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C. R. Mecanique 334 (2006) 399–407
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Upper error bounds on calculated outputs of interest for linear and nonlinear structural problems

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Received 25 October 2005; accepted after revision 4 April 2006

Available online 22 June 2006

Presented by Évariste Sanchez-Palencia

Abstract

This Note introduces new strict upper error bounds on outputs of interest for linear as well as time-dependent nonlinear structural problems calculated by the finite element method. Small-displacement problems without softening, such as (visco)plasticity problems, are included through the standard thermodynamics framework involving internal state variables. ***To cite this article: P. Ladevèze, C. R. Mecanique 334 (2006).***

Résumé

Bornes supérieures de l'erreur sur une quantité d'intérêt calculée par éléments finis en mécanique linéaire et non-linéaire des structures. La Note introduit de nouvelles bornes supérieures de l'erreur relative à une quantité d'intérêt calculée par éléments finis en mécanique linéaire et non-linéaire des structures. Sont considérés les problèmes en petites perturbations du type (visco)plastique sans adoucissement dans le cadre de la thermodynamique classique avec variables internes. ***Pour citer cet article : P. Ladevèze, C. R. Mecanique 334 (2006).***

Keywords: Computational solid mechanics; Verification; Output of interest; Constitutive relation error; Finite elements; Nonlinear mechanics

Mots-clés : Mécanique des solides numérique ; Vérification ; Quantité d'intérêt ; Erreur en relation de comportement ; Eléments finis ; Non-linéaire

1. Introduction

Today more than ever, modeling and simulation are central to any Mechanical Engineering activity. A constant concern both in industry and in research has always been the verification of models which, today, can attain very high levels of complexity. The novelty of the situation is that over the last twenty-five years truly quantitative tools for assessing the quality of a FE model have appeared; this topic is now known as 'model verification'. Of course, the original continuum mechanics model remains the reference (Fig. 1). The state of the art can be found in [1,2].

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1631-0721/$ – see front matter
doi:10.1016/j.crme.2006.04.004

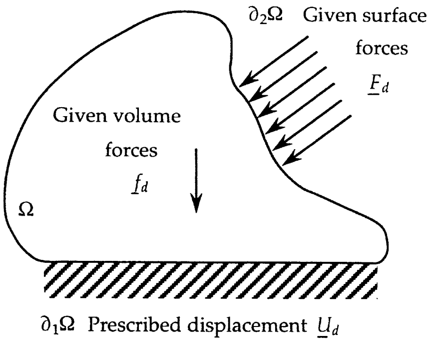

Fig. 1. Schematic representation of the environment (i.e., the prescribed conditions).

Until 1990, only global error estimators were available through three different families introduced by Ladevèze (1975), Babuška and Rheinboldt (1978), and Zienkiewicz and Zhu (1987). Since 1990, a key issue has become the evaluation of the quality of the outputs of interest resulting from a finite element analysis. This objective was beyond the reach of earlier error estimators, which provided only global information which was totally insufficient for dimensioning purposes in mechanical design (where the dimensioning criteria involve local values of stresses, displacements, stress intensity factors, ...). Among the numerous works on the linear case, we can mention as the earliest ones: Peraire and Patera, Rannacher et al., Strouboulis and Babuška, Oden and Prudhomme, Ladevèze et al.; further references can be found in [2]. The main idea which emerged then was that an output of interest could be written globally, thus allowing the reuse of global error estimators; however, accurate error estimation required the finite element solution of what is called the 'adjoint problem'. Extensions to the nonlinear case appeared in the early 1990s with Johnson, Rannacher et al., Ramm et al.; these approaches consisted in getting back to the linear case through linearization during each time step.

Unfortunately, most of these estimates are not guaranteed to be upper or lower bounds, which is a very serious drawback for robust design. Consequently, one of today's research challenges is to derive upper error bounds for the calculated values of outputs of interest. Even in the linear case, relatively few works have proposed answers: Ladevèze et al., Strouboulis and Babuška, Peraire et al., Diez and Huerta, De Almeida et al. Outside of the FE context, and only for the linear case, there are some quite old works, such as [3] and [4]. These, which use analytical Green functions, have serious limitations and seem quite remote from the present concern, in which numerical aspects are central.

This Note introduces new upper error bounds of a calculated output of interest for linear as well as time-dependent nonlinear problems. These are probably the first strict upper bounds to be published for the nonlinear case. Small-displacement problems without softening, such as (visco)plasticity, are included through the standard thermodynamics framework involving internal state variables. Classical convexity properties are assumed. This work completes the a posteriori error estimation method developed particularly at LMT-Cachan (see [2]), which is based on the concept of Constitutive Relation Error (CRE) and on quasi-explicit techniques for the construction of associated admissible FE solutions.

