VI International Conference on Adaptive Modeling and Simulation
ADMOS 2013
J. P. Moitinho de Almeida, P. Díez, C. Tiago and N. Parés (Eds)

EXPLICIT EXPRESSIONS OF DUAL LOADS FOR ACCURATE ERROR ESTIMATION AND BOUNDING IN GOAL ORIENTED ADAPTIVITY

J.J. Ródenas*, E. Nadal*, O.A. González-Estrada†, F.J. Fuenmayor*, S.P.A. Bordas†, and P. Kerfriden†

*Centro de Investigación en Tecnología de Vehículos (CITV)
Universitat Politècnica de València ,C/ Vera, S/n, E-46022-Valencia, Spain
e-mail: {jjrodena, ffuenmay}@mcm.upv.es, ennaso@upvnet.upv.es

†Institute of Mechanics & Advanced Materials,
Cardiff University, School of Engineering, Queen's Building, The Parade, Cardiff CF24 3AA
Wales, UK.
e-mail: {bordass, estradaoag}@cardiff.ac.uk, pierre.kerfriden@gmail.com

Key words: Quantities of Interest, Error estimator, Goal oriented adaptivity

Abstract. Recently, Goal Oriented Adaptivity (GOA) has been an active research area because of its advantages in terms of computational cost and accuracy. This technique consists in solving two Finite Element (FE) problems: the primal one, which is the actual problem and the dual one, which is an auxiliary problem depending on the Quantity of Interest (QoI).

To improve the quality of the error estimate in the QoI we consider a recovery-based procedure which enforces local equilibrium for an accurate stress representation. The proposed procedure requires the explicit expressions for the dual loads which, traditionally, are not obtained in the FE framework. Our objective in this paper is to obtain those explicit expressions for the dual problem for the extraction of linear QoI in the context of linear elasticity. The ZZ-type error estimator is used to evaluate the error in the QoI at element level, yielding a high quality, as shown in the numerical tests.

1 Introduction

The Finite Element (FE) solution is a numerical approximation to the unknown exact solution of a Boundary Value Problem (BVP), thus, there exists an *error* due to the discretization. The most widely used way to estimate the discretization error is to evaluate it in terms of the global energy. A great effort has been devoted since the very beginning by researchers in order to obtain good approximations or even sharp upper bounds for the global error measurement in energy norm [1, 2, 3, 4, 5, 6, 7].

These error estimators were based on the evaluation of an approximation to the true error in energy norm. However, for practitioners this quantity is, in general, not very useful from an industrial point of view. In practice, analysts run simulations in order to evaluate stresses, displacements, *etc...* in a particular area of the domain. In the late 90s, a new paradigm appeared [8, 9, 10] where, instead of evaluating the error of the solution in terms of energy, the error is evaluated in terms of a Quantity of Interest (QoI) in a Domain of Interest (DoI). That is, some relevant quantity are considered as the main output. Then, we directly control the error of the QoI in the DoI. The error estimation of a QoI requires solving two problems simultaneously, the first one is called primal problem and is the one we are interested in. The second problem, called dual or adjoint problem, serves to extract the information for the error in the QoI. Both problems are geometrically identical and differ on the applied loads. Those of the dual problem depend on the DoI and the QoI. The construction of the dual problem will be explained later in more detail.

Our approach to obtain estimations of the error in the QoI, in contrast to previous techniques, is based on the use of equilibrated recovered fields obtained for the solution of both, the primal and the dual problem. The proposed procedure begins with the evaluation of displacement recovered fields considering: the fulfilment of boundary and internal equilibrium equations, Dirichlet constraints and, for singular problems, the splitting of the displacement and stress fields into singular and smooth parts, as described in [11]. Similar recovery techniques considering stresses were previously used to obtain upper bounds of the error in energy norm in [12, 13]. For the recovery procedure we need the analytical expressions defining the loads for the primal and dual problems. Thus, for the dual problem, we must obtain the analytical expressions related to the QoI required during the recovery process.

Numerical tests using 2D benchmark problems with exact solution are used to investigate the quality of the proposed technique. Results for different quantities of interest show that the technique provides excellent error estimates which can be used in goal oriented adaptive procedures.

2 Problem Statement

2.1 Primal problem

In this section we briefly present the model for the 2D linear elasticity problem. Denote, in vectorial form, $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ as the stresses and strains, $\mathbf{D}$ as the elasticity matrix of the constitutive relation $\boldsymbol{\sigma} = \mathbf{D}\boldsymbol{\varepsilon}$, and $\mathbf{u}$ the unknown displacement field, which take values in $\Omega \subset \mathbb{R}^2$. $\mathbf{u}$ is the solution of the boundary value problem given by:

$$\begin{aligned}
\mathbf{S}\mathbf{u} &= -\mathbf{b} && \text{in } \Omega && (1)\\
\boldsymbol{\epsilon}(\mathbf{u}) &= \mathbf{L}\mathbf{u} && \text{in } \Omega && (2)\\
\mathbf{G}\boldsymbol{\sigma}(\mathbf{u}) &= \mathbf{t} && \text{on } \Gamma_N && (3)\\
\mathbf{u} &= \bar{\mathbf{u}} && \text{on } \Gamma_D, && (4)
\end{aligned}$$

