theta}{2})\cos(\frac{3\theta}{2}) \\ \sigma_{22}^I = \frac{1}{(2\pi r)^{1/2}} \cos(\frac{\theta}{2})(1+\sin(\frac{\theta}{2})\sin(\frac{3\theta}{2})) \end{cases}$$

$$\begin{cases} \sigma_{11}^{II} = -\frac{1}{(2\pi r)^{1/2}} \sin(\frac{\theta}{2})(2+\cos(\frac{\theta}{2})\cos(\frac{3\theta}{2})) \\ \sigma_{12}^{II} = \frac{1}{(2\pi r)^{1/2}} \cos(\frac{\theta}{2})(1-\sin(\frac{\theta}{2})\sin(\frac{3\theta}{2})) \\ \sigma_{22}^{II} = \frac{1}{(2\pi r)^{1/2}} \sin(\frac{\theta}{2})\cos(\frac{\theta}{2})\cos(\frac{3\theta}{2}) \end{cases}$$

Note: the expression of the fields of displacement and singular constraints established in 2D – plane deformations can extend to the case 2D – axisymmetric [bib12]. The singular functions are however valid only asymptotically, in other words the distance *R* at the bottom of crack must remain small compared to the ray of the bottom of crack.

1.2 Extension to the case 3D

In addition to the outline views of opening and slip plan, a third mode of slip antiplan (characterized by K_{III}) can be defined. Singular fields associated with the mode III are identified by solving the equilibrium equations of infinite a plan medium fissured for displacements only according to the axis x_3 :

$$\begin{cases} u_{S1}^m = 0 \\ u_{S2}^m = 0 \\ u_{S3}^m = \dfrac{4(1+\nu)}{E}\left(\dfrac{r}{2\pi}\right)^{1/2}\sin\left(\dfrac{\theta}{2}\right) \end{cases} \quad \text{and} \quad \begin{cases} \sigma_{31}^m = -\dfrac{1}{(2\pi r)^{1/2}}\sin\left(\dfrac{\theta}{2}\right) \\ \sigma_{32}^m = \dfrac{1}{(2\pi r)^{1/2}}\cos\left(\dfrac{\theta}{2}\right) \end{cases}$$

In the three-dimensional case, one can show that the asymptotic behavior of displacements and constraints is the sum of the solutions correspondents to the modes I and II (in plane deformations) and with the mode III (antiplan), and of four other particular solutions, but which are more regular than the preceding ones [bib9]. The principal term of the singular fields thus remains unchanged, and the field of displacement in 3D is expressed then in the following way:

$$u(s) = u_R + K_I(s)\, u_S^I + K_{II}(s)\, u_S^{II} + K_{III}(s)\, u_S^{III}$$

where s is the curvilinear X-coordinate along the bottom of crack and u_S^I, u_S^{II} and u_S^{III} are singular displacements defined in the preceding paragraph (expressed, for each point of the bottom of crack, in an adapted local reference mark).

1.3 Formula of IRWIN and rate of refund of energy G

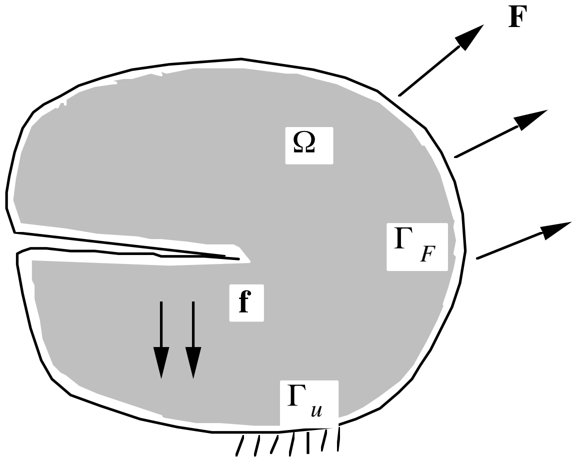
In linear elasticity, the stress intensity factors are connected to the rate of refund of energy G by the formula of IRWIN:

$$G = \frac{1-\nu^2}{E}\left(K_I^2 + K_{II}^2\right) \text{ in plane deformations}$$

$$G = \frac{1}{E}\left(K_I^2 + K_{II}^2\right) \text{ in plane constraints}$$

$$G(s) = \frac{1-\nu^2}{E}\left(K_I^2(s) + K_{II}^2(s)\right) + \frac{K_{III}^2(s)}{2\mu} \text{, with } \mu = \frac{E}{2(1+\nu)} \text{, in 3D}$$

One can show that this relation remains valid in the presence of initial constraints (thus in elasticity closely connected).
The rate of refund of energy G is defined by the opposite of the derivative of the potential energy compared to the propagation of the bottom of crack. In *Code_Aster*, G is calculated by the method theta [bib5 and R7.02.01 documentation] which is a Lagrangian method of derivation of the potential energy.



Thus, transformations are considered $M \rightarrow M + \eta\theta(M)$ area of reference Ω_0 in a field Ω_η who correspond to propagations of the crack. With these families of configuration of reference thus defined Ω_η correspond of the families of deformed configurations whose crack was propagated. Potential energy definite on Ω_η is brought back on Ω_0.

