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Error Estimation and Quality Control

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ABSTRACT

This chapter provides a description of the error assessment tools available for general Finite Element Analysis, in particular those for solid and structural mechanics. The text focuses in goal-oriented error estimation, in terms of general quantities of interest rather that in energy norm. However, the energy norm estimates are also discussed because they are seen as basic tools that must be used for assessing the error in arbitrary functional outputs of the solution. Attention is paid to the classification of the different methodologies and their main characteristics.

KEY WORDS: Error estimation, quality control, verification and validation, energy norm, goal-oriented adaptivity

1. INTRODUCTION

The Verification and Validation keywords pertain to the quality analysis of the numerical solution provided by the Finite Element Method (FEM). Validation refers to the discrepancy between the model (physical/mathematical) and reality (or experiments). This chapter is concentrated in the Verification concept, which concerns the errors introduced by the numerical solver. More precisely, the methodologies assessing the error associated with the finite element discretization are briefly reviewed.

Thus, it is assumed in the following that the error is the difference between the exact and the numerical solutions of some mathematical problem (typically a boundary value problem, that is, a partial differential equation plus some properly posed boundary conditions). Among the different error sources, the discretization errors are the main focus in this chapter, but the solution is also affected by different mistakes and blunders. The latter may come both from the programmer of the code (they are then referred as code bugs) or the user, who sometimes misunderstands the data set to be entered into the code or misinterprets the results furnished by the code. It is beyond of the scope of this chapter analyzing these error sources.

The error introduced by the numerical discretization, the finite element mesh, is assessed using either a priori and a posteriori error estimates. A priori estimates are mathematical expressions relating some measure of the error with the parameters of the discretization, namely, the characteristic element size, h, and the degree of the polynomial approximation inside the elements, p. Unknown constants are involved in the expressions, independent of h

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and p but depending on the exact solution. A priori estimates are essential tools to analyze the FEM, in particular its convergence behavior. Nevertheless, a priori estimates are not providing information of the actual error for a concrete solution corresponding to a given mesh. This chapter is concentrateed in a posteriori error assessment. These tools require using the approximate solution (they must be used after the finite element computation is performed, a posteriori) and provide information on the actual error associated with this approximation.

The first attempts in a posteriori error assessment did provide approximations of the error measured in energy norm. In the last decade, a huge effort has been produced in assessing the error in arbitrary quantities of interest. This research is extremely useful since it relates with goal-oriented error adaptivity. That is, finding the optimal mesh producing the result specified by the user with the prescribed accuracy at a minimum cost. Moreover, a recently open line of research concentrates in providing certificates of the approximate solution or, conversely, guaranteed bounds in which the exact solution lies.

The remainder of the chapter is devoted to describe the main goals and endeavors of the error assessment techniques, to schematically classify the principal estimators and to review their characteristics and potential.

2. PROBLEM STATEMENT

The different approaches to error estimation for the finite element numerical approximations are presented in the framework of linear elasticity. This section briefly introduces the notation used in this chapter, summarizes the basic goals and states some properties of the error that are useful in the following.

2.1. Basic equations

The body under study occupies the domain Ω with boundary $\partial\Omega$, see figure 1. The boundary $\partial\Omega$ is divided in two disjoint parts, Γ_N and Γ_D. In the Dirichlet part of the boundary, Γ_D, the displacement is set to be equal to a given value $\boldsymbol{u}_D$. A body load $\boldsymbol{b}$ is applied in Ω and a traction $\boldsymbol{t}$ is applied on the Neumann part of the boundary, Γ_N. The unknown displacement field $\boldsymbol{u}$ and the corresponding stresses $\boldsymbol{\sigma}(\boldsymbol{u})$ are found by solving the following boundary value problem:

$$-\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}(\boldsymbol{u}) = \boldsymbol{b} \qquad \text{in } \Omega, \tag{1a}$$

$$\boldsymbol{\sigma}(\boldsymbol{u})\cdot\boldsymbol{n} = \boldsymbol{t} \qquad \text{on } \Gamma_N, \tag{1b}$$

$$\boldsymbol{u} = \boldsymbol{u}_D \qquad \text{on } \Gamma_D. \tag{1c}$$

The variational or weak form of problem (1) requires introducing the following functional spaces. The space of admissible displacements $\mathcal{U}$ (a subspace of $\mathcal{H}^1(\Omega)$ of functions fulfilling (1c)) and the space of virtual displacements, $\mathcal{V}$ (also known as trial functions, similar to $\mathcal{U}$ but vanishing on Γ_D). Thus the weak form is readily expressed as find $\boldsymbol{u}\in\mathcal{U}$ such that

$$a\big(\boldsymbol{u},\boldsymbol{v}\big) = l\big(\boldsymbol{v}\big), \text{ for all } \boldsymbol{v}\in\mathcal{V}, \tag{2}$$

where

$$a\big(\boldsymbol{u},\boldsymbol{v}\big) := \int_\Omega \boldsymbol{\sigma}(\boldsymbol{u}) : \boldsymbol{\epsilon}(\boldsymbol{v})\, d\Omega \quad , \quad l\big(\boldsymbol{v}\big) := \int_\Omega \boldsymbol{b}\cdot\boldsymbol{v}\, d\Omega + \int_{\Gamma_N} \boldsymbol{t}\cdot\boldsymbol{v}\, d\Gamma,$$

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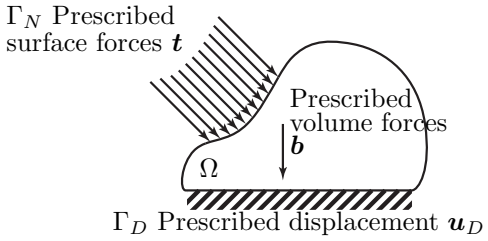