The first key point of this approach is the integration of an output of interest in terms of finite variations; this leads to the introduction of what is called the 'mirror problem at time T', which is very similar to the initial problem, as a substitute for the adjoint problem. Of course, the mirror problem coincides with the adjoint problem in the linear case. Another key point concerns the convexity properties, which constitute the true 'engine' of our approach for deriving upper error bounds. These properties lead to the basic relations between the dissipation-type constitutive relation error and the solution error. In the end, upper error bounds are derived on the basis of the data and the FE solutions of both the reference problem and the mirror problem over the time-space domain being studied.

This Note presents only the basic aspects. Numerical illustrations will be shown in upcoming papers. Preliminary results for the viscoelastic case were shown in [5].

2. The reference problem to be solved—notations

Initially, the structure being studied occupies a domain Ω bounded by $\partial\Omega$. We assume small displacements, quasi-static loading and isothermal conditions. The time interval of interest is denoted $[0, T]$.

At any time t belonging to $[0, T]$, the structure is placed in an "environment" characterized by a displacement $\underline{U}_d$ on a part $\partial_1\Omega$ of the boundary of Ω, a traction force density $\underline{F}_d$ on $\partial_2\Omega$ (the part of $\partial\Omega$ complementary to $\partial_1\Omega$), and a body force density $\underline{f}_d$ in the domain Ω.

The problem which describes the evolution of the structure over $[0, T]$ is to find the displacement field $\underline{U}(\underline{M}, t)$ and the stress field $\sigma(\underline{M}, t)$, with $t \in [0, T]$ and $\underline{M} \in \Omega$, which verify:

- the kinematic constraints:

$$\underline{U} \in \mathcal{U}^{[0,T]}; \qquad \underline{U}|_{\partial_1\Omega} = \underline{U}_d \quad \text{on }]0, T[\tag{1}$$

- the equilibrium equations (principle of virtual work):

$$\sigma \in \mathcal{S}^{[0,T]}; \quad \forall t \in]0, T[\ \forall \underline{U}^* \in \mathcal{U}_{\text{ad},0}$$
$$\int_\Omega \text{Tr}\big[\sigma \varepsilon(\underline{U}^*)\big]\,\mathrm{d}\Omega = \int_\Omega \underline{f}_d \cdot \underline{U}^*\,\mathrm{d}\Omega + \int_{\partial_2\Omega} \underline{F}_d \cdot \underline{U}^*\,\mathrm{d}S \tag{2}$$

- the constitutive relation:

$$\forall t \in [0, T]\ \forall \underline{M} \in \Omega \quad \sigma|_t = \boldsymbol{A}\big(\varepsilon(\dot{\underline{U}}|_\tau); \tau \leqslant t\big) \tag{3}$$

  where $\varepsilon(\underline{U})$ denotes the strain associated with the displacement ($\varepsilon(\underline{U})_{ij} = \frac{1}{2}(U_{i,j} + U_{j,i})$). $\mathcal{U}^{[0,T]}$ is the space containing the displacement field $\underline{U}$ defined over $\Omega \times]0, T[$, and $\mathcal{S}^{[0,T]}$ is the space containing the stresses, also defined over $\Omega \times]0, T[$. Finally, $\mathcal{U}_{\text{ad},0}$ is the vector space of the prescribed virtual velocities. Operator $\boldsymbol{A}$, which is given and generally single-valued, characterizes the mechanical behavior of the material.

Let us denote $\mathcal{U}_{\text{ad}}^{[0,T]}$ the space of the displacements which verify the kinematic constraints (1) and $\mathcal{S}_{\text{ad}}^{[0,T]}$ the space of the stresses which are solutions of the equilibrium equations (2).

3. Upper error bound for an output of interest in elasticity

Let us start with the simplest family of problems, i.e., elasticity problems. We focus on the final state of the structure at $t = T$; thus, the problem to be solved does not depend on time. Moreover, the constitutive relation (3) becomes:

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

where $\boldsymbol{K}$ denotes the Hooke's tensor, which is symmetric and positive definite. The spaces of the admissible displacements and stresses are $\mathcal{U}_{\text{ad}}$ and $\mathcal{S}_{\text{ad}}$ respectively. The densities $\underline{U}_d, \underline{f}_d, \underline{F}_d$ are known at $t = T$.

