Estimators of error in quantities of interest

Summary:

In this document, one presents the framework of the estimate of error in quantity of interest. This framework is used with explicit estimators in residue like with estimators in smoothing. A certain number of quantities of interest are detailed, in particular their writing in term of loading for the dual problem.

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1.1 Equations

An elastic solid, related to a Cartesian reference mark of $\mathbb{R}^3$, occupies, in its natural state and before deformation, a related limited open field Ω of $\mathbb{R}^3$ of regular border $\partial\Omega$ of outgoing normal $\vec{n}$. This contour is the union of two disjoined parts Γ_U and Γ_F such as $\Gamma_U \cup \Gamma_F = \partial\Omega$ and $\Gamma_U \cap \Gamma_F = \emptyset$.

That is to say $\vec{u}(x) = u_1(x)\vec{e}_1 + u_2(x)\vec{e}_2 + u_3(x)\vec{e}_3$ the displacement of a point M of Ω coordinates $x = (x_1, x_2, x_3)$. On contour Γ_U, a displacement $\vec{u}(x) = \vec{0}$ is imposed and a surface effort $\vec{F}(x)$ is imposed on Γ_F. The solid is also subjected to a voluminal effort $\vec{f}(x)$. The study is placed within the framework of linear elasticity and the assumption of the small disturbances, without viscous damping.

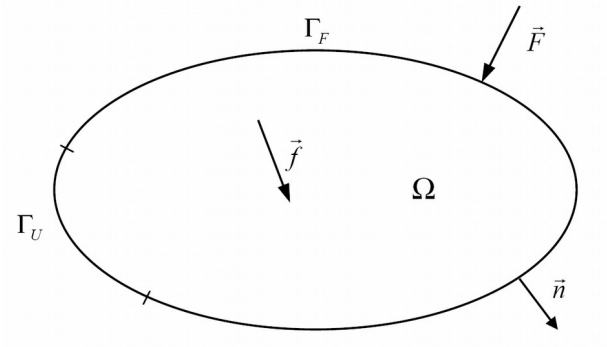

Figure 1.1-a : Not deformed configuration

In the continuation, we adopt the indicielle notation for the vectors and the tensors, as well as the rule of summation of Einstein on the repeated dumb indices. Thus, the following linear system:

$$\begin{cases} a_{11}x_1 + a_{12}x_2 = b_1 \\ a_{21}x_1 + a_{22}x_2 = b_2 \end{cases} \qquad \textbf{éq. 1.1-1}$$

can be written:

$$a_{ij}x_j = b_i \qquad \textbf{éq. 1.1-2}$$

The derivative of $i^{ème}$ component of a vector $\vec{v}$ compared to $j^{ème}$ component of the coordinates of space will be written $v_{i,j}$.

The symmetrical tensor of the constraints σ_{ij} is connected to the linearized symmetrical tensor of the deformations ε_{ij} by the relation:

$$\sigma_{ij} = a_{ijkl}\varepsilon_{kl} \qquad \textbf{éq. 1.1-3}$$

where a_{ijkl} is the tensor of the moduli of elasticity. It satisfies the relations with:

- symmetry: $a_{ijkh} = a_{jikh} = a_{ijhk} = a_{khij}$;

- positivity of the associated quadratic form: for any symmetrical real tensor of the second order X_{ij}, $\begin{cases} \exists \alpha_0 > 0, & \text{tel que} \quad X_{ij}\, a_{ijkh}(x)\, X_{kh} \geq \alpha_0\, X_{ij}\, X_{ij} \\ \forall\, X_{ij} = X_{ji}, & \forall\, x \in \Omega \end{cases}$.

The tensor of the deformations is connected to displacement by the relation:

$$\varepsilon(u) = \frac{1}{2}\left(grad(u) + grad^T(u)\right) \qquad \textbf{éq. 1.1-4}$$

For a homogeneous and isotropic material, the law of behavior is the law of Hooke:

$$\sigma = \lambda\, \mathrm{tr}(\varepsilon)\, I + 2\,\mu\, \varepsilon \qquad \textbf{éq. 1.1-5}$$

where λ and μ are the coefficients of Lamé.

The equilibrium equations, with the assumption of the small disturbances, are written:

$$div\, \sigma + \vec{f} = \vec{0} \qquad \textbf{éq. 1.1-6}$$

The boundary conditions previously defined are written:

$$\vec{u}(x) = \vec{0} \quad sur \quad \Gamma_U \qquad \textbf{éq. 1.1-7}$$

$$\sigma(x)\vec{n}(x) = \vec{F}(x) \quad sur \quad \Gamma_F \qquad \textbf{éq. 1.1-8}$$

The whole of the equations éq. 1.1-4 with éq. 1.1-8 constitute the problem (P_1) :

$$\begin{cases} \sigma_{ij,j} + f_i = 0 & dans \quad \Omega \\ \sigma_{ij} = a_{ijkh}\, \varepsilon_{kh} & dans \quad \Omega \\ \varepsilon_{ij}(u) = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) & \\ u_i(x) = 0 & sur \quad \Gamma_U \\ \sigma_{ij}\, n_j(x) = F_i(x) & sur \quad \Gamma_F \end{cases} \qquad \textbf{éq. 1.1-9}$$

1.2 Variational formulation

Space V is defined as the space of the functions v acceptable, sufficiently regular definite on Ω and with values in $\mathbb{R}^3$:

$$V = \left\{ v \in H^1(\Omega) \quad et \quad v = 0 \quad sur \quad \Gamma_U \right\}$$

The standards which are dependent for him are the following ones:

Normalizes L^2	$\|v\|^2_{L^2(\Omega)} = \int_\Omega v \cdot v \; d\Omega$
Normalizes H^1	$\|v\|^2_{H^1(\Omega)} = \int_\Omega \left(v \cdot v + \nabla\, v : \nabla\, v\right) d\Omega$
Pseudo norm H^1	$\|v\|^2_{H^1(\Omega)} = \int_\Omega \nabla\, v : \nabla\, v \; d\Omega$
Normalizes in energy	$\|v\|^2_e = \int_\Omega \sigma(v) : \varepsilon(v) \; d\Omega$

The equilibrium equation is multiplied by a function $v \in V$ sufficient regular then integrated on the field Ω :

$$0 = \int_\Omega \sigma_{ij,j} v_i \, d\Omega + \int_\Omega f_i v_i \, d\Omega \quad \textbf{éq. 1.2-1}$$

$$0 = \int_\Omega \left(\sigma_{ij} v_i\right)_{,j} d\Omega - \int_\Omega \sigma_{ij} v_{i,j} \, d\Omega + \int_\Omega f_i v_i \, d\Omega \quad \textbf{éq. 1.2-2}$$

The application of the formula of Green gives:

$$\int_\Omega \left(\sigma_{ij} v_i\right)_{,j} d\Omega = \int_{\partial\Omega} \sigma_{ij} n_j v_i \, d\Gamma \quad \textbf{éq. 1.2-3}$$

The properties of symmetry of the tensor of the constraints imply:

$$\sigma_{ij} v_{i,j} = \sigma_{ij} \varepsilon_{ij}(v) \quad \textbf{éq. 1.2-4}$$

What makes it possible to write:

$$\int_{\partial\Omega} \sigma_{ij} n_j v_i \, d\Gamma - \int_\Omega a_{ijkh} \varepsilon_{kh}(u) \, \varepsilon_{ij}(v) \, d\Omega + \int_\Omega f_i v_i \, d\Omega = 0 \quad \textbf{éq. 1.2-5}$$

The first term of the second member is null on Γ_U and it remains:

$$\int_{\Gamma_F} F_i v_i \, d\Gamma - \int_\Omega a_{ijkh} \varepsilon_{kh}(u) \varepsilon_{ij}(v) \, d\Omega + \int_\Omega f_i v_i \, d\Omega = 0 \quad \textbf{éq. 1.2-6}$$

The variational formulation of the problem (P_1) is written [bib1]:

$$\begin{cases} Trouver \quad u \in V \quad tel\ que \\ \quad a(u,v) = l(v) \qquad \forall v \in V \end{cases} \quad \textbf{éq. 1.2-7}$$

with:

$$a(u,v) = \int_\Omega a_{ijkh} \, \varepsilon_{kh}(u) \, \varepsilon_{ij}(v) \, d\Omega \quad \textbf{éq. 1.2-8}$$

$$l(v) = \int_{\Gamma_F} F_i v_i \, d\Gamma + \int_\Omega f_i v_i \, d\Omega \quad \textbf{éq. 1.2-9}$$

1.3 Discretization by finite elements

That is to say Ω^h a partition of Ω in N elements. A space finite elements $V^h \subset V$ is built starting from continuous, polynomial functions by pieces, and of degree p_E on each element E. Discretization of the problem (P_1) by the method of Galerkin provides the problem (P_h) [bib1]:

$$\begin{cases} Trouver \quad u^h \in V^h \quad tel\ que \\ \quad a(u^h, v^h) = l(v^h) \qquad \forall v^h \in V^h \end{cases} \quad \textbf{éq. 1.3-1}$$

1.4 Error of discretization

The digital error e approximation finite elements u^h is defined by:

$$e = u - u^h$$ **éq. 1.4-1**

Like u and u^h are elements of V then $e \in V$. The error satisfies the equation with the residue obtained while replacing u by $u^h + e$ in the variational formulation of the problem (P_h) :

$$a(e, v) = l(v) - a(u^h, v) = R_h^u(v) \quad \forall v \in V$$ **éq. 1.4-2**

As the bilinear form is definite positive, the residue R_h^u is a linear form limited on V who belongs to his dual V'. The standard of the residue is such as:

$$\|R_h^u\|_{V'} = \sup_{v \in V \setminus 0} \frac{|R_h^u(v)|}{\|v\|_e}$$ **éq. 1.4-3**

The residue measures the not-checking of certain properties of the equations of the problem and characterizes the unbalances and thus the error of discretization. It is easy to deduce from the equation 1.4-2 a new property. The function v^h is used as function test:

$$R_h^u(v^h) = l(v^h) - a(u^h, v^h) \quad \forall v^h \in V^h$$ **éq. 1.4-4**

Then by using the discretized form of the variational formulation, the property of orthogonality or property of Galerkin is obtained:

$$a(e, v^h) = R_h^u(v^h) = 0 \quad \forall v^h \in V^h$$ **éq. 1.4-5**

The equation 1.4-2 indicate that the error is solution of a problem of elasticity whose loading in effort is the residue of balance. This problem is as complicated to solve and expensive as the initial problem. Thus, instead of determining the error itself, in fact estimates will be sought.

1.5 Estimate of error *a priori*

As its name indicates it, the estimate *a priori* is done before calculation finite elements because it does not utilize the approximation finite elements u^h. Thus the functional analysis and the digital analysis allow, in many cases and under certain assumptions of regularity, to get results of estimate *a priori* ; i.e. the prediction of the asymptotic rate of convergence of the finite elements error. For more details, the works of Ciarlet [bib1] or Strang and Fix [bib2] could be consulted.

