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CONSTRUCTION OF ADMISSIBLE FIELDS AND GOAL-ORIENTED ERROR ESTIMATION: PERFORMANCES ON ENGINEERING EXAMPLES

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Abstract. Nowadays, a major interest in research activities concerns methods that aim at providing a reliable mean to control and assess the numerical quality of specific quantities, i.e. strict and accurate local error bounds. A general method for robust goal-oriented error estimation relies on the concept of constitutive relation error (CRE), associated to admissible stress fields and classical extraction techniques. This paper first deals with the comparison between different techniques used for constructing admissible stress fields, which are usually required in methods providing for robust global/goal-oriented error estimation. In this work, a new hybrid technique, called the *element equilibration + star-patch technique* (EESPT), is compared with the two other main existing techniques, namely the *element equilibration technique* (EET), and the *star-patch equilibration technique* (SPET) in terms of quality of associated error estimates, computational cost and simplicity of practical implementation into existing finite element codes. Besides, an enhanced version of the EESPT method has been revisited and demonstrates its relevance to produce sharper estimators. In a second part, we analyze goal-oriented error estimators constructed from the CRE. Two- and three-dimensional numerical experiments are carried out to investigate the performance of each estimator for the calculation of guaranteed error bounds on specific quantities of interest.

1 INTRODUCTION

The growing interest in the use of numerical simulation has intensively spurred the development of practical and efficient tools allowing to assess the quality of numerical approximate solutions obtained through the finite element method (FEM). First research works dealt with the development of effective global error estimation methods, providing an appraisal of the global measure of the discretization error by means of global energy

norms [1]. From now on, both researchers and engineers are motivated by the desire to evaluate numerical quality of specific quantities of practical interest, which are relevant for industrial decision making and certification. Various goal-oriented error estimation methods have been emerging for few years, applied to both linear and non-linear problems.

Nevertheless, only a few error estimators lead to robust and relevant error estimates ensuring the recovery of strict upper bounds of the exact error both for global or goal-oriented estimation. Such error estimators are currently based on the post-processing of the FE solution to build an admissible one. More precisely, a complex and key task concerns the derivation of a statically admissible stress field, whose construction relies on recovery techniques. A first technique relies on a dual formulation of the reference problem, which can be brought back to the calculation of another global solution of the reference problem leading straightforwardly to an admissible stress field. Despite its remarkable accuracy, this technique is not appropriate for error estimation, as it requires the use of a completely different formulation involving a costly global computation. A second technique, called the *element equilibration techniques* (EET) [1, 2], is based on the computation of equilibrated tractions through the use of an energetic relation, called prolongation condition, prior to the calculation of a statically admissible stress field through the fine resolution of problems defined at the element scale. Despite its affordable computational cost, this method is reckoned to be difficult to implement into a standard FE framework. A third technique, called the *star-patch equilibration technique* (SPET) [3], alleviates this difficulty since it relies on the partition of unity concept and, hence, leads to the fine resolution of self-balanced problems defined over stars or patches of elements, resulting in a higher computational cost. However, the practical implementation of this flux-free method is facilitated, as it does not require any flux-equilibration procedure. Eventually, the recently introduced and last technique, called the *element equilibration + star-patch technique* (EESPT) [2, 4], is an hybrid technique, as it benefits from components of both EET and SPET methods. Hence, this technique tends to be a fairly good trade-off between easiness of implementation, computational cost and quality of the error estimate. In this work, we aim at comparing performances of those classical balance techniques on industrial numerical examples. Besides, an enhanced version of the construction of equilibrated tractions involved in the EET and EESPT methods extends ideas first tackled in [5] in order to improve the set of balanced tractions in local regions. It consists in the local minimization of the complementary energy through a weakened prolongation condition in order to improve the quality of equilibrated tractions. The major breakthrough is the introduction of geometric and error criteria to define specific zones for optimizing the tractions, with the objective to obtain sharper bounds without noticeably increasing the computational cost.

As regards robust goal-oriented error estimation, a general method, initially developed in [6], has been prone to considerable developments. This technique, based on classical and powerful tools, such as extraction techniques and, more recently, handbook techniques and projection procedures [7], provides high-quality local error bounds on specific quantities

of interest. It also requires the resolution of an auxiliary problem, often referred to as dual (or adjoint) problem, involving extraction operators (or extractors). The resulting bounds are defined by means of two global error estimates with respect to the energy norm of the (quasi-)exact discretization error of reference and adjoint problems, respectively. An overview of the main features of this method is presented in this work.

The paper is organized as follows. Section 2 presents basics on error estimation in order to introduce the concept of admissible solution. Section 3 describes the main features of the three equilibration techniques which are considered to set up admissible stress fields; it particularly focuses on the new hybrid technique EESPT. Section 4 deals with the enhanced version of the EESPT technique, while Section 5 presents the key aspects of the goal-oriented error estimation based on extraction techniques. Section 6 shows numerical results on two- and three-dimensional applications.