3.1. The output of interest α

The quantity of interest α is a goal-oriented quantity, such as the mean value of a stress or displacement component over an element or a set of elements. Von Mises' stress is another possibility . Such an output of interest can be written globally:

$$\alpha_{\text{ex}} = \int_\Omega \text{Tr}\big[\sigma_{\text{ex}}\widetilde{\Sigma}\big]\,\mathrm{d}\Omega \tag{5}$$

where 'ex' denotes the exact value and $\widetilde{\Sigma}$ is the extractor which defines α. Here, for the sake of simplicity, we do not consider convex nonlinear functionals of the stress, but such extensions would not involve serious difficulties. The α-error is $|\alpha_{\text{ex}} - \alpha_h|$ where α_h is the value obtained from a finite element solution.

3.2. The data and associated admissible FE solutions

The prescribed displacement and forces are known. Let us assume that the finite element solution was calculated using a displacement approach. Thus, the finite element displacement-stress pair $(\underline{U}_h, \sigma_h)$ is known and the stress σ_h is FE-equilibrated.

The principle behind our approach consists in associating a new, admissible displacement-stress pair (i.e., belonging to $\boldsymbol{\mathcal{U}}_{\mathrm{ad}} \times \boldsymbol{\mathcal{S}}_{\mathrm{ad}}$), denoted $(\widehat{\underline{U}}_h, \hat{\sigma}_h)$, to the data and the finite element displacement-stress pair. This new entity also verifies what we call the 'prolongation conditions', which are relations with the finite element solution. This is achieved through a general quasi-explicit technique which is now well-known (see [2]). For the displacement, we generally take $\widehat{\underline{U}}_h = \underline{U}_h$.

In order to get a good bound, a common practice is to calculate what is called the adjoint problem, which is very classical in this case: it consists in an elasticity problem with a prestrain $\widetilde{\Sigma}$. Its finite element solution, which can be obtained with a refined mesh, is denoted $(\underline{\widetilde{U}}_h, \tilde{\sigma}_h)$, and the associated admissible FE solution is $(\widehat{\underline{\widetilde{U}}}_h, \hat{\tilde{\sigma}}_h)$.

3.3. Basic results concerning the error

Let us first recall the Prager–Synge theorem (1947), which links the constitutive relation error to the classical error in the solution:

$$\Phi^*(\sigma_{\mathrm{ex}} - \hat{\sigma}_h) + \Phi(\varepsilon_{\mathrm{ex}} - \hat{\varepsilon}_h) = \left[E^h_{\mathrm{CRE}}\right]^2 \tag{6}$$

$$\Phi^*(\sigma_{\mathrm{ex}} - \hat{\sigma}_{h,m}) = \frac{1}{4}\left[E^h_{\mathrm{CRE}}\right]^2 \quad \text{with } \hat{\sigma}_{h,m} \equiv \frac{1}{2}\left[\hat{\sigma}_h + \boldsymbol{K}\varepsilon\left(\widehat{\underline{U}}_h\right)\right] \tag{7}$$

where Φ and Φ^* are the global potentials (dual convex functions) of the constitutive relation:

$$\Phi^*(\sigma) \equiv \int_\Omega \varphi^*(\sigma)\,\mathrm{d}\Omega, \qquad \Phi(\varepsilon) \equiv \int_\Omega \varphi(\varepsilon)\,\mathrm{d}\Omega$$

$$\varphi^*(\sigma) \equiv \frac{1}{2}\,\mathrm{Tr}\left[\sigma \boldsymbol{K}^{-1}\sigma\right], \qquad \varphi(\varepsilon) \equiv \frac{1}{2}\,\mathrm{Tr}\left[\varepsilon \boldsymbol{K}\varepsilon\right]$$

The constitutive relation error is:

$$\left[E^h_{\mathrm{CRE}}\right]^2 \equiv \Phi^*(\hat{\sigma}_h) + \Phi(\hat{\varepsilon}_h) - \int_\Omega \mathrm{Tr}[\hat{\sigma}_h \hat{\varepsilon}_h]\,\mathrm{d}\Omega$$

The main result is the following:

Theorem 1. *The following upper bound holds*:

$$|\alpha_{\mathrm{ex}} - \alpha_h - \alpha_{hh}| \leqslant E^h_{\mathrm{CRE}} \cdot \widetilde{E}^h_{\mathrm{CRE}} \tag{8}$$

where E^h_{CRE} and $\widetilde{E}^h_{\mathrm{CRE}}$ are the constitutive relation errors related to the reference problem and the adjoint problem respectively. α_{hh} is a correction defined by:

$$\alpha_{hh} \equiv \int_\Omega \mathrm{Tr}\left[\left(\hat{\sigma}_h - \boldsymbol{K}\varepsilon\left(\widehat{\underline{U}}_h\right)\right)\boldsymbol{K}^{-1}\hat{\tilde{\sigma}}_{h,m}\right]\mathrm{d}\Omega + \int_\Omega \mathrm{Tr}\left[\left(\boldsymbol{K}\varepsilon\left(\widehat{\underline{U}}_h\right) - \sigma_h\right)\widetilde{\Sigma}\right]\mathrm{d}\Omega$$

