Detection of the singularities and calculation of a map of size of elements

Summary:

One proposes here a method which aims at improving the treatment of the singularities in the strategies of adaptation of grid with the software LOBSTER (in the case of refinement) or with software GMSH (case of mending of meshes). This mechanism allows, on the one hand to detect the finite elements connected to singular zones and on the other hand to obtain, for a given total error, the size of the finite elements of the new grid in the event of mending of meshes.
This functionality is accessible in the order CALC_ERREUR by the options of calculation SING_ELEM (constant field by element) or SING_ELNO (field with the nodes by element). This option is valid only in mechanics. It is necessary to have calculated beforehand an estimator of error in mechanics and the deformation energy on each element. In any rigour, this method is valid only in elasticity.

Contents

1 Introduction

The objective of the option suggested here is to improve the treatment of the singularities in the strategies of adaptation of grid suggested in Code_Aster . Indeed, the presence of singularities (present in practice in any real structural analysis by finite elements) implies two kinds of difficulties which one will describe here as “theoretical” and of “practices”.

The “theoretical” difficulties come owing to the fact that the contribution to the error in energy of the elements touching a singularity is form $C h^{\alpha}$ (C a constant, h size of the element and α the order of the singularity) while the contribution of the elements except singularity is form $C h^{q}$ (q depending only on the degree of interpolation of the functions of form of the element). The adaptation of the grid must take into account this difference to be most effective possible. For example, to divide the contribution of the error by 4, it will be necessary to in the case of take elements 16 times smaller a crack ($\alpha=1/2$) and of the elements 2 times smaller in the case except crack with quadratic elements ($p=2$).

The “practical” difficulties come owing to the fact that, in zones of singularities, the contributions to the error in energy are important. If one aims at obtaining an error in weak energy, these zones thus should be very strongly refined. However, one can wonder about the influence of these errors in energy on physical quantities which interest the engineer (displacement in such point, maximum constraint in such sensitive area, etc…). In other words, it is not because the zones of singularities cause important errors on the energy which they have a great influence on calculation apart from these zones. **In practice, the estimators of error quickly indicate the only zones of singularities as being refining: the zones of singularities mask the other errors, for example a zone with strong gradient which one would wish to refine.**

The Laboratory of Mechanics and CAO de Saint-Quentin developed a method making it possible, on the one hand, to detect the singularities, and on the other hand, to determine, for a given total error, the size of the finite elements of the new grid in the event of mending of meshes.

The use of this two information can be under consideration under two angles:

- The finite elements considered as “singular” by the method can be excluded from the process of cutting,
- the new size of the finite elements is given to a remaillor so that this one builds the new grid by as well as possible respecting this new map of size. Currently, the software LOBSTER cuts out the element once (for example into 2D, a triangle is divided into 4 but not more). To continue cutting, it is necessary to call on LOBSTER again. An evolution is thus to envisage so that one can divide several times an element and thus as well as possible respect the map of size of the new grid. It is however possible to use the free maillor GMSH who takes directly a map of size as starter.

Note:

This document shows for the unit the note resulting from a CRECO between the LMCAO and the department AMA whose reference is quoted in bibliography ([bib1]).

2 Detection of the singularities

2.1 Principle of the method

When the exact solution of the studied problem present of the singularities, the order of convergence of the solution finite elements is modified and thus also that of the estimator of error. Let us consider, for example, a problem of plane elasticity discretized with triangular elements of degree p.
If the exact solution U_{ex} is regular, one knows that ([bib2], [bib3]):

$$\|u-u_h\|_\Omega=\|e\|_\Omega\le C\,h^p \qquad \text{éq 2.1-1}$$

Where $\|e\|_\Omega\le C\,h^p$ is the contribution to the error in energy, that is to say:

$$\|e\|_\Omega\le\frac{1}{2}\int_\Omega \varepsilon(e_h)\;K\;\varepsilon(e_h)\,d\Omega \qquad \text{éq 2.1-2}$$

On the other hand, if the exact solution presents a singularity, for example if, locally in the vicinity of a point M_0, the field of displacement is form (with r and θ polar coordinates in the vicinity of the point M_0):

$$U_{ex}=r^\alpha V(\theta)+W \quad avec \quad 0<\alpha<1 \qquad \text{éq 2.1-3}$$

Then, it is shown that [Strang & Fix, 1976]:

$$\|e_h\|_\Omega\le C\,h^\alpha \qquad \text{éq 2.1-4}$$

It results from it that the rate of convergence of the total error in energy becomes independent of the degree p finite elements used and it is the same of that of the measurement of the error (for example, if $p=1\,\mathrm{ou}\,2$ then $\alpha=1/2$ for a crack).

