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Evaluation of the local quality of stresses in 3D finite element analysis

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Abstract

This article deals with the local quality on stresses produced during finite element analysis in 3D linear elasticity. We use an estimation technique based on the concept of error in constitutive relation, which yields excellent estimates of the local errors without requiring the approximate calculation of Green functions. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Finite element method; A posteriori error estimation; Local error; Stress

1. Introduction

The cost of manufacturing actual prototypes and the widespread availability of computer hardware and numerical tools and methods have led designers to the intensive development of virtual prototyping. However, in order to be able to make consistent and safe decisions, one must ensure that these virtual prototypes provide a sufficiently refined representation of physical reality. Methods have been developed over many years to evaluate the global quality of finite element analyses [1-3]. For linear problems, all these methods provide a global energy-based estimate of the discretization error. Most of the time, such global information is totally insufficient for dimensioning purposes in mechanical design because, in many common situations, the dimensioning criteria involve local values (stresses, displacements, intensity factors, ...). Therefore, it is necessary to evaluate also the quality of these local quantities calculated by finite element analysis. Such an estimation of the local quality of a finite element numerical model remains a widely open investigation field. A first approach, proposed by Babuška and Strouboulis [4,5], is based on the concept of pollution error. Another approach is to use extraction operators [6–10], which depend on the type of local quantity considered. In general, these extraction operators are determined approximately using a finite

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element method. In [7], Ladevéze et al. proposed an alternative approach in 2D elasticity which enables one to evaluate on each element *E* the error in energy $\|\sigma_{ex} - \sigma_h\|_E$ between the exact stress σ_{ex} and the finite element stress σ_h . This approach is based on the concept of error in constitutive relation and on a new technique of construction of statically admissible stress fields detailed in [11]. We know that for any statically admissible stress field $\hat{\sigma}_h$ the global error in energy $\|\sigma_{ex} - \sigma_h\|_Q$ on the whole structure Ω is bounded by $\|\hat{\sigma}_h - \sigma_h\|_Q$. The main advantage of the new construction is that it leads to improved statically admissible fields $\hat{\sigma}_h$ for which, experimentally, the energy over an element $\|\hat{\sigma}_h - \sigma_h\|_E$ is an upper bound of the error in energy $\|\sigma_{ex} - \sigma_h\|_E$ [11]. The aim of this paper is to study the extension of the approach proposed by Ladevèze to 3D elastic calculations. In Section 2, we briefly review the basic concepts of error estimators in constitutive relation for elasticity. The principle of the evaluation of $\|\sigma_{ex} - \sigma_h\|_E$ is presented in Section 3. In Section 4, we develop the technique of the construction of improved statically admissible fields $\hat{\sigma}_h$ for 3D elasticity. Currently, it is available for 4-node tetrahedral elements. In Section 5, we study in detail the local effectivity indexes using several examples

$$\zeta_E = rac{\|\hat{\sigma}_{\mathrm{h}} - \sigma_{\mathrm{h}}\|_E}{\|\sigma_{\mathrm{ex}} - \sigma_{\mathrm{h}}\|_E}.$$

An analysis of these first 3D examples shows, as had already been pointed out in 2D in [7], that the indexes ζ_E are such that $C \leq \zeta_E$, where C is numerically of the order of 1. In particular, for the dimensioning zones—i.e., the zones with high stresses— $\|\hat{\sigma}_h - \sigma_h\|_E$ is a very good evaluation of $\|\sigma_{ex} - \sigma_h\|_E$.

2. Error in constitutive relation

2.1. Reference problem

Let us consider an elastic structure within a domain Ω bounded by $\partial \Omega$. The external actions on the structure are represented by

- a prescribed displacement \underline{U}_d on a subset $\partial_1 \Omega$ of the boundary,
- a volume force density \underline{f}_{d} defined in Ω ,
- a surface force density \underline{F}_{d} defined on $\partial_{2}\Omega = \partial\Omega \partial_{1}\Omega$.