Proof. The adjoint problem is here the previous elasticity one, the structure being submitted to the prestrain $\widetilde{\Sigma}$; zero-value displacement and traction are prescribed on the boundary $\partial\Omega$. The starting point is:

$$\begin{aligned}\alpha_{\mathrm{ex}} - \alpha_h &= \int_\Omega \mathrm{Tr}\left[(\sigma_{\mathrm{ex}} - \sigma_h)\widetilde{\Sigma}\right]\mathrm{d}\Omega \\ &= \int_\Omega \mathrm{Tr}\left[\varepsilon\left(\underline{U}_{\mathrm{ex}} - \widehat{\underline{U}}_h\right)\left(\hat{\tilde{\sigma}}_h - \boldsymbol{K}\varepsilon\left(\widehat{\underline{\widetilde{U}}}_h\right)\right)\right]\mathrm{d}\Omega + \int_\Omega \mathrm{Tr}\left[\left(\hat{\sigma}_h - \boldsymbol{K}\varepsilon\left(\widehat{\underline{U}}_h\right)\right)\varepsilon\left(\widehat{\underline{\widetilde{U}}}_h\right)\right]\mathrm{d}\Omega \\ &\quad + \int_\Omega \mathrm{Tr}\left[\left(\boldsymbol{K}\varepsilon\left(\widehat{\underline{U}}_h\right) - \sigma_h\right)\widetilde{\Sigma}\right]\mathrm{d}\Omega\end{aligned}$$

Introducing $\hat{\tilde{\sigma}}_{h,m}$ as in (7), we get: $\alpha_{\mathrm{ex}} - \alpha_h - \alpha_{hh} = \int_\Omega \mathrm{Tr}[(\sigma_{\mathrm{ex}} - \hat{\sigma}_{h,m})\boldsymbol{K}^{-1}(\hat{\tilde{\sigma}}_h - \boldsymbol{K}\varepsilon(\widehat{\underline{\widetilde{U}}}_h))]\,\mathrm{d}\Omega$.
Using identity (7), we obtain the final upper bound. □

Remarks

- The bound defined by the second member of (8) is half of the previous bound (see [2]).
- The value of the error bound depends on the meshes used to solve the reference and adjoint problems. It is always possible, by refining the mesh of the adjoint problem alone, to control the value of the α-error.
- The orthogonality property related to the FE solution is not used.

4. Upper error bound of an output of interest for (visco)plasticity problems

4.1. The reference problem to be solved—notations

We are going to rewrite the reference problem (1), (2), (3) using some global notations within the framework of classical thermodynamics with internal variables. Let us introduce the following generalized quantities:

$$s = \begin{bmatrix} \sigma \\ \mathbb{Y} \end{bmatrix}, \qquad \dot{e}_p = \begin{bmatrix} \dot{\varepsilon}_p \\ -\dot{\mathbb{X}} \end{bmatrix}, \qquad \dot{e}_e = \begin{bmatrix} \dot{\varepsilon}_e \\ \dot{\mathbb{X}} \end{bmatrix} \tag{9}$$

where the additional internal variables are the n-vectors $\mathbb{X}$ and $\mathbb{Y}$. The dissipation bilinear form over the time-space domain is:

$$(\dot{e}_p, s) \mapsto \int_0^T \int_\Omega s \cdot \dot{e}_p \, d\Omega \, dt = \int_0^T \int_\Omega \left(\mathrm{Tr}[\sigma \dot{\varepsilon}_p] - \mathbb{Y} \cdot \dot{\mathbb{X}}\right) d\Omega \, dt$$

The reference problem is thus to find $(\dot{e}_p, s) \in \boldsymbol{\mathcal{S}}^{[0,T]}$ such that:

- $\dot{e} = \dot{e}_e + \dot{e}_p$: K-admissible
- s: S-admissible
- state equations: $e_e = \boldsymbol{\Lambda}(s)$
- state evolution laws: $\dot{e}_p = \boldsymbol{B}(s)$
- initial conditions: $s = 0$, $e = 0$ at $t = 0$ (10)