Γ_N and Γ_D denote the Neumann and Dirichlet boundaries with $\partial\Omega = \overline{\Gamma_N \cup \Gamma_D}$ and $\Gamma_N \cap \Gamma_D = \emptyset$, $\mathbf{b}$ are body loads and $\mathbf{t}$ are the tractions imposed along Γ_N. $\mathbf{S} = \mathbf{L}^T\mathbf{D}\mathbf{L}$, being $\mathbf{L}$ the differential operator, and $\mathbf{G}$ is the projection operator that projects the stress field into tractions over any boundary with outward normal vector $\mathbf{n} = \{n_x \; n_y\}^T$:

$$\mathbf{L} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{bmatrix} \tag{5}$$

$$\mathbf{G} = \begin{bmatrix} n_x & 0 & n_y \\ 0 & n_y & n_x \end{bmatrix} \tag{6}$$

Consider the initial stresses $\boldsymbol{\sigma}_0$ and strains $\boldsymbol{\varepsilon}_0$, the symmetric bilinear form $a : (V + \bar{\mathbf{u}}) \times V \rightarrow \mathbb{R}$ and the continuous linear form $\ell : V \rightarrow \mathbb{R}$ defined by:

$$a(\mathbf{u},\mathbf{v}) := \int_\Omega \boldsymbol{\sigma}^T(\mathbf{u})\boldsymbol{\varepsilon}(\mathbf{v})\mathrm{d}\Omega = \int_\Omega \boldsymbol{\sigma}^{\mathrm{T}}(\mathbf{u})\mathbf{D}^{-1}\boldsymbol{\sigma}(\mathbf{v})\mathrm{d}\Omega \tag{7}$$

$$\ell(\mathbf{v}) := \int_\Omega \mathbf{v}^T\mathbf{b}\mathrm{d}\Omega + \int_{\Gamma_\mathrm{N}} \mathbf{v}^{\mathrm{T}}\mathbf{t}\mathrm{d}\Gamma + \int_\Omega \boldsymbol{\sigma}^{\mathrm{T}}(\mathbf{v})\boldsymbol{\varepsilon}_0\mathrm{d}\Omega - \int_\Omega \boldsymbol{\varepsilon}^{\mathrm{T}}(\mathbf{v})\boldsymbol{\sigma}_0\mathrm{d}\Omega. \tag{8}$$

With these notations, the variational form of the problem reads [14]:

$$\text{Find } \mathbf{u} \in (V + \bar{\mathbf{u}}) : \forall \mathbf{v} \in V \quad a(\mathbf{u},\mathbf{v}) = \ell(\mathbf{v}) \tag{9}$$

where V is the standard test space for the elasticity problem such that $V = \{\mathbf{v} \mid \mathbf{v} \in [H^1(\Omega)]^2, \mathbf{v}|_{\Gamma_D}(\mathbf{x}) = \mathbf{0}\}$.

Let $\mathbf{u}^h$ be a finite element approximation of $\mathbf{u}$. The solution for the discrete counterpart of the variational problem in (9) lies in a subspace $(V^h + \bar{\mathbf{u}}) \subset (V + \bar{\mathbf{u}})$ associated with a mesh of finite elements of characteristic size h, and it is such that:

$$\forall \mathbf{v}^h \in V^h \subset V \qquad a(\mathbf{u}^h, \mathbf{v}^h) = \ell(\mathbf{v}^h). \tag{10}$$

Consider the linear elasticity problem given in (9) and its approximate FE solution $\mathbf{u}^h \in V^h \subset V$. This problem is related to the original problem to be solved, that henceforth will be called the *primal problem*.

2.2 Dual problem

Now, let us define $Q : V \rightarrow \mathbb{R}$ as a bounded linear functional representing some quantity of interest, acting on the space V of admissible functions for the problem at hand. The objective is to estimate the error in $Q(\mathbf{u})$ when calculated using the value of the approximate solution $\mathbf{u}^h$:

$$Q(\mathbf{u}) - Q(\mathbf{u}^h) = Q(\mathbf{u} - \mathbf{u}^h) = Q(\mathbf{e}). \tag{11}$$

As will be shown later, $Q(\mathbf{v})$ may be interpreted as the work associated with a displacement field $\mathbf{v}$ and a distribution of forces specific to each type of quantity of interest. If we particularise $Q(\mathbf{v})$ for $\mathbf{v} = \mathbf{u}$, this force distribution will allow us to extract information concerning the quantity of interest associated with the solution of the problem in (9).

A standard procedure [15] to evaluate $Q(\mathbf{e})$ consists in solving the auxiliary *dual* problem (also called *adjoint* or *extraction* problem) defined as:

$$\text{Find } \mathbf{w} \in V : \forall \mathbf{v} \in V \quad a(\mathbf{v}, \mathbf{w}) = Q(\mathbf{v}). \tag{12}$$

An exact representation for the error $Q(\mathbf{e})$ in terms of the solution of the dual problem can be simply obtained by substituting $\mathbf{v} = \mathbf{e}$ in (12) and remarking that for all $\mathbf{w}_Q^h \in V^h$, due to the Galerkin orthogonality, $a(\mathbf{e}, \mathbf{w}_Q^h) = 0$ such that:

$$Q(\mathbf{e}) = a(\mathbf{e}, \mathbf{w}) = a(\mathbf{e}, \mathbf{w}) - \cancelto{0}{a(\mathbf{e}, \mathbf{w}^h)} = a(\mathbf{e}, \mathbf{w} - \mathbf{w}^h) = a(\mathbf{e}, \boldsymbol{\epsilon}). \tag{13}$$