In order to obtain a good prediction of the optimized grids, the preceding observations lead us to use a rate of convergence q_E by element such as the estimator of error ε_E check:

$$\varepsilon_E=O\left(h^{q_E}\right) \qquad \text{éq 2.1-5}$$

A way simple to define these local coefficients consists in taking:

- $q_E=\alpha$ if the element E is connected to a singularity of order α ;
- $q_E=q$ for all the other finite elements where q does not depend that type of finite elements used.

The method presented thereafter thus comprises three phases:

- detection of the singular zones, in fact singular nodes of the grid;
- digital evaluation of the coefficient q_E for the elements connected to the nodes considered as singular (for the other elements, one fixes then $q_E=q$);
- calculation of the coefficient of modification of size r_E .

2.2 Detection of the singular nodes

The idea is to use the site errors. Indeed, the experiments show that these site errors present a peak in the vicinity of a singularity. For each node i grid, one thus compares the average error $\bar{m}^i$

elements connected to the node i with the average error $\bar{M}$ on the whole of the structure. The node i is regarded as singular if:

$$\bar{m}^i \geq \beta \bar{M} \quad \text{éq 2.2.1-1}$$

with

$$\bar{m}^i = \sqrt{\frac{\sum_{\text{E connecté à i}} \varepsilon_E^{\,2}}{\sum_{\text{E connecté à i}} mes(E)}} \quad \text{and} \quad \bar{M} = \sqrt{\frac{\sum_{E \in \text{structure}} \varepsilon_E^{\,2}}{\sum_{E \in \text{structure}} mes(E)}} \quad \text{éq 2.2.1-2}$$

where β is a coefficient larger than 1 and $mes(E)$ surface in 2D or volume in 3D of the element E. The digital experiments showed that the singular nodes are well detected while fixing $\beta=2$ in dimension 2, $\beta=3$ in dimension 3 for linear finite elements and $\beta=2$ in dimension 3 for quadratic finite elements.

Notice 1:

From a digital point of view, the detection of the singular nodes differs between the cases 2D and 3D. The conditions given thereafter for this detection are not based on a particular theory but rather on the experience gained in this field by the Laboratory of Mechanics and CAO de Saint-Quentin.

In 2D: a node ***I*** *is regarded as singular if he meets the 3 following conditions:*

$$\bar{m}_1^i \geq \beta \bar{M}$$
$$\bar{m}_1^i \geq \bar{m}_2^i \quad \text{éq 2.2.1-3}$$
$$\bar{m}_1^i \geq 3 \,\text{Min}\left(\bar{m}_2^i, \bar{m}_3^i\right)$$

Where $\bar{m}_1^i$ *,* $\bar{m}_2^i$ *and* $\bar{m}_3^i$ *are the averages of the error for the elements belonging to layers 1.2 and 3, respectively, compared to the node* i *considered.*

The layers are defined as follows:
Lay down 1: elements which have node I to test,
2 sleep: elements in contact (face, edge or node) with an element of layer 1,
3 sleep: elements in contact (face, edge or node) with an element of layer 2.

In 3D: the node i *is regarded as singular if he meets the condition* $\bar{m}_1^i \geq \beta \bar{M}$ *and if one of the nodes connected to the node* i *considered meets the condition* $\bar{m}_i^{\text{Noeud connecté à i}} \geq \beta \bar{M}$*. Contrary to the case 2D, the node* i *is singular only if one of its neighbors is also (one forgets the singular nodes isolated to keep only the singular edges).*

Notice 2:

In 2D, only the nodes tops are examined. In 3D, only the nodes tops located on an edge of the structure are examined (only for reasons of time calculation; this condition could thus be modified).

