A non-intrusive approach to get strict and sharp error bounds on local FE quantities for evolution problems

Abstract In this work, we set up a non-intrusive procedure that yields for strict and high-quality error bounds of quantities of interest in linear evolution problems solved by means of the Finite Element Method (FEM). The non-intrusive feature is achieved by introducing, via a partition of unity, enrichment functions in the solution of the adjoint problem (handbook techniques). The resulting goal-oriented error estimation method is thus easy to implement in a FE code and enables to consider truly pointwise quantities of interest.

Key words: Verification, Local error, Strict bounds, Handbook techniques, Pointwise quantities of interest.

1 Introduction

In the widespread numerical simulations carried out nowadays, a major concern remains the control of the quality of the numerical solutions obtained through approximate methods. Today, research intensely focuses on goal-oriented error estimation, i.e. assessment of the error on local quantities which are relevant for design purposes. The most accomplished works deal with linear static problems and give effective local error bounds [1, 2]. However, very few works on the subject are dedicated to evolution and non-linear problems; furthermore these usually lead to bounds which lack reliability because they are not guaranteed and/or not sharp, which is a serious drawback for robust design. In the framework of linear viscoelasticity problems described through internal variables and solved with the Finite Element Method (FEM), we introduced in [3] a method that yields for strict and effective error bounds on local quantities. This method leans on classical extraction techniques (leading to the solution of an adjoint problem), the concept of dissipation error and convexity properties. It takes history effects into account and may lead to very sharp error bounds provided that the adjoint problem is solved accurately. A simple but intrusive way of reaching such an accurate solution consisted in a local refinement of the time/space mesh being used for the adjoint problem.

In this paper, we go a step further by setting up a non-intrusive procedure to solve the adjoint problem precisely, in the sense that we keep unchanged the discretization parameters (mesh, operators) defined for the reference (or primal) problem [4]. We use for that handbook techniques [5] that consist in introducing enrichment functions via the Partition of Unity Method (PUM) when solving the adjoint problem with the FEM. These functions correspond to locally (quasi-)exact solutions of the adjoint problem; they are computed analytically or numerically in a (semi-)infinite domain. As a result, we get high-quality error bounds at reasonable cost without any remeshing. Furthermore, the method enables to consider truly pointwise quantities of interest in space and time by using as enrichment functions the well-known and possibly infinite energy Green functions.

2 Reference problem and dissipation error

We consider the structure Ω, with boundary ∂Ω, given in Fig. 1. It is subject over the time interval [0, T] to prescribed time-dependent mechanical solicitations (U_d, f_d, F_d).

Figure 1: Structure and its environment (left) and rheological model used (right).

We choose a material with a linear viscoelastic behavior defined by the generalized Maxwell model. Such a
material model can be easily described by means of the generalized internal variables \((n\text{-vectors}):\)

\[
s = \begin{bmatrix} \sigma_1 \\ \vdots \\ \sigma_n \end{bmatrix} \quad e^c = \begin{bmatrix} e_1^c \\ \vdots \\ e_n^c \end{bmatrix} \quad e^p = \begin{bmatrix} e_1^p \\ \vdots \\ e_n^p \end{bmatrix} \quad e = e^c + e^p
\]

where \(e^c_i\) and \(e^p_i\) are respectively the elastic and anelastic part of the total strain \(e_i = \epsilon(y)\) in the spring/damper set \(i\) (Fig. 1), whereas \(\sigma_i\) are the dual variables related to the Cauchy stress tensor \(\sigma\) by \(\sum_i \sigma_i = \sigma\). Under the assumptions of quasi-static, isothermal and small perturbations state, the reference problem consists in finding a solution \((e, s)\) that verifies the compatibility equations, the equilibrium equations, the initial conditions, and the constitutive relations which are split into two parts

\[
\begin{aligned}
e^c &= \Lambda(s) \quad \text{and} \quad \sum_{i=1}^n \sigma_i = \sigma \quad \text{(state equations)} ;
\end{aligned}
\]

\[
\begin{aligned}
\dot{e}^p &= B(s) \quad \text{(evolution laws).}
\end{aligned}
\]

The exact solution of the reference problem, denoted by \((e_{ex}, s_{ex})\), can not usually be reached. We thus compute an approximate solution of the problem, denoted by \((\tilde{e}_h, \tilde{s}_h)\), using the FEM associated to a backward-Euler scheme. Therefore, we define the discretization error \(E_{\text{diss}}\) is then a global measurement of the non-verification, for a given admissible solution \((\tilde{e}_h, \tilde{s}_h)\), of the evolution laws:

\[
E_{\text{diss}}^2(\tilde{e}_h, \tilde{s}_h) = \frac{1}{2} \int_0^T \int_{\Omega} \sum_{i=1}^n \sigma_i \epsilon_i \dot{\Sigma} \cdot (\dot{\tilde{e}}_h - B(\tilde{s}_h)) \cdot B^{-1} (\dot{\tilde{e}}_h - B(\tilde{s}_h)) \, d\Omega \, dt.
\]