Therefore, the error in evaluating $Q(\mathbf{u})$ using $\mathbf{u}^h$ is given by:

$$Q(\mathbf{u}) - Q(\mathbf{u}^h) = Q(\mathbf{e}) = a(\mathbf{e}, \boldsymbol{\epsilon}) = \int_\Omega \left(\boldsymbol{\sigma}_p - \boldsymbol{\sigma}_p^h\right) \mathbf{D}^{-1} \left(\boldsymbol{\sigma}_d - \boldsymbol{\sigma}_d^h\right) \mathrm{d}\Omega, \tag{14}$$

where $\boldsymbol{\sigma}_p$ is the stress field associated with the solution of the primal problem and $\boldsymbol{\sigma}_d$ is the one associated with the dual problem. Using the Zienkiewicz and Zhu (ZZ) error estimator [16] and (14) we can derive an estimate for the error in the QoI which reads:

$$Q(\mathbf{e}) \approx Q(\mathbf{e}_{es}) = \int_\Omega \left(\boldsymbol{\sigma}_p^* - \boldsymbol{\sigma}_p^h\right) \mathbf{D}^{-1} \left(\boldsymbol{\sigma}_d^* - \boldsymbol{\sigma}_d^h\right) \mathrm{d}\Omega, \tag{15}$$

where $\boldsymbol{\sigma}_p^*$ and $\boldsymbol{\sigma}_d^*$ represent the recovered stress fields for the primal and dual problems, respectively. Here, we expect to have a sharp estimate of the error in the QoI if the recovered stress fields are accurate approximations to their exact counterparts.

In order to obtain accurate representations of the exact stress fields both for the primal and dual solutions, we propose the use of a locally equilibrated displacement recovery technique, called SPR-CD, based on the ideas in [17, 11, 13]. This technique, which is an enhancement of the Superconvergent Patch Recovery (SPR) proposed in [18], enforces the fulfillment of the internal, boundary equilibrium equations and Dirichlet boundary conditions locally on patches. For problems with singularities the stress field is also decomposed into two parts: smooth and singular, which are separately recovered.

3 Quantities of Interest

The recovery procedure based on the SPR technique and denoted as SPR-CD, fully described in [19], relies on the *a priori* known values of $\mathbf{b}$, $\mathbf{t}$, $\boldsymbol{\varepsilon}_0$, $\boldsymbol{\sigma}_0$ and Dirichlet boundary conditions to impose the internal and boundary equilibrium equations and the exact displacements over Γ_D. Regarding the loads, these values are already available for the primal problem ($\mathbf{b}_p$ and $\mathbf{t}_p$). However, the body forces $\mathbf{b}_d$, boundary tractions $\mathbf{t}_d$, etc... are not known for the dual problem. We can easily derive expressions associated to certain linear QoIs, *e.g.* the mean values of displacements and stresses in a sub-domain of interest Ω_i, which can be interpreted in terms of $\mathbf{b}_d$ and $\mathbf{t}_d$. This approach was first introduced in [20] and presented later in [21]. Similarly, in [22] the authors defined the relation between the natural quantities of interest and dual loading data.

3.1 Mean displacement in Ω_i

Let us assume that the objective is to evaluate the mean value of the displacements along the direction α in a sub-domain of interest $\Omega_i \subset \Omega$. The functional for the quantity of interest can be written as:

$$Q(\mathbf{u}) = \bar{u}_\alpha|_{\Omega_i} = \frac{1}{|\Omega_i|}\int_{\Omega_i} \mathbf{u}^T \mathbf{c}_{u_\alpha} \mathrm{d}\Omega, \tag{16}$$

where $|\Omega_i|$ is the volume of Ω_i and $\mathbf{c}_{u_\alpha}$ is a vector used to select the appropriate combination of components of $\mathbf{u}$. For example, $\mathbf{c}_{u_\alpha} = \{1, 0\}^T$ if α is parallel to the x-axis. Now, considering $\mathbf{v} \in V$ in (16) results in:

$$Q(\mathbf{v}) = \int_{\Omega_i} \mathbf{v}^T \left(\frac{\mathbf{c}_{u_\alpha}}{|\Omega_i|}\right) \mathrm{d}\Omega = \int_{\Omega_\mathrm{i}} \mathbf{v}^\mathrm{T} \mathbf{b}_\mathrm{d} \mathrm{d}\Omega. \tag{17}$$

Note that the term $\mathbf{c}_{u_\alpha}/|\Omega_i|$ formally corresponds to a vector of body forces in the problem defined in (9). Therefore, we can say that $\mathbf{b}_d = \mathbf{c}_{u_\alpha}/|\Omega_i|$ is a constant vector of body loads that applied in the sub-domain of interest Ω_i can be used in the dual problem to extract the mean displacements.