We designate the material's Hooke's operator by **K**. Thus, the problem can be formulated as follows: find a displacement field \underline{U} and a stress field σ defined on Ω which verify

• the kinematic constraints

$$\underline{U} \in \mathscr{U} \quad \underline{U}||_{\partial_1 \Omega} = \underline{U}_{\mathrm{d}},\tag{1}$$

• the equilibrium equations

$$\sigma \in \mathscr{S} \quad \forall \underline{U}^* \in \mathscr{U}_{\mathrm{ad},0},\tag{2}$$

$$\int_{\Omega} \operatorname{Tr}[\sigma \varepsilon(\underline{U}^*)] \, \mathrm{d}\Omega = \int_{\Omega} \underline{f}_{-\mathrm{d}} \underline{U}^* \, \mathrm{d}\Omega + \int_{\partial_2 \Omega} \underline{F}_{-\mathrm{d}} \underline{U}^* \, \mathrm{d}S, \tag{3}$$

• the constitutive relation

$$\sigma = \mathbf{K}\varepsilon(\underline{U}). \tag{4}$$

 \mathscr{U} is the space in which the displacement field $(\mathscr{U} = [H^1(\Omega)]^3)$ is sought, \mathscr{S} the space of the stress $(\mathscr{S} = [L^2(\Omega)]^6)$, \mathscr{U}_0 the space of the fields in \mathscr{U} which are zero on $\partial_1 \Omega$ and where $\varepsilon(\underline{U})$ represents the linearized deformation associated with the displacement

 $\varepsilon(\underline{U}) = \frac{1}{2}(\operatorname{grad} \underline{U} + \operatorname{grad} \underline{U}^{\mathrm{T}}).$

The solution to the reference problem is designated by $(\underline{U}_{ex}, \sigma_{ex})$.

2.2. Definition of the error in constitutive relation

The approach based on the error in constitutive relation relies on a partitioning of the above equations into two groups:

- the admissibility conditions Eqs. (1) and (3),
- the constitutive relation Eq. (4).

In practice, the constitutive relation is often the least reliable of all the equations of the reference problem. Therefore, it is natural to consider approximate solutions which verify the admissibility conditions exactly and to quantify quality by the extent to which the constitutive relations are verified. This leads us to the introduction of the following definition:

We say that fields $\hat{s} = (\hat{U}, \hat{\sigma})$ are admissible if

- field $\underline{\hat{U}}$ verifies (1) ($\underline{\hat{U}}$ is kinematically admissible),
- field $\hat{\sigma}$ verifies (3) ($\hat{\sigma}$ is statically admissible).

One can then define a measure of the error in constitutive relation by

$$\hat{e}_{\rm h}(\hat{s}) = \|\hat{\sigma} - \mathbf{K}\varepsilon(\underline{\hat{U}})\|_{\Omega} \tag{5}$$

with $\| \bullet \|_{\Omega} = \int_{\Omega} \operatorname{Tr}[\bullet \mathbf{K}^{-1} \bullet] d\Omega$ and a relative error by

$$\hat{\varepsilon}_{\rm h} = \frac{\|\hat{\sigma} - \mathbf{K}\varepsilon(\underline{\hat{U}})\|_{\Omega}}{\|\hat{\sigma} + \mathbf{K}\varepsilon(\underline{\hat{U}})\|_{\Omega}}.$$
(6)

2.3. Errors in finite element discretization

Classically, if one discretizes the reference problem using a displacement-type finite element method, one obtains the following problem:

Find the kinematically admissible finite element displacement field \underline{U}_{h} such that

$$\forall \underline{U}_{h}^{*} \in \mathscr{U}_{h0} \int_{\Omega} \operatorname{Tr}[\varepsilon(\underline{U}_{h}) \mathbf{K}\varepsilon(\underline{U}_{h}^{*})] \, \mathrm{d}\Omega = \int_{\Omega} \underline{f}_{\mathrm{d}} \, \underline{U}_{h}^{*} \, \mathrm{d}\Omega + \int_{\partial_{2}\Omega} \underline{F}_{\mathrm{d}} \, \underline{U}_{h}^{*} \, \mathrm{d}S, \tag{7}$$

where U_{h0} is the space of finite element displacement fields which are zero on $\partial_1 \Omega$.

