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ERROR ESTIMATION IN QUANTITIES OF INTEREST FOR XFEM USING RECOVERY TECHNIQUES

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ABSTRACT

Error estimators that measure the error in a quantity of interest defined by the analyst, instead of the energy norm, have become increasingly popular as they provide an error indicator for goal oriented adaptivity procedures. We propose an a posteriori recovery-based error estimation technique which considers the stress intensity factor K typical of singular problems as the quantity of interest for the extended finite element method. The recovery procedure relies on the use of an enhanced superconvergent patch recovery technique to evaluate highly accurate recovered stress fields for the primal and dual problems, which are then used to obtain a sharp error estimate. The results indicate an accurate estimation of the error in K for benchmark problems with exact solution.

1 INTRODUCTION

The validation and quality assessment of the results obtained using numerical simulations is a critical area of research, specially relevant in sectors as nuclear power generation, chemical and aerospace.

In the context of linear elastic fracture mechanics, the failure of structures is characterized by the stress intensity factors (SIF) associated with the crack propagation phenomena. A standard SPR recovery technique used to obtain an error measure of the J-integral, which is closely related to the value of the SIF, has been previously presented for the finite element (FE) context in [1]. However, it does not consider any equilibrium constraints or the singularity near the crack tip, thus the obtained recovered stress field is not well suited for this kind of problems.

We proposed a procedure that relies on the enhanced superconvergent patch recovery technique presented in [2] to evaluate highly accurate recovered stress fields of the primal and dual problems, which are then used to obtain a sharp error estimate in extended finite element approximations. The primal problem is simply the problem at hand and the dual problem is used to extract information related to the quantity of interest. To formulate the dual problem we consider the linear equivalent domain integral representing K to obtain the applied loads of the dual FE approximation. The high accuracy of the recovered stress fields for both the primal and dual solutions is obtained by decomposing the raw stress field obtained from the finite element approximations into singular and smooth parts, and enforcing the fulfilment of boundary and internal equilibrium equations.

2 ERROR ESTIMATION IN QUANTITIES OF INTEREST

Consider the linear elasticity problem including a crack and its approximate FE solution $\mathbf{u}^h \in V^h \subset V$ as the *primal problem* to be solved.

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 goal is to estimate the error in $Q(\mathbf{u})$ when calculated using the value of the approximate solution $\mathbf{u}^h$:

$$Q(\mathbf{u}) - Q(\mathbf{u}^h) = Q(\mathbf{u} - \mathbf{u}^h) = Q(\mathbf{e}) \tag{1}$$

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

$$\text{Find } \mathbf{w}_Q \in V : a(\mathbf{v}, \mathbf{w}_Q) = Q(\mathbf{v}) \quad \forall \mathbf{v} \in V. \tag{2}$$

It can be proven that the error in evaluating $Q(\mathbf{u})$ using $\mathbf{u}^h$ is given by

$$Q(\mathbf{u}) - Q(\mathbf{u}^h) = Q(\mathbf{e}) = a(\mathbf{e}, \mathbf{e}_Q) = \int_\Omega \left(\boldsymbol{\sigma}_p - \boldsymbol{\sigma}_p^h\right) \mathbf{D}^{-1} \left(\boldsymbol{\sigma}_d - \boldsymbol{\sigma}_d^h\right) \mathrm{d}\Omega \tag{3}$$

where $\boldsymbol{\sigma}_p$ is the stress field associated with the primal solution and $\boldsymbol{\sigma}_d$ is the one associated with the dual solution. Using the expression for the Zienkiewicz-Zhu error estimator in [3] with (3) we can derive an estimate for the error in the QoI which reads

$$Q(\mathbf{e}) \approx Q(\mathbf{e}_{es}) = \int_\Omega \left(\boldsymbol{\sigma}_p^* - \boldsymbol{\sigma}_p^h\right) \mathbf{D}^{-1} \left(\boldsymbol{\sigma}_d^* - \boldsymbol{\sigma}_d^h\right) \mathrm{d}\Omega \tag{4}$$

2.1 Recovery technique

As noted above, a widely used technique to control the error in the energy norm in the FE discretization is the Zienkiewicz-Zhu error estimator [3], which is based on the recovery of an enhanced stress field $\boldsymbol{\sigma}^*$. It results clear that the accuracy of such estimation relies on the quality of the recovered field. In this work we consider the SPR-CX recovery technique, which is an enhancement of the error estimator introduced in [4]. The technique incorporates the ideas in [5] to guarantee locally on patches the exact satisfaction of the equilibrium equations, and the extension in [2] to singular problems.