2.3 Evaluation about the singularity

For each singular node i detected, the order of the singularity, i.e. the value of q_E who will be used for the elements connected to the node i, is given by identifying the value of the density of energy of the solution finite elements in the vicinity of the node i with the theoretical value in the vicinity of a singular point.

2.3.1 Case of dimension 2

In this case, one calculates average energy finite elements, in discs A of center i and of ray r :

$$\bar{e}_h(r)=\frac{1}{2\,mes(A)}\int_A \varepsilon(u_h)\;K\;\varepsilon(u_h)\,dA$$ éq 2.3.1-1

While identifying, by a method of least squares, this average energy with the theoretical value in the vicinity of a singularity of order α :

$$e(r)=k\,r^{2(\alpha-1)}+c$$ éq 2.3.1-2

a value numerically is obtained $\bar{\alpha}$ near to α .

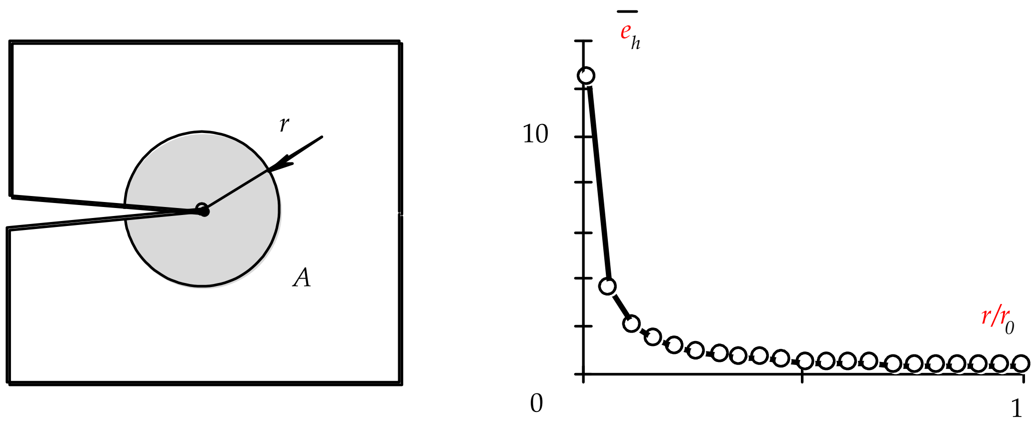

Figure 2.3.1-a: Digital evaluation of α

In practice the digital experiments show that it is enough to carry out the identification in a zone corresponding to 3 layers of elements around the singular point and to evaluate $\bar{e}^h(r)$ for 5 to 8 values of r regularly distributed in this zone (we took 10 values).

2.3.2 Case of dimension 3

In 3D the situation is more complex. The point singular, generally, are not isolated and it is thus frequent to be in the presence of singular edges. Let us consider, for example, the case of a cube embedded on a face and subjected to tractive efforts: all the points of the edges of the embedded face are singular [Figure 2.3.2-b].

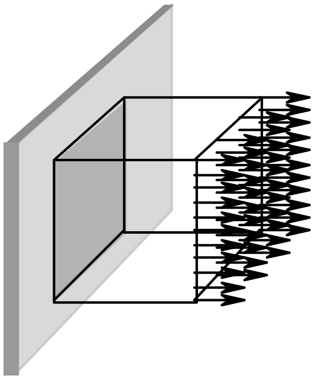

Figure 2.3.2-b: Cubic embedded in traction

In this situation, the evaluation of average energy in balls A of increasing ray and centered on a singular node does not allow to identify q_E . Indeed, as the ray increases the extent of the singular zone contained in the ball A increase and one does not obtain a fast decrease of $\overline{e}_h$ [Figure 2.3.2-c].

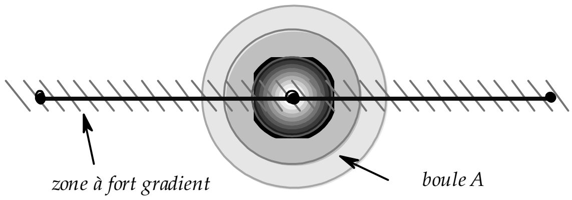

Figure 2.3.2-c: Energy in concentric balls

When the singular points are not isolated, the coefficient should be identified q_E in calculating the density of energy in coaxial cylinders built on the edges whose ends were regarded as singular [Figure 2.3.2-d] and cf notices [§ 2.2].