$\boldsymbol{\Lambda}$ is assumed to be linear: most viscoplastic materials are in this category (see [6]); this material description is called 'normal'. $\boldsymbol{B}$ could be nonlinear and multivalued, as in plasticity, but here we consider the family of standard materials whose state evolution laws can be expressed with two potentials, which are dual convex functions such that for $(t, \underline{M}) \in [0, T] \times \Omega$:

$$\forall (\dot{e}_p, s) \in \boldsymbol{\mathcal{S}} \quad \varphi^*(s) + \varphi(\dot{e}_p) - s \cdot \dot{e}_p \geqslant 0$$
$$\varphi^*(s) + \varphi(\dot{e}_p) - s \cdot \dot{e}_p = 0 \iff \dot{e}_p = \boldsymbol{B}(s)$$

Then, the constitutive relation error related to $(\dot{e}_p, s) \in \boldsymbol{\mathcal{S}}^{[0,T]}$ is:

$$[E_{\mathrm{CRE}}]^2 = \int_0^T \int_\Omega \left[\varphi^*(s) + \varphi(\dot{e}_p) - s \cdot \dot{e}_p\right] d\Omega \, dt \tag{11}$$

4.2. The associated admissible FE solution

In the dissipation error framework, the concept of admissibility must be modified:

Definition 1. A pair $(\dot{e}_p, s) \in \boldsymbol{\mathcal{S}}^{[0,T]}$ is admissible if:

(i) the state equations are verified ($e_e = \boldsymbol{\Lambda}(s)$).
(ii) $\dot{e} = \dot{e}_e + \dot{e}_p$ and s verify the kinematic constraints and the equilibrium equations.

Let $(\dot{e}_h, s_h)$ be the FE solution of the reference problem. Assuming linear behavior during each time step, we can extend the FE solution, originally defined at discrete instants, across the whole time-space domain. We assume that $\dot{e}_h$ is kinematically admissible and that σ_h verifies the FE equilibrium at any instant belonging to $]0, T[$. Using the same technique as in elasticity, we define a displacement-stress pair $(\underline{\widehat{U}}_h, \hat{\sigma}_h)$ which is admissible, in the classical sense, over $[0, T] \times \Omega$. However, for (visco)plasticity with the constraint $\mathrm{Tr}[\dot{\varepsilon}_p] = 0$, the previous displacement must be modified so that $\mathrm{Tr}[\hat{\dot{\varepsilon}}_p] = 0$. The additional internal variables $(\widehat{\mathbb{X}}_h, \widehat{\mathbb{Y}}_h)$, which must verify the state equations, can be easily constructed by solving local problems. The details can be found in [2].

4.3. The output of interest and the associated 'mirror' problem

The output of interest can be defined by:

$$\alpha_{\mathrm{ex}} = \int_0^T \int_\Omega \left[\mathrm{Tr}\left[\sigma_{\mathrm{ex}} \delta \dot{\tilde{\Sigma}}\right] - \mathbb{Y}_{\mathrm{ex}} \cdot \delta \dot{\tilde{\mathbb{X}}}\right] \mathrm{d}\Omega \, \mathrm{d}t = \int_0^T \int_\Omega s_{\mathrm{ex}} \cdot \delta \dot{\tilde{e}}_\Sigma \, \mathrm{d}\Omega \, \mathrm{d}t \tag{12}$$

where the extractor is: $\delta \dot{\tilde{e}}_\Sigma = \left[\begin{smallmatrix} \delta \dot{\tilde{\Sigma}} \\ -\delta \dot{\tilde{\mathbb{X}}} \end{smallmatrix}\right]$ with $\delta \dot{\tilde{e}}_\Sigma = 0$ at $t = T$.

Here, δ is a symbol indicating that $\delta \dot{\tilde{e}}_\Sigma$ must be interpreted as a finite, but relatively small, variation. *However, we do not carry out any linearization*. The adjoint problem is replaced by what we call the 'mirror' problem, which is similar to the reference problem except that time goes backwards: $\tau \equiv T - t$. This mirror problem, written with δ-quantities, is defined by:

Find $(\delta \dot{\tilde{e}}_p, \delta \tilde{s}) \in \boldsymbol{\mathcal{S}}^{[0,T]}$ such that:

- $\delta \dot{\tilde{e}} = \delta \dot{\tilde{e}}_e + \delta \dot{\tilde{e}}_p$: K-admissible
- $\delta \tilde{s} - \delta \tilde{s}_\Sigma$: S-admissible
- state equations: $\delta \tilde{e}_e = \boldsymbol{\Lambda}(\delta \tilde{s})$
- state evolution laws: $\delta \dot{\tilde{e}}_p = \widetilde{\boldsymbol{B}}(\delta \tilde{s}) \equiv \boldsymbol{B}(s_h + \delta \tilde{s}) - \boldsymbol{B}(s_h)$
- initial conditions: $\delta \tilde{s} = 0, \delta \dot{\tilde{e}} = 0$ at $\tau = 0$ (13)

where $s_h(\tau)$ is the FE solution of the reference problem and $\delta \dot{\tilde{e}}_\Sigma = \widetilde{\boldsymbol{B}}(\delta \tilde{s}_\Sigma) + \boldsymbol{\Lambda}(\delta \dot{\tilde{s}}_\Sigma)$.

Let $(\dot{\tilde{e}}_h, \tilde{s}_h)$ be the FE solution of the mirror problem and $(\hat{\dot{\tilde{e}}}_h, \hat{\tilde{s}}_h)$ the associated admissible FE solution over $[0, T] \times \Omega$. From now on, all these quantities will be defined by reference to the initial time t.

4.4. Basic results concerning the error

4.4.1. Link between the constitutive relation error and the error in the solution

Let us first introduce what we call the φ-tangent potential at x:

$$\overline{\varphi}(x' - x) \equiv \varphi(x') - \varphi(x) - y \cdot (x' - x) \geqslant 0$$

where φ, φ^* are two dual convex functions and (x, y) is such that $\varphi(x) + \varphi^*(y) - x \cdot y = 0$.

We give a new version of the fundamental link between the constitutive relation error and the error in the solution derived in [6]:

Theorem 2. *Let $(\dot{e}_{p,\mathrm{ex}}, s_{\mathrm{ex}})$ be the exact solution and $(\hat{\dot{e}}_{p,h}, \hat{s}_h)$ an arbitrary admissible solution of the reference problem. We have*:

$$\overline{\Phi}^*\left(s_{\mathrm{ex}} - \boldsymbol{B}^{-1}(\hat{\dot{e}}_{p,h})\right) + \overline{\Phi}\left(\dot{e}_{p,\mathrm{ex}} - \boldsymbol{B}(\hat{s}_h)\right) + \int_0^T |\dot{a}| E_F(s_{\mathrm{ex}} - \hat{s}_h) \, \mathrm{d}t = \left[E_{\mathrm{CRE}}^h\right]^2 \tag{14}$$

with:

- $\Phi \equiv \int_0^T \int_\Omega a(t)\varphi \,\mathrm{d}\Omega \,\mathrm{d}t, \qquad \Phi^* \equiv \int_0^T \int_\Omega a(t)\varphi^* \,\mathrm{d}\Omega \,\mathrm{d}t$
- $\left[E^h_{\mathrm{CRE}}\right]^2 = \int_0^T \int_\Omega a(t)\left[\varphi^*(\hat{s}_h) + \varphi(\hat{\dot{e}}_{p,h}) - \hat{s}_h \cdot \hat{\dot{e}}_{p,h}\right] \mathrm{d}\Omega \,\mathrm{d}t$
- $a(t)$: *arbitrary function such that* $a(t) \geqslant 0, \dot{a} \leqslant 0, a(T) = 0$

In some applications, it is interesting to restrict the time interval to a subinterval $[T', T]$. An identity similar to (14) holds, with the additional term $a(T')E_F^+|_{T'}$ on the right-hand side, where E_F^+ is an upper bound of $E_F(s_{\mathrm{ex}} - \hat{s}_h)|_{T'}$.

Proposition 1. *An upper bound of the free energy $E_F(s_{\mathrm{ex}} - \hat{s}_h)$ at t is $E_F^+(t)$, solution of*:

- $E_F^+(0) = 0$
- $\dfrac{\mathrm{d}}{\mathrm{d}t}(E_F^+) + \omega(E_F^+, t) = \int_\Omega \left[\varphi^*(\hat{s}_h) + \varphi(\hat{\dot{e}}_{p,h}) - \hat{s}_h \cdot \hat{\dot{e}}_{p,h}\right] \mathrm{d}\Omega \qquad (15)$

where ω is a function such that:

$$\omega\big(E_F^+(\Delta s), t\big) \leqslant \inf_{\Delta s \in \mathcal{S}_{\mathrm{ad},0}} \int_\Omega \left[\overline{\varphi}^*\big(\Delta s + \hat{s}_h - \boldsymbol{B}^{-1}(\hat{\dot{e}}_{p,h})\big) + \overline{\varphi}\big(\boldsymbol{B}(\Delta s + \hat{s}_h) - \boldsymbol{B}(\hat{s}_h)\big)\right] \mathrm{d}\Omega \qquad (16)$$

$\boldsymbol{\mathcal{S}}_{\mathrm{ad},0}$ *being the space of the statically admissible generalized stresses under homogeneous conditions.*

The proof essentially uses Theorem 2, written locally in time.

