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NEW BOUNDING TECHNIQUES FOR GOAL-ORIENTED ERROR ESTIMATION IN FE SIMULATIONS

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Abstract. In this work, we propose new bounding techniques that enable to derive accurate and strict error bounds on outputs of interest computed from numerical approximation methods such as the finite element method. These techniques are based on Saint-Venant's principle and exploit specific homotheticity properties in order to improve the quality of the bounds computed from the classical bounding technique. The capabilities of the proposed approaches are illustrated through two-dimensional numerical experiments carried out on a linear elasticity problem.

1 INTRODUCTION

In the context of finite element (FE) model verification, research and engineering activities focus on the development of robust goal-oriented error estimation methods designed to achieve strict and high-quality error bounds associated to specific quantities of interest. A general method [1] consists in using extraction techniques as well as robust global error estimation methods, and involves the global solution of an auxiliary problem, also known as dual or adjoint problem. The derivation of accurate local error bounds entails a fine resolution of this auxiliary problem. Nevertheless, the classical bounding technique may provide low-quality error bounds on specific quantities of interest, particularly when the global estimated errors related to both reference (primal) and adjoint (dual) problems are mainly concentrated in disjoint regions. The main source of overestimation presumably stems form the Cauchy-Schwarz inequality, especially when the zone of interest is located far from the predominant contributions of the global estimate associated to reference problem. This observation has spurred the development of new bounding techniques able to circumvent, or at least alleviate, this serious drawback by optimizing the sharpness and practical relevance of the classical computed bounds. In this work, we propose and analyze new improved bounding techniques based on non-classical and innovative tools, such as homotheticity properties [2]. These techniques are carefully tailored for the derivation of inequalities between appropriate quantities over two homothetic domains contained in the whole structure. Such relations are based on Saint-Venant's principle and seem to be limited to solely linear problems. The classical and enhanced techniques can be combined with an intrusive approach (local refinement techniques) or a non-intrusive one (handbook techniques [3]) to get a reliable solution of the adjoint problem.

The paper is organized as follows. Section 2 presents both reference and adjoint problems and defines the discretization error. Section 3 recalls basics on goal-oriented error estimation using extraction (or adjoint-based) techniques and the concept of constitutive relation error through the construction of admissible solutions. Section 4 describes the main features of the improved bounding techniques, while Section 5 provides some numerical experiments conducted on a linear elasticity problem with comparative results between conventional and alternative bounding techniques.

2 REFERENCE AND ADJOINT PROBLEMS

2.1 Reference problem and discretization error

Let us consider a mechanical structure occupying an open bounded domain $\Omega \subset \mathbb{R}^d$ (d being the space dimension), with Lipschitz boundary $\partial\Omega$. The prescribed loading acting on Ω consists of: a displacement field $\underline{U}_d$ on part $\partial_u\Omega \subset \partial\Omega$ ($\partial_u\Omega \neq \varnothing$); a traction force density $\underline{F}_d$ on the complementary part $\partial_f\Omega$ of $\partial\Omega$ such that $\overline{\partial_u\Omega \cup \partial_f\Omega} = \partial\Omega$, $\partial_u\Omega \cap \partial_f\Omega = \varnothing$; a body force field $\underline{f}_d$ within Ω. Structure Ω is assumed to be made of an isotropic, homogeneous material with linear and elastic behavior characterized by Hooke's tensor $\boldsymbol{K}$. Assuming a quasi-static loading, an isothermal case and a small perturbations state, the reference problem consists of finding a displacement/stress pair $(\underline{u}, \sigma)$ in the space domain Ω, which verifies:

- the kinematic conditions:

$$\underline{u} \in \boldsymbol{\mathcal{U}}; \quad \underline{u} = \underline{U}_d \quad \text{on } \partial_u\Omega; \quad \varepsilon(\underline{u}) = \frac{1}{2}\left(\nabla \underline{u} + \nabla^T \underline{u}\right) \quad \text{in } \Omega; \tag{1a}$$

- the weak form of equilibrium equations:

$$\sigma \in \boldsymbol{\mathcal{S}}; \quad \forall\, \underline{u}^* \in \boldsymbol{\mathcal{U}}_0, \quad \int_\Omega \operatorname{Tr}\left[\sigma\, \varepsilon(\underline{u}^*)\right] \mathrm{d}\Omega = \int_\Omega \underline{f}_d \cdot \underline{u}^* \,\mathrm{d}\Omega + \int_{\partial_f\Omega} \underline{F}_d \cdot \underline{u}^* \,\mathrm{d}S; \tag{1b}$$

- the constitutive relation:

$$\sigma = \boldsymbol{K}\, \varepsilon\big(\underline{u}\big) \quad \text{in } \Omega, \tag{1c}$$

where $\varepsilon(\underline{u})$ represents the classical linearized strain tensor corresponding to the symmetric part of the gradient of displacement field $\underline{u}$. Affine spaces $\boldsymbol{\mathcal{U}} = \left\{\underline{u} \in [\mathcal{H}^1(\Omega)]^d\right\}$ and $\boldsymbol{\mathcal{S}} = \left\{\sigma \in \mathcal{M}_s(d) \cap [\mathcal{L}^2(\Omega)]^{d^2}\right\}$ guarantee the existence of finite-energy solutions, $\mathcal{M}_s(d)$

representing the space of symmetric square matrices of order d. Lastly, $\boldsymbol{\mathcal{U}}_0 \subset \boldsymbol{\mathcal{U}}$ denotes the vectorial space associated to $\boldsymbol{\mathcal{U}}$.