The corresponding stress field is

 $\sigma_{\rm h} = \mathbf{K} \varepsilon (\underline{U}_{\rm h}). \tag{8}$

The method to evaluate the errors due to the finite element discretization consists of reconstructing, starting from the finite element data and solution, an admissible pair $\hat{s} = (\hat{U}_h, \hat{\sigma}_h)$. Since the finite element field is kinematically admissible, one takes

$$\underline{\hat{U}}_{\rm h} = \underline{U}_{\rm h}.\tag{9}$$

On the contrary, the stress field σ_h is not statically admissible. Techniques to reconstruct admissible stress fields have been under development for several years [2,12]. They enable one to obtain a field $\hat{\sigma}_h$ which verifies the equilibrium equations exactly (3). We will discuss these techniques in the next section.

The error in constitutive relation associated with the admissible pair $\hat{s} = (\hat{U}_h, \hat{\sigma}_h)$ is

$$\hat{\boldsymbol{c}}_{h} = \|\hat{\boldsymbol{\sigma}}_{h} - \mathbf{K}\boldsymbol{\varepsilon}(\underline{U}_{h})\|_{\Omega} = \|\hat{\boldsymbol{\sigma}}_{h} - \boldsymbol{\sigma}_{h}\|_{\Omega}.$$
(10)

2.4. Property of the global error in constitutive relation

Using the Prager–Synge theorem [13], one shows easily that

$$\|\sigma_{\rm ex} - \sigma_{\rm h}\|_{\varrho} \leqslant \hat{\boldsymbol{e}}_{\rm h}.\tag{11}$$

Thus, the error in constitutive relation is an upperbound of the discretization error. In other words, the global effectivity index (ratio of the estimated error to the true error) is always greater than 1. If one introduces the stress field:

$$\sigma_{\rm h}^* = \frac{1}{2} (\hat{\sigma}_{\rm h} + \sigma_{\rm h}), \tag{12}$$

one also obtains

$$\|\sigma_{\rm ex} - \sigma_{\rm h}^*\|_{\Omega} = \frac{1}{2} \,\hat{e}_{\rm h}.\tag{13}$$

3. Estimation of the local errors on stresses

For an element E of the mesh, the local error in energy on E can be defined as

$$e_{\operatorname{enr},E} = \frac{\|\sigma_{\operatorname{ex}} - \sigma_{\operatorname{h}}\|_{E}}{\operatorname{mes}(E)^{\frac{1}{2}}}$$
(14)

with $\| \bullet \|_E = \int_E \operatorname{Tr}[\bullet \mathbf{K}^{-1} \bullet] dE$.

One way of evaluating this quantity is to consider the similar quantity calculated from the admissible stress field $\hat{\sigma}_{h}$:

$$\hat{\boldsymbol{e}}_{\mathrm{enr},E} = \frac{\|\hat{\boldsymbol{\sigma}}_{\mathrm{h}} - \boldsymbol{\sigma}_{\mathrm{h}}\|_{E}}{\mathrm{mes}(E)^{\frac{1}{2}}}.$$
(15)

This strategy was proposed by Ladevèze in [7]. For 2D elastic calculations, $\hat{e}_{enr,E}$ was shown to be a very good evaluation of $e_{enr,E}$ provided that $\hat{\sigma}_{h}$ be constructed using the improved technique proposed in [11]. Furthermore, with this new construction one can observe experimentally that

 $e_{\operatorname{enr},E} \leqslant C \hat{e}_{\operatorname{enr},E},$ (16)

where C is numerically close to 1. It is important to point out that the use of the improved construction of statically admissible fields described in [11] is the crucial feature of the proposed method because the associated error estimator in constitutive relation has excellent local behavior. To illustrate this point, let us reexamine one of the examples presented in [7], i.e., the test case represented in Fig. 1. For this example, the global effectivity index is $\zeta = 2.99$. Fig. 2 shows the histogram of the local effectivity indexes. One can

observe that the local effectivity indexes all lie between 1.76 and 8.1. For the purpose of comparison, the same example was treated using the ZZ2 estimator, which provides an excellent global effectivity index: $\zeta = 0.968$.

However, Figs. 3 and 4 show that the local effectivity indexes are much more scattered, since they vary between 0.3 and 35.3. Furthermore, for a large number of elements, these indexes are much less than 1.