2 BASICS ON ERROR ESTIMATION AND ADMISSIBLE SOLUTIONS

2.1 The reference problem and associated discretization error

Let us consider a mechanical structure represented by an open bounded domain Ω, with boundary $\partial\Omega$. The prescribed volume and surface mechanical solicitations acting on structure Ω are: a displacement field $\underline{U}_d$ on part $\partial_1\Omega \neq \varnothing$; a traction force density $\underline{F}_d$ on the complementary part $\partial_2\Omega$ of $\partial\Omega$ such that $\overline{\partial_1\Omega \cup \partial_2\Omega} = \partial\Omega$, $\partial_1\Omega \cap \partial_2\Omega = \varnothing$; a body force field $\underline{f}_d$ within Ω. Structure Ω is composed of an isotropic, homogeneous material with linear and elastic behavior characterized by Hooke's tensor $\boldsymbol{K}$. Given a quasi-static loading, an isothermal case and a small perturbations state, the reference mechanical problem consists in finding a displacement/stress pair $(\underline{u},)$ in the space domain Ω, which verifies:

- the kinematic conditions: $\underline{u} \in \boldsymbol{\mathcal{U}}$; $\quad \underline{u}_{|\partial_1\Omega} = \underline{U}_d$; $\quad (\underline{u}) = \dfrac{1}{2}\big(\nabla(\underline{u}) + \nabla^T(\underline{u})\big)$; $\qquad (1)$
- the equilibrium equations: $\quad \in \boldsymbol{\mathcal{S}}$;

$$\forall\, \underline{u}^* \in \boldsymbol{\mathcal{U}}_0, \quad \int_\Omega \mathrm{Tr}\left[\ (\underline{u}^*)\right] \mathrm{d}\Omega = \int_\Omega \underline{f}_d \cdot \underline{u}^* \,\mathrm{d}\Omega + \int_{\partial_2\Omega} \underline{F}_d \cdot \underline{u}^* \,\mathrm{d}S; \qquad (2)$$

- the constitutive relation: $\quad (M) = \boldsymbol{K}\left(\underline{u}(M)\right) \quad \forall\, M \in \Omega, \qquad (3)$

where $(\underline{u})$ represents the classical linearized strain tensor corresponding to the symmetric part of the gradient of displacement field $\underline{u}$. Affine spaces $\boldsymbol{\mathcal{U}} = \{\underline{u} \in [\mathcal{H}^1(\Omega)]^3\}$ and $\boldsymbol{\mathcal{S}} = \{\ \in \mathcal{M}_s(3) \cap [\mathcal{L}^2(\Omega)]^6\}$ guarantee the existence of finite-energy solutions, $\mathcal{M}_s(n)$ representing the space of symmetric square matrices of order n. $\boldsymbol{\mathcal{U}}_0 \subset \boldsymbol{\mathcal{U}}$ denotes the vectorial space associated to $\boldsymbol{\mathcal{U}}$.

In practical applications, the exact solution of the reference problem, hereafter denoted $(\underline{u},)$, remains usually out of reach and only an approximate solution, referred to as $(\underline{u}_h, _h)$, can be obtained through numerical approximation methods (such as the finite element method (FEM) associated with a space mesh $\mathcal{M}_h$ mapping physical domain Ω). Such a numerical approximation is sought in a discretized space $\boldsymbol{\mathcal{U}}_h \times \boldsymbol{\mathcal{S}}_h \subset \boldsymbol{\mathcal{U}} \times \boldsymbol{\mathcal{S}}$. A

displacement-type FEM leads to a displacement field $\underline{u}_h$ verifying kinematic constraints (1), while a stress field $_h$ can be derived from the constitutive relation (3). The resulting discretization error, denoted $\underline{e}_h = \underline{u} - \underline{u}_h$, can be measured by means of the classical energy norm $\|\bullet\|_{u,\Omega} = \left(\int_\Omega \mathrm{Tr}\left[\boldsymbol{K}\left(\bullet\right)\left(\bullet\right)\right] \mathrm{d}\Omega\right)^{1/2}$, providing a global discretization error $\|\underline{e}_h\|_{u,\Omega}$. Besides, local measures defined with respect to a specified quantity of interest $I(\underline{u})$ of the problem enable one to capture local errors $e_h^{\mathrm{loc}} = I(\underline{u}) - I(\underline{u}_h)$.

2.2 The construction of an admissible solution

Verification research activities focus on the setting up of robust error estimation methods. The construction of what is called an "admissible solution" is currently an essential and key step in order to obtain guaranteed error bounds. An admissible pair $(\underline{\hat{u}}_h, \hat{}_h)$ verifies all the equations of the reference problem, apart from constitutive relation (3). On the one hand, a kinematically admissible displacement field is generally obtained by taking merely $\underline{\hat{u}}_h$ equal to $\underline{u}_h$. On the other hand, the derivation of a statically admissible stress field can be achieved by using various techniques. Such an admissible stress field $\hat{}_h$ can be deduced from the data and the FE stress field $_h$ alone. Section 3 focuses on the key points of the three existing techniques suitable to error estimation, namely the *element equilibration technique* (EET), the *star-patch element technique* (SPET) and the *element-equilibration + star-patch technique* (EESPT). Starting from an admissible solution $(\underline{\hat{u}}_h, \hat{}_h)$ provided by one of the previously mentioned balance techniques, one can measure the residual on constitutive relation (3), called the constitutive relation error (CRE) and hereafter referred to as $e_{\mathrm{cre}}(\underline{\hat{u}}_h, \hat{}_h) = \|\hat{}_h - \boldsymbol{K}\left(\underline{\hat{u}}_h\right)\|_{,\Omega}$, with $\|\bullet\|_{,\Omega} = \left(\int_\Omega \mathrm{Tr}\left[\bullet\ \boldsymbol{K}^{-1}\ \bullet\right] \mathrm{d}\Omega\right)^{1/2}$. Assessing the CRE $e_{\mathrm{cre}}(\underline{\hat{u}}_h, \hat{}_h)$ provides a guaranteed upper bound of the global discretization error $\|\underline{e}_h\|_{u,\Omega}$, as the well-known Prager-Synge theorem leads to the following bounding inequality:

$$\|\underline{e}_h\|_{u,\Omega}^2 = \|\underline{u} - \underline{\hat{u}}_h\|_{u,\Omega}^2 \leqslant \|\underline{u} - \underline{\hat{u}}_h\|_{u,\Omega}^2 + \| - \hat{}_h\|_{,\Omega}^2 = e_{\mathrm{cre}}^2(\underline{\hat{u}}_h, \hat{}_h), \tag{4}$$

which conveys the guaranteed nature of the CRE $e_{\mathrm{cre}}(\underline{\hat{u}}_h, \hat{}_h)$. Now, let us focus on the principles of the EET and SPET methods and the main aspects of the EESPT method.