In practical applications, the exact solution of the reference problem, hereafter denoted $(\underline{u}_{ex}, \sigma_{ex})$, remains usually out of reach and only an approximate solution, referred to as $(\underline{u}_h, \sigma_h)$, can be obtained through numerical approximation methods (such as the FE method (FEM) associated with a space mesh Ω_h mapping Ω). Such a numerical approximation is searched 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 (1a) and a stress field σ_h computed *a posteriori* from constitutive relation (1c).

The resulting discretization error, denoted $\underline{e}_h = \underline{u}_{ex} - \underline{u}_h$, can be assessed in terms of:

- a global measure defined with respect to the classical energy norm $\|\bullet\|_{u,\Omega} = \left(\int_\Omega \text{Tr}\left[\boldsymbol{K}\,\varepsilon(\bullet)\,\varepsilon(\bullet)\right] \mathrm{d}\Omega\right)^{1/2}$, providing a global discretization error $e_\Omega = \|\underline{e}_h\|_{u,\Omega}$;
- a local measure defined with respect to a specific output of interest $I(\underline{u})$ of the problem, providing a local error $e_I = I(\underline{u}_{ex}) - I(\underline{u}_h)$. Under the assumption of a linear quantity of interest with respect to displacement $\underline{u}$, it merely reads: $e_I = I(\underline{e}_h)$.

2.2 Adjoint problem

The quantity of interest, hereafter denoted I, is a goal-oriented output, such as the mean value of a stress component over a local region or the displacement value at a specific point, for instance. These meaningful quantities of practical interest to engineers are usually defined by means of extraction techniques, i.e. by expressing the local quantity I being considered in the global form involving global extraction operators, also called extractors. In this work, for the sake of simplicity, the quantity of interest is represented as a linear functional $\mathcal{L}$ of displacement field $\underline{u}$ on a finite support under the following global form:

$$I = \mathcal{L}(\underline{u}) = \int_\Omega \left(\text{Tr}\left[\tilde{\sigma}_\Sigma\,\varepsilon(\underline{u})\right] + \underline{\tilde{f}}_\Sigma \cdot \underline{u}\right) \mathrm{d}\Omega, \tag{2}$$

where so-called extractors $\tilde{\sigma}_\Sigma$ and $\underline{\tilde{f}}_\Sigma$, known analytically, can be mechanically viewed as a prestress field and a body force field, respectively. In the following, let $I_{ex} = \mathcal{L}(\underline{u}_{ex})$ and $I_h = \mathcal{L}(\underline{u}_h)$ be the unknown exact value of the quantity of interest I being studied and its approximate value obtained through the FEM, respectively.

Once the quantity of interest has been put into such a global form, the classical approach then consists of introducing an auxiliary problem, also called adjoint problem, which is similar to the reference problem, except that the external mechanical loading $(\underline{F}_d, \underline{f}_d)$ is replaced by the extractors on the one hand, and the non-homogeneous Dirichlet boundary conditions are changed to homogeneous kinematic constraints on the other hand. The adjoint problem consists of finding a displacement/stress pair $(\underline{\tilde{u}}, \tilde{\sigma})$, in the space domain Ω, which verifies:

- the kinematic conditions:

$$\underline{\tilde{u}} \in \boldsymbol{\mathcal{U}}_0; \tag{3a}$$

- the weak form of equilibrium equations:

$$\tilde{\sigma} \in \boldsymbol{\mathcal{S}}; \quad \forall \underline{u}^* \in \boldsymbol{\mathcal{U}}_0, \quad \int_\Omega \mathrm{Tr}\left[\tilde{\sigma}\varepsilon(\underline{u}^*)\right] \mathrm{d}\Omega = \mathcal{L}(\underline{u}^*) = \int_\Omega \Big(\mathrm{Tr}\left[\tilde{\sigma}_\Sigma\, \varepsilon(\underline{u}^*)\right] + \underline{\tilde{f}}_\Sigma \cdot \underline{u}^*\Big)\, \mathrm{d}\Omega; \tag{3b}$$

- the constitutive relation:

$$\tilde{\sigma} = \boldsymbol{K}\,\varepsilon\big(\underline{\tilde{u}}\big) \quad \text{in } \Omega. \tag{3c}$$

For similar reasons to the reference problem, the exact solution $(\underline{\tilde{u}}_{ex}, \tilde{\sigma}_{ex})$ of the adjoint problem remains out of reach in most practical applications, and one can only obtain an approximate solution, denoted $(\underline{\tilde{u}}_h, \tilde{\sigma}_h)$. This last solution lies in a discretized FE space associated with a space mesh $\tilde{\Omega}_h$, mapping the physical domain Ω.

3 BASICS ON GOAL-ORIENTED ERROR ESTIMATION BASED ON CONSTITUTIVE RELATION ERROR

We review here the classical procedure based on the concept of constitutive relation error (CRE) to obtain strict local error bounds on functional outputs.