One should note that the good local behavior of the estimator of the error in constitutive relation is due to the improved method of building admissible fields, described in [11] for 2D problems, which includes an essential step of optimization.

In order to show this last point clearly, let us consider the simple example of a fixed-fixed beam in traction (Fig. 5) and focus on the local errors in zone ω .

Let us perform a finite element analysis with the mesh represented on (Fig. 6).

In order to evaluate the discretization errors, let us use the classical estimator of the error in constitutive relation, which is strictly identical to the residual estimators of the "ErpBp + k" family developed in [14–16]. In this case, the resulting local effectivity index on ω is

$$\frac{\|\hat{\sigma}_{\rm h} - \sigma_{\rm h}\|_{\omega}}{\|\sigma_{\rm ex} - \sigma_{\rm h}\|_{\omega}} = 0.19,\tag{17}$$

which is unsatisfactory, while on the overall structural level one gets a global effectivity index of 3.2, which is quite good.



Fig. 2. Histogram for the error in constitutive relation.





Fig. 4. Comparison for values close to 1.



Fig. 5. Fixed-fixed beam.

Conversely, if one uses the improved method proposed in [11], one gets

$$\frac{\|\hat{\sigma}_{\rm h} - \sigma_{\rm h}\|_{\omega}}{\|\sigma_{\rm ex} - \sigma_{\rm h}\|_{\omega}} = 2.9,\tag{18}$$

leading to an effectivity index equal to 2.1. Thus, clearly, the technique for improving the construction of the admissible fields described in [11] for the 2D case is the key feature of the method we are proposing.



Fig. 6. Mesh of the beam.

In the next section, we propose the extension of this improved construction to the case of 3D elastic calculations. The local properties of the associated estimator will be studied in Section 5 using several examples.

4. Construction of admissible fields in 3D

4.1. Principle of the construction

The technique to build stress fields $\hat{\sigma}_h$ which verify the equilibrium equation (3) exactly has become a classic [2,12]. It involves two stages: the first stage consists of constructing on the sides of the elements surface force densities $\underline{\hat{F}}_h$ to represent the stress vectors $\hat{\sigma}_h \underline{n}_E$ as

$$[\hat{\sigma}_{h}\underline{n}_{E}]|_{\Gamma} = \eta_{E}\underline{\hat{F}}_{h} \quad \text{with } \Gamma \in \partial E, \tag{19}$$

where η_E is a function, constant on each side, whose value is either 1 or -1 and such that on the side common to two adjacent elements *E* and *E'*: $\eta_E + \eta_{E'} = 0$.

Moreover, these force densities are generated in such a way that, on each element *E* in the mesh, the volume loads \underline{f}_{d} and the surface loads $\eta_{E} \underline{\hat{F}}_{h}$ are in equilibrium on *E*. The detail of this construction procedure can be found in [12].

The second stage consists of constructing, element by element, a solution to the equilibrium equations:

$$\begin{cases} \underline{\operatorname{div}}\hat{\sigma}_E + \underline{f}_{\mathrm{d}} = 0 & \text{in } E, \\ \hat{\sigma}_E \, \underline{n}_E = \eta_E \underline{\hat{F}}_{\mathrm{h}} & \text{on } \partial E. \end{cases}$$
(20)

Then, field $\hat{\sigma}_{h}$ is obtained by $\forall E \ \hat{\sigma}_{h}|_{E} = \hat{\sigma}_{E}$.

For a given set of densities, of all the solutions of (20) the best field $\hat{\sigma}_{h|_{E}}$ is the one which is solution to the minimization problem:

$$\min_{\hat{\sigma}_E \text{ verifying (20)}} \| \hat{\sigma}_E - \sigma_h \|_E.$$
(21)