3 TECHNIQUES FOR CONSTRUCTING ADMISSIBLE STRESS FIELDS

Let us define $\mathcal{E}$, $\mathcal{N}$, $\mathcal{I}$, $\mathcal{N} \setminus \mathcal{I}$ and $\mathcal{J}$ the set of elements, nodes, vertices, non-vertex nodes and edges of the FE mesh $\mathcal{M}_h$, respectively. $\mathcal{E}_\Gamma^{\mathcal{J}} \subset \mathcal{E}$ represents the set of elements connected to edge Γ, respectively. $\mathcal{J}_i^{\mathcal{I}} \subset \mathcal{J}$ represents the set of edges connected to vertex i. $\mathcal{N}_E^{\mathcal{E}} \subset \mathcal{N}$ and $\mathcal{N}_\Gamma^{\mathcal{J}} \subset \mathcal{N}$ stand for the set of nodes associated with element E and edge Γ, respectively. $\mathcal{I}_E^{\mathcal{E}} \subset \mathcal{I}$ and $\mathcal{I}_\Gamma^{\mathcal{J}} \subset \mathcal{I}$ designate the set of vertices connected to element E and edge Γ. $\mathcal{N}_E^{\mathcal{E}} \setminus \mathcal{I}_E^{\mathcal{E}} \subset \mathcal{N} \setminus \mathcal{I}$ denotes the set of non-vertex nodes connected to element E. Finally, the FE displacement field $\underline{u}_h$ is assumed to belong to the FE interpolation space $\boldsymbol{\mathcal{U}}_h^p$ of degree less than or equal to p. $\mathcal{U}_h^p$ corresponds to its one-dimensional correspondent.

3.1 The element equilibration technique EET - standard method

The first technique, called the *element equilibration technique* (*EET*), initially introduced by Ladevèze [1], uses the FE properties of the stress field $\underline{\sigma}_h$ through an energy relation, called *prolongation condition*, connecting the searched admissible stress field $\hat{\underline{\sigma}}_h$ to the FE stress field $\underline{\sigma}_h$ under the form:

$$\int_E (\hat{\underline{\sigma}}_h - \underline{\sigma}_h) \, \underline{\nabla} \varphi_i \, \mathrm{d}\Omega = \underline{0} \quad \forall \, E \in \mathcal{E}, \; \forall \, i \in \mathcal{N}_E^{\mathcal{E}}, \tag{5}$$

where $\varphi_i \in \mathcal{U}_h^p$ is the FE shape function associated with node i.

Classically, the EET can be decomposed into two stages: first, construction of tractions $\underline{\hat{F}}_h$ in equilibrium with the external loading $(\underline{F}_d, \underline{f}_d)$ on element boundaries ∂E of the spatial mesh $\mathcal{M}_h$; second, calculation of an admissible stress field $\hat{\underline{\sigma}}_h$ in equilibrium with these equilibrated tractions $\underline{\hat{F}}_h$ and body force field $\underline{f}_d$ at the element level:

$$\hat{\underline{\sigma}}_{h|E} \in \boldsymbol{\mathcal{S}}_{\underline{\hat{F}}_h} \quad \Longleftrightarrow \quad \begin{cases} \hat{\underline{\sigma}}_{h|E} \in \boldsymbol{\mathcal{S}} \\ \underline{\mathrm{div}} \, \hat{\underline{\sigma}}_{h|E} + \underline{f}_d = \underline{0} \quad \text{in } E \\ \hat{\underline{\sigma}}_{h|E} \, \underline{n}_E = \eta_E \, \underline{\hat{F}}_h \quad \text{on } \partial E \end{cases} \tag{6}$$

Tractions $\underline{\hat{F}}_h$ are intended to reproduce the stress vectors $\hat{\underline{\sigma}}_{h|E} \underline{n}_E$ on edges ∂E of element $E \in \mathcal{E}$: $\hat{\underline{\sigma}}_{h|E} \underline{n}_E = \eta_E \, \underline{\hat{F}}_h \quad \text{on} \, \partial E$, where $\underline{n}_E$ is the outgoing normal vector to element E and $\eta_E = \pm 1$ are functions ensuring the continuity of the stress vector across ∂E. Besides, these tractions $\underline{\hat{F}}_h$ are built in equilibrium with the external loading $(\underline{F}_d, \underline{f}_d)$.

The procedure for calculating tractions $\underline{\hat{F}}_h$ on the element edges of the mesh $\mathcal{M}_h$ is quasi-explicit in the following sense: first, prescribed constraints $\eta_E \, \underline{\hat{F}}_h = \underline{F}_d$ are enforced on $\partial E \subset \partial_2 \Omega$; second, prolongation condition (5) leads to local problems $\mathcal{P}_i^{\mathcal{N}}$ associated with each node $i \in \mathcal{N}$. Problem $\mathcal{P}_i^{\mathcal{N}}$ is a linear system, whose unknown quantities over edges $\Gamma \in \mathcal{J}_i^{\mathcal{I}}$ are projections $\underline{\hat{b}}_{|\Gamma}^{(i)}$ of traction $\underline{\hat{F}}_{h|\Gamma}$ over the FE shape function φ_i. The existence of solutions to problem $\mathcal{P}_i^{\mathcal{N}}$ follows from the FE equilibrium properties. In the case of multiple solutions of local problems $\mathcal{P}_i^{\mathcal{N}}$, the least-squares minimization of a cost function $J(\underline{\hat{b}}^{(i)})$ involving known quantities $\underline{b}_{|\Gamma}^{(i)}$, which are the projections of the FE stress vector $\underline{\sigma}_h \, \underline{n}$, over edges $\Gamma \in \mathcal{J}_i^{\mathcal{I}}$, on the FE shape function φ_i, is performed to ensure uniqueness of the solution. Eventually, force fluxes $\underline{\hat{F}}_{h|\Gamma}$ are sought along each edge $\Gamma \in \mathcal{J}$ in the FE space $\boldsymbol{\mathcal{U}}_{h|\Gamma}^p$ and are recovered from the projections $\underline{\hat{b}}_{|\Gamma}^{(i)}$ associated to each node $i \in \mathcal{N}_\Gamma^{\mathcal{J}}$ by merely solving a set of linear local problems defined over each edge $\Gamma \in \mathcal{J}$.