Figure 1. Representation of the structure

being $\boldsymbol{\epsilon}(\cdot)$ the strain operator. Recall that the Hooke tensor $\mathbb{C}$ relates stresses and strains,

$$\boldsymbol{\sigma}(\boldsymbol{u}) = \mathbb{C} : \boldsymbol{\epsilon}(\boldsymbol{u}). \tag{3}$$

It is useful expressing the bilinear form $a(\cdot,\cdot)$ in terms of stresses instead of displacements by formally introducing $\overline{a}(\cdot,\cdot)$ such that

$$\overline{a}(\boldsymbol{\sigma},\boldsymbol{\tau}) := \int_\Omega \boldsymbol{\sigma} : \mathbb{C}^{-1} : \boldsymbol{\tau}\, d\Omega.$$

Note that, with this definition, $a(\boldsymbol{u},\boldsymbol{v}) = \overline{a}\big(\boldsymbol{\sigma}(\boldsymbol{u}),\boldsymbol{\sigma}(\boldsymbol{v})\big)$.

A finite element mesh of characteristic size h discretizing Ω induces the functional spaces $\mathcal{U}^h \subset \mathcal{U}$ and $\mathcal{V}^h \subset \mathcal{V}$. The finite element approximation to $\boldsymbol{u}$, $\boldsymbol{u}^h \in \mathcal{U}^h$, is such that

$$a(\boldsymbol{u}^h,\boldsymbol{v}) = l(\boldsymbol{v}), \text{ for all } \boldsymbol{v} \in \mathcal{V}^h.$$

A posteriori error estimation techniques aim at assessing the error committed in the approximation of $\boldsymbol{u}$, $\boldsymbol{e} := \boldsymbol{u} - \boldsymbol{u}^h$, where $\boldsymbol{e} \in \mathcal{V}$ is the solution of the residual equation

$$a(\boldsymbol{e},\boldsymbol{v}) = l(\boldsymbol{v}) - a(\boldsymbol{u}^h,\boldsymbol{v}) =: R(\boldsymbol{v}), \text{ for all } \boldsymbol{v} \in \mathcal{V}. \tag{4}$$

Remark 1. *The right-hand side of equation* (4) *is the weak residual associated with the trial function* $\boldsymbol{v}$*. Error estimation techniques based on solving this equation or making use of it are hence named residual type error estimators. It is worth noting also that the weak residual is also expressed in terms of the elementary strong residual* $\boldsymbol{r}_{el} = \boldsymbol{b} + \boldsymbol{\nabla}\cdot\boldsymbol{\sigma}(\boldsymbol{u}^h)$ *(which can be evaluated in the interior of the elements* Ω_k*,* $k = 1, 2, \ldots, n_{el}$*, of the mesh) and the singular residual,* $\boldsymbol{r}_{sing}$*. The singular residual is defined as the jump of the normal component of* $\boldsymbol{\sigma}(\boldsymbol{u}^h)$ *on the interelement edges* γ *(sides in 3D) in* Γ_{int}*,* $\boldsymbol{r}_{sing} = [\![\boldsymbol{\sigma}(\boldsymbol{u}^h)\cdot\boldsymbol{n}]\!]_{\Gamma_{int}}$ *and as the non verification of the Neumann boundary condition on the element edges* γ *in* Γ_N*,* $\boldsymbol{r}_{sing} = \boldsymbol{t} - \boldsymbol{\sigma}(\boldsymbol{u}^h)\cdot\boldsymbol{n}$*. The resulting expression is*

$$R(\boldsymbol{v}) = \sum_{k=1}^{n_{el}} \int_{\Omega_k} \boldsymbol{r}_{el}\cdot\boldsymbol{v}\, d\Omega + \sum_{\gamma\in\Gamma_{int}\bigcup\Gamma_N} \int_\gamma \boldsymbol{r}_{sing}\cdot\boldsymbol{v}\, d\Gamma. \tag{5}$$

These two components of the residual reveal the existence of two different error sources, the elementary and singular residuals. The former is associated with the lack of verification of the differential equation in the interior of the elements, the latter with the non verification of the continuity requirements of the stress field. The main rationale of the explicit residual error estimates consists in evaluating this two terms separately.

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The energy norm of the error, $\|\boldsymbol{e}\|$, is taken as a global measure of the error. This is the norm induced by $a(\cdot,\cdot)$ or $\overline{a}(\cdot,\cdot)$ when applied to stresses, namely

$$\|\boldsymbol{e}\|^2 = a(\boldsymbol{e},\boldsymbol{e}) = \overline{a}(\boldsymbol{\sigma}_e,\boldsymbol{\sigma}_e) = |||\boldsymbol{\sigma}_e|||^2,$$

where $\boldsymbol{\sigma}_e$ is the error in stresses $\boldsymbol{\sigma}_e := \boldsymbol{\sigma}(\boldsymbol{u}) - \boldsymbol{\sigma}(\boldsymbol{u}^h)$.

2.2. Assessing the energy norm of the error

A first step in a posteriori assessment is estimating the error measured in the energy norm, that is obtaining a good approximation of $\boldsymbol{\sigma}_e$ and computing $\|\boldsymbol{e}\|$. This translates in finding a new stress field $\boldsymbol{\sigma}^\star$ based on the information at hand, that is $\boldsymbol{\sigma}(\boldsymbol{u}^h)$, and such that $\boldsymbol{\sigma}^\star$ approximates the actual stresses $\boldsymbol{\sigma}(\boldsymbol{u})$ much better than $\boldsymbol{\sigma}(\boldsymbol{u}^h)$. Thus, a computable error estimate is readily obtained

$$\boldsymbol{\sigma}_e \approx \boldsymbol{\sigma}_e^\star = \boldsymbol{\sigma}^\star - \boldsymbol{\sigma}(\boldsymbol{u}^h),$$

yielding also the corresponding energy norm estimate $|||\boldsymbol{\sigma}_e^\star|||^2 = \overline{a}(\boldsymbol{\sigma}_e^\star,\boldsymbol{\sigma}_e^\star) \approx \|\boldsymbol{e}\|^2$.