The surface forces are considered $\boldsymbol{F}$ and voluminal $\boldsymbol{f}$ applied respectively to Γ_F and Ω_0. One notes $\Psi(\varepsilon(\boldsymbol{u}))$ density of free energy, $\boldsymbol{u}$ the field of displacement, T the field of temperature and θ the field of vectors describing the direction of transport in $\eta=0$, Λ the tensor of elasticity and σ^0 the initial stress field, then the general expression of the rate of refund of energy G [bib5] is:

$$
\begin{aligned}
G = & \int_\Omega \left[\sigma(\boldsymbol{u}):(\nabla \boldsymbol{u}.\nabla\theta) - \Psi(\varepsilon(\boldsymbol{u}))\operatorname{div}\theta\right] d\Omega & \leftarrow \textit{terme classique} \\
& - \int_\Omega \frac{\partial \Psi}{\partial T}(\nabla T.\theta)\, d\Omega & \leftarrow \textit{terme dû à la thermique} \\
& + \int_\Omega \left[(\nabla \boldsymbol{f}.\theta)\boldsymbol{u} + \boldsymbol{f}.\boldsymbol{u}\operatorname{div}\theta\right] d\Omega & \leftarrow \textit{terme dû aux forces volumiques } \boldsymbol{f} \textit{ sur } \Omega \\
& - \int_\Omega \left[(\Lambda^{-1}:\sigma(\boldsymbol{u})):(\nabla \sigma^0.\theta)\right] d\Omega & \leftarrow \textit{terme dû à la contrainte initiale} \\
& + \int_{\Gamma_F} \left[(\nabla \boldsymbol{F}.\theta)\boldsymbol{u} + \boldsymbol{F}.\boldsymbol{u}\left(\operatorname{div}\theta - \boldsymbol{n}.\frac{\partial\theta}{\partial \boldsymbol{n}}\right)\right] d\Gamma & \leftarrow \textit{terme dû aux forces surfaciques } \boldsymbol{F} \textit{ sur } \Gamma_F \\
& - \int_{\Gamma_u} \left[(\sigma.\boldsymbol{n}).(\nabla \boldsymbol{u}.\theta)\right] d\Gamma & \leftarrow \textit{terme dû aux déplacements imposés sur } \Gamma_u
\end{aligned}
$$

In linear elasticity, G can be regarded as the symmetrical bilinear shape of the field of displacement $\boldsymbol{u}$. Density of energy elastic $\Psi(\varepsilon(\boldsymbol{u}))$ is written:

$$\Psi(\varepsilon(\boldsymbol{u})) = \frac{1}{2}\varepsilon(\boldsymbol{u}):\Lambda:\varepsilon(\boldsymbol{u}) = \frac{1}{2}B(\boldsymbol{u},\boldsymbol{u})$$

while noting:

B the symmetrical bilinear form defined by: $B(\boldsymbol{u},\boldsymbol{v}) = \varepsilon(\boldsymbol{u}):\Lambda:\varepsilon(\boldsymbol{u})$

and the bilinear form $g_{cla}(.,.)$ associated at the end classic of G is defined by:

$$g_{cla}(\boldsymbol{u},\boldsymbol{v}) = \frac{1}{2}\int_\Omega \left[\frac{\partial B}{\partial \nabla \boldsymbol{u}}.(\nabla \boldsymbol{v}.\nabla\theta) + \frac{\partial B}{\partial \nabla \boldsymbol{v}}.(\nabla \boldsymbol{u}.\nabla\theta) - B(\boldsymbol{u},\boldsymbol{v})\operatorname{div}\theta\right] d\Omega$$

The construction of the other terms (forces voluminal and surface, thermal, initial constraints and imposed displacements) is defined in each under-part.

One has $G=g(\boldsymbol{u},\boldsymbol{u})$ if $\boldsymbol{u}$ is solution of the elastic problem.

1.4 Decoupling of the modes of rupture

To uncouple the three modes from rupture and to calculate the three factors of intensity of the constraints associated, the symmetrical bilinear form is used $g(.,.)$ and decomposition of the field of displacement $\boldsymbol{u}$ in parts regular and singular [bib7]. To simplify the presentation, one places oneself initially in the case plan, but the properties spread without difficulty with the case 3D.

$$\begin{cases} g(\boldsymbol{u},\boldsymbol{u}_S^I)=g(\boldsymbol{u}_R+K_I\boldsymbol{u}_S^I+K_{II}\boldsymbol{u}_S^{II},\boldsymbol{u}_S^I)=g(\boldsymbol{u}_R,\boldsymbol{u}_S^I)+K_I\,g(\boldsymbol{u}_S^I,\boldsymbol{u}_S^I)+K_{II}\,g(\boldsymbol{u}_S^{II},\boldsymbol{u}_S^I) \\ g(\boldsymbol{u},\boldsymbol{u}_S^I)=g(\boldsymbol{u}_R+K_I\boldsymbol{u}_S^I+K_{II}\boldsymbol{u}_S^{II},\boldsymbol{u}_S^{II})=g(\boldsymbol{u}_R,\boldsymbol{u}_S^{II})+K_I\,g(\boldsymbol{u}_S^I,\boldsymbol{u}_S^{II})+K_{II}\,g(\boldsymbol{u}_S^{II},\boldsymbol{u}_S^{II}) \end{cases}$$