Afterwards, the construction of such balanced tractions allows to seek the local restriction $\hat{\underline{\sigma}}_{h|E}$ of an admissible stress field $\hat{\underline{\sigma}}_h$ to each element $E \in \mathcal{E}$ as the solution of a self-equilibrated local problem $\mathcal{P}_E^{\mathcal{E}}$ (6), for which the pre-computed tractions $\underline{\hat{F}}_{h|\partial E}$ and body force field $\underline{f}_{d|E}$ act as prescribed external loading over each element $E \in \mathcal{E}$. Although the resolution of problem (6) was originally performed analytically by searching the admissible stress field in a piecewise polynomial basis [1], numerical methods, such as

the displacement-type FEM combined with a p-refinement or h-refinement technique, are henceforth employed to achieve an accurate approximation of the exact strictly admissible stress field. The p-approach with an additional degree $k = 3$ is commonly favored to solve numerically local problems (6), as it commonly provides quasi-admissible stress fields leading to accurate error bounds.

In spite of its affordable computational cost, the EET faces a major drawback related to its difficult and complex implementation inherent to the construction of equilibrated tractions.

3.2 The star-patch equilibration technique SPET - flux-free method

The second technique, called the *star-patch equilibration technique* (*SPET*), originally introduced in the field of fluid mechanics, has been adapted to solid mechanics by Parés, Díez and Huerta [3] under the name *flux-free technique*. This technique gets around the need of flux-equilibration procedure, resulting in an implementation easier than the first technique. Its specificity is the introduction of a partition of unity leading to the resolution of self-equilibrated local problems defined on sets of elements, also called *patches* or *stars*.

Starting from equilibrium equations (2) and replacing $\underline{u}$ by $\underline{e}_h + \underline{u}_h$, one obtains the global problem defining the discretization error $\underline{e}_h = \underline{u} - \underline{u}_h$ that reads: Find $\underline{e}_h \in \boldsymbol{\mathcal{U}}_0$ such that:

$$\begin{aligned}\int_\Omega \mathrm{Tr}\left[\boldsymbol{K}\left(\underline{e}_h\right)\left(\underline{u}^*\right)\right]\mathrm{d}\Omega &= -\int_\Omega \mathrm{Tr}\left[\boldsymbol{K}\left(\underline{u}_h\right)\left(\underline{u}^*\right)\right]\mathrm{d}\Omega + \int_\Omega \underline{f}_d \cdot \underline{u}^*\,\mathrm{d}\Omega + \int_{\partial_2\Omega} \underline{F}_d \cdot \underline{u}^*\,\mathrm{d}S \\ &= \mathcal{R}_h(\underline{u}^*) \quad \forall\, \underline{u}^* \in \boldsymbol{\mathcal{U}}_0, \end{aligned} \tag{7}$$

where $\mathcal{R}_h$ represents the weak residual functional associated with the FE approximation. This residual equation expresses the extent to which a numerical solution fails to verify the the FE equilibrium equations.

Introducing the partition of unity, defined by the linear FE shape functions $\lambda_i \in \mathcal{U}_h^1$ based on vertices $i \in \mathcal{I}$, into (7) leads to the definition of a set of local problems defined over patches Ω_i of elements surrounding each vertex $i \in \mathcal{I}$: Find $\underline{e}_i \in \boldsymbol{\mathcal{U}}_{0|\Omega_i}$ such that:

$$\int_{\Omega_i} \mathrm{Tr}\left[\boldsymbol{K}\left(\underline{e}_i\right)\left(\underline{u}^*\right)\right]\mathrm{d}\Omega = \mathcal{R}_h(\lambda_i\,\underline{u}^*) \quad \forall\, \underline{u}^* \in \boldsymbol{\mathcal{U}}_{0|\Omega_i}, \tag{8}$$

where $\boldsymbol{\mathcal{U}}_{0|\Omega_i}$ is the restriction of $\boldsymbol{\mathcal{U}}_0$ to patch Ω_i: $\boldsymbol{\mathcal{U}}_{0|\Omega_i} = \left\{\underline{u}^* \in \boldsymbol{\mathcal{U}}_{|\Omega_i}, \underline{u}^*_{|\partial_1\Omega\cap\Omega_i} = \underline{0}\right\}$.