3.2 Mean displacement along Γ_i

For the case where the quantity of interest is the functional that evaluates the mean value of the displacements along a given boundary Γ_i the expression reads:

$$Q(\mathbf{u}) = \bar{u}_\alpha|_{\Gamma_i} = \frac{1}{|\Gamma_i|}\int_{\Gamma_i} \mathbf{u}^T \mathbf{c}_{u_\alpha} \mathrm{d}\Gamma, \tag{18}$$

$|\Gamma_i|$ being the length of Γ_i and $\mathbf{c}_{u_\alpha}$ a vector used to select the appropriate component of $\mathbf{u}$. Again, considering $\mathbf{v} \in V$ in (18) we have:

$$Q(\mathbf{v}) = \int_{\Gamma_i} \mathbf{v}^T \left(\frac{\mathbf{c}_{u_\alpha}}{|\Gamma_i|}\right) \mathrm{d}\Gamma = \int_{\Gamma_\mathrm{i}} \mathbf{v}^\mathrm{T} \mathbf{t}_\mathrm{d} \mathrm{d}\Gamma \tag{19}$$

Note that the term $\mathbf{c}_{u_\alpha}/|\Gamma_i|$ can be interpreted as a vector of tractions applied along the boundary in the problem defined in (9). Thus, $\mathbf{t}_d = \mathbf{c}_{u_\alpha}/|\Gamma_i|$ is a vector of tractions applied on Γ_i that can be used in the dual problem to extract the mean displacements along Γ_i.

3.3 Mean stresses and strains in Ω_i

In the case that our QoI is the mean stress (or strains) in Ω_i we can define the QoI (20) where $\mathbf{c}_{\sigma_\alpha}^T$ is a vector to choose any linear combination of the stress (strain) components.

$$Q(\mathbf{u}) = \bar{\sigma}_\alpha|_{\Omega_i} = \frac{1}{|\Omega_i|}\int_{\Omega_i} \mathbf{c}_{\sigma_\alpha}^T \boldsymbol{\sigma} \mathrm{d}\Omega = \int_{\Omega_\mathrm{i}} \frac{\mathbf{c}_{\sigma_\alpha}^\mathrm{T}}{|\Omega_\mathrm{i}|}\boldsymbol{\sigma}\mathrm{d}\Omega \tag{20}$$

Comparing the last integral in (20) with (8) we can define $\boldsymbol{\epsilon}_{0,d} = \mathbf{c}_{\sigma_\alpha}^T/|\Omega_i|$ corresponding to the term of initial strains that we need to apply in the dual problem to extract the value of $\bar{\sigma}_\alpha|_{\Omega_i}$. A similar formulation can be derived for the case of the mean strains in Ω_i such that $\boldsymbol{\sigma}_{0,d} = \mathbf{c}_{\epsilon_\alpha}^T/|\Omega_i|$. Note that the loads for the dual problem of this QoI could also be obtained applying the divergence theorem, yielding tractions along the boundary of the DoI which are equivalent to the initial strains.

3.4 Mean tractions along Γ_i

Let $\mathbf{t} = \{t_n, t_t\}^T$, with t_n and t_t the normal and tangential components of the tractions vector $\mathbf{t}$. Let us assume that we want to evaluate, for example, the mean normal tractions along boundary Γ_i. The functional that defines the mean tractions along the boundary Γ_i can be expressed as

$$Q(\mathbf{u}) = \bar{\mathbf{t}}_n = \frac{1}{|\Gamma_i|}\int_{\Gamma_i} \mathbf{t}^T\mathbf{c}\mathrm{d}\Gamma \tag{21}$$

Using (21) and considering the extraction vector $\mathbf{c}$ and the rotation matrix $\mathbf{R}_\Gamma$ that aligns the tractions normal to the boundary Γ_i we have:

$$\begin{aligned}\bar{\mathbf{t}}_n &= \frac{1}{|\Gamma_i|}\int_{\Gamma_i} \mathbf{t}^T\mathbf{c}\mathrm{d}\Gamma = \frac{1}{|\Gamma_\mathrm{i}|}\int_{\Gamma_\mathrm{i}} \begin{Bmatrix} t_n & t_t \end{Bmatrix} \begin{Bmatrix} 1 \\ 0 \end{Bmatrix} \mathrm{d}\Gamma = \\ &= \frac{1}{|\Gamma_i|}\int_{\Gamma_i} \begin{Bmatrix} t_x & t_y \end{Bmatrix} \mathbf{R}_\Gamma^T \begin{Bmatrix} 1 \\ 0 \end{Bmatrix} \mathrm{d}\Gamma = \int_{\Gamma_\mathrm{i}} \begin{Bmatrix} t_x & t_y \end{Bmatrix} \frac{\mathbf{R}_\Gamma^\mathrm{T}}{|\Gamma_\mathrm{i}|} \begin{Bmatrix} 1 \\ 0 \end{Bmatrix} \mathrm{d}\Gamma = \int_{\Gamma_\mathrm{i}} \begin{Bmatrix} t_x & t_y \end{Bmatrix} \mathbf{u}_\mathrm{d}\mathrm{d}\Gamma\end{aligned} \tag{22}$$

In (22) the term $\mathbf{u}_d = \mathbf{R}_\Gamma^T\mathbf{c}/|\Gamma_i|$ corresponds to a vector of displacements used as Dirichlet boundary conditions for the dual problem used to extract the mean value of the normal tractions along Γ_i.