By duality, this is equivalent to seeking a displacement field \underline{V}_E defined on E such that

$$\underline{V}_{E} \in \mathscr{U}(E) \quad \text{and} \quad \forall \underline{V}^{*} \in \mathscr{U}(E) \int_{E} \operatorname{Tr}[\varepsilon(\underline{V}_{E})\mathbf{K}\varepsilon(\underline{V}^{*})] \, \mathrm{d}E = \int_{E} \underline{f}_{\mathrm{d}} \underline{V}^{*} \, \mathrm{d}E + \int_{\partial E} \eta_{E} \underline{\hat{F}}_{\mathrm{h}} \underline{V}^{*} \, \mathrm{d}\Gamma, \tag{22}$$

where $\mathscr{U}(E)$ designates the space of restrictions to E of the fields in \mathscr{U} . Then, $\hat{\sigma}_E$ is given by

$$\hat{\boldsymbol{\sigma}}_E = \mathbf{K} \varepsilon(\underline{V}_E). \tag{23}$$

Thus, one can obtain an approximation of $\hat{\sigma}_E$ by solving Problem (22) by a classical finite element method on *E*. In practice, it is sufficient, in order to obtain a good approximation, to consider either a discretization of *E* with a single element but an interpolation of degree p + k, where *p* is the degree of interpolation used in the finite element analysis and *k* a positive integer, or a subdivision of element *E* along with an interpolation of degree p + k' (generally, k' < k).

The essential step is the construction of densities $\underline{\hat{F}}_{h}$, as this conditions the quality of the resultant field $\hat{\sigma}_{h}$ and, consequently, the quality of the error estimator in constitutive relation.

4.2. Construction of densities

The new version of the error estimators in constitutive relation was introduced for two dimensions in [11]. It consists of constructing better quality densities. The object of this section is to present the extension of this method to 3D calculations.

Let us consider tetrahedral elements with an interpolation of degree p described using hierarchical shape functions. On a side Γ , these shape functions are designated by λ_1 , λ_2 , λ_3 for the linear part and ω_i $(i \in 4, 5, ..., N)$ for terms up to degree p (N = (p+1)(p+2)/2).

Let us introduce the three functions ψ_1, ψ_2, ψ_3 such that

$$\begin{cases} \psi_{\alpha} = \lambda_{\alpha} - \sum_{i=4}^{N} a_{\alpha}^{i} \omega_{i} \\ \int_{\Gamma} \psi_{\alpha} \omega_{i} \, \mathrm{d}\Gamma = 0 \, (\alpha = 1, 2, 3 \text{ and } i = 4, 5, \dots, N). \end{cases}$$
(24)

On a side Γ , a density of degree p:

$$\underline{\hat{F}}_{\mathrm{h}}|_{\Gamma} = \sum_{\alpha=1}^{3} \underline{\hat{F}}_{\alpha} \lambda_{\alpha} + \sum_{i=4}^{N} \underline{\hat{F}}_{i} \omega_{i}$$
(25)

has a unique decomposition of the form

$$\underline{\hat{F}}_{\mathrm{h}}|_{\Gamma} = \underline{\hat{H}}|_{\Gamma} + \underline{\hat{R}}|_{\Gamma} \tag{26}$$

with

$$\begin{cases} \int_{\Gamma} \underline{\hat{R}} |_{\Gamma} \omega_i d\Gamma = 0 & \text{if } i = 4, \dots, N, \\ \int_{\Gamma} \underline{\hat{H}} |_{\Gamma} \lambda_\alpha d\Gamma = 0 & \text{if } \alpha = 1, 2, 3. \end{cases}$$
(27)

Because of (24) and (27), $\underline{\hat{H}}|_{\Gamma}$ has zero resultant and moment on Γ and $\underline{\hat{R}}|_{\Gamma}$ is of the form

$$\underline{\hat{R}}|_{\Gamma} = \sum_{\alpha=1}^{3} \underline{R}_{\alpha} \psi_{\alpha} \text{ where } \underline{R}_{\alpha} \text{ are constant vectors.}$$
(28)

Using the weak prolongation condition:

For any element E and for any shape function ϕ_k not associated with a vertex E

$$\int_{E} (\hat{\sigma}_{h} - \sigma_{h}) \underline{\operatorname{grad}}(\phi_{k}) d\Omega = \underline{0},$$
(29)

we determine part $\underline{\hat{H}}|_{\Gamma}$ using the classical techniques described in [2,12].