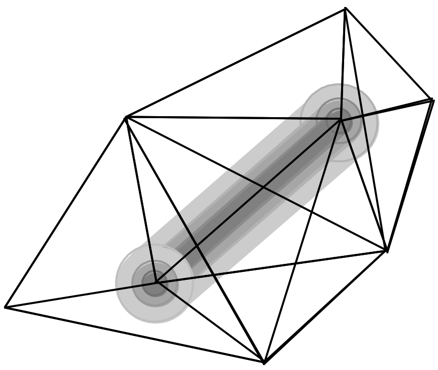

Figure 2.3.2-d: Energy in coaxial cylinders

2.4 Extension to the zones of stress concentration

In practice, we noted that the preceding method, clarification on cases presenting of the singularities also makes it possible to take into account correctly the zones with strong gradients of constraints even if mathematically these zones do not correspond to singularities.

3 Construction of an optimal grid

3.1 General information

The objective of a procedure of adaptation is to guarantee to the user a level of precision on the total error while minimizing the costs of calculation. To evaluate the errors of discretization, one uses a relative total measurement of the error ε and associated local contributions ε_E with:

$$\varepsilon^2=\sum_E \varepsilon_E{}^2 \qquad \text{éq 3.1-1}$$

The idea is to use the results of this first analysis finite elements and the estimators of errors to determine an optimal grid T^* i.e. a grid which makes it possible to respect desired precision the while minimizing the costs of calculation. One builds then the grid T^* using an automatic maillor and one carries out one second analysis finite elements.

3.2 Definition of optimality

For a given total error ε_0, a grid T^* is optimal compared to a measurement of error ε if:

$$\begin{array}{ll} \varepsilon^*=\varepsilon_0 & \text{précision demandée} \\ N^* & \text{nombre d'éléments de } T^* \text{ est minimum} \end{array} \qquad \text{éq 3.2-1}$$

This criterion of optimization naturally results in minimizing the costs of calculation.

3.3 Determination of an optimal grid

To determine the characteristics of the optimal grid T^*, the method consists in calculating on each element E grid T a coefficient of modification of sizes:

$$r_E=\frac{h_E^*}{h_E} \qquad \text{éq 3.3-1}$$

Where h_E is the current size of the element E and h_E^* the size (unknown) which it is necessary to impose on the elements T^* in the zone of E to ensure optimality [Figure 3.3-a]. A possible choice to define the size of an element h_E is to take the size of largest with dimensions of this element. The determination of the optimal grid is thus brought back to the determination, on the initial grid T, of a map of coefficients of modification of size.

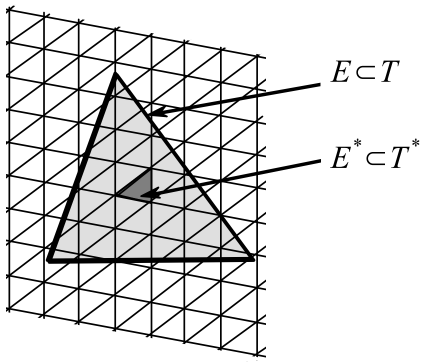

Figure 3.3-a: Definition of the sizes

The calculation of the coefficients r_E is based on the rate of convergence of the error:

$$\varepsilon = O\left(h^q\right) \quad \text{éq 3.3-2}$$

where q depends on the type of finite element used but also on the regularity of the exact solution of with the dealt problem. For the "classical" estimators of error, one supposes that the rate of convergence of the estimator of error is equal to the order of convergence of the solution finite elements. For the estimators in quantity of interest, this rate of convergence is equal to the double about convergence of the solution finite elements ([bib4]).

Thereafter, to calculate the coefficient of modification of size r_E, one distinguishes the case from the regular solution (q depends only on p, degree of interpolation of the functions of form of the element) of the case of the singular solution (q depends only on α, order of the singularity of the field of displacement).

3.4 "Classical" estimators of error

One designates by "classical" estimators of error the estimators who provide a standard (standard -L^2, standard -H^1, standard in energy) of the error in solution.