The stress field $\boldsymbol{\sigma}^\star$ is said to be statically admissible if it is continuous (at least in the normal components to the discontinuity surface, that is without traction jumps) and it fulfills the equilibrium equations (1a) and (1b). This is equivalent to say that for all the virtual displacements $\boldsymbol{v} \in \mathcal{V}$

$$\overline{a}(\boldsymbol{\sigma}^\star,\boldsymbol{\sigma}(\boldsymbol{v})) = l(\boldsymbol{v}). \tag{6}$$

Note that the solution of (6) is not unique because $\boldsymbol{\sigma}^\star$ is not assumed to fulfill any compatibility condition, in other words $\boldsymbol{\sigma}^\star$ does not necessarily derive from a displacement field following (3).

A statically admissible stress field $\boldsymbol{\sigma}^\star$ produces an energy norm estimate $|||\boldsymbol{\sigma}_e^\star|||$ larger than (or equal to) $\|\boldsymbol{e}\|$. The error estimation technique providing this kind of error approximation is referred as an upper bound error estimator. The upper bound property of the statically admissible stress field is readily derived by considering $\boldsymbol{v} = \boldsymbol{e}$ in (2) and (6), thus

$$\overline{a}(\boldsymbol{\sigma}(\boldsymbol{u}),\boldsymbol{\sigma}_e) = l(\boldsymbol{e}) = \overline{a}(\boldsymbol{\sigma}^\star,\boldsymbol{\sigma}_e)$$

and subtracting $\overline{a}(\boldsymbol{\sigma}(\boldsymbol{u}^h),\boldsymbol{\sigma}_e)$ in both sides

$$\overline{a}(\boldsymbol{\sigma}_e,\boldsymbol{\sigma}_e) = \overline{a}(\boldsymbol{\sigma}_e^\star,\boldsymbol{\sigma}_e),$$

which yields $|||\boldsymbol{\sigma}_e||| \leq |||\boldsymbol{\sigma}_e^\star|||$ by simply considering the Cauchy-Schwarz inequality.

Thus, the key issue in any error estimation technique is to produce a properly enhanced stress field $\boldsymbol{\sigma}^\star$. Moreover, if $\boldsymbol{\sigma}^\star$ is build up such that it is statically admissible, then this additional feature confers to the estimator the upper bound property. The strategies producing the enhanced stresses $\boldsymbol{\sigma}^\star$ are classified into two categories: recovery type estimators and implicit residual type estimators, which are discussed in sections 3 and 4.

It is worth remarking that, in general, the enhanced stress $\boldsymbol{\sigma}^\star$ and the corresponding stress error $\boldsymbol{\sigma}_e^*$ can only be used to evaluate the energy norm of the error, and no other quantities. In particular, any magnitude based on the displacement error cannot be evaluated using $\boldsymbol{\sigma}^\star$.

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2.3. Quantities of interest, adjoint problem and error representation

Assessing the energy norm of the error is not sufficient for many applications. In practice, the finite element user is interested in specific magnitudes extracted from the global solution by some post-process. These magnitudes are referred as *quantities of interest* or *functional outputs*. Goal-oriented error assessment strategies aim at estimating the error committed in these quantities and possibly providing bounds for it.

The quantities of interest considered here are linear functional outputs of the solution, $l^{\mathcal{O}}(\boldsymbol{u})$. In particular, those expressed in the form

$$l^{\mathcal{O}}(\boldsymbol{u}) = \int_{\Omega} \boldsymbol{b}^{\mathcal{O}} \cdot \boldsymbol{u}\, d\Omega + \int_{\Gamma_N} \boldsymbol{t}^{\mathcal{O}} \cdot \boldsymbol{u}\, d\Gamma + a(\boldsymbol{u}, \boldsymbol{\chi}^{\mathcal{O}}), \tag{7}$$

where $\boldsymbol{b}^{\mathcal{O}}$, $\boldsymbol{t}^{\mathcal{O}}$ and $\boldsymbol{\chi}^{\mathcal{O}}$ are given functions characterizing the quantity of interest. Note that $l^{\mathcal{O}}(\cdot)$ has the same structure as the right-hand side of (2). The extension to nonlinear outputs is discussed in Xuan et al., 2006.

This expression is pretty general and accounts for a large variety of quantities of interest. The first term in (7) is a weighted average of the displacements, being $\boldsymbol{b}^{\mathcal{O}}$ the weight. Note that this average is restricted to the support of $\boldsymbol{b}^{\mathcal{O}}$ which is in practice the way of indicating the zone of interest. Similarly, the second term in (7) accounts for averaged displacements along a part of the Neumann boundary. Note that displacements on the Dirichlet boundary, Γ_D, are known a priori and therefore it makes not sense to include in the quantity of interest averaged displacements on Γ_D. On the contrary, tractions on Γ_D are generally interesting for the end-users, as they are reaction forces on the supports. In fact, this kind of quantities are accounted by the third term in (7). At first sight, the third term in (7) only represents an average of the stresses in the interior of the domain of study. However, a proper choice of function $\boldsymbol{\chi}^{\mathcal{O}}$ allows also representing traction averages along Γ_D. This is readily demonstrated by noting that

$$\int_{\Gamma_D} \boldsymbol{\chi}^{\mathcal{O}} \cdot (\boldsymbol{\sigma}(\boldsymbol{u}) \cdot \boldsymbol{n})\, d\Gamma = a(\boldsymbol{u}, \boldsymbol{\chi}^{\mathcal{O}}) - \int_{\Gamma_N} \boldsymbol{t} \cdot \boldsymbol{\chi}^{\mathcal{O}}\, d\Gamma - \int_{\Omega} \boldsymbol{b} \cdot \boldsymbol{\chi}^{\mathcal{O}}\, d\Omega. \tag{8}$$

Equation (8) is obtained after the usual algebraic manipulation, using the weighted residuals technique into the original equation (1), taking $\boldsymbol{\chi}^{\mathcal{O}}$, which does not vanish on Γ_D, as weighting function. It is clear from (8) that the third term in (7) is a traction average on Γ_D plus a computable term involving part of the data.