Part $\underline{\hat{R}}|_{\Gamma}$, which, in practice, consists of three constant vectors \underline{R}_{α} per side Γ , can be determined by minimizing the error in constitutive relation. We designate by \mathscr{R} the set of $\underline{\hat{R}}$ such that

(1) for any side Γ included in $\partial_2 \Omega$: $\underline{\eta}_E(\underline{\hat{H}}|_{\Gamma} + \underline{\hat{R}}|_{\Gamma}) = \underline{F}_d$,

(2) for any element E of the mesh, $\underline{\hat{R}}$ is in equilibrium with the volume forces f_{d} .

Then, for $\underline{\hat{R}} \in \mathcal{R}$, there is at least one admissible stress field $\hat{\sigma}$ such that $[\hat{\sigma}|_{\underline{E}} \underline{n}_{\underline{E}}]|_{\Gamma} = \eta_{\underline{E}}(\underline{H}|_{\Gamma} + \underline{R}|_{\Gamma})$.

Let us call $\mathscr{S}_{\mathscr{R}}$ the set of these admissible stress fields. The best field achievable, $\hat{\sigma}$, is solution to the problem:

$$\min_{\hat{\sigma}\in\mathscr{S}_{\mathscr{A}}}\hat{e}_{\mathrm{h}}(\underline{U}_{\mathrm{h}},\hat{\sigma}),\tag{30}$$

which is equivalent to

$$\min_{\hat{\boldsymbol{\sigma}}\in\mathscr{S}_{\mathscr{R}}} \left[\frac{1}{2} \int_{\Omega} \mathrm{Tr}[\hat{\boldsymbol{\sigma}}\mathbf{K}^{-1}\hat{\boldsymbol{\sigma}}] \,\mathrm{d}\Omega - \int_{\partial_{1}\Omega} \hat{\boldsymbol{\sigma}}_{\underline{n}} \underline{U}_{\mathrm{d}} \,\mathrm{d}\Gamma \right].$$
(31)

This problem is a global problem defined on domain Ω . It can be solved at reasonable cost by introducing local problems defined on each element E [11]. Here, in order to simplify the presentation, we will limit ourselves to the case where f_{d} is constant on each element of the mesh, but the method can be extended to the general case.

Let us consider the densities $\underline{\hat{R}}_{|\Gamma}$ on the sides Γ of ∂E .

We write

$$\underline{f}_{E}^{R} = -\frac{1}{\mathrm{mes}(E)} \int_{\partial E} \eta_{E} \hat{\underline{R}} \mathrm{d}\Gamma - \mathscr{I}_{G}^{-1} \left(\int_{\partial E} \underline{GM} \wedge \eta_{E} \hat{\underline{R}} \mathrm{d}\Gamma \right) \wedge \underline{GM},\tag{32}$$

where \mathscr{I}_{G}^{-1} is the inertia operator for element *E*.

By construction, we have

For any solid motion \underline{U}_{S} on E

$$\int_{\partial E} \eta_E \underline{\hat{R}} \underline{U}_S \, \mathrm{d}\Gamma + \int_E \underline{f}_E^R \underline{U}_S \, \mathrm{d}E = 0.$$
(33)

Because of (24) and (27) we have For any solid motion \underline{U}_{S} on E

$$\int_{\partial E} \eta_E(\hat{\underline{R}} + \hat{\underline{H}}) \underline{U}_S \,\mathrm{d}\Gamma + \int_E \underline{f}_E^R \underline{U}_S \,\mathrm{d}E = 0.$$
(34)

Therefore, the set of stress fields $\hat{\sigma}_E$ which are in equilibrium on E with loads $\eta_E(\underline{\hat{R}} + \underline{\hat{H}})$ and \underline{f}_E^R is non-empty. We call it $\mathscr{S}_{ad|E}^R$ and $\hat{\sigma}_E$ belongs to $\mathscr{S}_{ad|E}^R$ if For any displacement field \underline{U}^* regular on E

$$\int_{E} \operatorname{Tr}[\hat{\sigma}_{E} \varepsilon(\underline{U}^{*})] dE = \int_{E} \underline{f}_{E}^{R} \underline{U}^{*} dE + \int_{\partial E} \eta_{E}(\underline{\hat{R}}|_{\partial E} + \underline{\hat{H}}|_{\partial E}) \underline{U}^{*} d\Gamma.$$
(35)