3.4.1 Case of the regular solution

Initially, we suppose that the exact solution is sufficiently regular so that the value of q does not depend that type of finite elements used and is equal to the degree of interpolation used p (p 1 for linear finite elements and 2 for quadratic finite elements is worth). In this case, to predict the optimal sizes, it is written that the report of the sizes is related to the report of the contributions to the error by:

$$\frac{\varepsilon_E^*}{\varepsilon_E} = \left[\frac{h_E^*}{h_E}\right] = r_E^p \quad \text{éq 3.4.1-1}$$

where ε_E^* represent the contribution of the elements of T^* located in the zone E, i.e.:

$$\varepsilon_E^* = \left[\sum_{E^* \subset E} \varepsilon_{E^*}^2\right]^{1/2} \quad \text{éq 3.4.1-2}$$

ε_E^* is the error of the element E^* calculated on the grid T.

The square of the error on the grid T^* can thus be evaluated by:

$$\sum_E \left(\varepsilon_E^*\right)^2=\sum_E r_E^{2p}\,\varepsilon_E^2 \qquad \text{éq 3.4.1-3}$$

and the number of elements of T^* by:

$$N^*=\sum_E \frac{1}{r_E^d} \qquad \text{éq 3.4.1-4}$$

Where d is the dimension of space in practice (, $d=2$ or 3).

Indeed, $r_E=\frac{h_E^*}{h_E}=\left(\frac{V}{N_E{}^*}\right)^{1/d}\left(\frac{N}{V}\right)^{1/d}$ with N the number of element of T in E (thus 1), N_E^* the number of element of T^* in the zone of E . One thus has $N_E^*=\frac{1}{r_E^d}$, that is to say $N^*=\sum_E N_E^*=\sum_E \frac{1}{r_E^d}$ the full number of elements of T^* .

The problem to be solved is thus:

$$\text{Minimiser}\quad N^*=\sum_E \frac{1}{r_E^d}\quad \text{avec}\quad \sum_E r_E^{2p}\,\varepsilon_E^2=\varepsilon_0^2 \qquad \text{éq 3.4.1-5}$$

It is about a problem of optimization with a constraint on the variables of optimization.
By introducing a multiplier of Lagrange, noted A , the problem [éq 3.4.1-5] amounts returning extremum the Lagrangian one:

$$L\left(\left\{r_E\right\}_{E\in T}\ ;\ A\right)=\sum_E \frac{1}{r_E^d}+A\left(\sum_E r_E^{2p}\,\varepsilon_E^2-\varepsilon_0^2\right) \qquad \text{éq 3.4.1-6}$$

The conditions of extremality give:

$$\frac{\partial L}{\partial r_E}=\frac{-d}{r_E^{d+1}}+2\,A\,p\,\varepsilon_E^2 r_E^{2p-1}=0\quad \forall E\in T \qquad \text{éq 3.4.1-7}$$

From where:

$$r_E=\left[\frac{d}{2\,A\,p\,\varepsilon_E^2}\right]^{1/(2p+d)} \qquad \text{éq 3.4.1-8}$$

While deferring in the second equation of [éq 3.4.1-5], one from of deduced A :

$$A=\frac{d}{2\,p}\left[\frac{\sum_E \varepsilon_E^{2d/(2p+d)}}{\varepsilon_0^2}\right]^{(2p+d)/2p} \qquad \text{éq 3.4.1-9}$$

One replaces the expression of A thus obtained in the equation [éq 3.4.1-8] to obtain r_E :

$$r_E = \frac{\varepsilon_0^{1/p}}{\varepsilon_E^{2/(2p+d)} \left[\sum_E \varepsilon_E^{2d/(2p+d)} \right]^{1/2p}}$$ éq 3.4.1-10

3.4.2 Case of the singular zones

To predict the optimal sizes, a rate of convergence is used q_E defined by element:

$$\frac{\varepsilon_E^*}{\varepsilon_E} = \left[\frac{h_E^*}{h_E} \right]^{q_E} = r_E^{q_E}$$ éq 3.4.2-1

where ε_E^* represent the contribution of the elements of T^* located in the zone E , i.e.:

$$\varepsilon_E^* = \left[\sum_{E^* \subset E} \varepsilon_{E^*}^2 \right]^{1/2}$$ éq 3.4.2-2