The expression (7) allows also determining pointwise quantities by using functions of the Dirac delta type although in practice smeared versions are preferred (averages in neighborhoods of the point) in order to avoid singularities.

The objective of the goal-oriented error assessment is to estimate the value of $l^{\mathcal{O}}(\boldsymbol{e})$ which, for linear outputs, coincides with $l^{\mathcal{O}}(\boldsymbol{u}) - l^{\mathcal{O}}(\boldsymbol{u}_H)$.

As pointed out in the previous section, the enhanced stresses $\boldsymbol{\sigma}^{\star}$ can only be used to assess the energy norm of the error. Thus, an error representation is needed to express the error in the quantity of interest in terms of the energy error. This error representation requires introducing an auxiliary problem, denoted as *adjoint* or *dual* problem by different authors . This problem reads: find $\boldsymbol{\psi} \in \mathcal{V}$ such that

$$a(\boldsymbol{v}, \boldsymbol{\psi}) = l^{\mathcal{O}}(\boldsymbol{v}), \text{ for all } \boldsymbol{v} \in \mathcal{V}. \tag{9}$$

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Note that the adjoint solution $\boldsymbol{\psi}$ lies in the space $\mathcal{V}$ (that is vanishes on Γ_D) and that, for the sake of clarity, the order of the arguments in $a(\cdot,\cdot)$ is switched with respect to the original equation (2). The numerical solution of the adjoint problem (9), $\boldsymbol{\psi}^h$, has the associated error $\boldsymbol{\varepsilon} := \boldsymbol{\psi} - \boldsymbol{\psi}^h$. These auxiliary functions are introduced such that the following error representation holds:

$$l^{\mathcal{O}}(\boldsymbol{e}) = a(\boldsymbol{e}, \boldsymbol{\psi}) = a(\boldsymbol{e}, \boldsymbol{\varepsilon}).$$

This error representation allows bounding the error in terms of the energy norm of the errors in the direct and adjoint problem. This is a direct consequence of the Cauchy-Schwarz inequality, namely

$$|l^{\mathcal{O}}(\boldsymbol{e})| = |a(\boldsymbol{e}, \boldsymbol{\varepsilon})| \leq \|\boldsymbol{e}\| \, \|\boldsymbol{\varepsilon}\|. \tag{10}$$

An obvious error bound for the quantity of interest follows: $l^{\mathcal{O}}(\boldsymbol{e})$ ranges between $\pm\|\boldsymbol{e}\| \, \|\boldsymbol{\varepsilon}\|$. Thus, an upper bound of the quantity of interest (in absolute value) is obtained if upper bounds for $\|\boldsymbol{e}\|$ and $\|\boldsymbol{\varepsilon}\|$ are available. The sharpness of this upper and lower bounding of the error in the quantity of interest is improved by considering the so-called parallelogram identity:

$$l^{\mathcal{O}}(\boldsymbol{e}) = \frac{1}{4}\|\kappa\boldsymbol{e} + \frac{1}{\kappa}\boldsymbol{\varepsilon}\|^2 - \frac{1}{4}\|\kappa\boldsymbol{e} - \frac{1}{\kappa}\boldsymbol{\varepsilon}\|^2 \tag{11}$$

standing for any non-zero factor κ. It follows from (11) that an upper bound for $l^{\mathcal{O}}(\boldsymbol{e})$ is obtained by combining an upper bound for $\|\kappa\boldsymbol{e} + \frac{1}{\kappa}\boldsymbol{\varepsilon}\|$ and a lower bound for $\|\kappa\boldsymbol{e} - \frac{1}{\kappa}\boldsymbol{\varepsilon}\|$ (using zero as a lower bound is a not sharp but robust option). Conversely a lower bound for $l^{\mathcal{O}}(\boldsymbol{e})$ is obtained by combining a lower bound for $\|\kappa\boldsymbol{e} + \frac{1}{\kappa}\boldsymbol{\varepsilon}\|$ and an upper bound for $\|\kappa\boldsymbol{e} - \frac{1}{\kappa}\boldsymbol{\varepsilon}\|$. In practice, if the lower bounds are properly assessed, this alternative is much sharper than using only (10) and usually allows determining the sign of $l^{\mathcal{O}}(\boldsymbol{e})$ because both upper and lower bounds may have the same sign.

Note that the energy norm assessment and energy bounds for the direct (or primal) and adjoint problems (or the combined problems yielding $\kappa\boldsymbol{e} \pm \frac{1}{\kappa}\boldsymbol{\varepsilon}$) are the basic underlying tools for goal oriented assessment.

3. RECOVERY ESTIMATES

The so-called *recovery* or *flux projection* error estimates use a simple postprocess technique to recover an enhanced stress field, $\boldsymbol{\sigma}^\star$, as introduced in 2.2. Using the pioneering idea introduced in Zienkiewicz and Zhu, 1987, $\boldsymbol{\sigma}^\star$ is straightforwardly computed as a least squares fitting of $\boldsymbol{\sigma}(\boldsymbol{u}^h)$.