Solvability and well-posedness of problems (8) is ensured by the introduction of projector $\Pi : \boldsymbol{\mathcal{U}}_0 \to \boldsymbol{\mathcal{U}}_{h,0}^1$ onto linear FE space $\boldsymbol{\mathcal{U}}_{h,0}^1$ into the right-hand side term of (8), especially for an interpolation degree $p = 1$ (see [2] for full details). Replacing the r.h.s term by $\mathcal{R}_h(\lambda_i\,(\underline{u}^* - \Pi\underline{u}^*))$ into (8) before using the well-known Galerkin orthogonality property leads to a new set of local problems $\mathcal{P}_i^{\mathcal{I}}$ over each patch Ω_i in the form: Find $\underline{e}_i \in \boldsymbol{\mathcal{U}}_{0|\Omega_i}$ such that:

$$\int_{\Omega_i} \mathrm{Tr}\left[\boldsymbol{K}\left(\underline{e}_i\right)\left(\underline{u}^*\right)\right]\mathrm{d}\Omega = \mathcal{R}_h(\lambda_i\,(\underline{u}^* - \Pi\underline{u}^*)) \quad \forall\, \underline{u}^* \in \boldsymbol{\mathcal{U}}_{0|\Omega_i}. \tag{9}$$

Such local problems (9) defined at the patch scale are self-equilibrated, which constitutes a serious advantage for implementation purposes. In practice, the fine resolution of local problems (9) is performed using a classical displacement FEM along with a p-approach, i.e. using the original FE mesh $\mathcal{M}_h$ with a $p+3$ discretization over each patch Ω_i. Numerical solutions $\underline{e}_i$ of problems (9) allow to obtain both a global error estimate, which is a guaranteed upper bound of the energy norm of the discretization error, and an admissible stress field over each element $E \in \mathcal{E}$:

$$\|\underline{e}_h\|_{u,\Omega} \leqslant \left(\sum_{E\in\mathcal{E}} \left\| \sum_{i\in\mathcal{I}_E^{\mathcal{E}}} \underline{e}_{i|E} \right\|_{u,E}^2 \right)^{1/2} \quad ; \quad \hat{}_{h|E} = {}_{h|E} + \boldsymbol{K} \left(\sum_{i\in\mathcal{I}_E^{\mathcal{E}}} \underline{e}_{i|E} \right), \tag{10}$$

with $\|\bullet\|_{u,E} = \left(\int_E \mathrm{Tr}\left[\boldsymbol{K} \left(\bullet_{|E} \right) \left(\bullet_{|E} \right) \right] \mathrm{d}\Omega \right)^{1/2}$. Though rather accurate and simple, the SPET may present a serious drawback inherent to the high calculation cost of problem $\mathcal{P}_i^{\mathcal{I}}$ (9) for three-dimensional computations, as problems $\mathcal{P}_i^{\mathcal{I}}$ (9) are defined at the patch scale, contrary to problems $\mathcal{P}_E^{\mathcal{E}}$ (6) defined at the element scale.

3.3 The element equilibration and star-patch technique EESPT - hybrid method

This last technique, formerly studied in Ladevèze *et al* [2, 4], is a hybrid and appealing method in the sense that it takes advantage of the ingredients of both EET and SPET methods introduced in Section 1, namely the prolongation condition and partition of unity concept. Similarly to the EET method, the procedure to construct an admissible stress field is carried out in two main steps: first, construction of a set of tractions $\underline{\hat{F}}_h$ in equilibrium with the external loading $(\underline{F}_d, \underline{f}_d)$ on element edges ∂E of the spatial mesh $\mathcal{M}_h$; second, calculation of an admissible stress field $\hat{}_h$ solution of static local problems $\mathcal{P}_E^{\mathcal{E}}$ (6) over each element $E \in \mathcal{E}$ where the equilibrated tractions $\underline{\hat{F}}_h$ act as Neumann boundary conditions. The second stage is similar to that involved in the EET method. Therefore, we now focus on the key points related to the traction recovering step.

Given that the restriction of prolongation condition (5) to linear FE shape function $\lambda_i \in \mathcal{U}_h^1$ is sufficient to satisfy equilibrium condition between tractions and body force field, it can be reformulated in the global form; using then the weak form of the equilibrium equations satisfied by $\hat{}_h$ leads to:

$$\sum_{E\in\mathcal{E}} \left[\int_{\partial E} \eta_E \, \underline{\hat{F}}_h \cdot \underline{v}_h^* \, \mathrm{d}S - \int_E \left(\mathrm{Tr}\left[{}_h \left(\underline{v}_h^* \right) \right] - \underline{f}_d \cdot \underline{v}_h^* \right) \mathrm{d}\Omega \right] = 0 \quad \forall \, \underline{v}_h^* \in \boldsymbol{\mathcal{V}}_h^1. \tag{11}$$

where $\boldsymbol{\mathcal{V}}_h^1$ represents the space of piecewise linear polynomial functions which are continuous over each element $E \in \mathcal{E}$ and possibly discontinuous across the inter-element edges.

By using the partition of unity defined by the linear FE shape functions $\lambda_i \in \mathcal{U}_h^1$, let us now consider the following set of local problems $\mathcal{P}_i^{\mathcal{I}}$ defined over patch Ω_i of elements $E \in \mathcal{E}_i^{\mathcal{I}}$ associated to each vertex $i \in \mathcal{I}$: Find $\lambda_i \, \underline{\hat{F}}_h^{(i)}$ such that:

$$a(\lambda_i \, \underline{\hat{F}}_h^{(i)}, \underline{v}_h^*) = \mathcal{Q}_{\Omega_i}(\lambda_i \, \underline{v}_h^*) \quad \forall \, \underline{v}_h^* \in \boldsymbol{\mathcal{V}}_h^1, \tag{12}$$

$$\text{where} \quad a(\lambda_i \, \underline{\hat{F}}_h^{(i)}, \underline{v}_h^*) = \sum_{\Gamma \in \mathcal{J}_i^{\mathcal{I}}} \int_\Gamma \lambda_i \, \underline{\hat{F}}_h^{(i)} \cdot \left(\sum_{E \in \mathcal{E}_\Gamma^{\mathcal{J}}} \eta_E \, \underline{v}_{h|E}^* \right) \mathrm{d}S$$

$$\text{and} \quad \mathcal{Q}_{\Omega_i}(\lambda_i \, \underline{v}_h^*) = \int_{\Omega_i} \Big(\mathrm{Tr}\left[{}_h \, (\lambda_i \, \underline{v}_h^*) \right] - \underline{f}_d \cdot \lambda_i \, \underline{v}_h^* \Big) \, \mathrm{d}\Omega.$$