The time function \(a(t)\), which is positive over \([0, T]\), enables to get a weighted dissipation error that takes the history effects encountered in evolution problems into account [3]. A first property of \(E_{\text{diss}}(\tilde{e}_h, \tilde{s}_h)\) is that it represents a global discretization error estimator which accounts for all sources of error (time and space discretizations in our case). Another property, which is the true engine to get strict local error bounds, is the link between \(E_{\text{diss}}(\tilde{e}_h, \tilde{s}_h)\) and the exact solution \((e_{ex}, s_{ex})\); it is on the form \(G(s_{ex} - \tilde{s}_h) = E_{\text{diss}}^2(\tilde{e}_h, \tilde{s}_h)\) where \(G\) is a given functional based on free energy and pseudo-potentials of dissipation.

3 The non-intrusive goal-oriented error estimation method

The first step consists in writing the considered quantity of interest \(I\) in a global form:

\[
I = \int_0^T \int_{\Omega} \sum_{i=1}^n \text{Tr}[\sigma_i \epsilon_i \dot{\Sigma}] \, d\Omega \, dt = \langle \langle s, \dot{\hat{s}}_{\Sigma} \rangle \rangle = -\langle \langle \hat{e}, \dot{\hat{s}}_{\Sigma} \rangle \rangle.
\]

The \(n\)-vectors \(\dot{\hat{s}}_{\Sigma}\), known analytically, represent the extraction function. Following the procedure described in [7], we then define a new problem, called adjoint problem, which is reverse in time but remains similar to the reference problem except that the loading now consists in the prestress \(\dot{\hat{s}}_{\Sigma} = \sum_{i=1}^n \dot{\Sigma}_i\). In the same way as for the reference problem, we compute a FE solution \((\tilde{e}_h, \tilde{s}_h)\) and an admissible solution \((\hat{e}_h, \hat{s}_h)\) for the adjoint problem. Note that the time/space mesh used to solve the adjoint problem can be chosen independently from the one defined for the reference problem. The following result thus yields (technical details can be found in [3]):

\[
|I_{ex} - I_h - I_{hh}| \leq 2 \left( \frac{1}{2} E_{\text{diss}}^2(\tilde{e}_h, \tilde{s}_h) + F_0(\Delta_h) \right)^{\frac{1}{2}} \left( F_2(\tilde{\hat{e}}_h) \right)^{\frac{1}{2}}
\]

where \(I_{ex}\) (resp. \(I_h\)) is the unknown exact value (resp. FE value) of the quantity of interest \(I\), \(I_{hh}\) is a correction term computed from the approximate solutions of both reference and adjoint problems, \(F_0\) and \(F_2\) are some functions known analytically, \(\Delta_h\) is a computable term that is not explicit, and \(\hat{\Delta}_h = -B(\hat{s}_h) - \hat{e}_h\). As a result, we obtain from (4) some strict bounds \(\xi_{inf}\) and \(\xi_{sup}\) of \(I_{ex}\), and \(I_h + I_{hh}\) can be viewed as a new approximation of \(I_{ex}\). Bounds \(\xi_{inf}\) and \(\xi_{sup}\) are sharp provided that term \(F_2(\hat{\Delta}_h)\)
is small enough, i.e. when the adjoint problem is solved correctly. This can be reached by refining locally the time/space mesh used to solve the adjoint problem. However, this intrusive technique may lead to large modifications in a FE code and requires high computational costs due to the fact that the solution of the adjoint problem usually presents high gradients in some localized zones of the domain $[0, T] \times \Omega$.

We propose here a procedure based on the handbook techniques developed in [5]. It consists in introducing enrichment functions, via the Partition of Unity Method (PUM), in the set of basis functions describing the approximate displacement field of the adjoint problem. The enrichment functions are singular solutions $(\tilde{\varphi}^\text{hand}, \tilde{\psi}^\text{hand})$ of the adjoint problem loading over an infinite (or semi-infinite) domain; they are usually computed analytically in time and numerically in space and constitute a library of pre-calculated solutions.