Note that the computed stresses $\boldsymbol{\sigma}(\boldsymbol{u}^h)$ are discontinuous across the interelement edges or sides. The corresponding traction jumps are in fact the basis for the singular residual, $\boldsymbol{r}_{\text{sing}}$, as shown in (5), and one of the error sources. Note also that the stresses inside the elements are computed from the derivatives of the displacements and therefore they are of lower polynomial degree: for linear elements stresses are piecewise constant, for quadratic elements stresses are linear... This is related with the interior residual $\boldsymbol{r}_{\text{el}}$: for instance, for linear elements $\boldsymbol{r}_{\text{el}} = \boldsymbol{b}$. It is clear that in order to enhance the stresses one has to smooth out the discontinuities (suppress traction jumps) and to increase the polynomial degree of the stress approximation inside the elements.

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This objective is easily reached by describing the stresses with the same functional description used for the displacements. A discrete space for the stresses $\mathcal{S}^h$ is introduced such that every component of the stress field is described using the same interpolation as the components of $\mathcal{U}^h$: functions in $\mathcal{S}^h$ are of the same type as functions in $\mathcal{U}^h$ (continuous and piecewise polynomial).

Thus, the recovered stress $\boldsymbol{\sigma}^\star$ is selected in $\mathcal{S}^h$ such that it minimizes the error $\boldsymbol{\sigma}^\star - \boldsymbol{\sigma}(\boldsymbol{u}^h)$ in a least squares sense. Following this basic idea, different fitting criteria have been introduced by different authors. Among the more popular it is worth mentioning the SPR (Super Patch Recovery) introduced in Zienkiewicz and Zhu, 1987. The SPR is based on the local polynomial fitting of the stress field in patches of elements. The locally fitted stress is evaluated at the nodal points to determine the nodal values of $\boldsymbol{\sigma}^\star \in \mathcal{S}^h$.

A different approach to recovery estimates was introduced in Wiberg et al., 1996 for structural dynamics. In this context the stress recovery does not suffice to compute the error; the error in displacements and velocities is also required. Thus, a technique enhancing the displacement approximation provided by the FEM is introduced. This technique follows the same rationale: the displacements $\boldsymbol{u}^h$ are less regular than expected (mathematically speaking they are $\mathcal{C}^0$ and not $\mathcal{C}^1$) and their local polynomial degree is eventually too low. The enhanced displacements $\boldsymbol{u}^\star$ are build-up as a post-process of $\boldsymbol{u}^h$ increasing the regularity requirements and the enriching the degree of the local polynomial description. This is essentially performed at every element of the mesh assessing the local curvatures of the solution, fitting a least squares polynomial in a patch of elements centered in the element under study. Recently, this approach has been found to be applicable in the goal-oriented framework where, in order to assess the error in the quantity of interest using the representation $l^{\mathcal{O}}(\boldsymbol{e}) = R(\boldsymbol{\varepsilon})$, an approximation of the error in the adjoint problem, $\boldsymbol{\varepsilon}$, is needed in terms of displacements (stresses are not sufficient), see Díez and Calderón, 2007.

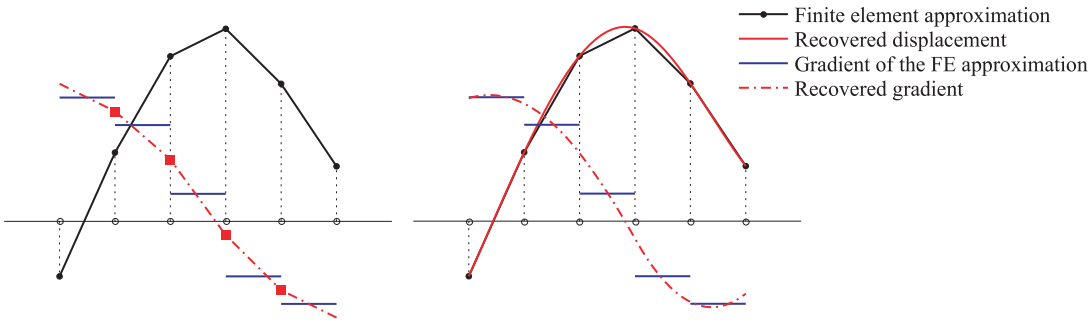

Figure 2. Illustration of the flux projection (left) and enhancement of displacement (right) recovery estimates

4. RESIDUAL TYPE ESTIMATES

As suggested by their name, residual type estimators assess the error using the residual, either using expression (5) (explicit residual estimates) or solving approximately (4) (implicit residual estimates).

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4.1. Explicit estimates

Explicit estimates are based on the decomposition of the weak residual discussed in remark 1. The computable elementary residual $\boldsymbol{r}_{\rm el}$ and singular residual $\boldsymbol{r}_{\rm sing}$ are seen as the two sources of error. Explicit estimates are based on postprocessing these two quantities and getting an approximation to the error. Thus, the estimate does not require solving any local problem and is computed directly from the finite element approximation. The input data of the problem to be solved is required to compute the elementary residual, and the part of the singular residual associated with the Neumann boundary. Note that this information is not used in the recovery estimates discussed in section 3, which are computed using only $\boldsymbol{\sigma}(\boldsymbol{u}^h)$ and no use is made of the data of the original problem.