A function $\tilde{\eta}(h, d, u)$ is an estimate of error *a priori* if:

$$\|u - u^h\| \leq \tilde{\eta}(h, d, u)$$ (1.5.1)

where $\|\cdot\|$ is a standard on the fields of displacements, h size of the elements, d a set of facts of the case and u the exact solution.

The convergence of the method finite elements used can be obtained if:

$$\lim_{h \to 0} \tilde{\eta}(h, d, u) = 0$$ (1.5.2)

and the rate of convergence, if there exists a reality $q>0$ such as:

$$\|u-u^h\|\leq h^q\ \bar{\eta}(d,u) \tag{1.5.3}$$

Estimators of error *a priori* do not allow to quantify the errors on the solution finite elements because they utilize the exact solution which is generally not known. In addition, these estimates are valid only in the asymptotic mode, mode which is with difficulty atteignable for calculations 3D. For the formulations using of the elements of the isoparametric type [bib2], in the case of a regular solution and for the standard in energy of the error, $q=p$, where p is the degree of interpolation of the finite elements. On the other hand, in the case of a singular solution, $q=\min(p,\alpha)$ where α is the order of the singularity of the solution of the problem (for a crack, for example, $\alpha=\frac{1}{2}$).

2 Estimators of errors *a posteriori*

2.1 Definition of the estimators *a posteriori*

In estimate *a posteriori*, the objective is not to find an estimate of the function error e but to determine an estimate of a measurement of the error. Thus the estimators who were developed these thirty last years provide a reliable and precise estimate of the error in total standards, such as the standards H^1, standards L^2 or standards in energy, postprocessing of the solution finite elements. This choice of total standards is imposed by the bilinear form. When the form is definite positive and symmetrical, as it is the case here, that induces a scalar product for which the associated standard is the standard in energy; it is thus natural to estimate the error in this standard.

The basic principle of this kind of estimate is to use the solution approached to estimate the error of discretization. In opposition to the estimate *a priori*, estimates *a posteriori* can be made only once the calculated approximate solution.

A function $\eta(h,u^h,d)$ is an estimate of error *a posteriori* if:

$$\|u-u^h\|\leq\eta(h,u^h,d) \tag{2.1.1}$$

where $\|\cdot\|$ is a standard on the fields of displacements, h size of the elements, d a set of facts of the case and u^h the approximate solution. Moreover, if $\eta(h,d,u^h)$ can be localised in the form:

$$\eta(h,u^h,d)=\left(\sum_E \eta_E(u^h,d)^2\right)^{\frac{1}{2}} \tag{2.1.2}$$

then quantities $\eta_E(u^h,d)$, elementary contributions of the estimate of the total error $\eta(h,u^h,d)$, indicating buildings of error are called. They provide a base for the adaptation of grids.

Many estimators exist and can be classified in three categories:

- Estimators of errors based on the unbalances resulting from work from Babuška and Rheinboldt [bib3];
- Indicators of errors built starting from smoothed constraints resulting from work from Zienkiewicz and Zhu [bib4];
- Measurements of errors based on the concept of error in relation of behavior exits of work of Ladevèze [bib5].

These various estimators, controlled well today, will be introduced in a more or less detailed way. A more detailed review could be found in [bib6] with [bib10].

2.2 Quality of the estimators

When an estimator is defined, it is necessary to wonder about the criteria and the means making it possible to judge performances of this estimator. In a general way, it is necessary to seek to build an estimator of which the asymptotic behavior (when size h elements tends towards zero) follows that of the error. This behavior results in the existence of two constants C_1 and C_2, depend on the facts of the case and of the discretization but not of the size of the elements, checking the following relation (Ladevèze & Shovel, 2004):

$$C_1\eta \leq \|e\| \leq C_2\eta \text{ when } h \text{ tends towards zero} \qquad \textbf{éq. 2.2-1}$$

where η represent the estimate of measurement $\|e\|$ error e on the field considered. Thus to judge performances of the estimators, there exist various intrinsic criteria.

2.2.1 Index of effectiveness

The index of effectiveness γ is defined like the relationship between the error calculated by an estimator $e_{estimée}$ and the true error e_{vraie} :

$$\gamma = \frac{e_{estimée}}{e_{vraie}} \qquad \textbf{éq. 2.2.1-1}$$

Unless having an analytical solution, the true error is calculated like the difference between a solution obtained on a very fine grid (solution *overkill*) and the solution obtained on a given network. An index of effectiveness close to the unit characterizes a good estimator. If this property is reached when the size of the elements tends towards zero, the estimator is known as asymptotically exact. Nevertheless, the estimate must be sufficiently precise (γ near to 1) for rather coarse grids in order to be usable for the current discretizations in engineering. Lastly, it is desirable to over-estimate the error ($\gamma > 1$) to be able to be usable like criterion of stop in an adaptive process.

Systematic studies were carried out by Strouboulis and Haque [bib11] and by Babuška [bib12] on various CAS-tests having an analytical solution or for which a reference solution can be given on a very fine grid. All in all, this reveals that the quality of an estimator depends on the topology of the grid, of the regularity of the solution and the regularity (flatness) of the elements.

The only total evidence γ does not allow to give an account of the way in which the site error behaves: it may be, that in some cases, the estimator is satisfactory for this criterion without it not succeeding in locating the zones where the error in energy is important [bib13].

2.2.2 Index of robustness

In order to free itself from the local behavior of the estimator, another criterion was defined by Babuška and Rodriguez [bib14]. For a given triangulation T, the local index of effectiveness γ_ω relating to the under-field ω is defined by:

$$\gamma_\omega = \frac{e^\omega_{estimée}}{e^\omega_{vraie}} \qquad \textbf{éq. 2.2.2-1}$$

Babuška and Strouboulis showed that one could reach the asymptotic beach of variation numerically of γ_ω [bib15]:

$$0 < C^\omega_{inf} \leq \gamma_\omega \leq C^\omega_{sup} < \infty \qquad \textbf{éq. 2.2.2-2}$$

The variation with 1 of γ_ω is measured by the index R_ω defined by:

$$R_\omega = \max\left\{\left|1-C_{sup}^{\omega}\right|+\left|1-C_{inf}^{\omega}\right| \; ; \; \left|1-\frac{1}{C_{sup}^{\omega}}\right|+\left|1-\frac{1}{C_{inf}^{\omega}}\right|\right\} \qquad \textbf{éq. 2.2.2-3}$$

The index of robustness R is largest R_ω obtained by varying the position of the cell ω of its vicinity on the grids belonging to a class of triangulation. This approach makes it possible to highlight the error of discretization on a under-field but also the distortion of the elements of the grid and the regularity of the solution. Although having mathematical bases, this technique seems complicated to implement for complex grids used in engineering.

3 Site error

3.1 Error of pollution

3.1.1 Definition of the error of pollution

To define the error of pollution, we will provide a pragmatic definition while trying to understand which can be its behavior and thus its influence during an adaptive process. For that, we will study the convergence of the error in standard of energy in various situations:

- Convergence of the total error for a total uniform refinement;
- Convergence of the error in the zone of interest for a total refinement;
- Convergence of the total error for a local refinement;
- Convergence of the error in the zone of interest for a local refinement.

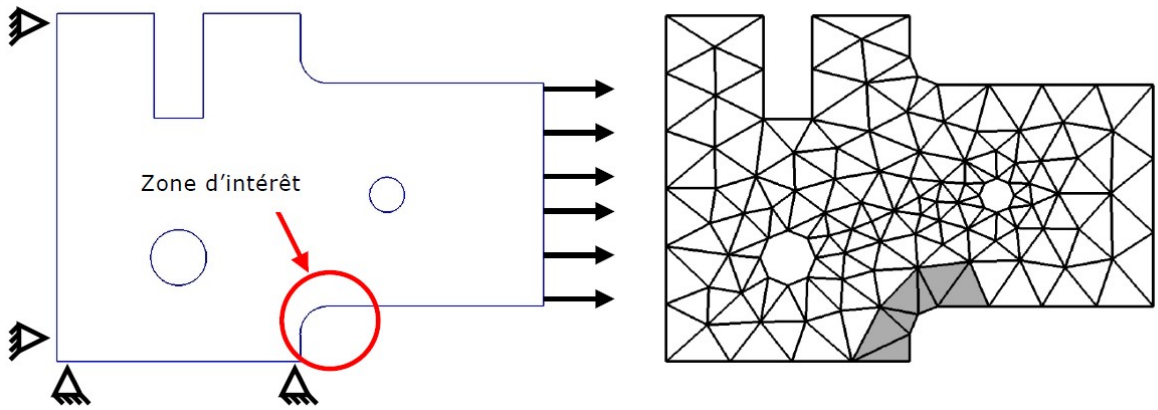

Figure 3.1.1-a : Geometry and grid (192 elements).

The problem to be solved is the problem whose geometry and grid are given by the figure 3.1.1-a. The imposed effort is unit, the Young modulus is equal to $E=1.0$ Pa and the Poisson's ratio are worth $\nu=0.3$. Finally modeling employed is a modeling in plane constraints. A series of approximations finite elements will be given on a succession of linear grids obtained by uniform refinement of the structure or uniform refinement of the zone of interest ω . The error in standard of energy is then calculated (thus without estimate) starting from a solution obtained on a very fine network (solution *overkill*) who will be our reference solution. Finally the absolute error is normalized by the standard in energy of the solution on the structure or the zone of interest according to the case. The results are presented in the figure 3.1.1-b.

For a total refinement, the total error converges "a little less quickly" than $p=1$; into dividing the size of the meshs by 10, the error is not divided by 10 (even into dividing the size by 16 the error is not divided by 10) (square markers). However this speed of convergence is reached only asymptotically. It should be noted that the curve represented seems to approach theoretical convergence starting from the last segment (for sizes meshs between 1/8 and 1/16). It is thus only the first part of a curve of convergence which is traced, when convergence in $p=1$ is not reached yet (pre-asymptotic mode).

When only the zone of interest is refined, the solution is not improved in the rest of the structure. The total error remains practically unchanged (round markers). This indicates that the error in the zone of interest contributes very little to the total error.