Thus, problem \mathbf{p}_E^R becomes:

Find $\hat{\sigma}_{E}^{R}$ solution to the minimization problem

$$\min_{\hat{\sigma}_E \in \mathscr{S}^R_{\mathrm{ad}|E}} \frac{1}{2} \int_E \mathrm{Tr}[\hat{\sigma}_E \mathbf{K}^{-1} \hat{\sigma}_E] \,\mathrm{d}E.$$
(36)

The solution to (36) is designated by $\hat{\sigma}_{E}^{R}$. This field is of the type

$$\hat{\sigma}_E^R = \hat{\sigma}_E^0 + \Sigma_E(R_E), \tag{37}$$

where R_E is the column of constant vectors \underline{R}_{α} defined on ∂E by relation (28) and where $\Sigma_E(R_E)$ is a linear term in R_E .

Field $\hat{\sigma}$ defined by $\hat{\sigma}|_E = \hat{\sigma}_E^R$ is statically admissible if and only if \underline{f}_E^R has the same moment and resultant as $\underline{f}_d|_E$.

This relation, which expresses the equilibrium between $\underline{\hat{R}}_{|\Gamma}$ on ∂E and \underline{f}_{d} on E, can also be written:

$$\mathbf{L}_E R_E = b_E \tag{38}$$

or, for the whole mesh

$$\mathbf{L}\mathbf{R} = b. \tag{39}$$

Therefore, in order to find the solution to (31), one needs only to minimize the complementary energy for all stress fields: $\hat{\sigma}_E^R = \hat{\sigma}_E^0 + \Sigma_E(R_E)$.

Except for terms which are independent of R, Eq. (31) is of the form

$$\min_{\mathbf{L}R=b}\left[\frac{1}{2}\mathbf{R}^{t}\mathbf{A}\mathbf{R}+B^{t}\mathbf{R}\right],\tag{40}$$

where matrices A, L and B are obtained by assembling elementary matrices. The introduction of Lagrange multipliers leads to the resolution of the linear system

$$\begin{bmatrix} \mathbf{A} & \mathbf{L} \\ \mathbf{L}^{t} & \mathbf{0} \end{bmatrix} \begin{bmatrix} R \\ \Lambda \end{bmatrix} = \begin{bmatrix} B \\ b \end{bmatrix}.$$
(41)

4.3. Practical implementation

The construction of matrices **A** and **B** requires the resolution of local problems (36). In practice, this resolution is performed in the same way as for problem (20): by duality on *E*, one reverts to a displacement problem which can be solved approximately by a finite element method. For tetrahedra of degree *p*, one may consider a discretization of *E* with either a single element but an interpolation of degree p + k, where *p* is the degree of interpolation used in the finite element analysis and *k* a positive integer, or a subdivision of element *E* along with an interpolation of degree p + k' (generally k' < k). The resolution of the global problem (40) is performed by an iterative method of the conjugate gradient type. In order to initialize the process, one first determines the set of densities using the standard procedure [12,17,18]. Furthermore, numerical experiments have shown that the optimization of densities needs to be performed only in the zones where this initialization is deficient: zones with large gradients or very ill-shaped elements.

5. Study of the quality of local estimations

We show examples modeled with linear tetrahedra (p = 1). The resolution of the local problems described in Section 4.2 was performed by subdividing each element *E* and increasing by 1 the degree of interpolation. In order to measure the local quality of our estimator, we introduced a local effectivity index ζ_E :

$$\zeta_E = \frac{\|\hat{\sigma}_{\rm h} - \sigma_{\rm h}\|_E}{\|\sigma_{\rm ex} - \sigma_{\rm h}\|_E}.\tag{42}$$

For problems for which σ_{ex} cannot be obtained analytically, we performed an analysis on an extremely fine mesh in order to obtain a good approximation of σ_{ex} .

5.1. Test case 1

The structure is a beam with square cross-section, built-in at one end and subjected to traction at the other end (Fig. 7). The mesh (Fig. 8) is coarse and consists of 38 linear tetrahedral elements.