The idea of explicit residual estimates uses (5) for $v = e - \Pi^h e$ (Π^h stands for the interpolation operator in $\mathcal{V}^h$) together with the Cauchy-Schwarz inequality and the a priori interpolation estimates. Cooking all these ingredients, the following expression is found (see Ainsworth and Oden, 2000 for a detailed derivation)

$$\|\boldsymbol{e}\|^2 \leq C \left(\sum_{k=1}^{n_{\rm el}} h_k^2 ||\boldsymbol{r}_{\rm el}||^2_{\mathcal{L}^2(\Omega_k)} + \sum_{\gamma \in \Gamma_{\rm int} \bigcup \Gamma_N} h_\gamma ||\boldsymbol{r}_{\rm sing}||^2_{\mathcal{L}^2(\gamma)} \right), \tag{12}$$

where C is a constant related with the interpolation estimates, generally unknown. Note that each residual is scaled with the local mesh sizes, h_k (element size) and h_γ (edge size), with different exponents arising also from the interpolation estimates. The right-hand side term in (12) is naturally decomposed into elementary contributions and, except for the unknown constant C, it is computable once $\boldsymbol{u}^h$ is obtained.

These estimates are computationally costless and very useful for adaptive procedures where it is important to identify the parts of the domain contributing to the error. Constant C is seen as a single (unknown) multiplicative factor and the local contributions of the elements are therefore properly assessed in a relative basis. Nevertheless, the global value of the error norm is only assessed up to the determination of C. Of course, C could also be estimated and even bounded but in general explicit estimates cannot produce guaranteed upper bounds for $\|\boldsymbol{e}\|$.

4.2. Implicit estimates

Implicit estimators aim at avoiding the disadvantages of explicit estimates by solving the original error equation (4) in a local basis. That is, typically in small domains (the elements or patches of elements) in which a local version of (4) is solved numerically. This requires locally increasing the resolution with respect to the original approximation in $\mathcal{U}^h$. The implicit estimates are classified in different categories, depending on

- the domain in which the local problem is stated: element residual methods (solved element by element) and subdomain residual methods (solved in patches of elements, either centered in nodes or elements)
- the boundary conditions imposed on the local problems: either Dirichlet or Neumann. Roughly speaking, the Dirichlet methods provide continuous approximations to the displacement error and lower bounds of the energy and the Neumann methods yield statically admissible stress fields and upper bounds of the energy error

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- the numerical method used to approximate the solution of the local problem: either a standard FE method providing a displacement based approximation of the error (producing the so-called asymptotic estimates which have bounding properties only with respect to a reference solution, not with respect to the exact error) or a dual approach yielding an approximation of the stress field exactly fulfilling the equilibrium equations (producing guaranteed or strict error bounds).

It is worth mentioning here the pioneering work of Ladevèze introducing the error estimators based in the concept of constitutive relation error, see Ladevèze and Leguillon, 1983. This family of error estimators is classified here in the implicit residual framework, together with the estimators solving elementary problems with Neumann boundary conditions, because it perfectly matches the category. The rationale for the presentation and the derivation of these techniques is however pretty different. Following this line of thought, based also in mechanical arguments, strategies to generalize these tools to nonlinear and transient problems have been suggested, see Chamoin and Ladevèze, 2008.

An alternative approach fitting also the implicit residual philosophy are the so-called *dual global solvers*. This strategy is based on the ideas introduced by Fraeijs de Veubeke, 1965. A statically admissible stress field $\boldsymbol{\sigma}^\star$ is obtained by means of a global computation over a discrete space $\mathcal{S}^h$ (where the stresses are interpolated). This requires solving a global optimization problem reading: find $\boldsymbol{\sigma}^\star \in \mathcal{S}^h$ such that the complementary energy $|||\boldsymbol{\sigma}^\star|||^2 = \overline{a}\big(\boldsymbol{\sigma}^\star, \boldsymbol{\sigma}^\star\big)$ is minimum, with the additional restriction of being statically admissible, see (6). Thus, the statically admissible stress field $\boldsymbol{\sigma}^\star$ produces an upper bound energy norm estimate, overestimating $\|\boldsymbol{e}\|$, see section 2.2. Moreover, this error bound is the sharper you can get in $\mathcal{S}^h$. Thus, estimates based on *dual global solvers* are generally sharp. Nevertheless, the global nature of the dual approximation makes them computationally expensive. Both the element residual methods and the subdomain residual methods are alternatives based on solving only local problems and, consequently, providing upper bounds of the error at an affordable computational cost.

4.3. Element residual method; equilibrated residual estimates

The local version of the error equation (4) in the element Ω_k of the mesh states that the restriction of the error $\boldsymbol{e}$ to Ω_k fulfills

$$a_k\big(\boldsymbol{e}, \boldsymbol{v}\big) = l_k\big(\boldsymbol{v}\big) - a_k\big(\boldsymbol{u}^h, \boldsymbol{v}\big) + \int_{\partial\Omega_k \setminus \partial\Omega} \big(\boldsymbol{\sigma}(\boldsymbol{u}) \cdot \boldsymbol{n}\big) \cdot \boldsymbol{v}\, d\Gamma \tag{13}$$

for all v taking values in Ω_k. Subscript k in the linear and bilinear forms indicates that the corresponding integrals are restricted to Ω_k. Note that the last term of the right-hand side stands for the local Neumann boundary conditions and depends on the unknown traction associated with the exact solution. Note also that the local error stress field $\boldsymbol{\sigma}(\boldsymbol{e})$ fulfills a variant of (13), substituting the left-hand side term by $\overline{a}_k\big(\boldsymbol{\sigma}(\boldsymbol{e}), \boldsymbol{\sigma}(\boldsymbol{v})\big)$.