3.1 Constitutive relation error

Starting from an admissible solution $(\underline{\hat{u}}_h, \hat{\sigma}_h)$ provided by one of the existing techniques [4], one can measure the global residual on constitutive relation (1c), called the CRE measure and denoted $e_{\mathrm{cre},\Omega} \equiv e_{\mathrm{cre},\Omega}(\underline{\hat{u}}_h, \hat{\sigma}_h) = \|\hat{\sigma}_h - \boldsymbol{K}\,\varepsilon(\underline{\hat{u}}_h)\|_{\sigma,\Omega}$, with $\|\bullet\|_{\sigma,\Omega} = \left(\int_\Omega \mathrm{Tr}\left[\,\bullet\;\boldsymbol{K}^{-1}\;\bullet\,\right]\,\mathrm{d}\Omega\right)^{1/2}$. Computing the CRE measure $e_{\mathrm{cre},\Omega}$ provides a guaranteed upper bound of the global discretization error $\|\underline{e}_h\|_{u,\Omega}$, as the well-known Prager-Synge hypercircle theorem leads to the following bounding inequality:

$$\|\underline{e}_h\|^2_{u,\Omega} = \|\underline{u}_{ex} - \underline{\hat{u}}_h\|^2_{u,\Omega} \leqslant \|\underline{u}_{ex} - \underline{\hat{u}}_h\|^2_{u,\Omega} + \|\sigma_{ex} - \hat{\sigma}_h\|^2_{\sigma,\Omega} = e^2_{\mathrm{cre},\Omega}, \tag{4}$$

which conveys the guaranteed nature of the CRE measure $e_{\mathrm{cre},\Omega}$ with respect to the global discretization error.

Introducing the average admissible field $\hat{\sigma}^m_h = \dfrac{1}{2}\left(\hat{\sigma}_h + \boldsymbol{K}\,\varepsilon(\underline{\hat{u}}_h)\right)$, one can directly deduce another fundamental relation, called the Prager-Synge's equality:

$$\|\sigma_{ex} - \hat{\sigma}^m_h\|_{\sigma,\Omega} = \frac{1}{2} e_{\mathrm{cre},\Omega}. \tag{5}$$

Equations (4) and (5) are key relations to derive guaranteed error bounds in both global and local robust error estimation methods.

In the same manner as for the reference problem, an admissible solution of the adjoint problem, hereafter referred to as $(\hat{\tilde{\underline{u}}}_h, \hat{\tilde{\sigma}}_h)$, can be derived from one of the existing equilibration techniques. Then, the associated CRE measure $\tilde{e}_{\text{cre},\Omega} \equiv e_{\text{cre},\Omega}(\hat{\tilde{\underline{u}}}_h, \hat{\tilde{\sigma}}_h)$ of the adjoint problem can be computed leading to a global estimate of the discretization error $\underline{\tilde{e}}_h = \underline{\tilde{u}}_{ex} - \underline{\tilde{u}}_h$ of the adjoint problem.

Now, let us focus on the main principles of the classical bounding technique involved in goal-oriented error estimation methods based on extraction techniques and the concept of CRE.

3.2 Basic identity and classical bounding technique

The expression of the quantity of interest I reformulated in the global form (2) as well as properties of both admissible solutions $(\hat{\underline{u}}_h, \hat{\sigma}_h)$ and $(\hat{\tilde{\underline{u}}}_h, \hat{\tilde{\sigma}}_h)$ lead to the following basic identity:

$$I_{ex} - I_h - I_{hh} = \langle \sigma_{ex} - \hat{\sigma}_h^m, \hat{\tilde{\sigma}}_h - \boldsymbol{K}\,\varepsilon(\hat{\tilde{\underline{u}}}_h) \rangle_{\sigma,\Omega}, \tag{6}$$

where $\langle \bullet, \circ \rangle_{\sigma,\Omega} = \int_\Omega \mathrm{Tr}\left[\bullet \boldsymbol{K}^{-1} \circ\right] \mathrm{d}\Omega$ is an energetic inner product defined on the stress field space $\boldsymbol{\mathcal{S}}$. I_{hh} can be viewed as a computable correction term involving known quantities of both reference and adjoint problems:

$$I_{hh} = \langle \hat{\tilde{\sigma}}_h^m, \hat{\sigma}_h - \boldsymbol{K}\,\varepsilon(\hat{\underline{u}}_h) \rangle_{\sigma,\Omega} + \mathcal{L}(\hat{\underline{u}}_h - \underline{u}_h), \tag{7}$$

where $\hat{\tilde{\sigma}}_h^m = \dfrac{1}{2}(\hat{\tilde{\sigma}}_h + \boldsymbol{K}\,\varepsilon(\hat{\tilde{\underline{u}}}_h))$. $I_h + I_{hh}$ can be interpreted as a new approximate solution of the exact value I_{ex} of the quantity of interest.

The fundamental equality (6), which does not call for any orthogonality property of the FE solutions and allows to build the finite-dimensional spaces associated to reference and adjoint problems independently, is the keystone of the classical bounding technique as well as the improved ones described in section 4.