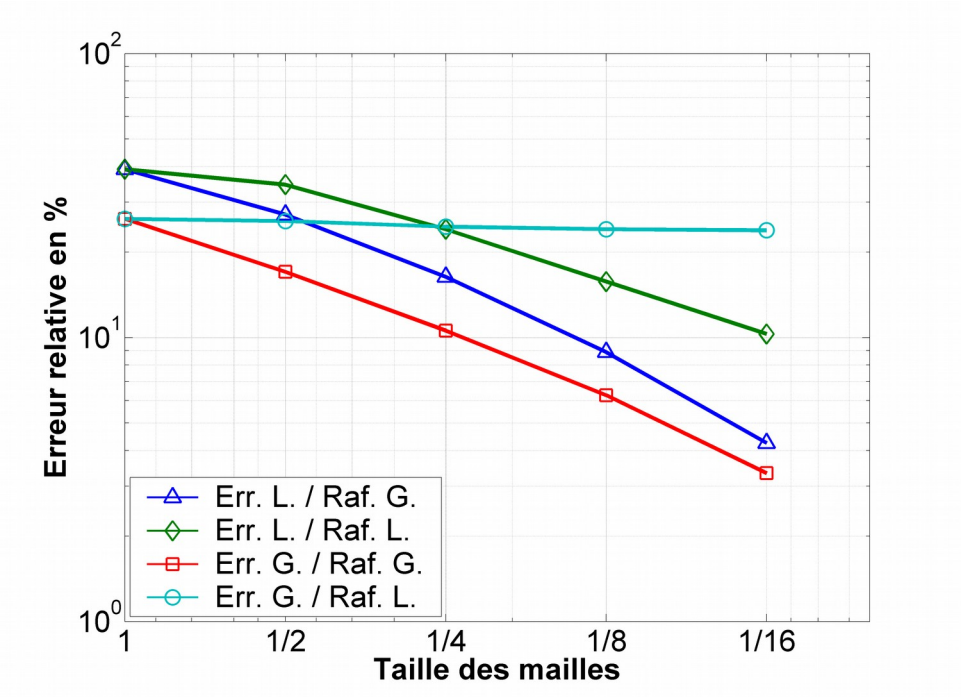

Figure 3.1.1-b : Description of the error of pollution: convergence of the error.

On the other hand by studying the curves relating to the error in the zone of interest, it is visible that significantly to improve the solution in this zone it is not enough to refine only this zone. Indeed the two curves (triangular markers rhombuses and markers) show a decrease of the site error but that obtained by local refinement shows a slower decrease: the two curves deviate. It thus seems that the error in the rest of the structure affects also the quality of the solution in the zone of interest. What means that the sum of the local contributions of the total estimators on under field ω do not represent the site error exactly. It thus seems that the true site error is made up of two parts: a local component and a complementary component resulting moreover from the structure. The consequence of this is that by refining only the zone of interest, the error in the rest of the structure does not decrease (i.e the complementary component remains constant). One can then imagine that the curve representing the site error with a local refinement (markers rhombuses) converges towards a nonworthless value if refinement is continued: this nonworthless value will represent the complementary component (the local component tending towards zero). The value of the complementary component is then called “error of pollution”.

A more formal definition can be given. The error of pollution was introduced by Babuška *et al.* [bib16], [bib17], [bib18]. They suppose that the error of discretization under field ω structure is made up:

- of a site error on ω , disregarding moreover structure;
- of an error of pollution or transported, resulting from the discretization in the rest of the structure.

The fundamental relation between the total error e and the solution Φ_E local problem of the error (solution resulting from *Equilibrated Residual Method* for example) is recalled:

$$a(e,v)=\sum_{E\in\Omega} a_E(\Phi_E,v) \quad \forall v\in V \qquad \textbf{éq. 3.1.1-1}$$

A site error e_ω^{loc} on a under-field ω can be defined by:

$$a\left(e_{\omega}^{loc}, v\right)=\sum_{E\subset\omega} a_E\left(\varphi_E, v\right) \quad \forall v\in V$$ **éq. 3.1.1-2**

Like the indicating function of site error φ_E does not depend that local residues on the approximation finite elements evaluated on the patch of elements $E*$, the site error e^{loc} depends only on the local residues on the patch $\tilde{\omega}$, constituted by the elements of ω and of the close elements. The component complementary to the true error is the error of pollution e_{ω}^{pol} :

$$a\left(e_{\omega}^{pol}, v\right)=\sum_{E\not\subset\omega} a_E\left(\varphi_E, v\right) \quad \forall v\in V$$ **éq. 3.1.1-3**

This part of the true error comes from the residues located apart from under field and is transported until under field, thus affecting the precision. The error e_{ω} in a under-field ω is thus the sum of the two components defined previously:

$$e_{\omega}=e_{\omega}^{loc}+e_{\omega}^{pol}$$ **éq. 3.1.1-4**

Within sight of the figure 3.1.1-b and of the preceding definition, it becomes obvious that the control of the error of pollution is paramount. Indeed, apart from the zone of interest, when the grid is coarse, it perhaps an important source of error of pollution. Consequently, a local refinement on under field must be counterbalanced by an adequate refinement apart from under field in order to controlling the error of pollution. We will see in the continuation that the estimators of error in quantity of interest allow to ensure this balance between local refinement and refinement apart from under field.

3.1.2 Estimate of the error of pollution

To estimate the error of pollution, various methods were proposed. Method suggested by Babuška (Babuška *et al.*, 1995) is related to the functions of Green which describe the interaction between various points of the field. The error of pollution is estimated with the error of approximation of the function of Green associated with certain points. Another method was used by Huerta and Díez (Huerta & Díez, 2000) and consists in finding an approximation of e_{ω}^{pol} by resolution of the problem defining this error. Other work can be also quoted (Ainsworth, 1999), (Oden & Feng, 1996). The industrial interest of the evaluation of this error being limited, we will not more develop these methods of estimate. Many work on the calculation of terminals of the error makes useless the estimate of the error of pollution because it is understood in the terminals. Moreover, for the estimate of a site error, as we indicated already, the estimators in quantity of interest allow to free itself from the error of pollution thanks to the dual problem.

3.2 Error in quantity of interest

3.2.1 Quantities of interest

The estimates of errors in standard of energy are too abstract to provide to the users computer codes sufficient information on the various aspects of the sought solution. It is then more useful to estimate an error in terms of quantities of interest; quantities having a physical direction (an average of displacements in an under-area of the physical field or an average of constraints on an interface or even, in the case of vibrations, one of the Eigen frequencies). Mathematically, they are characterized by linear functional calculuses or not within the space of functions to which the solutions belong.

Several examples are given: the average of a component of displacement on a field ω :

$$Q(v)=\frac{1}{|\omega|}\int_{\omega} v_x \, d\Omega$$ **éq. 3.2.1-1**

the average of a component of the tensor of the constraints on a field ω :

$$Q(v)=\frac{1}{|\omega|}\int_{\omega}\sigma_{xx}\,d\,\Omega$$ **éq. 3.2.1-2**

One then seeks to calculate the quantity ε^{Q} who can be expressed in the following form:

$$\varepsilon^{Q}=Q(u)-Q(u^{h})$$ **éq. 3.2.1-3**

If Q is linear, the following equality is checked:

$$\varepsilon^{Q}=Q(u-u^{h})=Q(e)$$ **éq. 3.2.1-4**

In the continuation, only the case of the linear functional calculuses will be considered because that corresponds to the framework of the simplified approach presented in the continuation. In a general way, treatment used for the nonlinear quantities (like the constraint of Von Mises or the integral J in breaking process) is the linearization [bib19] and [bib20].

3.2.2 Dual problem and fundamental relation

The error in quantity of interest can be estimated by using properties of duality of the operators intervening in the weak formulation of the problem of reference. From a mechanical point of view, that corresponds to the existence of a function solution of a dual problem, known as function of influence, representing the influence of the efforts of the problem of reference on total energy. The function of influence is then used as weighting of the residues of balance of the problem of reference.

A simplified approach is presented, insofar as the framework is limited to linear elasticity and the linear quantities of interest. This results in the fact that $Q(\cdot)$ is a linear form and that $a(\cdot,\cdot)$ is a bilinear form. This approach makes it possible to better understand the need for using the error on the function of influence and not only the function of influence.

The relation between the error in quantity of interest and the residue can be expressed by the introduction of an unknown function ω, called function of influence:

$$Q(e)=\omega(R_{h}^{u})$$ **éq. 3.2.2-1**

Moreover, one shows in [bib21] that the preceding relation becomes:

$$Q(e)=R_{h}^{u}(\omega)$$ **éq. 3.2.2-2**

By combining the preceding relationship to the equation of the residues:

$$a(e,v)=R_{h}^{u}(v)$$ **éq. 3.2.2-3**

a relation between the error on the problem of reference, the function of influence and the error in quantity of interest is obtained:

$$a(e,\omega)=Q(e)$$ **éq. 3.2.2-4**

This equality is necessarily checked when $\omega\in V$ is solution of the following problem:

$$\begin{cases}\text{Trouver } \omega\in V \text{ tel que}\\ a(v,\omega)=Q(v) \qquad \forall\ v\in V\end{cases}$$ **éq. 3.2.2-5**

This problem is called dual or assistant problem. It is noticed that if ω could be calculated in an exact way, then $Q(u)$ could be directly given starting from the facts of the case because:

$$Q(u)=a(u,\omega)=l(\omega) \qquad \text{éq. 3.2.2-6}$$

But unfortunately, it is also difficult to determine the function of influence ω to determine u in the primal problem. This is why an approximation finite elements $\omega^h \in V^h$ of ω who satisfied

$$a(v^h,\omega^h)=Q(v^h) \quad \forall\, v^h \in V^h \qquad \text{éq. 3.2.2-7}$$

is introduced. One also notes that in substituent e with v^h in the dual problem, one obtains:

$$Q(e)=a(e,\omega) \qquad \text{éq. 3.2.2-8}$$

To replace ω by ω^h in the preceding relation is not sufficient to obtain an estimate of $Q(e)$ because $a(e,\omega^h)=0$ (property of orthogonality). This is why it is necessary to evaluate the error on the function of noted influence $\varepsilon=\omega-\omega^h$. By introducing this error into the preceding relation, a representation of the error is obtained:

$$Q(e)=a(e,\varepsilon) \qquad \text{éq. 3.2.2-9}$$

In the case of nonlinear problems and/or of the nonlinear quantities of interest, which precedes does not apply. In this case, the primal problem is written:

$$\begin{cases} Trouver\ u\in V\ tel\ que \\ \quad A(u;v)=L(v) \qquad \forall\, v\in V \end{cases} \qquad \text{éq. 3.2.2-10}$$

where $A(\cdot;\cdot)$ is a semi-linear form such as the arguments which follow the semicolon are linear and $L(\cdot)$ a linear form continues on V.