Note that in this case $\bar{\mathbf{w}}_Q = \mathbf{u}_d \neq 0$, then (13) does not hold. We redefine the dual problem in (12), $\forall \mathbf{v} \in V$, such that:

$$\begin{aligned} a(\mathbf{v}, \mathbf{w}_Q) &= 0 \quad \text{in } \Omega \\ \mathbf{w}_Q &= \mathbf{u}_d \quad \text{on } \Gamma_i \end{aligned} \tag{23}$$

The dual solution can be expressed as $\mathbf{w}_Q = \mathbf{w}_Q^0 + \bar{\mathbf{w}}_Q$, where $\mathbf{w}_Q^0 = 0$ on Γ_i. Assuming that $\bar{\mathbf{w}}_Q = \mathbf{u}_d$ is in the FE solution space, the FE approximation for (23) is also decomposed into two parts $\mathbf{w}_Q^h = \mathbf{w}_Q^{h0} + \bar{\mathbf{w}}_Q$ where, again, $\mathbf{w}_Q^{h0} = 0$ on Γ_i. Therefore, we have for the dual problem:

$$\forall \mathbf{v} \in V \quad a(\mathbf{v}, \mathbf{w}_Q^0) = -a(\mathbf{v}, \bar{\mathbf{w}}_Q) \tag{24}$$

Substituting $\mathbf{v} = \mathbf{e}$ in (24), using the Galerkin orthogonality property, $a(\mathbf{e}, \mathbf{w}_Q^{h0}) = 0$, and considering that $\mathbf{e}_Q^0 = \mathbf{e}_Q$ we write:

$$a(\mathbf{e}, \mathbf{w}_Q^0 - \mathbf{w}_Q^{h0}) = a(\mathbf{e}, \mathbf{e}_Q^0) = a(\mathbf{e}, \mathbf{e}_Q) = -a(\mathbf{e}, \bar{\mathbf{w}}_Q) \tag{25}$$

Similarly, the QoI can also be rewritten by means of the divergence theorem. Thus, generalizing (22) $\forall \mathbf{v} \in V$ we have:

$$Q(\mathbf{v}) = \int_{\Gamma_i} (\mathbf{G}\boldsymbol{\sigma}(\mathbf{v}))^T \mathbf{u}_d \, \mathrm{d}\Gamma = \int_{\Omega_\mathrm{i}} \boldsymbol{\sigma}(\mathbf{v})^\mathrm{T} \epsilon(\mathbf{u}_\mathrm{d}) \, \mathrm{d}\Omega = \mathrm{a}(\mathbf{v}, \mathbf{u}_\mathrm{d}) \tag{26}$$

Thus, $Q(\mathbf{e}) = a(\mathbf{e}, \mathbf{u}_d) = a(\mathbf{e}, \bar{\mathbf{w}}_Q)$ and substituting in (25) we obtain the error for this QoI: $Q(\mathbf{e}) = -a(\mathbf{e}, \mathbf{e}_Q)$.

3.5 Generalized stress intensity factor in Ω_i

The Generalized Stress Intensity Factor (GSIF) K is the characterizing parameter in problems with singularities. The GSIF is a multiplicative constant that depends on the loading of the problem and linearly determines the intensity of the displacement and stress fields in the vicinity of the singular point. In the particular case that the corners that produce the singularities have an angle of 2π, this parameter is called the Stress Intensity Factor (SIF).

Let us consider the general singular problem of a V-notch domain subjected to loads in the infinite. The analytical solution for this singular elasticity problem can be found in [23] where, considering a polar reference system centred in the corner, the displacement and stress fields at points sufficiently close to the corner can be described as:

$$\mathbf{u}(r, \phi) = K_\mathrm{I} r^{\lambda_\mathrm{I}} \boldsymbol{\Psi}_\mathrm{I}(\lambda_\mathrm{I}, \phi) + K_\mathrm{II} r^{\lambda_\mathrm{II}} \boldsymbol{\Psi}_\mathrm{II}(\lambda_\mathrm{II}, \phi) \tag{27}$$

$$\boldsymbol{\sigma}(r, \phi) = K_\mathrm{I} \lambda_\mathrm{I} r^{\lambda_\mathrm{I}-1} \boldsymbol{\Phi}_\mathrm{I}(\lambda_\mathrm{I}, \phi) + K_\mathrm{II} \lambda_\mathrm{II} r^{\lambda_\mathrm{II}-1} \boldsymbol{\Phi}_\mathrm{II}(\lambda_\mathrm{II}, \phi) \tag{28}$$

where r is the radial distance to the corner, λ_m (with $m = \mathrm{I}, \mathrm{II}$) are the eigenvalues that determine the order of the singularity, $\boldsymbol{\Psi}_m$ and $\boldsymbol{\Phi}_m$ are sets of trigonometric functions that depend on the angular position ϕ, and K_m are the Generalised Stress Intensity Factors (GSIFs). For the evaluation of the GSIF we consider the expression shown in [24]:

$$K^{(1,2)} = -\frac{1}{C} \int_{\Omega^*} \left[\left(u_x^{(2)} \frac{\partial q}{\partial x} \right) \sigma_{xx}^{(1)} + \left(u_y^{(2)} \frac{\partial q}{\partial y} \right) \sigma_{yy}^{(1)} + \left(u_x^{(2)} \frac{\partial q}{\partial y} + u_y^{(2)} \frac{\partial q}{\partial x} \right) \sigma_{xy}^{(1)} \right.$$
$$\left. - \left(\sigma_{xx}^{(2)} \frac{\partial q}{\partial x} + \sigma_{xy}^{(2)} \frac{\partial q}{\partial y} \right) u_x^{(1)} - \left(\sigma_{xy}^{(2)} \frac{\partial q}{\partial x} + \sigma_{yy}^{(2)} \frac{\partial q}{\partial y} \right) u_y^{(1)} \right] \mathrm{d}\Omega, \tag{29}$$