Therefore,  

$$\tilde{\mathbf{u}} = \sum_{j=1}^{n_{\text{no}}^\text{PUM}} \psi_j \tilde{\varphi}^\text{hand}_j + \tilde{\mathbf{u}}^r$$

where $\psi_j$ is the classical FE shape function associated to node $j$, $n_{\text{no}}^\text{PUM}$ is the total number of nodes enriched by the PUM and $\tilde{\mathbf{u}}^r$ is a displacement field to be calculated. Note that the degrees of freedom associated to the PUM are known i.e. the enrichment is entirely determined; only the field $\tilde{\mathbf{u}}^r$ is unknown. The total solution then reads $(\tilde{\varphi}, \tilde{\psi}) = (\tilde{\varphi}^\text{PUM}, \tilde{\psi}^\text{PUM}) + (\tilde{\varphi}^r, \tilde{\psi}^r)$. It is composed of two terms: an enrichment term $(\tilde{\varphi}^\text{PUM}, \tilde{\psi}^\text{PUM})$ which locally equilibrates the loading of the adjoint problem but which does not verify all the boundary conditions on $\partial \Omega$: a FE term $(\tilde{\varphi}^r, \tilde{\psi}^r)$ which can be seen as a residual solution and that enables to verify all the boundary conditions on $\partial \Omega$.

The new problem we thus have to solve consists in finding the residual solution $(\tilde{\varphi}^r, \tilde{\psi}^r)$. It retains the same structure as the original adjoint problem except that the loading is much more regular. Due to the smoothness of the residual solution $(\tilde{\varphi}^r, \tilde{\psi}^r)$, we can compute an accurate approximate solution $(\hat{\varphi}^r, \hat{\psi}^r)$ using the FEM with the same time/space discretization as the one used for the reference problem. The method is called non-intrusive in this sense: we reuse the operators (factorized stiffness matrix, ...) of the reference problem and only the force vector has to be changed. Practically, the adjoint problem is solved in the same time as the reference problem. Eventually, we get an approximate solution $(\hat{\varphi}^r, \hat{\psi}^r)$ of the adjoint problem, such that $(\hat{\varphi}^r, \hat{\psi}^r) = (\tilde{\varphi}^\text{hand}, \tilde{\psi}^\text{hand}) + (\tilde{\varphi}^r, \tilde{\psi}^r)$. After computing an admissible residual solution $(\tilde{\varphi}^\text{hand}, \tilde{\psi}^\text{hand})$, the bounding result (4) holds with $\tilde{\varphi}^r = B(\hat{\psi}^r) - \tilde{\varphi}^r$ due to the fact that the evolution laws are verified by the handbook solutions. As regards term $I_{hh}$ involved in (4), it is calculated using overintegration.

The extension of the non-intrusive method to pointwise in space quantities of interest is straightforward. Indeed, the associated handbook functions correspond in that case to the well-known Green functions. One can introduce such functions, even though they are infinite-energy, into the approximate solution of the adjoint problem as they do not appear in the expression of the upper bound given in (4). The Green functions are here calculated analytically in space and time, using techniques based on strain nuclei and the image method (see [8] for details). An example of such a Green function is given in Fig. 2.

![Figure 2](image.png)

Figure 2: Spatial distribution of the stress field corresponding to a pointwise prestress loading over a 2D infinite domain: $\hat{\sigma}_{xx}^\text{hand}$ (left), $\hat{\sigma}_{yy}^\text{hand}$ (center), $\hat{\sigma}_{xy}^\text{hand}$ (right).

However, as the FE value $I_h$ of a pointwise quantity at some point $P$ within $\Omega$ is not always defined (due to possible discontinuities of the derivatives across element boundaries), we recast (4) into the form:

$$|I_{ex} - \hat{I}_h - \hat{I}_{hh}| \leq 2\left[\frac{1}{2} E_{\text{dis}}^2 (\hat{\varphi}^r, \hat{\psi}^r) + F_0(\Delta_h)\right]^{\frac{1}{2}} \cdot \left|F_2(\hat{x}_h)\right|^{\frac{1}{2}}$$

(5)

where $\hat{I}_h$ and $\hat{I}_{hh}$ are some quantities defined at any regular point $P$ using the admissible solution $(\hat{\varphi}^r, \hat{\psi}^r)$. 


Therefore, (5) provides some strict and guaranteed bounds of the exact value $I_{ex}$ of a pointwise quantity, such as a component of displacement or stress at a point.