The specificity of problems $\mathcal{P}_i^{\mathcal{I}}$ (12) is that the kernel of bilinear operator $a(\bullet, \bullet)$ is known beforehand, as it corresponds to the space $\bar{\boldsymbol{\mathcal{U}}}_{h,0|\Omega_i}^1 = \left\{ \underline{v}_h^* \in \bar{\boldsymbol{\mathcal{V}}}_h^1, \underline{v}_{h|\Gamma \in \mathcal{J}_i^{\mathcal{I}} \cap \partial\Omega}^* = \underline{0} \right\}$, where $\bar{\boldsymbol{\mathcal{V}}}_h^1$ defines the set of piecewise linear polynomial functions $\underline{v}_h^* \in \boldsymbol{\mathcal{V}}_h^1$ which are continuous over the whole patch Ω_i and a fortiori across edges $\Gamma \in \mathcal{J}_i^{\mathcal{I}}$. The *a priori* knowledge of this kernel makes this technique practical and readily implementable. Thus, solvability of problems (12) is ensured for a FE interpolation degree $p \geqslant 2$ by considering $\bar{\boldsymbol{\mathcal{U}}}_{h,0|\Omega_i}^1$ along with FE properties. A special treatment is required in the case $p = 1$, for which the r.h.s term of problems (12) is replaced by $\mathcal{Q}_{\Omega_i}(\lambda_i \, \underline{v}_h^*(\underline{x}_i))$, thus ensuring well-posedness (see [2] for more details).

Uniqueness of the solution of such problems is guaranteed by means of the minimization of a cost function of the form [2]: $J_{\Omega_i}(\lambda_i \, \underline{\hat{F}}_h^{(i)}) = \frac{1}{2} \sum_{\Gamma \in \mathcal{J}_i^{\mathcal{I}}} (\lambda_i \, \underline{\hat{F}}_h^{(i)} - \lambda_i \, \underline{F}_h^{(i)})_{|\Gamma}^2$, where the known quantity $\lambda_i \, \underline{F}_{h|\Gamma}^{(i)}$ depends on the projection of the FE stress field ${}_h$ over the edge $\Gamma \in \mathcal{J}_i^{\mathcal{I}}$ and the traction force density $\underline{F}_d$.

Eventually, searching $\lambda_i \, \underline{\hat{F}}_h^{(i)}$ in $\boldsymbol{\mathcal{U}}_{h|\Gamma}^p$ leads to equilibrated tractions $\underline{\hat{F}}_h$ along each edge $\Gamma \in \mathcal{J}$ merely defined as $\underline{\hat{F}}_{h|\Gamma} = \sum_{i \in \mathcal{I}_\Gamma^{\mathcal{J}}} (\lambda_i \, \underline{\hat{F}}_h^{(i)})_{|\Gamma}$. Let us recall that such tractions naturally satisfy (11). Furthermore, enforcement of conditions $\eta_E \, \underline{\hat{F}}_h = \underline{F}_d$ over edges $\Gamma \subset \partial_2\Omega$ can be achieved by adding these constraints in the constrained minimization problem. In the following, we focus on the main points dealing with the enhanced version.

4 IMPROVEMENT IN THE CONSTRUCTION OF EQUILIBRATED TRACTIONS

The principle, inspired from an idea developed in [5], is to optimize the quality of the computed admissible stress field by improving the recovering strategy for the construction of equilibrated tractions without impairing the corresponding computational cost too much. To do so, the original prolongation condition involved in the EET and EESPT has been weakened with the objective to confer a greater flexibility in the construction of balanced tractions, thus leading to the following energetic relation:

$$\int_E (\underline{\hat{\varepsilon}}_h - \underline{\varepsilon}_h) \cdot \underline{\nabla}\varphi_i \, \mathrm{d}\Omega = \underline{0} \quad \forall\, i \in \mathcal{N}_E^{\mathcal{E}} \setminus \mathcal{I}_E^{\mathcal{E}},\ \forall\, E \in \mathcal{E}_e, \tag{13}$$

where φ_i is the FE shape function associated with non-vertex node i and $\mathcal{E}_e \subset \mathcal{E}$ (similarly, $\mathcal{J}_e \subset \mathcal{J}$) is the set of elements (respectively edges) involved in the enhanced procedure. Various criteria, such as geometric or error estimate criteria, can be considered to *a priori* select part Ω_e, i.e. the set $\mathcal{E}_e$ of elements. Hence, the construction of balanced tractions along edges $\Gamma \in \mathcal{J}_e$ involved in the EET and EESPT methods needs to be adapted to this weakened prolongation. Densities $\underline{\hat{F}}_h$ along edges $\Gamma \in \mathcal{J}_e$ are still sought in $\boldsymbol{\mathcal{U}}^p_{h|\Gamma}$, but are henceforth decomposed in the form:

$$\underline{\hat{F}}_h = \underline{\hat{H}}_h + \underline{\hat{R}}_h \quad \text{on } \Gamma \in \mathcal{J}_e, \quad \text{with} \quad \int_\Gamma \underline{\hat{H}}_h \, \varphi_i = \underline{0} \quad \forall\, i \in \mathcal{I}_\Gamma^{\mathcal{J}_e}, \tag{14}$$

$$\int_\Gamma \underline{\hat{R}}_h \, \varphi_i = \underline{0} \quad \forall\, i \in \mathcal{N}_\Gamma^{\mathcal{J}_e} \setminus \mathcal{I}_\Gamma^{\mathcal{J}_e}. \tag{15}$$