Subsequently, the classical bounding procedure merely consists of applying the Cauchy-Schwarz inequality to (6) with respect to inner product $\langle \bullet, \circ \rangle_{\sigma,\Omega}$ and then using Prager-Synge's equality (5). This yields:

$$|I_{ex} - I_h - I_{hh}| \leqslant \frac{1}{2}\, e_{\text{cre},\Omega}\, \tilde{e}_{\text{cre},\Omega}. \tag{8}$$

Eventually, the derivation of strict lower and upper bounds $(\xi_{\text{inf}}, \xi_{\text{sup}})$ of I_{ex} (or, equivalently, of the local error $I_{ex} - I_h$) can be achieved straightforwardly, just having a global error estimation procedure at hand:

$$\xi_{\text{inf}} \leqslant I_{ex} \leqslant \xi_{\text{sup}}, \tag{9}$$

with

$$\begin{aligned} \xi_{\text{inf}} &= I_h + I_{hh} - \frac{1}{2}\, e_{\text{cre},\Omega}\, \tilde{e}_{\text{cre},\Omega}; \\ \xi_{\text{sup}} &= I_h + I_{hh} + \frac{1}{2}\, e_{\text{cre},\Omega}\, \tilde{e}_{\text{cre},\Omega}. \end{aligned} \tag{10}$$

Besides, owing to the independent natures of spatial discretizations associated to reference and adjoint problems, a convenient way to achieve accurate and sharp bounds of I_{ex} is to perform a local space refinement of the adjoint mesh $\tilde{\Omega}_h$ alone around the zone of interest ω in order to properly solve the adjoint problem while keeping a reasonable computational cost. In most common situations, the discretization error related to the adjoint problem is concentrated in the vicinity of the zone of interest, whereas that related to the reference problem may be scattered around zones which present some singularities or other error sources. However, when the error related to the reference problem is mostly located outside and far from the zone of interest, the classical bounding technique may yield large and low-quality local error bounds and thus makes useless bounding result (9). This is the point that we are revisiting here.

The proposed bounding techniques we present in the following section are intended to get around this serious drawback proper to the classical technique in order to sharpen the local error bounds.

4 IMPROVED BOUNDING TECHNIQUES

4.1 Homotheticity transfromation

Let us consider a reference subdomain, denoted ω_1 and included in Ω, defined by a point $\underline{O}$ and a geometric shape. The set of homothetic domains ω_λ associated to ω_1 is defined as:

$$\omega_\lambda = \mathcal{H}_{[\underline{O},\lambda]}(\omega_1) \tag{11}$$

where $\mathcal{H}_{[\underline{O};\lambda]}$ stands for the homothetic transformation operator centered in point $\underline{O}$, called homothetic center, and parameterized by a nonzero positive scalar $\lambda \in \,]0\,, \lambda_{\max}]$, also called magnification ratio, scale factor or similitude ratio, such that $\omega_\lambda \subset \Omega$ (see Figure 1). The geometric shape defining the set of homothetic domains ω_λ can be chosen arbitrarily. Nevertheless, these physical domains are supposed to be basic in practice, such as a circle or a rectangle in 2D, and a sphere or a rectangular cuboid (also called rectangular parallelepiped or right rectangular prism) in 3D, for instance.

For a given pair $(\omega_\lambda, \omega_{\bar{\lambda}})$ of homothetic domains included in Ω, represented in Figure 1 and parameterized by $(\lambda, \bar{\lambda})$, such that $\omega_\lambda \subset \omega_{\bar{\lambda}} \subset \Omega$, i.e. $\lambda \in \,]0\,, \bar{\lambda}]$, the position $\underline{v}_\lambda$ of a point $\underline{M}_\lambda$ along boundary $\partial\omega_\lambda$ can be defined from the position $\underline{v}_{\bar{\lambda}}$ of the corresponding point $\underline{M}_{\bar{\lambda}}$ along boundary $\partial\omega_{\bar{\lambda}}$ by the following relation:

$$\underline{v}_\lambda = \begin{cases} \dfrac{\lambda}{\bar{\lambda}}\, \underline{v}_{\bar{\lambda}}(\bar{s}) & \text{parameterized by } (\lambda, \bar{s}) \text{ in 2D;} \\ \dfrac{\lambda}{\bar{\lambda}}\, \underline{v}_{\bar{\lambda}}(\bar{s}_1, \bar{s}_2) & \text{parameterized by } (\lambda, \bar{s}_1, \bar{s}_2) \text{ in 3D,} \end{cases} \tag{12}$$

where $\bar{s}$ (resp. $\bar{s}_1$ and $\bar{s}_2$) represent the curvilinear abscissa along boundary $\partial\omega_{\bar{\lambda}}$ in 2D (resp. 3D).

Such a parameterization leads to various homotheticity properties [2] that are at the root of fundamental inequalities such as the one introduced in Section 4.3.

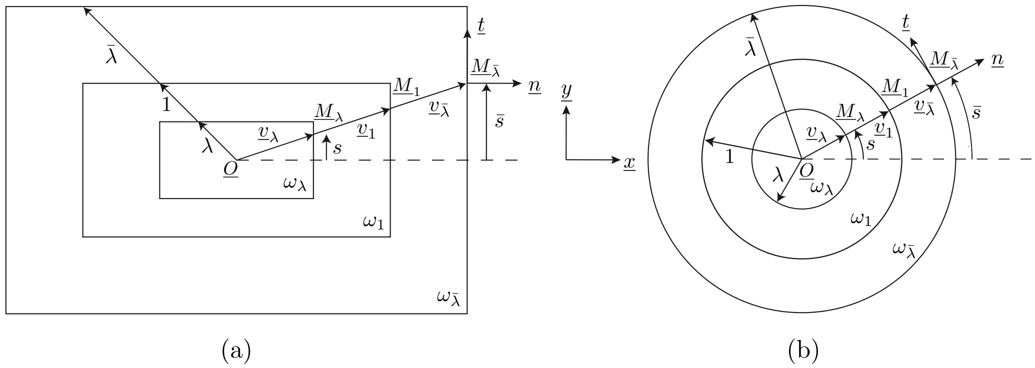

Figure 1: Examples of rectangular (a) and circular (b) homothetic domains in 2D.