One shows in plane linear thermoelasticity that $\boldsymbol{u}_S^I$ and $\boldsymbol{u}_S^{II}$ are orthogonal for the scalar product defined by the bilinear form $g(.,.)$ and that the terms utilizing the regular part are cancelled:

$$\begin{aligned} g(\boldsymbol{u}_S^I,\boldsymbol{u}_S^{II})= \quad g(\boldsymbol{u}_S^{II},\boldsymbol{u}_S^I)= \quad 0 \\ g(\boldsymbol{u}^R,\boldsymbol{u}_S^I)= \quad g(\boldsymbol{u}^R,\boldsymbol{u}_S^{II})= \quad 0 \end{aligned}$$

One thus has finally:

$$\begin{aligned} g(\boldsymbol{u},\boldsymbol{u}_S^I) &= K_I\,g(\boldsymbol{u}_S^I,\boldsymbol{u}_S^I) \\ g(\boldsymbol{u}^R,\boldsymbol{u}_S^{II}) &= K_{II}\,g(\boldsymbol{u}_S^{II},\boldsymbol{u}_S^{II}) \end{aligned}$$

Moreover, by writing the rate of refund of energy in the form:

$$G=g(\boldsymbol{u},\boldsymbol{u})=g(\boldsymbol{u}_R+K_I\boldsymbol{u}_S^I+K_{II}\boldsymbol{u}_S^{II},\boldsymbol{u}_R+K_I\boldsymbol{u}_S^I+K_{II}\boldsymbol{u}_S^{II})$$

one finds the formula of IRWIN by re-using the properties of orthogonality:

$$g(\boldsymbol{u},\boldsymbol{u})=K_I^2\,g(\boldsymbol{u}_S^I,\boldsymbol{u}_S^I)+K_{II}^2\,g(\boldsymbol{u}_S^{II},\boldsymbol{u}_S^{II})$$

with:

$$g(\boldsymbol{u}_S^I,\boldsymbol{u}_S^I) = g(\boldsymbol{u}_S^{II},\boldsymbol{u}_S^{II}) = \frac{1-\nu^2}{E} \text{ in C\_PLAN}$$

$$g(\boldsymbol{u}_S^I,\boldsymbol{u}_S^I) = g(\boldsymbol{u}_S^{II},\boldsymbol{u}_S^{II}) = \frac{1}{E} \text{ in D\_PLAN}$$

Finally, in a general way:

$$\begin{cases} K_I=E\,g(\boldsymbol{u},\boldsymbol{u}_S^I) \\ K_{II}=E\,g(\boldsymbol{u},\boldsymbol{u}_S^{II}) \end{cases} \quad \text{in C\_PLAN}$$

$$\begin{cases} K_I=\dfrac{E}{1-\nu^2}\,g(\boldsymbol{u},\boldsymbol{u}_S^I) \\ K_{II}=\dfrac{E}{1-\nu^2}\,g(\boldsymbol{u},\boldsymbol{u}_S^{II}) \end{cases} \quad \text{in D\_PLAN and in 3D}$$

and $K_{III}=2\mu \, . \, g(\boldsymbol{u},\boldsymbol{u}_S^{III})$ in 3D

Establishment of the calculation of the stress intensity factors in linear thermoelasticity in *Code_Aster* is realized starting from the expression of the rate of refund of energy G in linear elasticity, written in symmetrical bilinear form, by introducing the known expressions of singular displacements, and by using the method theta.

2 Establishment of K_I, K_{II} and K_{III} in linear thermoelasticity in *Code_Aster*

2.1 Types of elements and loadings

To calculate the stress intensity factors K_I and K_{II} (and possibly K_{III}) in linear elasticity, it is necessary to use the option `CALC_K_G` order `CALC_G`.

This option is valid as well for a crack with a grid (classical finite elements) as for a crack nonwith a grid (finite elements nouveau riches: method X-FEM). It is available in 2D (modelings '`C_PLAN`'and'`D_PLAN`'for a crack with a grid or not; modeling'`AXIS`'for a crack with a grid only) and in 3D, for linear or quadratic finite elements.

All the classical thermomechanical loadings are taken into account: thermal loadings, voluminal loadings (gravity, rotation,…), surface loadings (including on the lips of the crack).

Note:

> *One does not take account of the term due to the displacements imposed on* Γ_u *, one thus should not impose conditions of DIRICHLET on the lips of the crack.*

2.2 Environment necessary for the calculation of K_I, K_{II} and K_{III}

The order `CALC_G` allows to recover the model of the problem, the characteristics of material, the field of displacement. The field theta is recovered or calculated by the order `CALC_G`.