In order to obtain a solvable local problem, the unknown boundary traction $\boldsymbol{\sigma}(\boldsymbol{u}) \cdot \boldsymbol{n}$ on the boundary of Ω_k is replaced by some approximated value $\boldsymbol{g}_k$ that has to be determined on all the interelement edges. Thus, the local equation for the approximated stress error, $\boldsymbol{\sigma}_e^\star$ is

$$\overline{a}_k\big(\boldsymbol{\sigma}_e^\star, \boldsymbol{\sigma}(\boldsymbol{v})\big) = l_k\big(\boldsymbol{v}\big) - a_k\big(\boldsymbol{u}^h, \boldsymbol{v}\big) + \int_{\partial\Omega_k \setminus \partial\Omega} \boldsymbol{g}_k \cdot \boldsymbol{v}\, d\Gamma. \tag{14}$$

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In order to provide statically admissible stresses, the approximated traction $\boldsymbol{g}_k$ has to fulfill two properties

1. on the common edge of two contiguous elements Ω_k and $\Omega_{k'}$, $\boldsymbol{g}_k = -\boldsymbol{g}_{k'}$ (this is to guarantee the continuity of the traction associated with $\boldsymbol{\sigma}^\star$)
2. the boundary traction must be in equilibrium with the interior loads. This *compatibility condition* is needed to ensure that the problem (14) is solvable.

The compatibility condition requires $\boldsymbol{g}_k$ to fulfill

$$l_k(\boldsymbol{v}) - a_k(\boldsymbol{u}^h, \boldsymbol{v}) + \int_{\partial\Omega_k \setminus \partial\Omega} \boldsymbol{g}_k \cdot \boldsymbol{v} d\Gamma = 0 \tag{15}$$

for any rigid body motion $\boldsymbol{v}$ (in 2D, this means $\boldsymbol{v}$ taking the values of the two translations $\boldsymbol{t}_x$ and $\boldsymbol{t}_y$ and the rotation $\boldsymbol{\theta}$). If this condition is fulfilled, problem (14) is solvable (the solution exists, even if it is not unique). Any of the solutions of this problem produces an upper bound estimate.

The first idea to determine $\boldsymbol{g}_k$ was introduced by Bank and Weiser, 1985 and consists in taking $\boldsymbol{g}_k$ equal to the average of the numerical normal traction, computed from $\boldsymbol{\sigma}(\boldsymbol{u}^h)$. This is equivalent to assume that $\boldsymbol{\sigma}(\boldsymbol{u}) \cdot \boldsymbol{n} \approx \langle \boldsymbol{\sigma}(\boldsymbol{u}^h) \rangle_{\text{ave}} \cdot \boldsymbol{n}$ on the interelement edges. This option fulfills the continuity restriction but fails guaranteing the compatibility condition (15). To overcome this problem, Bank and Weiser, 1985 propose the following work-around: the test function $\boldsymbol{v}$ in problem (14) is taken in a restricted functional space of functions vanishing at the vertex nodes of element Ω_k. This simple approach only yields statically admissible estimates stresses $\boldsymbol{\sigma}_e^\star$ if the error on the nodes of the mesh is zero. This is not the general case and consequently if this strategy is used, the upper bound property cannot be guaranteed. An alternative also devised in Bank and Weiser, 1985 consists in replacing in the right-hand side of (14) $\boldsymbol{v}$ by $\boldsymbol{v} - \Pi^h \boldsymbol{v}$. This automatically guarantees that the local problem is compatible (or equilibrated) and preserves the global upper bound property. The global property is kept because subtracting $\Pi^h \boldsymbol{v}$ in the argument of $R(\cdot)$ (the right-hand side of (4)) does not change the error equation. This smart operation can also be seen as an implicit way of recovering a compatible traction $\boldsymbol{g}_k$.

This is the basis of the so-called *equilibrated residual estimates*. In fact, this family of estimators introduces efficient and practical algorithms for constructing equilibrated fluxes, that is recovering $\boldsymbol{g}_k$ by solving only local problems. The compatibility condition (15) is at the first sight a global restriction, involving the tractions on all the element boundaries. If the equilibrated residual methods are among the most popular implicit residual type estimators is because the computation of the tractions $\boldsymbol{g}_k$ is decoupled node to node. Using a smart representation of $\boldsymbol{g}_k$, the nodal contributions to $\boldsymbol{g}_k$ on all the edges converging in a given node are computed independently, and it requires solving a small linear system of equations as indicated in Ainsworth and Oden, 1993; Ladevèze and Leguillon, 1983; Ladevèze et al., 1991; Ladevèze and Maunder, 1996; Sauer-Budge et al., 2004; Parés et al., 2006.

4.4. Subdomain residual methods; flux-free estimates

The effectivity of the equilibrated residual method depends on the quality of the local tractions $\boldsymbol{g}_k$. For instance, the dual-global estimates are usually much sharper than the equilibrated residual estimates. Moreover, although computing $\boldsymbol{g}_k$ as indicated above is computationally

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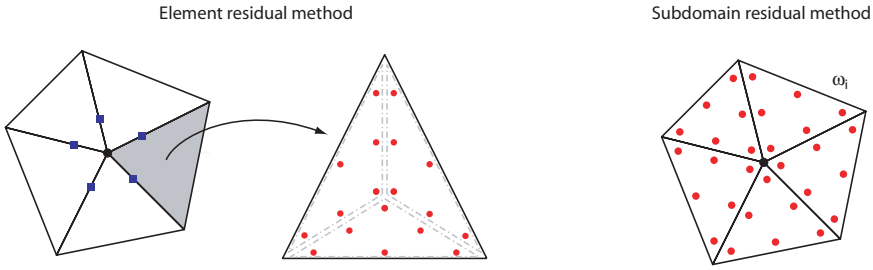

Figure 3. Illustration of the element residual method (left) and the subdomain residual method (right). In the element residual method the contribution to the tractions $\boldsymbol{g}_k$ of every node of the mesh (represented by the blue squares) are computed in a nodal basis. Then, the tractions $\boldsymbol{g}_k$ are used to solve the local elementary problems and the stresses inside the element fulfilling the equilibrium are determined. Subdomain residual method: a larger local problem is solved for each node of the mesh but no equilibrated tractions have to be computed. The red circles represent the degrees of freedom describing the approximated stresses.

inexpensive because the local problems are decoupled, the implementation of the equilibration techniques is often involved and difficult to generalize to different element types or space dimensions.