4.2 Principle

First, let us recall the expression of quantity q involved in basic identity (6) for building local error bounds :

$$q = \langle \sigma_{ex} - \hat{\sigma}_h^m, \hat{\tilde{\sigma}}_h - \boldsymbol{K}\,\varepsilon(\hat{\tilde{\underline{u}}}_h) \rangle_{\sigma,\Omega}, \tag{13}$$

where $\hat{\sigma}_h^m$ and $\hat{\tilde{\sigma}}_h - \boldsymbol{K}\,\varepsilon(\hat{\tilde{\underline{u}}}_h)$ are given quantities coming from reference and adjoint problems, respectively, and σ_{ex} is the unknown exact stress solution of the reference problem.

By considering a subdomain ω_λ of domain Ω and its complementary part $\Omega \setminus \omega_\lambda$, the approach consists in splitting quantity q into two distinct contributions q_{ω_λ} and $q_{\Omega \setminus \omega_\lambda}$:

$$q = q_{\omega_\lambda} + q_{\Omega \setminus \omega_\lambda},$$

where

$$q_{\omega_\lambda} = \langle \sigma_{ex} - \hat{\sigma}_h^m, \hat{\tilde{\sigma}}_h - \boldsymbol{K}\,\varepsilon(\hat{\tilde{\underline{u}}}_h) \rangle_{\sigma,\omega_\lambda}; \tag{14a}$$

$$q_{\Omega \setminus \omega_\lambda} = \langle \sigma_{ex} - \hat{\sigma}_h^m, \hat{\tilde{\sigma}}_h - \boldsymbol{K}\,\varepsilon(\hat{\tilde{\underline{u}}}_h) \rangle_{\sigma,\Omega \setminus \omega_\lambda}. \tag{14b}$$

When quantity $\hat{\tilde{\sigma}}_h - \boldsymbol{K}\,\varepsilon(\hat{\tilde{\underline{u}}}_h)$ involved in the CRE measure of the adjoint problem is mostly concentrated over part ω_λ, i.e. by choosing a subdomain ω_λ surrounding the zone of interest ω, part $q_{\Omega \setminus \omega_\lambda}$ can be accurately bounded by simply using the Cauchy-Schwarz inequality with respect to inner product $\langle \bullet, \circ \rangle_{u,\Omega \setminus \omega_\lambda}$ and the Prager-Synge's equality (5):

$$\left| q_{\Omega \setminus \omega_\lambda} \right| \leqslant \| \sigma_{ex} - \hat{\sigma}_h^m \|_{\sigma,\Omega \setminus \omega_\lambda} \, \tilde{e}_{\text{cre},\Omega \setminus \omega_\lambda} \leqslant \frac{1}{2} \, e_{\text{cre},\Omega} \, \tilde{e}_{\text{cre},\Omega \setminus \omega_\lambda}. \tag{15}$$

Given that the discretization error associated to the adjoint problem is mainly located around the zone of interest $\omega \subset \omega_\lambda$, $\tilde{e}_{\text{cre},\Omega \setminus \omega_\lambda}$ is a relatively small computable term. It follows that the main contribution to the local error comes from part q_{ω_λ}. Consequently, quantity q_{ω_λ} has to be bounded with a particular care in order to derive accurate local error bounds while preserving the guaranteed nature of the error estimate.

4.3 Fundamental inequality

Let us consider the space $\boldsymbol{\mathcal{V}}$ of functions satisfying homogeneous equilibrium conditions:

$$\boldsymbol{\mathcal{V}} = \left\{ \underline{v} \in \boldsymbol{\mathcal{U}} \text{ such that } \underline{\mathrm{div}}(\boldsymbol{K}\,\varepsilon(\underline{v})) = \underline{0} \text{ in } \Omega \right\}, \tag{16}$$

and let us introduce the Steklov constant, or Steklov eigenvalue, h defined in [5] as:

$$h = \max_{\underline{v} \in \boldsymbol{\mathcal{V}}_{|\omega_1}} \boldsymbol{\mathcal{S}}_1(\underline{v}), \tag{17}$$

with

$$\boldsymbol{\mathcal{S}}_1(\underline{v}) = \frac{\left\| \boldsymbol{K}\,(\underline{v} \otimes \underline{n})_{\mathrm{sym}} \right\|^2_{\sigma,\partial\omega_1}}{\|\underline{v}\|^2_{u,\omega_1}}, \tag{18}$$

where $(\bullet)_{\mathrm{sym}}$ represents the symmetric part of tensor of order 2 (or matrix) $\bullet$. Then, for any homothetic domain $\omega_\lambda \subset \Omega$ parametrized by $\lambda > 0$, one can derive a relation involving the product of constant h and parameter λ:

$$h\lambda = \max_{\underline{v} \in \boldsymbol{\mathcal{V}}_{|\omega_\lambda}} \boldsymbol{\mathcal{S}}_\lambda(\underline{v}), \tag{19}$$

with

$$\boldsymbol{\mathcal{S}}_\lambda(\underline{v}) = \frac{\left\| \boldsymbol{K}\,(\underline{v} \otimes \underline{n})_{\mathrm{sym}} \right\|^2_{\sigma,\partial\omega_\lambda}}{\|\underline{v}\|^2_{u,\omega_\lambda}}. \tag{20}$$