The approach consists in regarding the primal problem as a problem of minimization under constraint [bib19], [bib20]:

$$\begin{cases} Trouver\ u\in V\ tel\ que \\ Q(u)=\inf\limits_{z\in S} Q(z) \\ où \\ S=\{ z\in V;\ A(z;v)=L(v),\ \forall\, v\in \in V \} \end{cases} \qquad \text{éq. 3.2.2-11}$$

To solve the problem of minimization, the couple $(u,\omega)\in V\times V$ such as he is sought satisfies the primal problem and the dual problem:

$$\begin{cases} A(u;\tilde{v})=L(\tilde{v}) \qquad \forall\, \tilde{v}\in V \\ A'(u;v,\omega)=Q'(u;v) \quad \forall\, v\in V \end{cases} \qquad \text{éq. 3.2.2-12}$$

Finally, the relation between the error in quantity of interest ε^Q and the residue is given by:

$$\varepsilon^Q=Q(u)-Q(u^h)=R(u^h;\omega)+\Delta A+\Delta Q \qquad \text{éq. 3.2.2-13}$$

where ΔA and ΔQ the derivative second and third utilize of A and Q.

3.2.3 Estimate of the error in quantity of interest

From the fundamental relation 3.2.2-9, various techniques were developed in order to estimate the error in quantity of interest.

The simplest technique and most direct is to use the total estimators in standard of energy. By applying the theorem of Cauchy-Schwartz, a relation between the error in quantity of interest and the standards in energy of the errors to the primal problem and the dual problem can be found [bib22]:

$$|Q(e)| \leq \|e\|_e \|\varepsilon\|_e \qquad \textbf{éq. 3.2.3-1}$$

This expression thus enables us to easily estimate the error in quantity of interest by using any estimator of error in standard in energy, this without additional development in a computer code laying out total estimators. Although this estimate is simplest, it is also coarsest: she does not take into account the local interactions between the primal error and the dual error (schematically that wants to say that an error on displacement does not result in an error into quantity of interest). This can lead to heavy over-estimates of the error in quantity of interest.

A a little different approach, called *Dual Weighted Residual* (DWR) [bib19], consists in considering the exact expression of the error in quantity of interest:

$$Q(e) = a(e, \omega - \omega^h) = R_h^u(\omega - \omega^h) \qquad \textbf{éq. 3.2.3-2}$$

The dual problem is solved by using a method of high approximation of order. Another method, less expensive, consists in using functions of interpolation of order high definite on elementary patchs of the field. This approach leads to a guaranteed upper limit of the error.

An approach “exact terminals” (*exact bounds approach*) [bib23] uses the properties of the estimate based on the dual analysis. Thus thanks to a formulation in displacements of the finite element method, a lower limit of the exact deformation energy is obtained; thanks to a formulation in constraints, an upper limit of exact complementary energy is obtained. From a practical point of view, this method is very expensive since it implies to twice solve the primal problem and the dual problem.

Other methods exist to estimate the error in quantity of interest but from an industrial point of view, only the approach using of the total estimators in standard of energy seems to be convincing. It does not require an additional development to reach an indication of the error and it is also much less expensive.

3.2.4 Terminals of the error

3.2.4.1 A new expression for the error

Although very simple to obtain, the relation 3.2.3-1 product a consequent over-estimate of the error. Various techniques were proposed to cure this problem. Prudhomme and Oden employ the relation of the parallelogram for the problems with symmetrical bilinear forms which gives access to an upper limit and a lower limit of the error [bib24], [bib21].

If e and ε are the errors of the approximations finite elements, respectively of the solutions of the problems primal and dual then:

$$Q(e) = a(e, \varepsilon) = \frac{1}{4}\|e+\varepsilon\|_e^2 - \frac{1}{4}\|e-\varepsilon\|_e^2 \qquad \textbf{éq. 3.2.4.1-1}$$

The scalar factor is introduced $s \in R$

$$Q(e)=a(e,\varepsilon)=\frac{1}{4}\|se+s^{-1}\varepsilon\|_e^2-\frac{1}{4}\|se-s^{-1}\varepsilon\|_e^2$$ **éq. 3.2.4.1-2**

The scalar s is selected so that the quantities $\|se\|_e$ and $\|s^{-1}\varepsilon\|_e$ have the same amplitude, which implies to choose $s=\sqrt{\|\varepsilon\|_e/\|e\|_e}$.

Indeed e and ε can be of very different order of magnitude. The scalar s aim at "normalizing" the two terms, in order to avoid making a difference of two very close terms because that can induce an important digital error.

Formally, any existing estimator of errors can be used to evaluate the standards in energy of the relation of the parallelogram; more this estimate will be "just" better will be the quality of the estimator of error in quantity of interest.

3.2.4.2 Construction of the terminals

Total estimators η_{inf}^{+}, η_{sup}^{+}, η_{inf}^{-} and η_{sup}^{-} are defined such as:

$$\eta_{inf}^{+}\leq\|se+s^{-1}\varepsilon\|_e\leq\eta_{sup}^{+}$$ **éq. 3.2.4.2-1**

$$\eta_{inf}^{-}\leq\|se-s^{-1}\varepsilon\|_e\leq\eta_{sup}^{-}$$ **éq. 3.2.4.2-2**

By rewriting the two preceding inequalities as follows:

$$\frac{1}{4}\left(\eta_{inf}^{+}\right)^2\leq\frac{1}{4}\|se+s^{-1}\varepsilon\|_e^2\leq\frac{1}{4}\left(\eta_{sup}^{+}\right)^2$$ **éq. 3.2.4.2-3**

$$\frac{1}{4}\left(\eta_{inf}^{-}\right)^2\leq\frac{1}{4}\|se-s^{-1}\varepsilon\|_e^2\leq\frac{1}{4}\left(\eta_{sup}^{-}\right)^2$$ **éq. 3.2.4.2-4**

and by adding them:

$$\frac{1}{4}\left(\eta_{inf}^{+}\right)^2-\frac{1}{4}\left(\eta_{sup}^{-}\right)^2\leq\frac{1}{4}\|se+s^{-1}\varepsilon\|_e^2-\frac{1}{4}\|se-s^{-1}\varepsilon\|_e^2\leq\frac{1}{4}\left(\eta_{sup}^{+}\right)^2-\frac{1}{4}\left(\eta_{inf}^{-}\right)^2$$ **éq. 3.2.4.2-5**

a framing of the error in quantity of interest is obtained.

Then terminals η_{inf}^{Q}, η_{sup}^{Q} are introduced such as:

$$\eta_{inf}^{Q}=\frac{1}{4}\left(\eta_{inf}^{+}\right)^2-\frac{1}{4}\left(\eta_{sup}^{-}\right)^2$$ **éq. 3.2.4.2-6**

$$\eta_{sup}^{Q}=\frac{1}{4}\left(\eta_{sup}^{+}\right)^2-\frac{1}{4}\left(\eta_{inf}^{-}\right)^2$$ **éq. 3.2.4.2-7**

The error in quantity of interest $Q(e)$ is limited by η_{inf}^{Q} and η_{sup}^{Q} :

$$\eta_{inf}^{Q}\leq Q(e)\leq\eta_{sup}^{Q}$$ **éq. 3.2.4.2-8**

It is also possible to use the estimates η_{eei}^{Q} and η_{ees}^{Q} defined such as:

$$\eta_{eei}^{Q}=\frac{1}{4}\left(\eta_{inf}^{+}\right)^2-\frac{1}{4}\left(\eta_{inf}^{-}\right)^2 \qquad \text{éq. 3.2.4.2-9}$$

$$\eta_{ees}^{Q}=\frac{1}{4}\left(\eta_{sup}^{+}\right)^2-\frac{1}{4}\left(\eta_{sup}^{-}\right)^2 \qquad \text{éq. 3.2.4.2-10}$$

like estimate of the error in quantity of interest $Q(e)$.

Lastly, a last estimate can be obtained, by realising the terminals η_{inf}^{Q} and η_{sup}^{Q} or estimates η_{eei}^{Q} and η_{ees}^{Q}, noted η_{moy}^{Q} :

$$\begin{aligned}\eta_{moy}^{Q} &= \frac{1}{2}\left(\eta_{eei}^{Q}+\eta_{ees}^{Q}\right)\\ &= \frac{1}{2}\left(\eta_{inf}^{Q}+\eta_{sup}^{Q}\right)\\ &= \frac{1}{8}\left(\left(\eta_{inf}^{+}\right)^2+\left(\eta_{sup}^{+}\right)^2\right)-\frac{1}{8}\left(\left(\eta_{inf}^{-}\right)^2+\left(\eta_{sup}^{-}\right)^2\right)\end{aligned} \qquad \text{éq. 3.2.4.2-11}$$

The following figure summarizes the various possible combinations of the estimate of error in standard of energy to obtain an estimate or terminals of the error in quantity of interest. This shows which if one then has terminals for an estimator in standard of energy one has terminals for the error in quantity of interest.

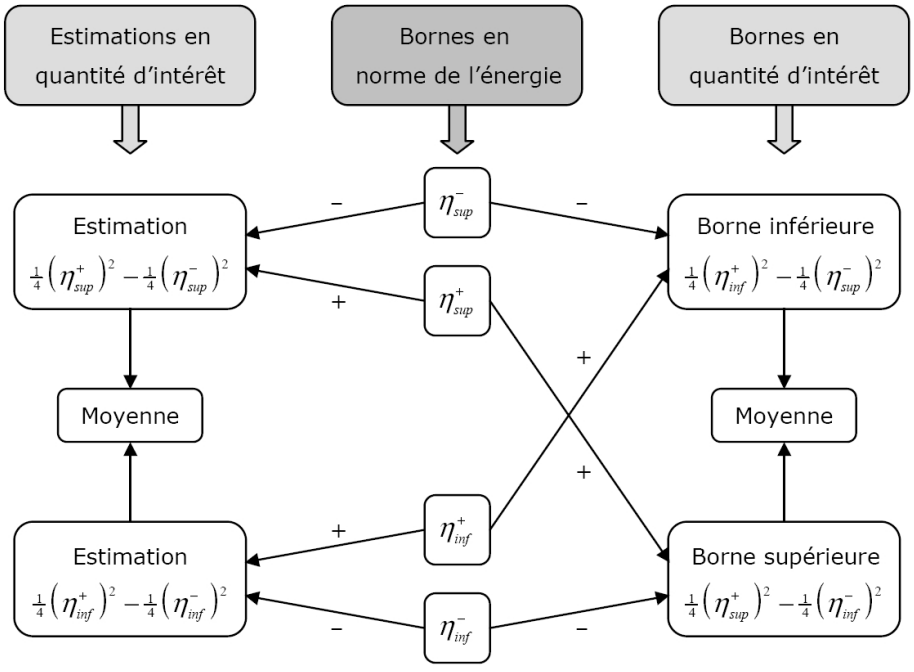

Figure 3.2.4.2-a : Estimates and terminals of the error in quantity of interest (Prudhomme *et al.*, 2003).

3.2.4.3 Estimates of the terminals of the error

In the preceding chapter, it was shown that terminals of the total error were accessible by using estimators in implicit residues. The broad outlines are given here to obtain terminals of the error in quantity of interest by using the implicit estimators. It should be noted that this is only one example and that other methods of estimate can provide terminals of the error in quantity of interest.