The square of the error on the grid T^* can thus be evaluated by:

$$\sum_E \left(\varepsilon_E^* \right)^2 = \sum_E r_E^{2q_E} \varepsilon_E^2$$ éq 3.4.2-3

and the number of elements of T^* is always evaluated by:

$$N^* = \sum_E \frac{1}{r_E^d}$$ éq 3.4.2-4

The new problem to be solved is thus:

$$\text{Minimiser} \quad N* = \sum_E \frac{1}{r_E^d} \quad \text{avec} \quad \sum_E r_E^{2q_E} \varepsilon_E^2 = \varepsilon_0^2$$ éq 3.4.2-5

who is a problem of optimization with a constraint on the variables of optimization.
By introducing a multiplier of Lagrange, noted A , the problem amounts returning extremum the Lagrangian one:

$$L\left(\left\{ r_E \right\}_{E \in T} \; ; \; A \right) = \sum_E \frac{1}{r_E^d} + A \left(\sum_E r_E^{2q_E} \varepsilon_E^2 - \varepsilon_0^2 \right)$$ éq 3.4.2-6

The conditions of extremality give:

$$\frac{\partial L}{\partial r_E} = -\frac{d}{r_E^{d+1}} + 2 A q_E \varepsilon_E^2 r_E^{2q_E - 1} = 0 \quad \forall E \in T$$ éq 3.4.2-7

From where:

$$r_E = \left[\frac{d}{2 A q_E} \varepsilon_E^2 \right]^{1/(2q_E + d)}$$ éq 3.4.2-8

While deferring in the second equation of [éq 3.4.2-5], one obtains a nonlinear equation in A (because q_E depends on the elements):

$$\sum_E \left[\left[\frac{d}{2 A q_E} \right]^{2 q_E/(2 q_E+d)} \varepsilon_E^{2d/(2 q_E+d)} \right] - \varepsilon_0^2 = 0 \qquad \text{éq 3.4.2-9}$$

It is solved by the method of Newton (the multiplier of Lagrange is initialized by taking the multiplier of Lagrange of the regular solution i.e. the expression [éq 3.4.2-9] with $q_E = p$). Once A calculated, one from of deduced r_E by the equation [éq 3.4.2-8].

3.5 Estimators of error in quantities of interest

One designates by estimators of error in quantities of interest the estimators who provide an error on a precise physical quantity (quantity of interest) on a selected zone.

3.5.1 Case of the regular solution

In the case of estimators in quantity of interest, the value of q is worth $2p$ [bib4] (p 1 for linear finite elements and 2 for quadratic finite elements is worth). To predict the optimal sizes, it is written that the report of the sizes is related to the report of the contributions to the error by:

$$\frac{\varepsilon_E^*}{\varepsilon_E} = \left[\frac{h_E^*}{h_E} \right]^{2p} = r_E^{2p} \qquad \text{éq 3.5.1-1}$$

where ε_E^* represent the contribution of the elements of T^* located in the zone E , i.e.:

$$\varepsilon_E^* = \sum_{E^* \subset E} \varepsilon_{E^*} \qquad \text{éq 3.5.1-2}$$

ε_E^* is the error of the element E^* calculated on the grid T .

The error on the grid T^* can thus be evaluated by:

$$\sum_E \varepsilon_E * = \sum_E r_E^{2p} \varepsilon_E \qquad \text{éq 3.5.1-3}$$

and the number of elements of T^* by:

$$N^* = \sum_E \frac{1}{r_E^d} \qquad \text{éq 3.5.1-4}$$

Where d is the dimension of space in practice (, $d=2$ or 3).

The problem to be solved is thus:

$$\text{Minimiser} \quad N^* = \sum_E \frac{1}{r_E^d} \quad \text{avec} \quad \sum_E r_E^{2p} \varepsilon_E = \varepsilon_0 \qquad \text{éq 3.5.1-5}$$

There still, it is about a problem of optimization with a constraint on the variables of optimization.