The relative global error estimate for this calculation is 10%. On Fig. 9, we show the contributions associated with the error calculation versus the element number. The local effectivity index is shown on Fig. 10. For this example, the local effectivity indexes ranged between 0.98 and 1.3.

For dimensioning purposes in mechanical design, only the high-stress zones are significant. We are interested only in the error affecting such zones. The stress intensity in an element E is defined by

$$I_{E} = \frac{\|\sigma_{h}\|_{E}}{\max_{E'} \|\sigma_{h}\|_{E'}}.$$
(43)

Let S_{α} be the set of elements of the mesh with a stress intensity greater than α :

$$\mathbf{S}_{\alpha} = \{E; I_E \geqslant \alpha\}. \tag{44}$$

The minimum corresponding effectivity index is

$$m_{\alpha} = \min_{E \in \mathbf{S}_{\alpha}} \zeta_{E}. \tag{45}$$

The evolution of m_{α} with α is shown on Fig. 11. In this example, the local error in constitutive relation is an upperbound of the exact local error in the zones where the stress is the highest.



Fig. 7. Beam: loading.



Fig. 8. Beam: mesh.



Fig. 9. Local contributions to the error.



Fig. 10. Local effectivity indexes.



5.2. Test case 2

In this example, the loading was less simple and the global error estimation was higher. The structure was subjected to uniform surface forces on one side (Fig. 12). The mesh, which consists of 194 elements, is given in Fig. 13. The global relative error was 34%. The measured global effectivity was 1.14.

Remark. As examples become more complex, one can observe that in the elements where the error is very small numerical perturbations can be significant (of the same order of magnitude as the quantities in the ratio), thus leading to inconsistent effectivity indexes. In order to overcome this difficulty and eliminate the elements with virtually no error, we adopted the following procedure: first, the elements in the mesh are sorted in the order of decreasing error $(E_1, E_2, ...)$ with $\hat{e}_{h, E_1} \ge \hat{e}_{h, E_2} \ge ...$; then, we determine the integer q such that $\sum_{i=1}^{q} \hat{e}_{h, E_i}^2 = 0.95 \hat{e}_h^2$. Local effectivity indexes are calculated on these elements alone.

In this example, the local effectivity indexes ranged between 0.77 and 1.70. The evolution of the minimum effectivity index m_{α} with α (Fig. 14) shows that in the zones where the stress is high the minimum effectivity index is close to 1 and greater than 1 in the most highly stressed zones.

5.3. Test case 3

Now we will present the more elaborate example of a flange, which can be used to fasten a part during machining. The flange was clamped along the lower surface to represent its connection to the machine tool. It was subjected to a pressure load along the perpendicular side to represent the cutting load. We considered two dimensioning zones, one corresponding to the reinforcements (Zone R) and the other to the clamping (Zone E) (Fig. 15).



Fig. 12. Arch: loading.



Fig. 13. Arch: mesh.

The mesh comprised 2828 elements (Fig. 16). The estimated global error was 41%. The "exact" global error was calculated and is equal to 36% (in order to obtain the "exact" solution, we generated a mesh with 22,624 10-node tetrahedral elements).





Fig. 15. Flange: Zones E and R.



Fig. 16. Flange: mesh.

The study of Zones R and E gave the following results:

- in the most highly-loaded zone, corresponding to the reinforcements: actual error: 7.79% estimation: 8.62% effectivity index: 1.1065
- in the zone near the clamping: actual error: 27.57% estimation: 29.70% effectivity index: 1.0769.

In all the cases studied, we observed that one can use the upperbound defined by Eq. (16), with C on the order of 1 in the zones where the stress intensity is highest.

6. Conclusions

In this paper, we have showed that the construction of improved statically admissible fields proposed in [11] can be extended to the case of 3D calculations in elasticity.

The examples presented here along with many other examples calculated by Ladevèze's team in Cachan show experimentally that, in many common situations, the local contributions associated with the new version of the estimator of the error in constitutive relation provide good estimates of the local quality of the stresses calculated by finite element analysis. In these situations, from a practical standpoint, these contributions can be used to evaluate the local errors.

Obviously, there can still be situations [19] in which an extraction technique must be used. Of course, this is also the case if one wishes to evaluate the local quality of other quantities, such as displacements or stress intensity factors.

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