With an aim of obtaining the hight delimiters previously definite, the functions ψ_E^u and ψ_E^ω, corresponding respectively to the errors e and ε, are calculated by introducing the local problems relating to the problems primal and dual. The following estimates are then obtained:

$$\eta_{sup}^{+}=\left\| s\,\psi_E^u+s^{-1}\psi_E^\omega\right\|_e \text{ and } \eta_{sup}^{-}=\left\| s\,\psi_E^u-s^{-1}\psi_E^\omega\right\|_e \qquad \textbf{éq. 3.2.4.3-1}$$

For the estimate of the lower limits, it is necessary to proceed in a similar way that for the estimate of the hight delimiters by building continuous functions than the interfaces from ψ_E^u and ψ_E^ω :

$$\eta_{inf}^{+}=\frac{\left|\left(s\,R_h^u+s^{-1}R_h^\omega\right)\left(s\,\chi^u+s^{-1}\chi^\omega\right)\right|}{\left\|s\,\chi_E^u+s^{-1}\chi_E^\omega\right\|_e} \text{ and } \eta_{inf}^{-}=\frac{\left|\left(s\,R_h^u-s^{-1}R_h^\omega\right)\left(s\,\chi^u-s^{-1}\chi^\omega\right)\right|}{\left\|s\,\chi_E^u-s^{-1}\chi_E^\omega\right\|_e} \qquad \textbf{éq. 3.2.4.3-2}$$

4 Estimate of the error in quantity of interest

4.1 Estimator of error in quantity of interest based on the explicit residues

The error in quantity of interest can be estimated starting from any estimator of the total error. Thus, an estimator of error in quantity of interest is built starting from the relation of the parallelogram and the estimator of error based on the explicit residues η of which the expression on each element η_E is [R4.10.02]:

$$\eta_E^2 = h_E^2 \|r_E\|_{L^2(E)}^2 + \frac{1}{2}\sum_{\Gamma \not\subset \Gamma_F} l_\Gamma \|t_\Gamma\|_{L^2(\Gamma)}^2 + \sum_{\Gamma \subset \Gamma_F} l_\Gamma \|t_\Gamma\|_{L^2(\Gamma)}^2 \qquad \textbf{éq. 4.1-1}$$

The use of the expression given by the inequality of Cauchy-Schwartz:

$$|Q(e)| \leq \|e\|_e \|\varepsilon\|_e \qquad \textbf{éq. 4.1-2}$$

with the estimator of type explicit residue an estimate of the error in quantity of interest gives easily while estimating $\|e\|_e$ and $\|\varepsilon\|_e$ but this estimate is coarse.

The relation of the parallelogram given by:

$$Q(e) = a(e,\varepsilon) = \frac{1}{4}\|e+\varepsilon\|_e^2 - \frac{1}{4}\|e-\varepsilon\|_e^2 = \frac{1}{4}\|s\,e+s^{-1}\varepsilon\|_e^2 - \frac{1}{4}\|s\,e-s^{-1}\varepsilon\|_e^2 \qquad \textbf{éq. 4.1-3}$$

with $s = \sqrt{\|\varepsilon\|_e / \|e\|_e}$ (cf §3.2.4), provides a more precise estimate because it allows a real coupling between the primal error and the dual error. The use of the estimate of the error of each of the two problems is not possible, the standard of a sum is not equal to the sum of the standards:

$$\|e+\varepsilon\|_e^2 = a(e+\varepsilon, e+\varepsilon) = \|e\|_e^2 + \|\varepsilon\|_e^2 + 2\,a(e,\varepsilon) \qquad \textbf{éq. 4.1-4}$$

$$\|e-\varepsilon\|_e^2 = a(e-\varepsilon, e-\varepsilon) = \|e\|_e^2 + \|\varepsilon\|_e^2 - 2\,a(e,\varepsilon) \qquad \textbf{éq. 4.1-5}$$

This is why it is necessary to set out again of the definition of the estimator of error in residue in order to evaluate directly $\|s\,e+s^{-1}\varepsilon\|_e^2$ and $\|s\,e-s^{-1}\varepsilon\|_e^2$. The error in solution $e = u - u^h$ being solution of a problem of elasticity of which the data in effort are the residues of balance, it is thus a question of formulating the problems of which $(s\ e+s^{-1}\varepsilon)$ and $(s\,e-s^{-1}\varepsilon)$ are solutions.

The primal problem and the dual problem are given by the following relations:

$$\begin{cases} a(u,v) = l(v) & \forall\ v \in V \\ a(v,\varepsilon) = Q(v) & \forall\ v \in V \end{cases} \qquad \textbf{éq. 4.1-6}$$

The residues associated with these problems are respectively given by:

$$\begin{cases} R_h^u(v) = l(v) - a(u^h, v) \\ R_h^\omega(v) = Q(v) - a(v, \omega^h) \end{cases} \qquad \textbf{éq. 4.1-7}$$

While replacing u by u^h+e and ω by $\omega^h+\varepsilon$ and by using the symmetry of $a(\cdot,\cdot)$, one obtains the equations controlling the errors e and ε :

$$\begin{cases} a(e,v)=R_h^u(v) \\ a(\varepsilon,v)=R_h^\omega(v) \end{cases} \quad \text{éq. 4.1-8}$$

By linear combination, there are the two following problems:

$$\begin{cases} a(s\,e+s^{-1}\varepsilon,v)=(s\,R_h^u+s^{-1}R_h^\omega)(v) \\ a(s\,e-s^{-1}\varepsilon,v)=(s\,R_h^u-s^{-1}R_h^\omega)(v) \end{cases} \quad \text{éq. 4.1-9}$$

Thus the digital error $(s\,e+s^{-1}\varepsilon)$ (and $(se-s^{-1}\varepsilon)$) is generated by the total residue $(s\,R_h^u+s^{-1}R_h^\omega)$ (respectively $(s\,R_h^u-s^{-1}R_h^\omega)$). In a way similar to the estimator in residue, there exists a constant C^+ (and C^-), independent of the size of the elements, such as:

$$\|s\,e+s^{-1}\varepsilon\|_e^2\le C^+\left[\sum_E h_E^2\|s\,r_E^u+s^{-1}r_E^\omega\|_{L^2(E)}^2+\sum_{\Gamma\not\subset\Gamma_U} l_\Gamma\|s\,t_\Gamma^u+s^{-1}t_\Gamma^\omega\|_{L^2(\Gamma)}^2\right] \quad \text{éq. 4.1-10}$$

$$\|s\,e-s^{-1}\varepsilon\|_e^2\le C^-\left[\sum_E h_E^2\|s\,r_E^u-s^{-1}r_E^\omega\|_{L^2(E)}^2+\sum_{\Gamma\not\subset\Gamma_U} l_\Gamma\|s\,t_\Gamma^u-s^{-1}t_\Gamma^\omega\|_{L^2(\Gamma)}^2\right] \quad \text{éq. 4.1-11}$$

Finally the estimator of error in quantity of interest ${}^{REQI}\eta_E$ is defined such as:

$${}^{REQI}\eta_E=\frac{1}{4}(\eta_E^+)^2-\frac{1}{4}(\eta_E^-)^2 \quad \text{éq. 4.1-12}$$

with η_E^+ and η_E^- defines by:

$$(\eta_E^+)^2=c^+\left[h_E^2\|s\,r_E^u+s^{-1}r_E^\omega\|_{L^2(E)}^2+\frac{1}{2}\sum_{\Gamma\not\subset\Gamma_F} l_\Gamma\|s\,t_\Gamma^u+s^{-1}t_\Gamma^\omega\|_{L^2(\Gamma)}^2+\sum_{\Gamma\subset\Gamma_F} l_\Gamma\|s\,t_\Gamma^u+s^{-1}t_\Gamma^\omega\|_{L^2(\Gamma)}^2\right] \quad \text{éq. 4.1-13}$$

$$(\eta_E^-)^2=c^-\left[h_E^2\|s\,r_E^u-s^{-1}r_E^\omega\|_{L^2(E)}^2+\frac{1}{2}\sum_{\Gamma\not\subset\Gamma_F} l_\Gamma\|s\,t_\Gamma^u-s^{-1}t_\Gamma^\omega\|_{L^2(\Gamma)}^2+\sum_{\Gamma\subset\Gamma_F} l_\Gamma\|s\,t_\Gamma^u-s^{-1}t_\Gamma^\omega\|_{L^2(\Gamma)}^2\right] \quad \text{éq. 4.1-14}$$

Taking into account the definitions of the terminals of the error in quantity of interest given in part 1, the estimator which we have just defined does not limit the error but gives some an approximate value:

$$Q(e)\approx\sum_E {}^{REQI}\eta_E \quad \text{éq. 4.1-15}$$

The estimator thus determined is thus connected more with an indicator of error allowing to guide a strategy of grid. This indicator is programmed in *Code_Aster*, it is available for all the types of elements 2D and 3D (except the pyramids) like for the linear and quadratic elements.

4.2 Estimator in quantity of interest based on smoothings of field

An estimator of error is built directly starting from the techniques of smoothing [R4.10.01] and of the fundamental relation between the error in quantity of interest, error on the solution of the primal problem and that on the solution of the dual problem:

$$Q(e)=a(e,\varepsilon)=\int_\Omega Tr\left[{}^T(\sigma(u)-\sigma(u^h))\;K^{-1}\;(\sigma(\omega)-\sigma(\omega^h))\right]d\,\Omega \quad \text{éq. 4.2-1}$$

The approach consists in building starting from the solutions finite elements u^h and ω^h continuous stress fields $\tilde{\sigma}(u^h)$ and $\tilde{\sigma}(\omega^h)$ nearest possible to the exact solutions. This operation of smoothing is carried out by the various techniques described in the first part. An upper limit is thus obtained [bib9]:

$$a(e,\varepsilon) \leq C \int_\Omega Tr\left[\left(\tilde{\varepsilon}(u)-\varepsilon(u^h)\right) K \left(\tilde{\varepsilon}(\omega)-\varepsilon(\omega^h)\right)\right] d\Omega \quad \textbf{éq. 4.2-2}$$

The local contributions of error in quantity of interest can be as follows defined:

$$^{ZZQI}\eta_E = \int_E Tr\left[\left(\tilde{\varepsilon}(u)-\varepsilon(u^h)\right) K \left(\tilde{\varepsilon}(\omega)-\varepsilon(\omega^h)\right)\right] d E \quad \textbf{éq. 4.2-3}$$

The estimator is the sum on the elements of the contributions and is written:

$$^{ZZQI}\eta = \sum_E {}^{ZZQI}\eta_E \quad \textbf{éq. 4.2-4}$$

This estimator is very simple to implement and practically does not require a development for a code equipped with techniques of smoothing. This indicator is programmed in *Code_Aster*, it is available for all the types of elements 2D.