By introducing a multiplier of Lagrange, noted A, the problem [éq 3.5.1-5] amounts returning extremum the Lagrangian one:

$$L\left(\{r_E\}_{E\in T};\mathrm{A}\right)=\sum_E \frac{1}{r_E^d}+A\left(\sum_E r_E^{2p}\varepsilon_E-\varepsilon_0\right) \qquad \text{éq 3.5.1-6}$$

The conditions of extremality give:

$$\frac{\partial L}{\partial r_E}=-\frac{d}{r_E^{d+1}}+2\,A\,p\,\varepsilon_E\,r_E^{2p-1}=0 \quad \forall E\in T \qquad \text{éq 3.5.1-7}$$

From where:

$$r_E=\left[\frac{d}{2\,A\,p\,\varepsilon_E}\right]^{1/(2p+d)} \qquad \text{éq 3.5.1-8}$$

While deferring in the second equation of [éq 3.5.1-5], one from of deduced A :

$$A=\frac{d}{2\,p}\left[\frac{\sum_E \varepsilon_E^{d/(2p+d)}}{\varepsilon_0}\right]^{(2p+d)/2p} \qquad \text{éq 3.5.1-9}$$

One replaces the expression of A thus obtained in the equation [éq 3.5.1-8] to obtain r_E :

$$r_E=\frac{\varepsilon_0^{1/2p}}{\varepsilon_E^{1/(2p+d)}\left[\sum_E \varepsilon_E^{d/(2p+d)}\right]^{1/2p}} \qquad \text{éq 3.5.1-10}$$

3.5.2 Case of the singular zones

To predict the optimal sizes, one forces now:

$$\frac{\varepsilon_E^*}{\varepsilon_E}=\left[\frac{h_E^*}{h_E}\right]^{2q_E}=r_E^{2q_E} \qquad \text{éq 3.5.2-1}$$

where ε_E^* represent the contribution of the elements of T^* located in the zone E , i.e.:

$$\varepsilon_E^*=\sum_{E^*\subset E}\varepsilon_{E^*} \qquad \text{éq 3.5.2-2}$$

The square of the error on the grid T^* can thus be evaluated by:

$$\sum_E \varepsilon_E^*=\sum_E r_E^{2q_E}\varepsilon_E \qquad \text{éq 3.5.2-3}$$

and the number of elements of T^* is always evaluated by:

$$N^* = \sum_E \frac{1}{r_E^d} \qquad \text{éq 3.5.2-4}$$

The new problem to be solved is thus:

$$\text{Minimiser} \quad N^* = \sum_E \frac{1}{r_E^d} \quad \text{avec} \quad \sum_E r_E^{2q_E} \varepsilon_E = \varepsilon_0 \qquad \text{éq 3.5.2-5}$$

who is a problem of optimization with a constraint on the variables of optimization.
By introducing a multiplier of Lagrange, noted A, the problem amounts returning extremum the Lagrangian one:

$$L\left(\{r_E\}_{E\in T} \ ; \ A\right) = \sum_E \frac{1}{r_E^d} + A\left(\sum_E r_E^{2q_E} \varepsilon_E - \varepsilon_0\right) \qquad \text{éq 3.5.2-6}$$

The conditions of extremality give:

$$\frac{\partial L}{\partial r_E} = -\frac{d}{r_E^{d+1}} + 2\,A\,q_E\,\varepsilon_E\,r_E^{2q_E} - 1 = 0 \quad \forall E \in T \qquad \text{éq 3.5.2-7}$$

From where:

$$r_E = \left[\frac{d}{2\,A q_E}\varepsilon_E\right]^{1/(2q_E+d)} \qquad \text{éq 3.5.2-8}$$

While deferring in the second equation of [éq 3.5.2-5], one obtains a nonlinear equation in A :

$$\sum_E \left[\left[\frac{d}{2\,A\,q_E}\right]^{2q_E/(2q_E+d)} \varepsilon_E^{d/(2q_E+d)}\right] - \varepsilon_0 = 0 \qquad \text{éq 3.5.2-9}$$

It is solved by the method of Newton (the multiplier of Lagrange is initialized by taking the multiplier of Lagrange of the regular solution i.e. the expression [éq 3.5.2-9] with $q_E = p$). Once A calculated, one from of deduced r_E by the equation [éq 3.5.2-8].