4.4.2. Upper error bound for an output of interest α

The starting point is the following relation, which can be easily proven.

Proposition 2. *Using the previous notations, the α-error is equal to*:

$$-\alpha_{\mathrm{ex}} + \alpha_h + \alpha_{hh} = \int_0^T \int_\Omega (s_{\mathrm{ex}} - \hat{s}_{h,m}) \cdot \big(\widetilde{\boldsymbol{B}}(\delta\hat{\tilde{s}}_h) - \delta\hat{\dot{\tilde{e}}}_{p,h}\big) \mathrm{d}\Omega \,\mathrm{d}t + \boldsymbol{C}(s_{\mathrm{ex}} - s_h, \delta\tilde{s}_\Sigma) - \boldsymbol{C}(s_{\mathrm{ex}} - s_h, \delta\hat{\tilde{s}}_h) \qquad (17)$$

where:

- $\alpha_{hh} \equiv -\int_0^T \int_\Omega \left[(\hat{\dot{e}}_h - \dot{e}_h) \cdot (\delta\tilde{s}_\Sigma - \delta\hat{\tilde{s}}_h) - (\hat{s}_h - s_h) \cdot \delta\hat{\dot{\tilde{e}}}_h + (\hat{s}_{h,m} - s_h) \cdot \big(\widetilde{\boldsymbol{B}}(\delta\hat{\tilde{s}}_h) - \delta\hat{\dot{\tilde{e}}}_{p,h}\big)\right] \mathrm{d}\Omega \,\mathrm{d}t$
- $\dot{e}_h = \boldsymbol{\Lambda}(\dot{s}_h) + \boldsymbol{B}(s_h)$; $\hat{s}_{h,m}$: *arbitrary*, $\delta\hat{\dot{\tilde{e}}}_{p,h|t} = \left[\delta\tilde{e}_{h,\tau} - \boldsymbol{\Lambda}(\delta\hat{s}_{h,\tau})\right]|_{\tau = T - t}$
- $\boldsymbol{C}(\Delta s, \delta s) = \int_0^T \int_\Omega [\Delta s \cdot \delta\dot{e}_p - \Delta\dot{e}_p \cdot \delta s] \,\mathrm{d}\Omega \,\mathrm{d}t$ *with* $\Delta\dot{e}_p = \widetilde{\boldsymbol{B}}(\Delta s)$, $\delta\dot{e}_p = \widetilde{\boldsymbol{B}}(\delta s)$

Remarks

– The idea behind this relation is related to the $\boldsymbol{C}$-terms: these are very small if the finite variations $(s_{\mathrm{ex}} - s_h)$ and $\delta\tilde{s}_\Sigma$ are small. Moreover, if the material model is linear, the $\boldsymbol{C}$-terms are equal to zero. If necessary, one can multiply α by a scalar less than 1. $\boldsymbol{C}$ is called the 'model nonlinearity indicator'.

– The generalized stress $\hat{s}_{h,m}$ is similar to the mean stress introduced in (7). In practice, we take an approximation of the minimization problem related to the cost function g:

$$g(s-\hat{s}_{h,m})=\int_0^T\big[a\overline{\varphi}^*\big(s-\boldsymbol{B}^{-1}(\hat{\dot{e}}_{p,h})\big)+a\overline{\varphi}\big(\boldsymbol{B}(s)-\boldsymbol{B}(\hat{s}_h)\big)+|\dot{a}|E_F(s-\hat{s}_h)\big]\,\mathrm{d}t \tag{18}$$

– The orthogonality conditions related to the FE solution are not used.

Upper bounds of I_1 and I_2 (see (17))
We only give the results here.