4.3 Estimator in quantity of interest based on the hierarchical bases

The starting point to build this estimator is still the fundamental relation of the error in quantity of interest:

$$Q(e) = a(e,\varepsilon) \quad \textbf{éq. 4.3-1}$$

The resolution of the primal problem and the dual problem with “rich” grids more (practically they are uniformly refined grids) makes it possible to obtain the improved solution $u*$ primal problem and the solution improved of the dual problem $\omega*$.

By considering that approximations $u*$ and $\omega*$ are sufficiently precise compared to the original approximations u^h and ω^h then the error in quantity of interest is given by:

$$Q(e) = a(e,\varepsilon) = a(u-u^h, \omega-\omega^h) \approx a(u*-u^h, \omega*-\omega^h) = Q(e*) \quad \textbf{éq. 4.3-2}$$

A local estimator of error in quantity of interest can be defined as follows:

$$^{BHQI}\eta_E = \int_E Tr\left[\left(\varepsilon(u*)-\varepsilon(u^h)\right) K \left(\varepsilon(\omega*)-\varepsilon(\omega^h)\right)\right] d E \quad \textbf{éq. 4.3-3}$$

The total estimator is the sum on the elements and is written as follows:

$$^{BHQI}\eta = \sum_E {}^{BHQI}\eta_E$$

This estimator can be of an interest limited for an industrial use taking into account the cost of generated calculation. Indeed the primal problem and the dual problem will have to be each one solved twice: once on the initial grid and once on a finer grid thus with a overcost of calculation. However this estimator can return the error in quantity of interest available for classes of problems for which no estimator available or is implemented (problems to the eigenvalues or of dynamics in *Code_Aster* for example).

5 Formulation of the quantity of interest

As we already saw in the first part, instead of evaluating a measurement of the error such as the standard in energy for example, it is more useful to consider the error on a quantity of interest having a physical direction. This quantity of interest (*quantity of interest* or *output*) can be represented by a linear functional calculus $Q(\cdot)$ defined on the space of the functions tests. The goal of the estimate in quantity of interest is thus to make sure of quality of $Q(u^h)$ by estimating the quantity:

$$\varepsilon^Q = Q(u-u^h) = Q(e) \qquad \text{éq. 5-1}$$

To obtain the estimate, the functional calculus should be used $Q(\cdot)$ like the loading of the dual problem defined by:

$$\begin{cases} Trouver\ \omega \in V\ tel\ que \\ \quad a(v,\omega) = Q(v) \qquad \forall\ v \in V \end{cases} \qquad \text{éq. 5-2}$$

Many physical quantities are used in design and must be controlled. These sizes can be, for examples, the average of a component of displacement or the average of a component of the constraints on a under-field (zone of interest):

$$Q(v) = \frac{1}{|\omega|}\int_\omega v_x \, d\Omega \qquad \text{éq. 5-3}$$

$$Q(v) = \frac{1}{|\omega|}\int_\omega \sigma_{xx} \, d\Omega \qquad \text{éq. 5-4}$$

These quantities are not usable directly like loading of the dual problem. It is necessary to express them in an adequate way in order to find the loading to be imposed on the local problem. The general form of these quantities is the following one [bib25]:

$$Q(v) = \int_\Omega f^Q \cdot v \, d\Omega + \int_{\Gamma_F} F^Q \cdot v \, d\Gamma - a(u^Q, v) \qquad \text{éq. 5-5}$$

where f^Q, F^Q and u^Q are given. In the continuation, we will see that simple quantities of interest result directly from this general form to constitute of them typical cases in which one or more terms are worthless.

5.1 Sizes associated with displacements

5.1.1 Component of displacement in a field

The first quantity related to displacement is the median value of a component of displacement under - field ω :

$$Q^{depl}(v) = \frac{1}{|\omega|}\int_\omega v_i \, d\Omega \quad i = 1,2 \text{ ou } 3 \qquad \text{éq. 5.1.1-1}$$

$Q^{depl}(v)$ can be written:

$$\int_\Omega f^Q \cdot v \, d\Omega \qquad \text{éq. 5.1.1-2}$$

who corresponds to the typical case where $F^Q=0$ and $u^Q=0$ and where f^Q is a constant vector on ω and no one elsewhere.

The dual problem to solve is written in the following way:

$$\int_\Omega \sigma_{ij}(v)\varepsilon_{ij}(\omega)\ d\Omega=\int_\Omega f_i^Q\ v_i\ d\Omega \quad \forall v\in V \qquad \textbf{éq. 5.1.1-3}$$

By using the property of symmetry of the tensor of the constraints and while deriving, one obtains:

$$\int_\Omega \left(\sigma_{ij}(\omega)\ v_i\right)_{,j}\ d\Omega-\int_\Omega \sigma_{ij,j}(\omega)\ v_i\ d\Omega=\int_\Omega f_i^Q\ v_i\ d\Omega \qquad \textbf{éq. 5.1.1-4}$$

Finally by using the formula of Stokes, one a:

$$\int_\Omega \left(\sigma_{ij,j}(\omega)+f^Q\right)\ v_i\ d\Omega-\int_{\partial\Omega}\sigma_{ij}(\omega)\ n_j\ v_i\ d\Omega=0 \qquad \textbf{éq. 5.1.1-5}$$

This enables us to write the local dual problem:

$$\begin{cases}\sigma_{ij,j}(\omega)+f_i^Q &= 0 \quad dans\ \ \Omega\\ u_i(x) &= 0 \quad sur\ \ \Gamma_U\\ \sigma_{ij}(\omega)\ n_j(x) &= 0 \quad sur\ \ \Gamma_F\end{cases} \qquad \textbf{éq. 5.1.1-6}$$

One notes thus that imposing $Q^{depl}(v)$ as loading of the dual problem amounts imposing a constant voluminal loading on ω. It should be noted that if one searches the error on the vector complete displacement, it will be necessary to solve as much dual problem than components (2 in dimension 2 and 3 in dimension 3).

5.1.2 Component of displacement on an edge

Another useful quantity related to displacement is the median value of a component of displacement on an edge $\gamma\subset\Gamma_F$:

$$Q^{depl}(v)=\frac{1}{|\gamma|}\int_\gamma v_i\ d\Gamma \quad i=1,2\ ou\ 3 \qquad \textbf{éq. 5.1.2-1}$$

$Q^{depl}(v)$ can be written:

$$\int_{\Gamma_F} F^Q\cdot v\ d\Gamma \qquad \textbf{éq. 5.1.2-2}$$

who corresponds to the typical case where $f^Q=0$ and $u^Q=0$ and where F^Q is a constant vector on γ and no one elsewhere and with for each v_i, $F_i^Q=\frac{1}{|\gamma|}$; other components of F^Q being worthless.

The local dual problem is written in the following way:

$$\begin{cases}\sigma_{ij,j}(\omega) &= 0 \quad dans\ \ \Omega\\ u_i(x) &= 0 \quad sur\ \ \Gamma_U\\ \sigma_{ij}(\omega)\ n_j(x) &= F_i^Q \quad sur\ \ \Gamma_F\end{cases} \qquad \textbf{éq. 5.1.2-3}$$

To impose $Q^{depl}(v)$ as loading of the dual problem amounts imposing a linear in dimension 2 and surface loading in dimension 3 restricted on Γ_F.

5.1.3 Normal displacement on a board

Finally the last quantity related to displacement is the average of normal displacement on a board $\gamma \subset \Gamma_F$:

$$Q^{depl}(v)=\frac{1}{|\gamma|}\int_\gamma v_n \, d\Gamma \qquad \textbf{éq. 5.1.3-1}$$

$Q^{depl}(v)$ can be written:

$$\int_{\Gamma_F} pn\cdot v \, d\Gamma \qquad \textbf{éq. 5.1.3-2}$$

where n is the normal vector at the edge γ and $p=\frac{1}{|\gamma|}$ on γ and no one elsewhere.

The local dual problem is written in the following way:

$$\begin{cases} \sigma_{ij,j}(\omega) &= 0 & dans \ \Omega \\ u_i(x) &= 0 & sur \ \Gamma_U \\ \sigma_{ij}(\omega)\, n_j(x) &= pn_i & sur \ \Gamma_F \end{cases} \qquad \textbf{éq. 5.1.3-3}$$

To impose $Q^{depl}(v)$ as loading of the dual problem amounts imposing a loading of linear in dimension 2 and surface pressure in dimension 3.

5.2 Sizes associated with the constraints

5.2.1 Component of the constraints in a field

We are interested now in the estimate of the error on the median value of a component of the constraints under - field ω :

$$Q^{sigma}(v)=\frac{1}{|\omega|}\int_\omega \sigma_{ij} \, d\Omega \quad i,j=1,2 \ ou \ 3 \qquad \textbf{éq. 5.2.1-1}$$

To determine $Q^{sigma}(v)$, it is enough to determine:

$$-a(u^Q,v)=\int_\Omega \sigma(v) : \Sigma(u^Q) \, d\Omega \qquad \textbf{éq. 5.2.1-2}$$

who corresponds to the typical case where $f^Q=0$ and $F^Q=0$ and where $\Sigma(u^Q)$ is a constant symmetrical operator on ω and no one elsewhere.

For that, it is enough to write that the component of the constraints is equal to the trace of the product between operators of which one is nonnull in ω :

$$Q^{sigma}(v)=\frac{1}{|\omega|}\int_\omega \sigma_{ij} \, d\Omega=\int_\omega \sigma : \Sigma \, d\Omega+\underbrace{\int_{\Omega\setminus\omega} \sigma : \Sigma \, d\Omega}_{=0}=\int_\Omega \sigma : \Sigma \, d\Omega \quad i,j=1,2 \ ou \ 3 \qquad \textbf{éq. 5.2.1-3}$$

with for each σ_{ij} , $\Sigma_{ij}=\frac{1}{|\omega|}$ for $i=j$; $\Sigma_{ij}=\frac{1}{2|\omega|}$ for $i\neq j$.