In the SPR-CX, a patch is defined as the set of elements connected to a vertex node. On each patch, a polynomial expansion for each one of the components of the recovered field is expressed in the form:

$$\sigma_i^*(\mathbf{x}) = \mathbf{p}(\mathbf{x})\mathbf{a}_i \quad i = xx, yy, xy \tag{5}$$

where $\mathbf{p}$ represents a polynomial basis and $\mathbf{a}$ are unknown coefficients. Usually, the polynomial basis is chosen equal to the finite element basis for the displacements.

Constraint equations are introduced via Lagrange multipliers into the linear system used to solve for the coefficients $\mathbf{A}$ on each patch in order to enforce the satisfaction of the:

- Internal equilibrium equation.
- Boundary equilibrium equation: A point collocation approach is used to impose the satisfaction of a polynomial approximation to the tractions along the Neumann boundary at the patch.
- Compatibility equation: This additional constraint is also imposed to further increase the accuracy of the recovered stress field.

For singular problems the exact stress field $\boldsymbol{\sigma}$ is decomposed into two stress fields, a smooth field $\boldsymbol{\sigma}_{smo}$ and a singular field $\boldsymbol{\sigma}_{sing}$. Then, the recovered field $\boldsymbol{\sigma}^*$ required to compute the ZZ error estimate can be expressed as the contribution of two recovered stress fields, one smooth $\boldsymbol{\sigma}^*_{smo}$ and one singular $\boldsymbol{\sigma}^*_{sing}$:

$$\boldsymbol{\sigma}^* = \boldsymbol{\sigma}^*_{smo} + \boldsymbol{\sigma}^*_{sing}. \tag{6}$$

For the recovery of the singular part, the expressions which describe the asymptotic fields near the crack tip are used. To evaluate $\boldsymbol{\sigma}^*_{sing}$ we first obtain estimated values of the stress intensity factors K_{I} and K_{II} using an equivalent domain integral method based in extraction functions [6]. Notice that the recovered part $\boldsymbol{\sigma}^*_{sing}$ is an equilibrated field as it satisfies the equilibrium equations.

Then, the field $\boldsymbol{\sigma}^*_{smo}$ is evaluated applying the enhancements of the SPR technique previously described, i.e. satisfaction of equilibrium and compatibility equations at each patch. Note that as both $\boldsymbol{\sigma}^*_{smo}$ and $\boldsymbol{\sigma}^*_{sing}$ satisfy the equilibrium equations, $\boldsymbol{\sigma}^*$ also satisfy equilibrium at each patch.

To obtain a continuous field, the recovered stresses $\boldsymbol{\sigma}^*$ are directly evaluated at an integration point $\mathbf{x}$ through the use of a partition of unity procedure [7]. The reader is referred to [8, 4] for more details.

3 NUMERICAL EXAMPLES

The Westergaard problem of an infinite plate loaded at infinity with biaxial tractions $\sigma_{x\infty} = \sigma_{y\infty} = \sigma_\infty$ and shear traction τ_∞, presenting a crack of length $2a$, is used to investigate the quality of the proposed technique as it has an exact analytical solution . The numerical model, which can be found in [2], corresponds to a finite portion of the domain where the applied projected stresses for mode I and mode II are evaluated from the analytical Westergaard solution.

To assess the performance of the proposed technique we consider the effectivity index of the error estimator θ and the effectivity in the quantity of interest θ_{QoI} defined as:

$$\theta = \frac{Q(\mathbf{e}_{es})}{Q(\mathbf{e})} \quad , \quad \theta_{QoI} = \frac{Q(\mathbf{u}^h) + Q(\mathbf{e}_{es})}{Q(\mathbf{u})} \tag{7}$$

where $Q(\mathbf{e})$ denotes the exact error in the quantity of interest, and $Q(\mathbf{e}_{es})$ the evaluated error estimate.

Table 1: Stress intensity factor K_{I} as QoI.

ndof	$Q(\mathbf{e}_{es})$	$Q(\mathbf{e})$	θ	θ_{QoI}
351	2.5264002	2.1144455	1.1948288	1.0026054
1289	0.4821894	0.5146442	0.9369373	0.9997947
4973	0.1140116	0.1216039	0.9375659	0.9999520
19637	0.0267482	0.0278142	0.9616742	0.9999933

In Tables 1 and 2, the proposed technique accurately captures the magnitude of the error. The global effectivity is close and converges to the theoretical value $\theta = 1$, with values that vary within the range [0.8, 1.1]. Despite equilibrium is not satisfied for the dual problem in the domain used for the extraction of K we obtain good results. As expected, the effectivity of the corrected QoI is highly accurate.

Table 2: Stress intensity factor K_{II} as QoI.

ndof	$Q(\mathbf{e}_{es})$	$Q(\mathbf{e})$	θ	θ_{QoI}
351	2.2885898	1.1272503	2.0302410	1.0073450
1289	0.2827324	0.2901661	0.9743812	0.9999530
4973	0.0699652	0.0689483	1.0147483	1.0000064
19637	0.0167546	0.0158745	1.0554407	1.0000056

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