The subdomain residual methods are introduced as an alternative to equilibrated residual methods such that:

- they preclude solving a global problem (the local equations are posed in different subdomains, patches of elements surrounding a node, also denoted as *stars*)
- they provide upper bound estimates
- they circumvent the necessity of finding proper tractions as boundary conditions for the local problems. The local boundary conditions are *natural* and the estimates are also said to be *flux-free*.

In order to localize the error equation (4), use is made of the partition of unity property. Let ϕ_i be the linear finite element interpolation function associated with the i-th vertex node of the mesh. Note that these functions sum up to the unity and that the support of ϕ_i is precisely the patch of elements containing this node, ω_i. Thus, a local version of (4) in ω_i, providing a local approximation $\boldsymbol{\sigma}_e^{\star i}$ of the stress error, is readily recovered as

$$\overline{a}_{\omega^i}\left(\boldsymbol{\sigma}_e^{\star i}, \boldsymbol{\sigma}(\boldsymbol{v})\right) = R(\phi_i \boldsymbol{v}) \tag{16}$$

for all $\boldsymbol{v}$ taking values in ω_i, being $\overline{a}_{\omega^i}(\cdot,\cdot)$ the restriction of $\overline{a}(\cdot,\cdot)$ to ω_i. The sum of the local approximations to the stress error $\boldsymbol{\sigma}_e^{\star i}$ provide a statically admissible stress field $\boldsymbol{\sigma}_e$ and its corresponding error norm is a sharp upper bound of the error, see Parés et al., 2006. The local problem (16) is automatically equilibrated in most of the cases because the right-hand side vanishes for $\boldsymbol{v}$ equal to a rigid body motion. In the unique case in which this equilibrium is not automatically guaranteed (linear elements for structural mechanics) a straightforward modification is introduced to ensure solvability, see Parés et al., 2006.

Similar approaches are developed taking $\overline{a}_{\omega^i}(\cdot,\cdot)$ as a locally weighted version of $\overline{a}(\cdot,\cdot)$, see Carstensen and Funken, 1999; Machiels et al., 2000; Morin et al., 2003. In this case the upper bound estimate is obtained adding the squared norms of the local contributions rather than

adding the functions and computing the norm afterwards. The estimates obtained following this rationale are not as sharp as the ones obtained taking $\overline{a}_{\omega^i}(\cdot,\cdot)$ as simple restriction of $\overline{a}(\cdot,\cdot)$.

4.5. Lower bounds for the energy using implicit Dirichlet estimates

Recall that in order to get sharp bounds of the error in the quantities of interest using (11), it is important to obtain lower bounds of the energy norm of the error. Any continuous approximation of the displacement error, $\boldsymbol{e}^\star \in \mathcal{V}$, is such that $R(\boldsymbol{e}^\star)\|\boldsymbol{e}^\star\|^{-1} \leq \|\boldsymbol{e}\|$. This is a direct consequence of taking $\boldsymbol{v} = \boldsymbol{e}^\star$ in (4) (this is only possible if $\boldsymbol{e}^\star$ is continuous) and use the Cauchy-Schwarz inequality. Thus, a lower bound is easily recovered after $\boldsymbol{e}^\star$.

The simplest way of guaranteeing continuity by solving local residual problems is to use homogeneous Dirichlet boundary conditions (prescribe displacements equal to zero) on the boundary of the local subdomains. This idea was used in Díez et al., 1998 solving such problems elementwise and then complementing the estimate by adding the contribution of a new family of subdomains overlapping the elements while keeping the lower bound property in the resulting error assessment.

The continuous estimate $\boldsymbol{e}^\star$ can also be obtained using the recovery techniques proposed in section 3 or postprocessing the local solution of the residual type estimates based on Neumann local problems as described in Díez et al., 2003. Obviously, the quality of the resulting lower bound depends on how well $\boldsymbol{e}^\star$ approximates $\boldsymbol{e}$, in particular, for $\boldsymbol{e}^\star = \boldsymbol{e}$, $R(\boldsymbol{e}^\star)\|\boldsymbol{e}^\star\|^{-1} = \|\boldsymbol{e}\|$ and the estimate is therefore exact.

5. CLOSURE

The main techniques assessing the error associated with the FE discretization have been briefly reviewed. The tools available are progressively being incorporated in the FE commercial codes. From the end-user viewpoint, it is extremely important to have at hand one of these tools in order to evaluate the quality of the FE solution provided by the code. Ideally, the paradigm for the FE practitioner is to certify the quality of the solution for a given quantity of interest. The subsequent step is to adapt the mesh and design the optimal FE discretization, giving the desired answer with the prescribed accuracy at the minimum cost.

Adaptive strategies use the local error assessment to find the optimal element size in every zone of the domain. This can be done converting the local error into a desired element size using ad-hoc expressions derived from a priori estimates, see Díez and Calderón, 2007; Vidal et al., 2008. Then, a new mesh has to be build-up from scratch. A different approach consists in detecting the elements that need to be refined and refine the mesh keeping the structure of the previous one. If both upper and lower bounds of the quantity of interest are available, this can be done in terms of the local contribution to the bound gap. This local contribution is found to be positive in all the elements and, consequently, it can be used to assess which elements have to be refined. A complete description of the adaptive procedures is provided in a companion chapter of this Encyclopedia.

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