The dual problem to solve is written in the following way:

$$\int_\Omega \sigma_i(v)\ \varepsilon_{ij}(\omega)\ d\Omega = \int_\Omega \sigma_{ij}(v)\ \Sigma_{ij}\ d\Omega \qquad \text{éq. 5.2.1-4}$$

While deriving, one obtains:

$$\int_\Omega \left(\left(\sigma_{ij}(\omega) - a_{ijkl}\Sigma_{kl}\right) v_i\right)_{,j}\ d\Omega - \int_\Omega \left(\sigma_{ij}(\omega) - a_{ijkl}\Sigma_{kl}\right)_{,j}\ v_i\ d\Omega = 0 \qquad \text{éq. 5.2.1-5}$$

Finally by using the formula of Stokes, one a:

$$\int_\Omega \left(\left(\sigma_{ij}(\omega) - a_{ijkl}\Sigma_{kl}\right) v_i\right)_{,j}\ d\Omega - \int_\Omega \left(\sigma_{ij}(\omega) - a_{ijkl}\Sigma_{kl}\right) n_j\ v_i\ d\Omega = 0 \qquad \text{éq. 5.2.1-6}$$

This enables us to write the local dual problem:

$$\begin{cases} \left(\sigma_{ij}(\omega) - a_{ijkl}\Sigma_{kl}\right)_{,j} & = & 0 & dans\ \ \Omega \\ u_i(x) & = & 0 & sur\ \ \Gamma_U \\ \left(\sigma_{ij}(\omega) - a_{ijkl}\Sigma_{kl}\right) n_j(x) & = & 0 & sur\ \ \Gamma_F \end{cases} \qquad \text{éq. 5.2.1-7}$$

One notes thus that imposing $Q^{sigma}(v)$ as loading of the dual problem amounts imposing an initial deformation Σ. It should be noted that if one searches the error on the complete tensor of the constraints, it will be necessary to solve as much dual problem than components (3 in dimension 2 and 6 in dimension 3).

5.2.2 Normal constraint on an edge

It can be interesting to consider the error on the normal constraint on an edge γ :

$$Q^{sigma}(v) = \int_\gamma n\cdot\sigma(v)n\ d\Omega \qquad \text{éq. 5.2.2-1}$$

This quantity does not arise in the general form. The introduction of an auxiliary function is necessary [bib25]. This function χ is defined such as $\chi|_\gamma = 1$ and equalizes to zero on the rest of $\partial\Omega$.

If $n^\gamma = n|_\gamma$, the function χ check the following equation:

$$\begin{aligned} a\left(u, \chi\ n^\gamma\right) &= \int_\Omega \sigma_{ij}(u)\varepsilon_{ij}(\chi\ n^\gamma)\ d\Omega \\ &= \int_{\partial\Omega} \sigma_{ij}(u)\ n_j(\chi\ n^\gamma)_i\ d\Omega - \underbrace{\int_\Omega \left(\sigma_{ij}(u)\right)_{,j}(\chi\ n^\gamma)_i\ d\Omega}_{=0} \\ &= \int_\gamma \sigma_{ij}(u)\ n_j(\chi\ n^\gamma)_i\ d\Omega \end{aligned} \qquad \text{éq. 5.2.2-2}$$

What shows that the quantity of interest can be written in an equivalent way:

$$Q^{sigma}(u) = \int_\gamma n\cdot\sigma(u)n\ d\Omega = a\left(u, \chi\ n^\gamma\right) =: \tilde{Q}(u) \qquad \text{éq. 5.2.2-3}$$

But as the preceding equality is not true that for one u individual, it should be noted that:

$$Q^{sigma}(v) = \int_\gamma n\cdot\sigma(v)n\ d\Omega \neq a\left(v, \chi\ n^\gamma\right) =: \tilde{Q}(v) \qquad \text{éq. 5.2.2-4}$$

For more facility, quantity $\tilde{Q}(v)$ will be used instead of the quantity $Q^{sigma}(v)$. Indeed it corresponds to use $u^Q = -\chi\ n^\gamma$.

The quantity of interest to use is thus written in the following way:

$$\tilde{Q}(v)=-a(u^Q,v)=\int_\Omega \sigma(v):\Sigma(-\chi\ n^\gamma)\ d\Omega \qquad \textbf{éq. 5.2.2-5}$$

who corresponds to the typical case where $f^Q=0$ and $F^Q=0$.

In a way similar to the case of the average of the constraints, the local dual problem is written:

$$\begin{cases} \left(\sigma_{ij}(\omega)-a_{ijkl}\Sigma_{kl}\right)_{,j} = 0 \quad dans \quad \Omega \\ u_i(x) = 0 \quad sur \quad \Gamma_U \\ \left(\sigma_{ij}(\omega)-a_{ijkl}\Sigma_{kl}\right) n_j(x) = 0 \quad sur \quad \Gamma_F \end{cases} \qquad \textbf{éq. 5.2.2-6}$$

To impose $\tilde{Q}(v)$ as loading of the dual problem amounts imposing a field of initial deformation calculated starting from the field of displacement $u^Q=-\chi\ n^\gamma$. This quantity of interest was not implemented in *Code_Aster*.

5.2.3 Constraint of Von Mises in a field

The constraint of Von Mises is a very useful mechanical quantity in term of dimensioning for the engineer. The difficulty to estimate the error on this quantity lies in the fact that its expression is not linear compared to displacement and thus unusable with the technique presented. The difficulty is overcome thanks to a linearization of the expression and under certain assumptions [bib21].

The tensor of the constraints σ can break up into the sum of a tensor deviatoric σ^d (whose trace is worthless) and of a spherical tensor σ^s (whose diagonal extra terms are worthless):

$$\sigma=\sigma^d+\sigma^s \qquad \textbf{éq. 5.2.3-1}$$

where σ^d and σ^s are defined by:

$$\sigma^d=\sigma-\frac{1}{3}tr(\sigma)\ \boldsymbol{I} \qquad \sigma^s=\frac{1}{3}tr(\sigma)\ \boldsymbol{I} \qquad \textbf{éq. 5.2.3-2}$$

The constraint of Von Mises, noted σ_{vm}, is defined by:

$$\sigma_{vm}=\sqrt{\frac{3}{2}\sigma^d:\sigma^d} \qquad \textbf{éq. 5.2.3-3}$$

In linear elasticity, the constraint depends linearly on displacement, which enables us to write:

$$\sigma^d(u)=\sigma^d(u^h)+\sigma^d(e) \qquad \textbf{éq. 5.2.3-4}$$

By using this in the definition of the constraint of Von Mises, one obtains:

$$\sigma_{vm}(u)=\sqrt{\frac{3}{2}\left(\left(\sigma^d(u^h)+\sigma^d(e)\right):\left(\sigma^d(u^h)+\sigma^d(e)\right)\right)} \qquad \textbf{éq. 5.2.3-5}$$

The preceding expression is rewritten in order to reveal a function whose limited development is known:

$$\begin{aligned}\sigma_{vm}(u) &= \sqrt{\frac{3}{2}\left(\sigma^d(u^h):\sigma^d(u^h)+2\,\sigma^d(u^h):\sigma^d(e)+\sigma^d(e):\sigma^d(e)\right)} \\ &= \sigma_{vm}(u^h)\sqrt{1+\frac{3}{2}\frac{2\,\sigma^d(u^h):\sigma^d(e)+\sigma^d(e):\sigma^d(e)}{\sigma^2_{vm}(u^h)}}\end{aligned}$$ **éq. 5.2.3-6**

The development limited to order 1 when e tends towards zero allows to obtain the following approximation:

$$\begin{aligned}\sigma_{vm}(u) &\approx \sigma_{vm}(u^h)\left(1+\frac{3}{2}\frac{\sigma^d(u^h):\sigma^d(e)}{\sigma^2_{vm}(u^h)}\right) \\ &\approx \sigma_{vm}(u^h)+\frac{3}{2}\frac{\sigma^d(u^h):\sigma^d(e)}{\sigma_{vm}(u^h)}\end{aligned}$$ **éq. 5.2.3-7**

Finally, an approximation of the error on the constraint of Von Mises is given:

$$\sigma_{vm}(u)-\sigma_{vm}(u^h)\approx\frac{3}{2}\frac{\sigma^d(u^h):\sigma^d(e)}{\sigma_{vm}(u^h)}$$ **éq. 5.2.3-8**

Thus, to estimate the error on the average of the constraint of Von Mises in a field:

$$\varepsilon^Q=\frac{1}{|\omega|}\int_\omega\left(\sigma_{vm}(u)-\sigma_{vm}(u^h)\right)d\,\Omega$$ **éq. 5.2.3-9**

the following functional calculus perhaps used:

$$Q^{vm}(v)=\frac{3}{2|\omega|}\int_\omega\frac{\sigma^d(u^h):\sigma^d(v)}{\sigma_{vm}(u^h)}\,d\,\Omega$$ **éq. 5.2.3-10**

As for the component of the constraints on a field, to determine $Q^{vm}(v)$, it is enough to determine:

$$-a\left(u^Q,v\right)=\int_\Omega\Sigma(u^Q):\sigma(v)\,d\,\Omega$$ **éq. 5.2.3-11**

What corresponds to the typical case where $f^Q=0$ and $F^Q=0$ and where $\Sigma\left(u^Q\right)$ is a constant symmetrical operator by element on ω and no one elsewhere. The fact that in the equation 5.2.3-10 appears $\sigma^d(v)$ and not $\sigma(v)$ require to rewrite the functional calculus $Q^{vm}(v)$ to reveal $\sigma(v)$:

$$Q^{vm}(v)=\frac{3}{2|\omega|}\int_\omega\frac{\sigma^d(u^h):\left(\sigma(v)-\sigma^s(v)\right)}{\sigma_{vm}(u^h)}\,d\,\Omega$$ **éq. 5.2.3-12**

$$Q^{vm}(v)=\frac{3}{2|\omega|}\int_\omega\frac{\sigma^d(u^h):\sigma(v)-\sigma^d(u^h):\sigma^s(v)}{\sigma_{vm}(u^h)}\,d\,\Omega$$ **éq. 5.2.3-13**

Lastly, the double contraction enters a tensor deviatoric and a spherical tensor being worthless, the functional calculus is written:

$$Q^{vm}(v)=\frac{1}{|\omega|}\int_\omega\left(\frac{3}{2\,\sigma_{vm}(u^h)}\sigma^d(u^h)\right):\sigma(v)\,d\,\Omega$$ **éq. 5.2.3-14**

with $\Sigma(u^Q)=\frac{3}{2\,\sigma_{vm}(u^Q)}\sigma^d(u^Q)$ and $u^Q=u^h$.

In a way similar to the case of the average of the constraints, the local dual problem is written:

$$\begin{cases}\left(\sigma_{ij}(\omega)-a_{ijkl}\Sigma_{kl}\right)_{,j} &= 0 \quad dans \quad \Omega\\ u_i(x) &= 0 \quad sur \quad \Gamma_U\\ \left(\sigma_{ij}(\omega)-a_{ijkl}\Sigma_{kl}\right)n_j(x) &= 0 \quad sur \quad \Gamma_F\end{cases} \qquad \textbf{éq. 5.2.3-15}$$

To impose $Q^{vm}(v)$ as loading of the dual problem amounts imposing a field of initial deformation.

5.3 Sizes related to the breaking process

5.3.1 Factors of intensity of the constraints

A method of calculating of K_I, K_{II} and K_{III} in 2D (plan and axisymmetric) and 3D is recalled; it is based on the extrapolation of the jumps of displacements on the lips of the crack. This method is applicable only to the case of the plane cracks, in homogeneous and isotropic materials; it is used in the order POST_K1_K2_K3.