Let $(\omega_\lambda, \omega_{\bar{\lambda}})$ be a pair of homothetic domains such that $\lambda \in \,]0\,,\bar{\lambda}]$, i.e. $\omega_\lambda \subset \omega_{\bar{\lambda}}$. The following key inequality holds [2]:

$$\|\sigma_{ex} - \hat{\sigma}_h\|^2_{\sigma,\omega_\lambda} \leqslant \left(\frac{\lambda}{\bar{\lambda}}\right)^{1/h} \|\sigma_{ex} - \hat{\sigma}_h\|^2_{\sigma,\omega_{\bar{\lambda}}} + \gamma_{\lambda,\bar{\lambda}}, \tag{21}$$

where

$$\gamma_{\lambda,\bar{\lambda}} \equiv \gamma_{\lambda,\bar{\lambda}}(\underline{\hat{u}}_h, \hat{\sigma}_h) = \int_{\lambda'=\lambda}^{\bar{\lambda}} \left[\left(\frac{\lambda'}{\lambda}\right)^{-1/h} \frac{1}{h\lambda'} e^2_{\mathrm{cre},\omega_{\lambda'}} \right] \mathrm{d}\lambda'. \tag{22}$$

Let us note that, using Prager-Synge's equality (5), unknown term $\|\sigma_{ex} - \hat{\sigma}_h\|_{\sigma,\omega_{\bar{\lambda}}}$ involved in the right-hand side term of fundamental inequality (21) is readily bounded as:

$$\|\sigma_{ex} - \hat{\sigma}_h\|^2_{\sigma,\omega_{\bar{\lambda}}} \leqslant \left(\|\sigma_{ex} - \hat{\sigma}^m_h\|_{\sigma,\omega_{\bar{\lambda}}} + \|\hat{\sigma}^m_h - \hat{\sigma}_h\|_{\sigma,\omega_{\bar{\lambda}}} \right)^2 \leqslant \frac{1}{4} \left(e_{\mathrm{cre},\Omega} + e_{\mathrm{cre},\omega_{\bar{\lambda}}} \right)^2 \tag{23}$$

It follows that fundamental result (21) can be rewritten in terms of perfectly known quantities as:

$$\|\sigma_{ex} - \hat{\sigma}_h\|^2_{\sigma,\omega_\lambda} \leqslant \left(\frac{\lambda}{\bar{\lambda}}\right)^{1/h} \frac{1}{4} \left(e_{\mathrm{cre},\Omega} + e_{\mathrm{cre},\omega_{\bar{\lambda}}} \right)^2 + \gamma_{\lambda,\bar{\lambda}}. \tag{24}$$

This last inequality is the key point to derive sharp bounds for part q_{ω_λ}.

4.4 Final bounding result

Applying the Cauchy-Schwarz inequality with respect to scalar product $\langle \bullet, \circ \rangle_{\sigma,\omega_\lambda}$ and then using the key inequality (24) introduced in the previous section leads to the following bounding result:

$$|q_{\omega_\lambda} - I_{hhh,\lambda}| \leqslant \left[\left(\frac{\lambda}{\bar{\lambda}} \right)^{1/h} \frac{1}{4} \left(e_{\mathrm{cre},\Omega} + e_{\mathrm{cre},\omega_{\bar{\lambda}}} \right)^2 + \gamma_{\lambda,\bar{\lambda}} \right]^{1/2} \tilde{e}_{\mathrm{cre},\omega_\lambda}. \tag{25}$$

Collecting both inequalities (25) and (15) for parts q_{ω_λ} and $q_{\Omega\backslash\omega_\lambda}$, respectively, one obtains:

$$|I_{ex} - I_h - I_{hh} - I_{hhh,\lambda}| \leqslant \tilde{e}_{\mathrm{cre},\omega_\lambda}\, \delta_{\lambda,\bar{\lambda}} + \frac{1}{2}\, e_{\mathrm{cre},\Omega}\, \tilde{e}_{\mathrm{cre},\Omega\backslash\omega_\lambda}, \tag{26}$$

where

$$\delta_{\lambda,\bar{\lambda}} \equiv \delta_{\lambda,\bar{\lambda}}(\underline{\hat{u}}_h, \hat{\sigma}_h) = \left[\left(\frac{\lambda}{\bar{\lambda}} \right)^{1/h} \frac{1}{4} \left(e_{\mathrm{cre},\Omega} + e_{\mathrm{cre},\omega_{\bar{\lambda}}} \right)^2 + \gamma_{\lambda,\bar{\lambda}} \right]^{1/2} \tag{27}$$

and

$$I_{hhh,\lambda} = \frac{1}{2} \langle \hat{\sigma}_h - \boldsymbol{K}\, \varepsilon(\underline{\hat{u}}_h), \hat{\tilde{\sigma}}_h - \boldsymbol{K}\, \varepsilon(\underline{\hat{\tilde{u}}}_h) \rangle_{\sigma,\omega_\lambda} \tag{28}$$

are fully calculable from the computed approximate solutions of both reference and adjoint problems.