Crack with a grid:

- In 2D, it is necessary to define the keyword `FOND_FISS`, which makes it possible to recover a concept of the type `fond_fiss` (produced by the order `DEFI_FOND_FISS`) where the basic node of crack and the normal with the crack are defined.
- In 3D, it is necessary to define the keyword `CRACK`, which makes it possible to recover a concept of the type `fiss_xfem` (produced by the order `DEFI_FISS_XFEM`) where the basic nodes of crack and the local bases along the bottom of crack are defined.
- When that the crack is laid out along an axis of symmetry, one can be satisfied to represent only half of the model, and to specify the symmetry of the loading by the keyword `SYME` (or if `FOND_FISS` the presence of symmetry is indicated is automatically detected). By default, one supposes that there is no symmetry. If one affects the value '`YES`'with the keyword `SYME`, that means that only mode I of rupture acts (opening of the lips of the crack) and one automatically affects the zero value to K_{II} (and possibly K_{III}).

Crack nonwith a grid (method X-FEM):

- In 2D as in 3D, the crack must be defined, for mechanical calculation and postprocessing, using the order `DEFI_FISS_XFEM`. The keyword `CRACK` must be well informed 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 the crack.

Let us insist on the need for assigning to all the elements (including those of the lips) the values of the YOUNG moduli E and of the Poisson's ratio ν , because they are used in the calculation of singular displacements. These values must be homogeneous on all the support of the field theta. In addition, if a loading is affected on the surface meshs (in 3D) or linear (in 2D) of the lips of the crack, the meshs of those must be correctly directed.

2.3 Bilinear form symmetrical G (. .)

2.3.1 Elementary classical term

$$TCLA=\sigma(\boldsymbol{u}):(\nabla \boldsymbol{u} \nabla \theta)-\Psi(\varepsilon(\boldsymbol{u}))\,\mathrm{div}\,\theta$$

Density of energy elastic $\Psi(\varepsilon(\boldsymbol{u}))$ can be written in linear thermoelasticity in the following form:

in `D_PLAN` and in `C_PLAN` :

$$2\Psi(\varepsilon(\boldsymbol{u}))=C_1(\varepsilon_{xx}^2+\varepsilon_{yy}^2)+2C_2\varepsilon_{xx}\varepsilon_{yy}+4C_3\varepsilon_{xy}^2-2\Psi_{th}$$

in `3D` :

$$2\Psi(\varepsilon(\boldsymbol{u}))=C_1(\varepsilon_{xx}^2+\varepsilon_{yy}^2+\varepsilon_{zz}^2)+2C_2(\varepsilon_{xx}\varepsilon_{yy}+\varepsilon_{xx}\varepsilon_{zz}+\varepsilon_{yy}\varepsilon_{zz})+4C_3(\varepsilon_{xy}^2+\varepsilon_{xz}^2+\varepsilon_{yz}^2)-2\Psi_{th}$$

with Ψ_{th} = Density of energy due to thermics:

$$\Psi_{th}=3K\alpha(T-T_{réf})\,tr\,\varepsilon-\frac{9}{2}K\alpha^2(T-T_{réf})^2$$

where:

$$\begin{aligned}3K &= \frac{E}{1-2\nu}\\ \alpha &= dilation\ thermique\\ \varepsilon &= tenseur\ de\ déformations\\ T_{réf} &= température\ de\ référence\end{aligned}$$

and with:

$$\begin{cases}C_1=\dfrac{(1-\nu)E}{(1+\nu)(1-2\nu)}=\lambda+2\mu\\ C_2=\dfrac{\nu E}{(1+\nu)(1-2\nu)}=\lambda\\ C_3=\dfrac{E}{2(1+\nu)}=\mu\end{cases}$$ in `D_PLAN` and in `3D` ; $$\begin{cases}C_1=\dfrac{E}{(1-\nu^2)}\\ C_2=\dfrac{\nu E}{(1-\nu^2)}\\ C_3=\dfrac{E}{2(1+\nu)}=\mu\end{cases}$$ in `C_PLAN`

While noting $\Psi(\varepsilon(\boldsymbol{u}))=\Psi(\boldsymbol{u},\boldsymbol{u})$, one has $2\Psi(\boldsymbol{u},\boldsymbol{v})=S1-S1TH$ with:

$$S1=C1\left(\frac{\partial u_k}{\partial x_k}\frac{\partial v_k}{\partial x_k}\right)+C2\left(\frac{\partial u_i}{\partial x_i}\frac{\partial v_j}{\partial x_j}(1-\delta_{ij})\right)+C3\left(\frac{\partial u_i}{\partial x_j}\frac{\partial v_i}{\partial x_j}(1-\delta_{ij})+\frac{\partial u_k}{\partial x_l}\frac{\partial v_l}{\partial x_k}(1-\delta_{kl})\right)$$

$$S1TH=3K\alpha((T_u-T_{réf})\,tr\,\varepsilon(\boldsymbol{v})+(T_v-T_{réf})\,tr\,\varepsilon(\boldsymbol{u}))-9K\alpha^2(T_u-T_{réf})(T_v-T_{réf})$$