The stress intensity factors are identified starting from the jump of displacements $[U]$ by a method of least squares on a segment length r_{max}. This is expressed by the problem of minimization according to:

$$K \quad \text{minimise} \quad F(k)=\frac{1}{2}\int_0^{r_{max}}\left(C[U(r)]-k\sqrt{r}\right)^2 dr \qquad \textbf{éq. 5.3.1-1}$$

To solve this problem, a value of k is sought such as the derivative of F cancel yourself:

$$F'(K)=\int_0^{r_{max}}\sqrt{r}\left(K\sqrt{r}-C[U(r)]\right)dr=0 \qquad \textbf{éq. 5.3.1-2}$$

The separation of the integral gives:

$$\int_0^{r_{max}} r\,K\,dr=\int_0^{r_{max}}\sqrt{r}\,C[U(r)]\,dr \qquad \textbf{éq. 5.3.1-3}$$

$$K\left[\frac{r^2}{2}\right]_0^{r_{max}}=\int_0^{r_{max}}\sqrt{r}\,C[U(r)]\,dr \qquad \textbf{éq. 5.3.1-4}$$

The formula clarifies to calculate K results directly:

$$K=\frac{2C}{r_{max}^2}\int_0^{r_{max}}\sqrt{r}[U(r)]dr \qquad \textbf{éq. 5.3.1-5}$$

By carrying out integration by a method of the trapezoids, the preceding relation becomes:

$$K=\frac{C}{r_{max}^2}\sum_{i=1}^{N}\left([U]_{i-1}\sqrt{r_{i-1}}+[U]_i\sqrt{r_i}\right)\left(r_i-r_{i-1}\right) \qquad \textbf{éq. 5.3.1-6}$$

where N is the number of nodes on the segment $[0\,,r_{max}]$. It is noted that K is the linear shape of the field of displacement for one r_{max} fixed, typically that corresponds to 4 or 5 elements.

To express the factors of intensity of the constraints in term of loading for the dual problem, we will use the equation 5.3.1-5.

While revealing the components of displacement on the upper lip $U_i^{sup}(r)$ and components of displacement on the lower lip $U_i^{inf}(r)$, one obtains:

$$K_i = \frac{2C}{r_{max}^2} \int_\Gamma \left(U_i^{sup}(r) - U_i^{inf}(r) \right) \sqrt{r}\, dr \qquad \textbf{éq. 5.3.1-7}$$

Contour Γ is made up by the two lips of the crack; Γ^{sup} is the upper lip and Γ^{inf} is the lower lip. This makes it possible to separate the preceding integral in two parts:

$$K_i = \frac{2C}{r_{max}^2} \left[\int_{\Gamma^{sup}} U_i(r) \sqrt{r}\, dr - \int_{\Gamma^{inf}} U_i(r)\, \sqrt{r}\, dr \right] \qquad \textbf{éq. 5.3.1-8}$$

In order to reveal the function test v, the components of displacements are written like the scalar product of two vectors:

$$K_i = \frac{2C}{r_{max}^2} \left[\int_{\Gamma^{sup}} v \cdot g_i(r) \sqrt{r}\, dr - \int_{\Gamma^{inf}} v \cdot g_i(r) \sqrt{r}\, dr \right] \qquad \textbf{éq. 5.3.1-9}$$

With $i = I, II, III$; g_I the normal vector with the plan of crack, g_{II} the normal vector at the bottom of crack and g_{III} the tangent vector at the bottom of crack. This thus means that the expression of the quantity of interest is valid in dimension 3 and thus allows the estimate of error of the factors of intensity of the constraints for the problems in dimension 3.

Finally by gathering all the terms, the following expression is obtained:

$$Q(v) = K_i(v) = \int_{\Gamma^{sup}} f^{sup} \cdot v\ dr + \int_{\Gamma^{inf}} f^{inf} \cdot v\ dr \qquad \textbf{éq. 5.3.1-10}$$

with:

$$f^{sup} = \frac{2C}{r_{max}^2} g_i(r) \sqrt{r} \text{ and } f^{inf} = -\frac{2C}{r_{max}^2} g_i(r) \sqrt{r} \qquad \textbf{éq. 5.3.1-11}$$

This expression corresponds to a linear loading in dimension 2 (surface in dimension 3) to impose on a partition of the lips of the crack on the basis of the point and length r_{max}. The choice of the ray r_{max} must be made so that it is in the singular zone and contain the possible elements of Barsoum.

6 Use and implementation in Code_Aster

The estimator of error in quantity of interest is implemented in *Code_Aster* in mechanics for all the elements, modelings C_PLAN, D_PLAN, AXIS and 3D.

To estimate the error in quantity of interest, we saw that it was necessary to solve an assistant problem whose loading in effort is the quantity of interest. The following table summarizes and gathers the loadings to be imposed in *Code_Aster*, by the means of the order AFFE_CHAR_MECA, for each quantity of interest. The table is given for 2D but the 3D results easily. For the component quantities of the constraints, the value to be indicated is 1.0 for the diagonal terms and 0.5 for the others.

	$Q(v)$	Keyword of AFFE_CHAR_MECA	Component
Average of a component of displacement on a contour	$\frac{1}{\lvert\gamma\rvert}\int_\gamma v_x \, d\Gamma$	FORCE_CONTOUR	FX=1.
	$\frac{1}{\lvert\gamma\rvert}\int_\gamma v_y \, d\Gamma$	FORCE_CONTOUR	FY=1.
Average of a component of displacement on under - field	$\frac{1}{\lvert\omega\rvert}\int_\omega v_x \, d\Omega$	FORCE_INTERNE	FX=1.
	$\frac{1}{\lvert\omega\rvert}\int_\omega v_y \, d\Omega$	FORCE_INTERNE	FY=1.
Average of normal displacement on a contour	$\frac{1}{\lvert\gamma\rvert}\int_\gamma v_n \, d\Gamma$	PRES_REP	PRES=1.
Average of a component of the constraints on under - field	$\frac{1}{\lvert\omega\rvert}\int_\omega \sigma_{xx} \, d\Omega$	PRE_EPSI	EPXX=1.
	$\frac{1}{\lvert\omega\rvert}\int_\omega \sigma_{yy} \, d\Omega$	PRE_EPSI	EPYY=1.
	$\frac{1}{\lvert\omega\rvert}\int_\omega \sigma_{xy} \, d\Omega$	PRE_EPSI	EPXY=0.5

When the quantities of interest are not linear or when their expression does not make it possible to easily express them in term of loading a particular treatment is necessary. For the non-linear quantities, the theory does not apply; this is why they should be linearized. The constraint of Von Mises is the typical example. The linearization brings us to the following formula:

$$Q^{vm}(v)=\frac{1}{\lvert\omega\rvert}\int_\omega \left(\frac{3}{2\,\sigma_{vm}(u^h)}\sigma^d(u^h)\right) : \sigma(v)\; d\Omega \qquad \textbf{éq. 6-1}$$

Thus one approaches the quantity of interest Von Mises by another linear quantity. The loading to be imposed in *Code_Aster* is a made up stress field:

$$\frac{3K}{2}\frac{\sigma^d(u^h)}{\sigma_{vm}(u^h)} \qquad \textbf{éq. 6-2}$$

When the definition of the quantity is not adapted to the expression of a loading, it is necessary, there too, to use a treatment which will be specific to each quantity of interest. For our applications, the factors of intensity of constraints (FIC) are interesting sizes. By using a method based on extrapolation of the jumps of displacements on the lips of the crack, one can express the FIC in the following way, with $C=1$ in plane constraint and $C=1-\nu^2$ in plane deformation:

$$K=\frac{2C}{r_{max}^2}\int_0^{r_{max}} \sqrt{r}\,[U(r)]\,dr \qquad \textbf{éq. 6-3}$$

What makes it possible to obtain the following expression:

$$Q(v)=K_i(v)=\int_{\Gamma^{sup}} f^{sup}\cdot v\ dr+\int_{\Gamma^{inf}} f^{inf}\cdot v\ dr \qquad \textbf{éq. 6-4}$$

with:

$$f^{sup}=\frac{2C}{r_{max}^2}g(r)\sqrt{r} \text{ and } f^{inf}=-\frac{2C}{r_{max}^2}g(r)\sqrt{r} \qquad \textbf{éq. 6-5}$$

with $g(r)$ vector which directs the crack.

In *Code_Aster*, this vector is known under the name of VECT_K1. One sees thus that it is necessary to impose an effort on each lip of the crack (and f^{inf}). The following table shows these two results.

	$Q(v)$	Keyword of AFFE_CHAR_MECA_F	Component
Average of the constraint of Von Mises	$\frac{1}{\lvert\omega\rvert}\int_\omega \sigma_{vm}\, d\,\Omega$	PRE_SIGM	Made up field
Stress intensity factor	$K_I \quad K_{II} \quad K_{III}$	FORCE_CONTOUR	F+ on lip sup. F- on lip inf.

The error analysis in quantity of interest passes by the resolution of an elastic design (corresponding to the dual problem) whose loading is on the one hand, the same one as that of the problem principal (or primal) on the conditions of Dirichlet (thus in imposed displacement), and on the other hand, that representing the selected quantity of interest. It is then necessary to provide this result in CALC_ERREUR via the keyword RESU_DUAL.

Lastly, various possible options in CALC_ERREUR are:
- 'QIZ1_ELEM' (respectively 'QIZ2_ELEM'): estimator of error in quantity of interest based on the method of Zhu-Zienkiewicz. The option should be calculated beforehand 'ERZ1_ELEM' or 'ERZ2_ELEM'.
- 'QIRE_ELEM' (by element) or 'QIRE_ELNO' (by element with the nodes): estimator of error in quantity of interest based on the residues in mechanics. The option should be calculated beforehand 'ERME_ELEM'.

Examples of application on industrial structures could be found in the thesis of J. DELMAS [bib26].

List of tests implementing the estimators of error in quantity of interest:

Test of the estimator of error in quantity of interest	sslv113c
test of the estimator of error in quantity of interest	sslv113d
Indicator of voluminal meshs error and functions	sslv153a
Detection of the singularities in a fissured plate (TRIA3)	ssnp130a
Estimators of error in quantities of interest for the calculation of the fic	zzzz257a
Estimators of error in quantities of interest for the calculation of the fic	zzzz257b
Estimators of error in quantities of interest for the calculation of the fic	zzzz257c
Estimators of error in quantities of interest for the calculation of the fic	zzzz257d

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8 Description of the versions of the document

Index Doc.	Version Aster	Author (S) or contributor (S), organization	Description of the modifications
With	8.3	J.DELMAS EDF/R & D /AMA	Initial text