4 Use in *Code_Aster*

4.1 Orders

The order of the singularity and the map of modification of size are calculated by the order `CALC_ERREUR` by activating the options `'SING_ELEM'` (constant field by element) or `'SING_ELNO'` (field with the nodes by element).

The option `'SING_ELEM'` calculate, on each element, two components:

- `'DEGREE'` : the order of the singularity i.e. the value of the coefficient q_E (which is worth p if the element is not connected to a singular node and which is worth α if not);
- `'REPORT'` : the relationship between the current size h_E and new size h_E^* finite element ($h_E / h_E^* = 1/r_E$);
- `'SIZE'` : new size h_E^* finite element ($h_E^* = r_E h_E$).

The calculation of this option requires, as a preliminary, the calculation of an estimator of error (it is the absolute component which is used and it is coded into hard in *Code_Aster*) and of the total deformation energy. If one of these options is not calculated, a message of alarm is transmitted and the option 'SING_ELEM' is not calculated.

The user can inform the optional keyword 'TYPE_ESTI' by indicating one of the options following:

- 'ERME_ELEM' for the estimator based on the residues;
- 'ERZ (1 or 2) _ELEM_SIGM' for the estimator based on the smoothed constraints (Zhu - Zienkiewicz version 1 or 2);
- 'QIRE_ELEM' for the estimator in quantity of interest based on the residues;
- 'QIZ (1 or 2) _ELEM_SIGM' for the estimator in quantity of interest based on the smoothed constraints (Zhu - Zienkiewicz version 1 or 2).

If this keyword is not then indicated the estimator based on the residues 'ERME_ELEM' by default (message of emitted alarm) is selected. If the two estimators of Zhu-Zienkiewicz are present, one chooses 'ERZ1_ELEM'.

For the total deformation energy, one uses:

- With STAT_NON_LINE : 'ETOT_ELEM' who is the total deformation energy on a finite element (valid for an elastic behavior and an elastoplastic behavior 'VMIS_ISOT_XXX').
- With MECA_STATIQUE : 'EPOT_ELEM' who is the potential energy of elastic strain on a finite element and integrated starting from displacements and temperature (valid only for one elastic behavior).

The user must also inform the keyword 'PREC_ERR' who allows to calculate the precision ε_0 equation [éq 2.2-1] in the following way: $\varepsilon_0 = \text{PREC\_ERR} * Erreur_{totale}$. The value of 'PREC_ERR' strictly lies between 0 and 1 (a fatal message is transmitted if this condition is not checked).

For the option 'SING_ELNO', it is about a recopy of the values of 'SING_ELEM' with the nodes of the element. The preliminary calculation of 'SING_ELEM' is thus necessary. If 'SING_ELEM' is absent, a message of alarm is transmitted and the option 'SING_ELNO' is not calculated.

4.2 Perimeter of use

The perimeter of use is the same one (but more reduced) than that of the estimator of error chosen namely:

- For the estimator in residue: finite elements of the continuous mediums in 2D (triangles and quadrangles) or 3D (only tetrahedrons) for an elastoplastic behavior,
- For the estimator of Zhu-Zienkiewicz: finite elements of the continuous mediums in 2D (triangles and quadrangles) for an elastic behavior.

In any rigour (cf [§2]), calculation about the singularity is obtained starting from theoretical energy at a peak of crack [éq 2.3.1-2], valid equation only in elasticity. The use of this option in elastoplasticity is thus to handle with prudence.

5 Bibliography

[1] COOREVITS P.: Mechanism of detection of the singularities. First part. Note of the Laboratory of Mechanics and CAO (Saint-Quentin).

[2] CIARLET P. - G.: The finite element method for elliptic problems, North-Holland, 1978.

[3] STRANG & FIX: Year analysis of the finite element method, Prentice hall, 1976.

[4] Estimators of error in quantities of interest. [R4.10.06]

6 Description of the versions of the document

Index Doc.	Version Aster	Author (S) or contributor (S), organization	Description of the modifications
With	8.4	V.Cano EDF/R & D /AMA	Initial text
B	9.4	J.Delmas EDF/R & D /AMA	Recasting of the document + addition of the estimators of error in quantities of interest