Proposition 3. *Let be* $I_1=\int_0^T\int_\Omega(s_{\mathrm{ex}}-\hat{s}_{h,m})\cdot(\widetilde{\boldsymbol{B}}(\delta\hat{\dot{s}}_h)-\delta\hat{\dot{\tilde{e}}}_{p,h})\,\mathrm{d}\Omega\,\mathrm{d}t$. *We have*:

$$I_1\leqslant 2\big[\big[E^h_{\mathrm{CRE}}\big]^2-\big[E^h_{\mathrm{CRE},m}\big]^2\big]^{1/2}\cdot\big[F^2(\overline{\mu}\,\dot{\tilde{a}}_h)\big]^{1/2}+F^1(\dot{\tilde{a}}_h) \tag{19}$$

with:

- $\big[E^h_{\mathrm{CRE},m}\big]^2=\int_\Omega\Big[\min_{y\in\mathcal{F}^{[0,T]}}g(y)\Big]\mathrm{d}\Omega,\quad \dot{\tilde{a}}_h=\widetilde{\boldsymbol{B}}(\delta\hat{\dot{s}}_h)-\delta\hat{\dot{\tilde{e}}}_h$
- $f(\dot{x})\equiv\sup_{y\in\mathcal{F}^{[0,T]}}\Big[\int_0^T y\cdot\dot{x}\,\mathrm{d}t-g(y)\Big]\quad\forall\dot{x}\in\mathcal{E}^{[0,T]}$, *Legendre–Fenchel transform of* g
- $f(\mu\,\dot{x})=f(0)+\mu f^1(\dot{x})+f^2(\mu\,\dot{x})$ *with* $\mu\geqslant 0$ $\lim_{\mu\to 0^+}\dfrac{f^2(\mu\,\dot{x})}{\mu}=0$
- $F(\cdot)=\int_\Omega f(\cdot)\,\mathrm{d}\Omega,\quad 1=\dfrac{[[E^h_{\mathrm{CRE}}]^2-[E^h_{\mathrm{CRE},m}]^2]}{F^2(\overline{\mu}\dot{\tilde{a}}_h)}$ (20)

An alternative consists in using the Legendre–Fenchel transform for the dissipation bilinear form written at $(t,\underline{M})\in[0,T]\times\Omega$. *This bound is similar and easier to obtain, but it is less effective. Another option is to work globally over* $[0,T]\times\Omega$.

Let be: $I_2\equiv\boldsymbol{C}(s_{\mathrm{ex}}-s_h,\delta\tilde{s}_\Sigma)-\boldsymbol{C}(s_{\mathrm{ex}}-s_h,\delta\hat{s}_h)$.
There are several means of deriving bounds of I_2. Let us introduce: $g_\Delta(\Delta s)\equiv g(\Delta s+\hat{s}_{h,m}-s_h)$ and define analytically, or at least numerically:

$$f_\Delta(\dot{a},-b)=\sup_{\substack{\Delta s\in\mathcal{F}^{[0,T]}\\ \Delta\dot{e}_p=\widetilde{\boldsymbol{B}}(\Delta s)}}\int_0^T\big[\Delta s\cdot\dot{a}-\Delta\dot{e}_p\cdot b-g_\Delta(\Delta s)\big]\,\mathrm{d}t \tag{21}$$

Writing $F_\Delta(\mu\delta\dot{\tilde{a}},-\mu\delta\tilde{b})=F_\Delta(0,0)+\mu F^1_\Delta(\delta\dot{\tilde{a}},-\delta\tilde{b})+F^2_\Delta(\mu\delta\dot{\tilde{a}},-\mu\delta\tilde{b})$, the following bound can be proved:

$$I_2\leqslant\big[\big[E^h_{\mathrm{CRE}}\big]^2-\big[E^h_{\mathrm{CRE},m}\big]^2\big]^{1/2}\big[F^2_\Delta(\overline{\mu}\delta\dot{\tilde{a}},-\overline{\mu}\delta\tilde{b})\big]^{1/2}+F^1_\Delta(\delta\dot{\tilde{a}},-\delta\tilde{b}),\quad 1=\frac{[[E^h_{\mathrm{CRE}}]^2-[E^h_{\mathrm{CRE},m}]^2]}{F^2_\Delta(\overline{\mu}\delta\dot{\tilde{a}},-\overline{\mu}\delta\tilde{b})} \tag{22}$$

F_Δ is small if the finite variations Δs and δs are small. A similar technique can be derived to get a strict lower bound.
Finally, we obtain a strict upper bound of $|\alpha_{\mathrm{ex}}-\alpha_h-\alpha_{hh}|$.

5. Conclusion

We derived a strict upper bound of the error in an output of interest for standard material models with convex properties. This bound requires the resolution of a small local problem in space defined over the time interval being studied, i.e., the calculation of the pseudo Legendre–Fenchel transform of g, f_Δ. This can be achieved analytically or, at least, numerically. Let us note that no properties of the finite element solutions are used in the process; therefore, other computational methods could be considered.

Unilateral contact with friction should also lend itself to this error framework.

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