Thus, this improved technique provides the following guaranteed lower and upper bounds $(\chi_{\mathrm{inf}}, \chi_{\mathrm{sup}})$ of I_{ex}:

$$\chi_{\mathrm{inf}} \leqslant I_{ex} \leqslant \chi_{\mathrm{sup}}, \tag{29}$$

with

$$\chi_{\mathrm{inf}} = I_h + I_{hh} + I_{hhh,\lambda} - \left| \tilde{e}_{\mathrm{cre},\omega_\lambda}\, \delta_{\lambda,\bar{\lambda}} + \frac{1}{2}\, e_{\mathrm{cre},\Omega}\, \tilde{e}_{\mathrm{cre},\Omega\backslash\omega_\lambda} \right|; \tag{30a}$$

$$\chi_{\mathrm{sup}} = I_h + I_{hh} + I_{hhh,\lambda} + \left| \tilde{e}_{\mathrm{cre},\omega_\lambda}\, \delta_{\lambda,\bar{\lambda}} + \frac{1}{2}\, e_{\mathrm{cre},\Omega}\, \tilde{e}_{\mathrm{cre},\Omega\backslash\omega_\lambda} \right|. \tag{30b}$$

These bounds depend on both parameters λ and $\bar{\lambda}$ associated to subdomains ω_λ and $\omega_{\bar{\lambda}}$, respectively. In order to get a practical minimizer, one seeks to reduce ratio $\lambda/\bar{\lambda}$ as much as possible by choosing: the smallest parameter λ such that domain ω_λ surrounds the zone of interest ω; the largest parameter $\bar{\lambda}$ such that domain $\omega_{\bar{\lambda}}$ remains a homothetic mapping of ω_λ (preserving its geometric shape) contained in Ω, and leading to sharp error bounds.

A second improved technique has been introduced and relies on similar homotheticity arguments, but differs from the first one presented in this paper in the way of bounding part q_{ω_λ}, which involves another fundamental inequality. The interested reader can refer to [2] for more information. This alternative bounding technique leads to guaranteed lower and upper bounds $(\zeta_{\text{inf}}, \zeta_{\text{sup}})$ of I_{ex}. Those bounds involve only one parameter $\bar{\lambda}$, which can be chosen such that subdomain $\omega_{\bar{\lambda}}$ recovers the zone where the solution of adjoint problem has stiff gradients.

5 NUMERICAL RESULTS

All numerical experiments have been performed assuming that the material remains isotropic, homogeneous, linear and elastic with Young's modulus $E = 1$ and Poisson's ratio $\nu = 0.3$. Furthermore, the two-dimensional examples are assumed to satisfy the plane-stress approximation. The balance technique used to derive a statically admissible stress field is the element equilibration technique (EET) combined with a p-refinement technique consisting of a $p + k$ discretization, p being the FE interpolation degree and k an additional degree equal to 3 (see [4]).

Performances of the proposed bounding techniques are illustrated through the two-dimensional cracked structure of Figure 2, which presents two round cavities. A homogeneous Dirichlet boundary condition is imposed to the bigger circular hole, whereas a unit internal constant pressure p_0 is applied to the smaller one. Furthermore, the top-left edge is subjected to a unit normal traction force density $\underline{t} = +\underline{n}$. Besides, a single edge crack emanates from the bottom of the smaller cavity. The two lips of this crack as well as the remaining sides are traction-free boundaries. The FE mesh Ω_h consists of 7 751 linear triangular elements and 4 122 nodes (i.e. 8 244 d.o.f.), see Figure 2. The reference mesh $\Omega_{\bar{h}}$ used to compute an "overkill" solution and to define a "quasi-exact" value, denoted I_{ex} for convenience, of the quantity of interest is built up by dividing each element into 256 elements; thereby, it is made of 1 984 256 linear triangular elements and 996 080 nodes (i.e. 1 992 160 d.o.f.).

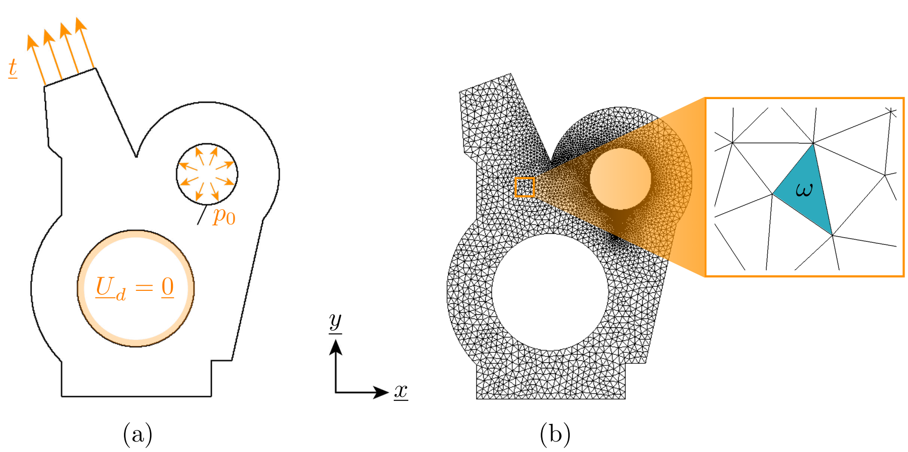

Figure 2: Cracked structure model problem (a) and associated finite element mesh (b).