First, part $\underline{\hat{H}}_h$ on $\Gamma \in \mathcal{J}_e$ can be determined in the same way as for the original construction, but using both weak prolongation condition (13) and relation (14) instead of strong prolongation condition (5). Second, calculation of part $\underline{\hat{R}}_h$ on $\Gamma \in \mathcal{J}_e$ is performed by minimizing the complementary energy (or, equivalently, the constitutive relation error) locally on part $\Omega_e \subset \Omega$ containing elements $E \in \mathcal{E}_e$ under the following constraints: Neumann boundary conditions over edges $\Gamma \in \mathcal{J}_e \cap \partial_2\Omega$; equilibrium conditions of tractions $\underline{\hat{H}}_h + \underline{\hat{R}}_h$ with body force field $\underline{f}_d$ over each element $E \in \mathcal{E}_e$; equilibrium conditions of tractions $\underline{\hat{H}}_h + \underline{\hat{R}}_h$ with body force field $\underline{f}_d$ and standard tractions $\underline{\hat{F}}_h^{Std}$ over each element $E \in \bar{\mathcal{E}}_e \setminus \mathcal{E}_e$, where $\bar{\mathcal{E}}_e \subset \mathcal{E}$ denotes the set of elements E connected to at least one edge $\Gamma \in \mathcal{J}_e$; therefore, $\bar{\mathcal{E}}_e \setminus \mathcal{E}_e$ contains all the elements connected to one and only one edge $\Gamma \in \mathcal{J}_e$; $\underline{\hat{F}}_h^{Std}$ are pre-calculated tractions over edges $\Gamma \in \partial E \setminus \mathcal{J}_e$ coming from the standard construction over element $E \in \bar{\mathcal{E}}_e \setminus \mathcal{E}_e$. The yielded tractions are optimized so that the resulting estimate is sharper than the one obtained by original version of the construction of balanced tractions.

5 GOAL-ORIENTED ERROR ESTIMATION

5.1 The extraction technique and associated adjoint problem

Let us now outline the main aspects of the general method dealing with goal-oriented error estimation. The objective consists in evaluating the discretization error in a specific quantity of interest I by means of extraction techniques, i.e. by expressing the local quantity I in the global form involving extraction operators or extractors. Let us consider a quantity of interest I represented by a linear functional Ł of displacement field $\underline{u}$, defined on space $\boldsymbol{\mathcal{U}}$, written in the following global form:

$$I = \text{Ł}(\underline{u}) = \int_\Omega \left(\mathrm{Tr}\left[\tilde{\underline{\sigma}}_\Sigma (\underline{u}) \right] + \tilde{\underline{f}}_\Sigma \cdot \underline{u} \right) \mathrm{d}\Omega, \tag{16}$$

where $\tilde{\ }_\Sigma$ and $\underline{\tilde{f}}_\Sigma$ are known quantities, called extractors, homogeneous to a stress field and a body force field, respectively. Then, the approach consists in introducing an adjoint problem, similar to the reference problem, but with a different mechanical loading involving not $(\underline{F}_d, \underline{f}_d)$ either, but extractors. The adjoint problem consists in finding a displacement/stress pair $(\underline{\tilde{u}}, \tilde{\ })$ in the space domain Ω, which verifies:

- the kinematic conditions: $\underline{\tilde{u}} \in \boldsymbol{\mathcal{U}}_0$; (17)
- the equilibrium equations: $\tilde{\ } \in \boldsymbol{\mathcal{S}}$; $\forall\, \underline{u}^* \in \boldsymbol{\mathcal{U}}_0$, $\displaystyle\int_\Omega \mathrm{Tr}\left[\tilde{\ }(\underline{u}^*)\right] \mathrm{d}\Omega = Ł(\underline{u}^*)$; (18)
- the constitutive relation: $\tilde{\ }(M) = \boldsymbol{K}\left(\underline{\tilde{u}}(M)\right) \quad \forall\, M \in \Omega$. (19)

As seen earlier in Section 2.1, one can compute an approximate solution, denoted $(\underline{\tilde{u}}_h, \tilde{\ }_h)$, using a FEM associated with a space mesh $\tilde{\mathcal{M}}_h$ which may differ from FE mesh $\mathcal{M}_h$ used to solve the reference problem. Subsequently, an admissible solution $(\underline{\hat{\tilde{u}}}_h, \hat{\tilde{\ }}_h)$ of the adjoint problem can be derived from one of the equilibration techniques presented in Sections 3 and 4. Eventually, one can compute the associated CRE $e_{\mathrm{cre}}(\underline{\hat{\tilde{u}}}_h, \hat{\tilde{\ }}_h)$.

5.2 The resulting bounds

Let I_{ex} and I_h be the unknown exact value of the quantity of interest I and its associated approximate value obtained through the FEM, respectively. Owing to the linearity of Ł, the discretization error in I reads $I_{ex} - I_h = Ł(\underline{u} - \underline{u}_h)$. Given admissible solutions $(\underline{\hat{u}}_h, \hat{\ }_h)$ and $(\underline{\hat{\tilde{u}}}_h, \hat{\tilde{\ }}_h)$ of reference and adjoint problems, respectively, the procedure described in [8] leads to the following bounding inequality:

$$|I_{ex} - I_h - I_{hh}| \leqslant \frac{1}{2}\, e_{\mathrm{cre}}(\underline{\hat{u}}_h, \hat{\ }_h)\, e_{\mathrm{cre}}(\underline{\hat{\tilde{u}}}_h, \hat{\tilde{\ }}_h), \tag{20}$$

where $I_{hh} = \dfrac{1}{2}\displaystyle\int_\Omega \mathrm{Tr}\left[(\ _h - \boldsymbol{K}(\underline{\hat{u}}_h))\, \boldsymbol{K}^{-1}\, (\hat{\ }_h + \boldsymbol{K}(\underline{\hat{\tilde{u}}}_h))\right] \mathrm{d}\Omega + Ł(\underline{\hat{u}}_h - \underline{u}_h)$ can be viewed as a correction term related to the independent nature of the spatial discretization associated to the reference and adjoint problems.