where indices *I*, *J*, *K* and *L* correspond to a summation on the 2 coordinates of space (resp. 3 coordinates) in 2D (resp. 3D); $T_{\mathbf{u}}$ is the temperature associated with the field with displacement $\mathbf{u}$ by the relation:

$$\sigma=\Lambda\left(\varepsilon(\boldsymbol{u})-\varepsilon^{th}\right)$$

where $\varepsilon_{ij}^{th}=\alpha(T-T_{réf})\delta_{ij}$ and σ the equilibrium equations check. T_v is the temperature associated with field of displacement $v=\boldsymbol{u}_s$ (singular functions). For the calculation of the rate of refund of energy, $T_v=T_u, v=u$, for the calculation of the factors of intensity of the constraints, one took $T_v=T_f$, i.e., one has taken singular solutions of a purely mechanical problem.

Note:

> *The use of the purely thermal singular solutions in the method G-theta to determine the factors of intensity of forced of a thermomechanical problem as programmed in Code_Aster involves implicitly the approximation in the calculation of K.*
>
> *The comparison between G calculated by `CALC_K_G` and `G_IRWIN` will provide an indicator of error. If the difference is very large, the calculation of K is not right. However, the values of G are right.*

In the same way, the term $\sigma(\boldsymbol{u}):(\nabla\boldsymbol{u}\nabla\theta)$ can be written:

$$\sigma(\boldsymbol{u}):(\nabla\boldsymbol{u}\nabla\theta)=S2-S2TH$$

with:

$$S2=C1\left[\frac{\partial u_k}{\partial x_k}\frac{\partial v_k}{\partial x_k}\frac{\partial\theta_k}{\partial x_k}+\frac{1}{2}\left(\frac{\partial u_i}{\partial x_i}\frac{\partial v_i}{\partial x_j}+\frac{\partial v_i}{\partial x_i}\frac{\partial u_i}{\partial x_j}\right)(1-\delta_{ij})\frac{\partial\theta_j}{\partial x_i}\right]$$
$$+C2\left[\frac{1}{2}\frac{\partial\theta_i}{\partial x_j}\left(\frac{\partial u_k}{\partial x_k}\frac{\partial v_j}{\partial x_i}+\frac{\partial v_k}{\partial x_k}\frac{\partial u_j}{\partial x_i}\right)(1-\delta_{jk})\right]$$
$$+C3\left[\frac{1}{2}\left(\frac{\partial u_k}{\partial x_i}\left(\frac{\partial v_k}{\partial x_j}+\frac{\partial v_j}{\partial x_k}\right)+\frac{\partial v_k}{\partial x_i}\left(\frac{\partial u_k}{\partial x_j}+\frac{\partial u_j}{\partial x_k}\right)\right)(1-\delta_{jk})\frac{\partial\theta_i}{\partial x_j}\right]$$

and:

$$S2TH=\frac{TH1}{2}3K\alpha(T_u-T_{réf})\left(\frac{\partial v_i}{\partial x_j}\frac{\partial\theta_j}{\partial x_i}\right)+\frac{THA}{2}3K\alpha(T_v-T_{réf})\left(\frac{\partial u_i}{\partial x_j}\frac{\partial\theta_j}{\partial x_i}\right)$$

where $\mathrm{TH1}=1$ in `D_PLAN` and in `3D` and $\mathrm{TH1}=\frac{1-2\nu}{1-\nu}$ in `C_PLAN`.

Finally the classical term is written:

$$TCLA=(S2-S2TH)-\frac{1}{2}(S1-S1TH)\,\mathrm{div}\,\theta$$

2.3.2 Thermal term

One makes the assumption that the characteristics of material (E,ν,α) do not depend on the temperature.

in `D_PLAN` and in `C_PLAN` : $TTHE=\frac{-\partial\Psi}{\partial T}(\nabla T.\theta)=\frac{1}{2}3K\alpha\,tr\,\varepsilon\left(\frac{\partial T}{\partial x}\theta_x+\frac{\partial T}{\partial y}\theta_y\right)$

in `3D` :

$TTHE = TTHE1 + TTHE2$ with

$$TTHE1 = \frac{1}{2} 3K\alpha \left(tr\,\varepsilon(\boldsymbol{u}) \left(\frac{\partial T_v}{\partial x}\theta_x + \frac{\partial T_v}{\partial y}\theta_y + \frac{\partial T_v}{\partial z}\theta_z \right) + tr\,\varepsilon(\boldsymbol{v}) \left(\frac{\partial T_u}{\partial x}\theta_x + \frac{\partial T_u}{\partial y}\theta_y + \frac{\partial T_u}{\partial z}\theta_z \right) \right)$$

and

$$TTHE2 = -9K\alpha^2 \left((T_u - T_{réf}) \left(\frac{\partial T_v}{\partial x}\theta_x + \frac{\partial T_v}{\partial y}\theta_y + \frac{\partial T_v}{\partial z}\theta_z \right) + (T_v - T_{réf}) \left(\frac{\partial T_u}{\partial x}\theta_x + \frac{\partial T_u}{\partial y}\theta_y + \frac{\partial T_u}{\partial z}\theta_z \right) \right)$$

For the calculation of the rate of refund of energy, $T_v = T_u, v = u$, for the calculation of the factors of intensity constraints, one took $T_v = T_f$, i.e., one took the singular solutions of a problem purely mechanics.