The quantity of interest being considered in this work is a linear function of displacement field $\underline{u}$ associated to reference problem. It is the average value of the component

σ_{xx} of the stress field $\boldsymbol{\sigma}$ in a local zone $\omega \subset \Omega$:

$$I = \langle \sigma_{xx} \rangle_\omega = \frac{1}{|\omega|} \int_\omega \sigma_{xx} \, \mathrm{d}\Omega, \tag{31}$$

where extraction domain ω corresponds to an element of FE mesh Ω_h illustrated in Figure 2 and $|\omega|$ represents its measure. The loading of the the adjoint problem involves an extractor corresponding to a uniform prestress field $\tilde{\boldsymbol{\sigma}}_\Sigma = \boldsymbol{K}\, \tilde{\boldsymbol{\varepsilon}}_\Sigma$ over element ω, where $\tilde{\boldsymbol{\varepsilon}}_\Sigma = \dfrac{1}{|\omega|} \underline{x} \otimes \underline{x}$.

The main contributions to the error estimate $e_{\mathrm{cre},\Omega}$ associated to reference problem are by a majority located near the crack tip, while that to the error estimate $\tilde{e}_{\mathrm{cre},\Omega}$ associated to adjoint problem are concentrated around the zone of interest ω. Therefore, the error estimates for both reference and adjoint problems are localized in disjoint regions.

The homothetic center $\underline{O}$ coincides with the center of the circle $\mathcal{C}_\omega$ circumscribed by element ω and the values of parameters λ and $\bar{\lambda}$ involved in the first improved technique are set to $2\, r_{\mathcal{C}_\omega}$ and $14\, r_{\mathcal{C}_\omega}$, respectively, where $r_{\mathcal{C}_\omega}$ corresponds to the radius of $\mathcal{C}_\omega$. The value of parameter $\bar{\lambda}_{\mathrm{opt}}$ involved in the second improved technique is set to $9\, r_{\mathcal{C}_\omega}$, which enables to achieve the sharpest bounds for quantity of interest I.

The results obtained for classical bounding technique as well as first and second improved variants are presented in terms of the normalized bounds $(\bar{\xi}_{\mathrm{inf}}, \bar{\xi}_{\mathrm{sup}})$, $(\bar{\chi}_{\mathrm{inf}}, \bar{\chi}_{\mathrm{sup}})$, $(\bar{\zeta}_{\mathrm{inf}}, \bar{\zeta}_{\mathrm{sup}})$, respectively, with respect to I_{ex}. Figure 3 shows the evolutions of the normalized lower and upper bounds of I_{ex} for quantity of interest I as functions of the number of elements $\tilde{N}_e$ contained in the FE mesh $\Omega_{\tilde{h}}$ associated to adjoint problem for the classical bounding technique as well as the two improved ones. The adjoint mesh $\Omega_{\tilde{h}}$ has been locally refined near the zone of interest ω, since the loading and the contributions to the global error estimate of the adjoint problem are highly localized in this region. One can see a slight improvement in the bounds obtained with the first improved technique compared to the classical one. As regards the second improved technique, a very clear improvement is observed allowing to achieve sharp local error bounds without refining too much the adjoint problem, thus keeping an affordable computing time.

6 CONCLUSION AND PROSPECTS

In this paper, we introduced new approaches related to the general framework of robust goal-oriented error estimation dealing with extraction techniques. These techniques are based on mathematical tools which are not classical in model verification. Various linear quantities of interest (such as the local average of a stress component, the pointwise value of a displacement component or a stress intensity factor) are considered in [2] to illustrate the effectivity of the proposed techniques. Those numerical experiments clearly demonstrate the efficiency of these methods to produce strict and relevant bounds on the errors in linear local quantities of interest compared to the classical bounding technique, especially when the discretization error related to the reference problem is not concentrated in

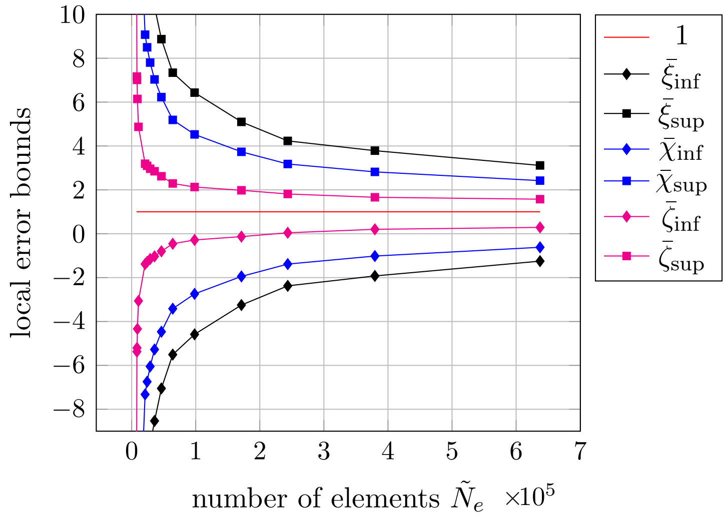

Figure 3: Evolutions of the lower and upper normalized bounds of I_{ex} for local quantity I_1, obtained using the classical bounding technique as well as first and second improvements, with respect to the number of elements $\tilde{N}_e$ associated to the discretization of the adjoint problem.

the local zone of interest. Nevertheless, the second proposed technique seems to achieve sharper local error estimates than the first one. Finally, such powerful methods may open up opportunities and help widen the field of robust goal-oriented error estimation methods. Both techniques could be easily extended to other quantities of interest but are restricted to linear problems, i.e. cases where Saint-Venant's principle is well established.

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