The resulting bound on the local error $I_{ex} - I_h$ is expressed as not only the product of two global error estimates, namely $e_{\mathrm{cre}}(\underline{\hat{u}}_h, \hat{\ }_h)$ and $e_{\mathrm{cre}}(\underline{\hat{\tilde{u}}}_h, \hat{\tilde{\ }}_h)$, related to reference and adjoint problems, respectively, but also using a calculable correction term I_{hh}. Hence, quantity $I_h + I_{hh}$ can be considered as a new approximate value of I_{ex}. Note also that the derivation of bounding relation (20) requires no orthogonality property of the FE solutions, contrary to classical procedures. A detailed description and proofs of the bound properties can be found in [8, 7].

6 NUMERICAL RESULTS

Performances of the proposed robust global estimators are illustrated through a two-dimensional weight sensor under bending, represented in Figure 1. The FE mesh, containing 11 807 linear triangular elements and 6 320 nodes (i.e. 12 640 d.o.f.), is

given in Figure 1. The mesh density increases toward the top and bottom regions of the two holes, which constitute the highest stress zones. The reference solution is obtained from a very fine mesh made of 3 326 963 linear triangular elements and 1 668 711 nodes (i.e. 3 337 422 d.o.f.) ("overkill solution"). The quasi-exact value of the energy norm $\|\underline{e}_h\|_{u,\Omega}$ of the discretization error (i.e. the reference error) is equal to 347.997.

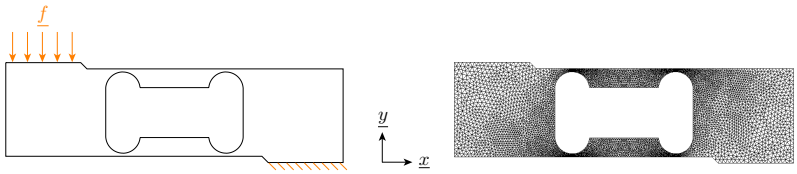


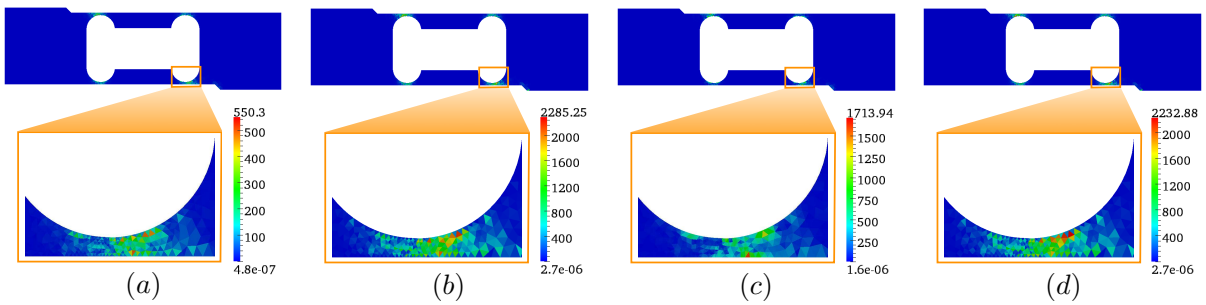
Figure 1: Weight sensor model problem (left) and associated finite element mesh (right).

Capabilities of the different techniques for global error estimation are reported in Table 1 and compared in terms of numerical quality and computational cost. It is observed that the SPET method gives better numerical accuracy, while EET and EESPT methods require lower computational cost, at least 4 times less expensive than that needed for the SPET method. Eventually, the EESPT method seems to be a fairly good trade-off, as it provides slightly better accuracy than the EET at similar CPU cost, and its implementation has been made simpler than that of the EET.

Table 1: Comparison of the error estimators given by the EET, the SPET, and the EESPT.

Methods	Estimate e_{cre}	Effectivity index $e_{\text{cre}}/\|\underline{e}_h\|_{u,\Omega}$	Normalized CPU time
EET	812.999	2.3362	1.000
SPET	556.629	1.5995	4.218
EESPT	812.801	2.3357	1.156

Figure 2 shows maps of the elementary contributions to the global reference error and that of the global estimates, obtained by the EET and SPET and EESPT methods, respectively. The largest contributions to the global reference error/estimate are located in the neighborhood of the highly-loaded zone.



(a) (b) (c) (d)

Figure 2: Maps of local contributions to the global reference error (a), the error estimates computed using the EET (b), the SPET (c), and the EESPT (d), and zoom around the highly-loaded region.

7 CONCLUSIONS

Assessment of the performances of various techniques to reconstruct admissible fields has been performed. Numerical results show that the hybrid EESPT method is a worthwhile technique allowing to obtain accurate error bounds at reasonable computing time with little effort, as the practical implementation is simpler than the EET method. However the EESPT, as well as the EET, gives less accurate estimate than the SPET, since the latter presents sharper upper bounds than the former. Nevertheless, the computational cost needed to compute the EESPT is much smaller than that required for the SPET. In addition, one can prove that the enhanced procedure applied to the EESPT (or EET) enables to recover better effectivity indices, i.e. sharper estimates, than the original construction, while keeping an affordable CPU time in the case of error estimate criteria. Those results confirm that accuracy of the yielded estimate is driven by the quality of the associated balanced tractions, especially in specific regions where the local contributions to the error are predominant. Besides, when willing to deal with goal-oriented error estimation, this improved procedure can be fairly used to obtain high-quality bounds on the local error on a given quantity of interest.

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