Note:

> *The use of the purely thermal singular solutions in the method G-theta to determine the factors of intensity of forced of a thermomechanical problem as programmed in Code_Aster involves implicitly the approximation in the calculation of K.*
>
> *The comparison between G calculated by `CALC_K_G` and `G_IRWIN` will provide an indicator of error. If the difference is very large, the calculation of K is not right. However, the values of G are right.*

2.3.3 Term forces voluminal

$$TFOR = (\nabla f . \theta)\, \boldsymbol{u} + f . \boldsymbol{u} \operatorname{div} \theta$$

In any rigour, this term is linear and nonquadratic in displacement. The construction of the associated symmetrical bilinear form is thus not commonplace. It is considered whereas there exists a dependence of the force to the field of displacement; one notes f_u forces voluminal associated with the field of displacement $\boldsymbol{u}$ for the elastic problem and f_v voluminal forces associated with the fictitious acceptable field $\boldsymbol{v}$. One can then build a symmetrical bilinear expression of $TFOR$ $(\boldsymbol{u}, \boldsymbol{v})$ as follows:

$$TFOR(\boldsymbol{u}, \boldsymbol{v}) = \frac{1}{2} [(\nabla f_u . \theta)\, \boldsymbol{v} + (\nabla f_v . \theta)\, \boldsymbol{u} + (f_u . \boldsymbol{v} + f_v . \boldsymbol{u}) \operatorname{div} \theta]$$

It will be noted well that $TFOR(\boldsymbol{u}, \boldsymbol{u}) = TFOR$.
As the expressions which we are brought to calculate are of the type $TFOR(\boldsymbol{u}, \boldsymbol{u})$ and $TFOR(\boldsymbol{u}, \boldsymbol{u_S})$, where $\boldsymbol{u}$ and $\boldsymbol{u_S}$ are respectively the field of displacement and the singular field, and that:

$$f_{u^s} = \operatorname{div}(\sigma(\boldsymbol{u_S})) = 0 \text{ on } \Omega$$

One limits oneself to write:

$$TFOR(\boldsymbol{u}, \boldsymbol{v}) = CS [(\nabla F_u . \theta)\, \boldsymbol{v} + F_u . \boldsymbol{v} \operatorname{div} \theta] \text{ with } \begin{cases} CS = 0.5 & v = u_S \\ CS = 1 & v = u \end{cases}$$

The same remark is valid for the thermal classical term, the additional term due to thermics and the terms due to the surface forces.

The voluminal terms of forces and initial constraint generate linear and nonquadratic terms in $\boldsymbol{u}$ and thus whose associated form bilinear is more delicate to build,
To do it, let us consider that the initial constraints and the voluminal forces also depend on the field of displacement; one introduces then

2.3.4 Term of initial constraint

$$TINI_1 = -\int_\Omega \left[(\Lambda^{-1}:\sigma(\boldsymbol{u})):(\nabla\sigma^0.\theta)\right] d\Omega$$

In any rigour, this term is linear and nonquadratic in displacement. The construction of the associated symmetrical bilinear form is thus not commonplace. One carries out the same reasoning as for the voluminal term of force, by considering that there exists a dependence of the force to the field of displacement; one notes σ_u^0 forces voluminal associated with the field of displacement $\boldsymbol{u}$ for the elastic problem and σ_v^0 voluminal forces associated with the fictitious acceptable field $\boldsymbol{v}$. One can then build a symmetrical bilinear expression of $TINI_1$ as follows:

$$TINI_1(\boldsymbol{u},\boldsymbol{v}) = -\frac{1}{2}\int_\Omega \left[(\Lambda^{-1}:\sigma_u):(\nabla\sigma_v^0.\theta)+(\Lambda^{-1}:\sigma_v):(\nabla\sigma_u^0.\theta)\right] d\Omega$$

with $\sigma_u = \Lambda : sym(\nabla\boldsymbol{u})+\sigma_u^0$ and $\sigma_v = \Lambda : sym(\nabla\boldsymbol{v})+\sigma_v^0$

In the presence of initial constraints, the formulation of the free energy and the forced relation/deformation are also modified.

$$\Psi(\varepsilon(\boldsymbol{u}),\boldsymbol{\sigma^0}) = \frac{1}{2}\left(\varepsilon(\boldsymbol{u})+\Lambda^{-1}:\sigma^0\right):\Lambda:\left(\varepsilon(\boldsymbol{u})+\Lambda^{-1}:\sigma^0\right) = \frac{1}{2}\left(\varepsilon(\boldsymbol{u})-\varepsilon_{ref}\right):\Lambda:\left(\varepsilon(\boldsymbol{u})-\varepsilon_{ref}\right)$$

$$\sigma = \Lambda:\varepsilon(\boldsymbol{u})+\sigma^0$$

with $\varepsilon_{ref} = -\Lambda^{-1}:\sigma^0$

That adds two dependent terms at the end classic $\sigma(\boldsymbol{u}):(\nabla\boldsymbol{u}\nabla\theta)-\Psi(\varepsilon(\boldsymbol{u}))\mathrm{div}\,\theta$:

- a term related to the addition of the initial constraint in the constraint: $TINI_2 = \sigma^0:(\nabla\boldsymbol{u}\nabla\theta)$
- a term related to the modification of the free energy: $TINI_3 = -\frac{1}{2}\left(2\varepsilon(\boldsymbol{u})-\varepsilon_{ref}\right):\sigma^0\,\mathrm{div}\,\theta$

One carries out the same reasoning and one builds the terms of associated bilinear form:

- $TINI_2(\boldsymbol{u},\boldsymbol{v}) = \frac{1}{2}\left(\sigma_v^0:\nabla\boldsymbol{u}+\sigma_u^0:\nabla\boldsymbol{v}\right).\nabla\theta$
- $TINI_3(\boldsymbol{u},\boldsymbol{v}) = -\frac{1}{4}\left(\left(2\varepsilon(\boldsymbol{u})\right):\sigma_v^0+\left(2\varepsilon(\boldsymbol{v})\right):\sigma_u^0+2\sigma_u^0:\Lambda^{-1}:\sigma_v^0\right)\mathrm{div}\,\theta$

Two cases arise: that is to say $\boldsymbol{v}=\boldsymbol{u}$ (determination of G), that is to say $\boldsymbol{v}=\boldsymbol{u}_S$ (determination of the factors of intensity of the constraints). In this second case, it should be remembered that the initial stress field is given before the appearance of crack, and thus is not a priori compatible with a singular field. Its contribution to displacements actually intervenes through the total constraint in balance with the field of displacement.
One thus writes:

$$\begin{cases}\boldsymbol{\sigma_v^0} = \boldsymbol{\sigma^0} & si\ \boldsymbol{v}=\boldsymbol{u}\\ \boldsymbol{\sigma_v^0} = 0 & si\ \boldsymbol{v}=\boldsymbol{u}_S\end{cases}$$

With final, for the calculation of the rate of refund of energy:

- $TINI_1(\boldsymbol{u},\boldsymbol{u})=-\int_\Omega \left[(\varepsilon(\boldsymbol{u})+\Lambda^{-1}:\sigma^0):(\nabla\sigma^0.\theta)\right] d\Omega$
- $TINI_2(\boldsymbol{u},\boldsymbol{u})=\int_\Omega \left(\sigma^0:\nabla\boldsymbol{u}\right).\nabla\theta\, d\Omega$
- $TINI_3(\boldsymbol{u},\boldsymbol{u})=-\frac{1}{2}\int_\Omega \left((2\varepsilon(\boldsymbol{u})):\sigma^0+\sigma^0:\Lambda^{-1}:\sigma^0\right)\mathrm{div}\,\theta\, d\Omega$

And for the factors of intensity of the constraints:

- $TINI_1(\boldsymbol{u},\boldsymbol{u_S})=-\frac{1}{2}\int_\Omega \left[(\varepsilon(\boldsymbol{u_S})):(\nabla\sigma^0.\theta)\right] d\Omega$
- $TINI_2(\boldsymbol{u},\boldsymbol{u_S})=\frac{1}{2}\int_\Omega \left(\sigma^0:\nabla\boldsymbol{u_S}\right).\nabla\theta\, d\Omega$
- $TINI_3(\boldsymbol{u},\boldsymbol{u_S})=-\frac{1}{2}\int_\Omega \left((\varepsilon(\boldsymbol{u_S})):\sigma^0\right)\mathrm{div}\,\theta\, d\Omega$

2.3.5 Term forces surface

The term forces surface is written:

$$TSUR=(\ \nabla \boldsymbol{F}.\theta)\,\boldsymbol{u}+\boldsymbol{F.u}(\ \mathrm{div}\,\theta-n.\frac{\partial\theta}{\partial n})$$

The term in $n.\frac{\partial\theta}{\partial n}$ because the gradient is null of θ is orthogonal with n. As for the term forces voluminal, the bilinear expression $TSUR(\mathrm{u},\mathrm{v})$ is obtained by considering that v is equal to displacement u (and thus $\mathrm{F}_v=\mathrm{F}_u$), that is to say with a singular field $\boldsymbol{u_S}$ (and thus $\mathrm{F}_v=0$). One has then:

$$TSUR(u,v)=CS[(\nabla F_u.\theta)v+F_u.v\,\mathrm{div}\,\theta] \text{ with } \begin{cases} CS=0.5 & v=u_S \\ CS=1 & v=u \end{cases}$$