where $u^{(1)}$, $\sigma^{(1)}$ are the displacement and stress fields from the FEM solution, $u^{(2)}$, $\sigma^{(2)}$ are the auxiliary fields associated with the extraction functions for the GSIFs in mode I or mode II, q is an arbitrary function used to define the extraction zone, which is one at the singular point and 0 on the boundaries. x_j refers to the local coordinates system at the crack tip. For more details we refer the reader to [24].

Rearranging terms of the integral in (29), we can obtain:

$$K^{(1,2)} = \int_{\Omega} \mathbf{u}^{(1)^T} \left(-\frac{1}{C}\right) \begin{bmatrix} \sigma_{xx}^{(2)} q_{,1} + \sigma_{xy}^{(2)} q_{,2} \\ \sigma_{xy}^{(2)} q_{,1} + \sigma_{yy}^{(2)} q_{,1} \end{bmatrix} + \boldsymbol{\sigma}^{(1)^T} \left(-\frac{1}{C}\right) \begin{bmatrix} u_x^{(2)} q_{,1} \\ u_y^{(2)} q_{,2} \\ u_y^{(2)} q_{,1} + u_x^{(2)} q_{,2} \end{bmatrix} \mathrm{d}\Omega \quad (30)$$

where $q_{,1} = \partial q / \partial x$ and $q_{,2} = \partial q / \partial y$. Rewriting the previous expression we obtain:

$$K^{(1,2)} = \int_{\Omega} \left(\mathbf{u}^{(1)^T} \mathbf{A} + \boldsymbol{\sigma}^{(1)^T} \mathbf{B} \right) \mathrm{d}\Omega \quad (31)$$

Thus, if we replace $\mathbf{u}$ by a vector of arbitrary displacements $\mathbf{v}$, the quantity of interest can be defined as:

$$Q(\mathbf{v}) = \int_{\Omega} \mathbf{v}^T \mathbf{b}_d \mathrm{d}\Omega + \int_{\Omega} \mathbf{L}\mathbf{v}^T \mathbf{D} \boldsymbol{\varepsilon}_{0d} \mathrm{d}\Omega \quad (32)$$

where $\mathbf{A}$ has been replaced by the dual body forces $\mathbf{b}_d$ and the term $\mathbf{B}$ has been replaced by the vector of initial strains $\boldsymbol{\varepsilon}_{0d}$. It must be taken into account that these expressions can be used either for mode I or mode II.

4 Numerical examples

To verify the influence of the analytical dual loads we compare the standard SPR with our new approach, called SPR-CD, using a singular problem. Plane strain and 2D linear elastic behavior are considered. A bilinear (Q4) h-adaptive refinement process, guided by the error in the quantity of interest, has been considered in all examples. To assess the performance of the recovery procedure and error indicators we have considered some quantities: *i*) the global effectivity θ that indicates the relation between the exact error $Q(\mathbf{e})$ and the estimated error $Q(\mathbf{e}_{es})$:

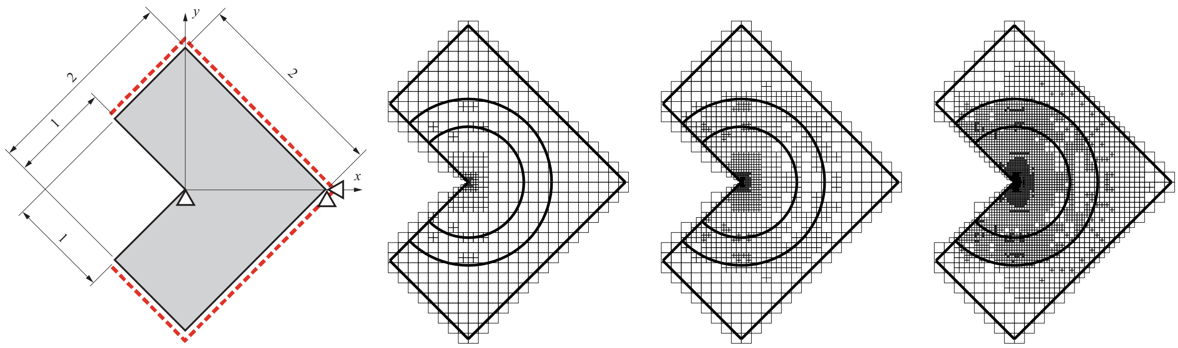
$$\theta = \frac{Q(\mathbf{e}_{es}) - Q(\mathbf{e})}{|Q(\mathbf{e})|}, \quad (33)$$

with positive values meaning overestimation of the error and negative values underestimation, and *ii*) the error in the QoI η_{QoI} which is the relation between the estimated and exact value of the QoI according to the next expression:

$$\eta_{QoI} = \frac{Q(\mathbf{u}^h) + Q(\mathbf{e}_{es})}{Q(\mathbf{u})} \quad (34)$$