## 4 Numerical results

We consider a L-shaped structure clamped at its base and subject to a prescribed displacement $U_{d}(t)$ along its upper right edge (Fig. 3). We assume plane stress state and take a Maxwell rheological model composed of three spring/damper sets. The FE solution is obtained by discretizing the structure spatially with 100 linear quadrangle elements and dividing the time interval $[0, T]$ ($T = 20$ s) into 20 time steps. We deal with the quantity of interest:

$$I = \dot{\epsilon}_{yy}^{p}(P)_{T}$$

where $P$ is a point that lies within an element of the mesh (Fig. 3).

![Figure 3: The structure being considered (left), its loading (center), and location of point P (right).](image)

Let us note that the calculation of $I_{ex}$, used as the reference value, is performed using a "quasi-exact" solution obtained by means of a very refined FE mesh ("overkill solution"). The loading of the associated adjoint problem consists of a prestress $\tilde{\sigma}_{\Sigma}$ at point $P$ in the form $\tilde{\sigma}_{\Sigma}(t)\delta(P)$. Evolution of $\tilde{\sigma}_{\Sigma}(t)$ is given in Fig. 4.

![Figure 4: Evolution of $\tilde{\sigma}_{\Sigma}$ with respect to time (left), nodes involved in the enrichment through the PUM (center), and definition of zone $\omega$ (right).](image)

The analytical enrichment functions we use, taking traction-free boundary conditions into account, are similar to those given in Fig. 2; they represent the exact solution of the adjoint problem loading over a semi-infinite domain. They are introduced in the approximate solution of the adjoint problem through the PUM applied at specific nodes of the mesh i.e. nodes close to the zone of application of the adjoint problem loading (these nodes are circled in Fig. 4). We then get the following bounds:

$$\bar{\xi}_{inf} = \frac{\xi_{inf}}{I_{ex}} = 0.96 \quad \bar{\xi}_{sup} = \frac{\xi_{sup}}{I_{ex}} = 1.04.$$  

which shows that the non-intrusive method is very effective and enables to obtain accurate bounds of localized quantities through the enrichment of only a few nodes of the space mesh (due to St-Venant principle).

In addition, one can seek lower and upper bounds of $I_{ex}(P)$ for any point $P$ within a specific local zone of interest $\omega \subset \Omega$ (Fig. 4). The procedure consists in sweeping zone $\omega$ and considering that the residual
solution $(\tilde{r}_h^e, \tilde{s}_h^e)$ of the adjoint problem does not depend on the localization of $P$ over $\omega$ (practically, this is verified if the enrichment zone is sufficiently large). Thus only the handbook function has to be changed when sweeping over $\omega$, and the following result yields:

$$| I_{ex}(P) - \hat{I}_h(P) - \hat{I}_{hh}(P) | \leq 2 \left[ \frac{1}{2} E^2_{diss}(\tilde{r}_h, \tilde{s}_h) + F_0(\Delta h) \right]^{\frac{1}{2}} \forall P \in \omega$$

The method provides the following bounds for the extremum $I_{ex}^{\max, \omega}$ of $I_{ex}$ over $\omega$:

$$\tilde{\xi}_{\text{inf}}^\omega = \frac{\xi_{\text{inf}}^\omega}{I_{ex}^{\max, \omega}} = 0.95 \quad \tilde{\xi}_{\text{sup}}^\omega = \frac{\xi_{\text{sup}}^\omega}{I_{ex}^{\max, \omega}} = 1.05$$

As a result, we are able to obtain high-quality lower and upper bounds for the extremum of $I_{ex}$ (or $L^\infty$-norm of $I_{ex}$) over a given zone, which constitutes useful information for design purposes.

5 Conclusion

We presented in this paper a method that provides for strict and high-quality error bounds of local quantities in linear viscoelasticity problems. It is made non-intrusive due to the fact that by using handbook techniques, the adjoint problem is solved precisely while keeping unchanged the discretization parameters and operators defined for the reference problem; only the loading has to be changed. As a result, the bounding process appears in a "black-box" manner for the analyst/designer whose only intervention consists in defining the quantity of interest. Furthermore, the non-intrusive technique enables one to easily tackle pointwise quantities by using Green’s functions. Several numerical tests in 2D and 3D clearly illustrated the interest and efficiency of the proposed method.

In summary, this work demonstrates that reliable local error bounds can be obtained at reasonable cost for linear evolution problems, a fact which was not really accepted by the scientific community until now. It should be mentioned that the goal-oriented error estimation method proposed here does not use the orthogonality properties of the FE solutions. Therefore, it could conceivably be applied to problems solved by approximate methods other than the FEM; it could moreover be applied to other linear parabolic problems. A forthcoming work will consist in extending this approach for dynamics, viscoplasticity and in the nonlinear regime including friction.

References