2.3.6 Term of modal dynamics

In the case of dynamic problems, an additional term $TDYN$ appears in the decomposition of rate of refund of energy expressed in the paragraph 1.3 :

$$TDYN=-\int_\Omega \frac{1}{2}\rho\,\dot{u}\,\ddot{u}.div\,\sigma.d\Omega-\int_\Omega \frac{1}{2}\rho\,\dot{u}\nabla\dot{u}.\theta.d\Omega+\int_\Omega \frac{1}{2}\rho\,\ddot{u}\nabla u.\theta.d\Omega$$

where $\dot{u}$ and $\ddot{u}$ are respectively the derivative first and second of the field of displacement u compared to time. For the harmonic problems, this term can be simplified [feeding-bottle 10]. While noting ω the pulsation of the studied clean mode and ρ the density, the bilinear form of the dynamic term is written as follows:

$$TDYN(u,v)=-\frac{1}{2}(\rho\,\omega^2 u_k v_{k,j}\theta_j+\rho\,\omega^2 v_k u_{k,j}\theta_j).$$

2.4 Fields of singular displacements and their derivative

Singular fields u_S^I, u_S^{II} and u_S^{III}, respectively associated with the modes I, II and III, are known explicitly like their derivative. They are written according to the polar coordinates in the reference mark related to the crack.
The successive introduction of these singular fields allows, as indicated in the §1, the elementary calculation of the stress intensity factors K_I, K_{II} and K_{III}.

2.5 Postprocessing of the results of K_I and K_{II}

2.5.1 For the problems 2D

Knowing the values of the stress intensity factors K_I and K_{II} for a given crack, formulas of AMESTOY - BUI and DANG-VAN, allow the calculation of the angle of propagation of the crack according to 3 criteria (K_I maximum, K_{II} and G maximum) [bib6].

That is to say Ω_m^η a field identical to Ω except that the crack is prolonged in the direction of angle m of a segment of right-hand side length η.

$$\Omega_m^0 \equiv \Omega$$

Are $K_I(\eta, m)$, $K_{II}(\eta, m)$, $G(\eta, m)$ stress intensity factors and the rate of refund of energy of Ω_m^η subjected to the same loading as Ω.

One poses:

$$\begin{aligned} K_I^*(m) &= \lim_{\eta\to 0} K_I(\eta, m) \\ K_{II}^*(m) &= \lim_{\eta\to 0} K_{II}(\eta, m) \\ G^*(m) &= \lim_{\eta\to 0} G(\eta, m) \end{aligned}$$

Criteria quoted by AMESTOY - BUI and DANG-VAN [bib6] are:

- to choose m_0 such as $K_I^*(m_0)$ that is to say maximum,
- to choose m_0 such as $K_{II}^*(m_0)$ that is to say no one,
- to choose m_0 such as $G^*(m_0)$ that is to say maximum.

These criteria give very nearby results [bib8].

The results are given in the form of a table of 4 coefficients K_{11}, K_{21}, K_{12} , K_{22} allowing to calculate K_I^* and K_{II}^* in all the cases of loading:

$$\begin{pmatrix} K_I^* \\ K_{II}^* \end{pmatrix} = \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} \begin{pmatrix} K_I \\ K_{II} \end{pmatrix}$$

Angle m (°)	K_{11}	K_{21}	K_{12}	K_{22}

0	1	0	0	1
10	0.9886	0.0864	— 0.2597	0.9764
20	0.9552	0.1680	— 0.5068	0.9071
30	0.9018	0.2403	— 0.7298	0.7972
40	0.8314	0.2995	— 0.9189	0.6540
50	0.7479	0.3431	— 1.0665	0.4872
60	0.6559	0.3696	— 1.1681	0.3077
70	0.5598	0.3788	— 1.2220	0.1266
80	0.4640	0.3718	— 1.2293	— 0.0453
90	0.3722	0.3507	— 1.1936	— 0.1988

$$K_{11}(-m)=K_{11}(m),\ K_{21}(-m)=-K_{21}(m),\ K_{12}(-m)=-K_{12}(m),\ K_{22}(-m)=K_{22}(m)$$

The research of the angle m_0 in `CALC_G` is made of 10 degrees in 10 degrees. The angle β of propagation is not calculated and is printed out (in the file `MESSAGE`) that if `INFORMATION` is worth 2.

2.5.2 For the 3D problems

The direction of propagation of a crack in 3D can be given by the principle of *Maximum Hoop Criterion Stress* (maximization of the circumferential constraint) [bib11]. The angle of propagation expresses itself then in the following way:

$$\beta=2\arctan\left[\frac{1}{4}.\left(\frac{K_I}{K_{II}}-sign(K_{II}).\sqrt{\left(\frac{K_I}{K_{II}}\right)^2+8}\right)\right]$$

The angle β, calculated systematically, is indicated in table result produced by the order `CALC_G` (column `BETA`).

3 Bibliography

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4 Description of the versions of the document

Index Doc.	Version Aster	Author (S) or contributor (S), organization		Description of the modifications
With	4	E.Visse	EDF/R & D /MMN	Text intial
B	7.4	E.Galenne	EDF/R & D /AMA	minor modifications
C	8.4	E.Galenne	EDF/R & D /AMA	Extension under the 3D, terms voluminal and thermal
D	9.4	E.Galenne	EDF/R & D /AMA	Card 11175 CALC_K_G into axisymmetric