4.1 Problem 1. L-Shape plate

The problem model is in Figure 1a. The model is loaded on the boundary with the tractions corresponding to the first symmetric term of the asymptotic expansion that describes the exact solution under mode I or II loading conditions around the singular vertex. The exact displacement and stress fields for the singular elastic problem can be found in [23]. Material parameters are elastic modulus $E = 1000$ and Poisson's ratio $\nu = 0.3$. As we are solving a singular problem, for the recovery we use the *singular+smooth* technique described in [11]. For this problem we consider the GSIF as the QoI, that is K_{I} or K_{II}. When K_{I} is the QoI the primal problem is loaded with $K_{\mathrm{I}} = 1$ and $K_{\mathrm{II}} = 0$, and with $K_{\mathrm{I}} = 0$ and $K_{\mathrm{II}} = 1$ when K_{II} is the QoI. In Figure 1 we present a set of h-adapted meshes for K_{I}. We represent in Figure 2, for K_{I} and K_{II}, the results of the proposed



(a) Problem model (b) Mesh 2 (c) Mesh 3 (d) Mesh 4

Figure 1: Problem 1. L-Shape plate. Sequence of the h-adaptive refinement process guided by the error in the QoI K_{I}.

recovery procedure (SPR-CD) using the analytical expressions of the dual loads, and the standard SPR. The smoother and more accurate behavior of the novel procedure,is clearly shown in both the effectivity of the error estimator and the indicator for the QoI.

5 Conclusions

In this work we have presented a methodology to obtain the analytical expressions for the loads of the dual problem, which are required by the equilibrated displacement recovery technique we are using to locally equilibrate the recovered dual stress field. The error estimation is performed by using a ZZ-type error estimator, thus, the quality of the recovered solutions is critical. Numerical results have shown the importance of equilibrating the recovered solutions for the primal and dual problem in order to provide the sharp error estimates presented.

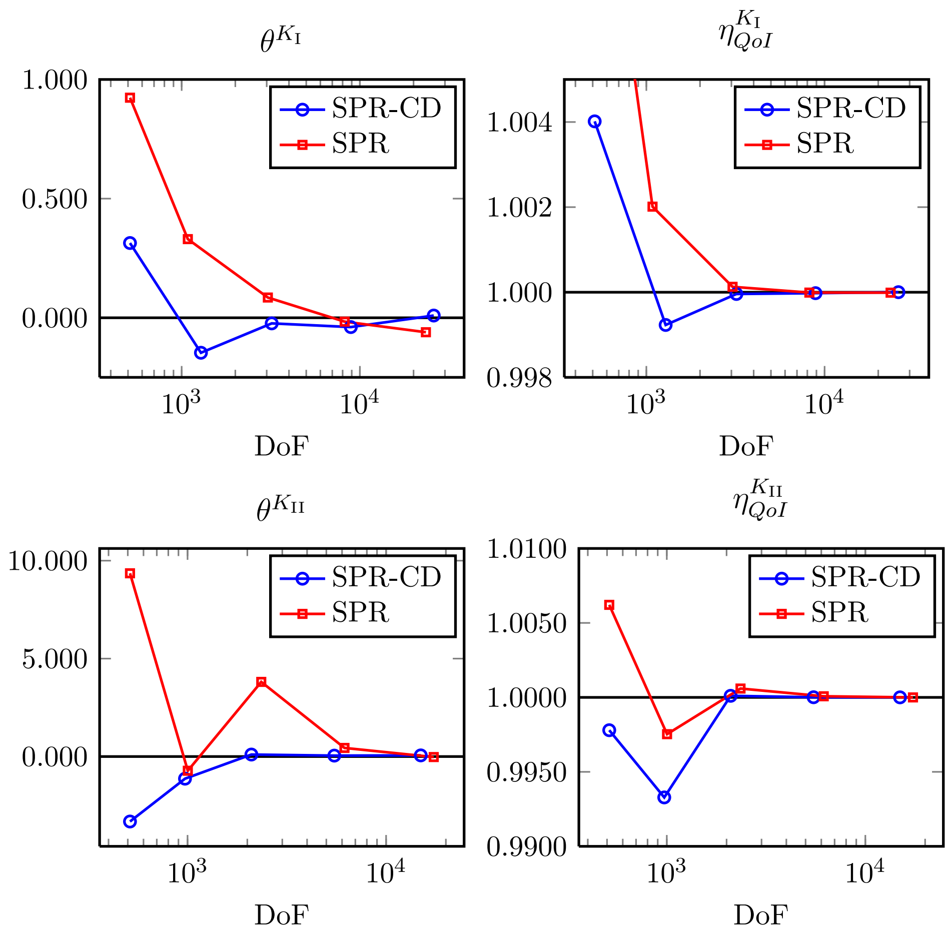


Figure 2: Problem 1. K_{I} and K_{II}. Evolution of the global effectivites

ACKNOWLEDGEMENTS

The authors acknowledge the support of the research project DPI2010-20542 of the Ministerio de Economía y Competitividad (Spain), the FPU program (AP2008-01086), the funding from Universitat Politècnica de València and Generalitat Valenciana (PROMETEO/2012/023), the EPSRC grant EP/G042705/1 and the Framework Programme 7 Initial Training Network Funding under grant number 289361 "Integrating Numerical Simulation and Geometric Design Technology."

REFERENCES

[1] Babuška I. Error-Bounds for Finite Element Method. *Numerische Mathematik* 1970; **16**:322–333.

[2] Babuška I, Rheinboldt WC. A-posteriori error estimates for the finite element method. *International Journal for Numerical Methods in Engineering* 1978;

12(10):1597–1615.

[3] Ladevèze P, Leguillon D. Error estimate procedure in the finite element method and applications. *SIAM Journal on Numerical Analysis* 1983; **20**(3):485–509.

[4] Díez P, Parés N, Huerta A. Recovering lower bounds of the error by postprocessing implicit residual a posteriori error estimates. *International Journal for Numerical Methods in Engineering* Mar 2003; **56**(10):1465–1488.

[5] Pereira OJBA, de Almeida JPM, Maunder EAW. Adaptive methods for hybrid equilibrium finite element models. *Computer Methods in Applied Mechanics and Engineering* 1999; **176**(1-4):19–39.

[6] Almeida OJB, Moitinho JP. A posteriori error estimation for equilibrium finite elements in elastostatic problems. *Computer Assisted Mechanics and Engineering Sciences* 2001; **8**(2-3):439–453.

[7] Moitinho JP, Maunder EAW. Recovery of equilibrium on star patches using a partition of unity technique. *International journal for ...* 2009; **79**:1493–1516.

[8] Ainsworth M, Oden JT. *A posteriori Error Estimation in Finite Element Analysis*. John Wiley & Sons: Chichester, 2000.

[9] Paraschivoiu M, Peraire J, Patera AT. A posteriori finite element bounds for linear-functional outputs of elliptic partial differential equations. *Computer Methods in Applied Mechanics and Engineering* 1997; **150**(1-4):289–312.

[10] Ladevèze P, Rougeot P, Blanchard P, Moreau JP. Local error estimators for finite element linear analysis. *Computer Methods in Applied Mechanics and Engineering* 1999; **176**(1-4):231–246.

[11] Ródenas JJ, González-Estrada OA, Tarancón JE, Fuenmayor FJ. A recovery-type error estimator for the extended finite element method based on singular+smooth stress field splitting. *International Journal for Numerical Methods in Engineering* 2008; **76**(4):545–571.

[12] Díez P, Ródenas JJ, Zienkiewicz OC. Equilibrated patch recovery error estimates: simple and accurate upper bounds of the error. *International Journal for Numerical Methods in Engineering* 2007; **69**(10):2075–2098.

[13] Ródenas JJ, González-Estrada OA, Díez P, Fuenmayor FJ. Accurate recovery-based upper error bounds for the extended finite element framework. *Computer Methods in Applied Mechanics and Engineering* 2010; **199**(37-40):2607–2621.

[14] Verfürth R. A review of a posteriori error estimation techniques for elasticity problems. *Computational Methods in Applied Mechanics and Engineering* 1999; **176**:419–440.

[15] Oden JT, Prudhomme S. Goal-oriented error estimation and adaptivity for the finite element method. *Computers & Mathematics with Applications* 2001; **41**(5-6):735–756.

[16] Zienkiewicz OC, Zhu JZ. A simple error estimator and adaptive procedure for practical engineering analysis. *International Journal for Numerical Methods in Engineering* 1987; **24**(2):337–357.

[17] Ródenas JJ, Tur M, Fuenmayor FJ, Vercher A. Improvement of the superconvergent patch recovery technique by the use of constraint equations: the SPR-C technique. *International Journal for Numerical Methods in Engineering* 2007; **70**(6):705–727.

[18] Zienkiewicz OC, Zhu JZ. The superconvergent patch recovery and a posteriori error estimates. Part 1: The recovery technique. *International Journal for Numerical Methods in Engineering* 1992; **33**(7):1331–1364.

[19] Nadal E, González-Estrada OA, Ródenas JJ, Bordas SPA, Fuenmayor FJ. Error estimation and error bounding in energy norm based on a displacement recovery technique. *6th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2012)*, Eccomas, 2012.

[20] Ródenas JJ. Goal Oriented Adaptivity: Una introducción a través del problema elástico lineal. *Technical Report*, CIMNE, PI274, Barcelona, Spain 2005.

[21] González-Estrada OA, Ródenas JJ, Nadal E, Bordas SPA, Kerfriden P. Equilibrated patch recovery for accurate evaluation of upper error bounds in quantities of interest. *Adaptive Modeling and Simulation. Proceedings of V ADMOS 2011*, Aubry D, Díez P, Tie B, Parés N (eds.), CINME: Paris, 2011.

[22] Verdugo F, Díez P, Casadei F. Natural quantities of interest in linear elastodynamics for goal oriented error estimation and adaptivity. *Adaptive Modeling and Simulation. Proceedings of V ADMOS 2011*, Aubry D, Díez P, Tie B, Parés N (eds.), CIMNE: Paris, 2011.

[23] Szabó BA, Babuška I. *Finite Element Analysis*. John Wiley & Sons: New York, 1991.

[24] Ródenas JJ, Giner E, Tarancón JE, González-Estrada OA. A recovery error estimator for singular problems using singular+smooth field splitting. *Fifth International Conference on Engineering Computational Technology*, Topping BHV, Montero G, Montenegro R (eds.), Civil-Comp Press: Stirling, Scotland, 2006.