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Locally equilibrated stress recovery for goal oriented error estimation in the extended finite element method

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ABSTRACT

Goal oriented error estimation and adaptive procedures are essential for the accurate and efficient evaluation of finite element numerical simulations that involve complex domains. By locally improving the approximation quality, for example, by using the extended finite element method (XFEM), we can solve expensive problems which could result intractable otherwise. Here, we present an error estimation technique for enriched finite element approximations that is based on an equilibrated recovery technique, which considers the stress intensity factor as the quantity of interest. The locally equilibrated superconvergent patch recovery is used to obtain enhanced stress fields for the primal and dual problems defined to evaluate the error estimate.

1. Introduction

In continuum mechanics, stresses and strains are usually the main quantities to describe the behaviour of a component under certain loads. However, when the component is affected by a crack these parameters are not sufficient to properly describe the behaviour of the component in the Linear Elasticity (LE) framework. For instance, under the LE assumptions, the stress field at the crack tip will take infinite values, and in the surroundings of the crack tip, due to the high stress value, the small deformations assumption does not hold. Linear Elastic Fracture Mechanics (LEFM) assumptions are considered valid for brittle fracture [1,2]. One characterising parameter used to give a more realistic description of the behaviour around the crack tip is the *stress intensity factor* (SIF), which focuses in the local stress state at the crack tip [2] and can be considered an energy-based quantity. Hence, to properly describe the behaviour at the crack tip in LEFM is necessary to accurately evaluate the SIF. It results interesting to evaluate an error measure for the SIF to be able to control its level of accuracy [3,4].

Since the beginning of the use of numerical simulations many methods have been developed to control the discretisation error of finite element approximations, mostly based on the evaluation of global error in energy norm of the Finite Element (FE) solution. These methods can be broadly classified in residual based [5], recovery based [6] and dual analysis [7,8]. The numerical results in [9–11] showed that a recovery technique with a standard superconvergent patch recovery (SPR) [12], applied in problems with smooth solution, was more robust than the residual estimates considered. However, a more interesting approach is to control the error in a particular quantity relevant for the design process [13–16]. This quantity could be defined as a bounded functional that describes the displacement or stresses in a given area of the domain, or for the case of fracture mechanics, the SIF that characterises the crack. This approach, referred to as goal oriented, is usually based on the use of duality techniques that involve the formulation of an *adjoint* or *dual* problem directly related to the quantity of interest (QoI). Residual methods have been frequently used to evaluate the error in quantities of interest although examples involving recovery techniques can be found in [17,3], and considering dual analysis in [18]. In [19] an enhanced version of the SPR technique was used to obtain accurate estimations of the error in different QoI in the context of linear elasticity problems solved with the FEM. In [3], recovery and residual based estimates of the error in evaluating the *J*-integral (directly related to the SIF) for finite element (FE) approximations in the context of LEFM were presented. The authors showed that the most accurate error estimates for the *J*-integral were obtained with the recovery based estimators.

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Refs. [16,15] showed that the error in the quantity of interest can be expressed in terms of errors in energy norm, and that if these errors in energy norm can be bounded we could also bound the error in the quantity of interest. On the other hand, it is usually difficult to obtain guaranteed error bounds of the quantities of interest while maintaining the accuracy of the estimate. The need of such a bound is also arguable in an engineering context as the reliability of an a posteriori error estimate, which is quantified by its local effectivity, can be verified beforehand on a number of practical cases. Here, we are interested in increasing the effectivity of the error estimate used to guide adaptive algorithms rather than error bounding.

In the context of LEFM, the extended finite element method (XFEM) [20] has been successfully used to enrich the finite element approximation in order to represent the particular features of cracks, namely, the discontinuity along the crack faces and the singularity at the crack tip. This method helps to overcome some of the difficulties when modelling crack propagation, such as the need for remeshing to obtain conforming meshes to the crack topology. Recent advanced numerical approaches for the purpose of XFEM and fracture analysis also include Mixed Discrete Least Squares Meshless (MDLSM) [21], and XIGA [22]. Error estimators in energy norm for XFEM and other partition of unity methods have been proposed in [23–26] using recovery techniques, and in [27,4,28] using the residual approach. A goal oriented approach for enriched finite element approximations based on the constitutive relation error has been presented in [29]. In [30] goal oriented error estimators based on the explicit residual method were introduce for the XFEM framework. In [31], adaptive techniques based on energy norm and goal oriented error estimation have been investigated for enriched finite element approximations.

In this paper, we propose a goal oriented error estimation technique for XFEM approximations that is based on the enhanced recovery technique previously presented in [25,26] and the consideration of the SIF, typical of LEFM, as the quantity of interest. One of the key features of the recovery-based error estimators is that the solution is recovered patch-wise in a basis richer than the one used for the FE approximation. As shown in [23,32], when XFEM is used, the basis used for the recovery should include the singular terms, which is not common in standard recovery techniques. Therefore, error estimates in quantities of interest will also require a careful consideration of the singular character of the XFEM solution, and the use of extended recovery approaches becomes a necessity to obtain accurate estimates. To improve the quality of the recovered stresses for the primal and dual problems, and therefore, the accuracy of the error estimate, we consider equilibrium constraints locally in patches of elements and the splitting of the recovered stress field into *singular* and *smooth* parts, which is the fundamental idea in the recovery process to describe the singular behaviour of the solution.

The paper is organised as follows. In Section 2, we introduce the problem under consideration and its corresponding enriched approximation. In Section 3, we show useful analytical definitions of QoI for the enforcement of equilibrium conditions. The recovery process is described in Section 4. We discuss the formulation of the dual problem when considering the stress intensity factor as the quantity of interest in the goal oriented approach. Numerical results are provided in Section 5 and conclusion are drawn in Section 6.

2. Problem statement and XFEM for LEFM

In this section, we introduce the 2D LEFM problem. We denote by $\mathbf{u}$ the displacement, by $\boldsymbol{\sigma}$ the Cauchy stress and by $\boldsymbol{\varepsilon}$ the strain, all these fields defined over the domain $\Omega \subset \mathbb{R}^2$, of boundary denoted by $\partial\Omega$. Γ_N and Γ_D refer to the parts of the boundary where the Neumann and Dirichlet conditions are applied, and Γ_C to the free traction surface describing a crack such that $\partial\Omega = \Gamma_N \cup \Gamma_D \cup \Gamma_C$ and $\Gamma_N \cap \Gamma_D \cap \Gamma_C = \emptyset$. We denote by $\mathbf{b}$ the body loads, $\mathbf{t}$ the tractions imposed along Γ_N and $\boldsymbol{\sigma}_0$, $\boldsymbol{\varepsilon}_0$ the initial stresses and strains. The displacement field $\mathbf{u}$ is the solution of the problem given by

$$\mathbf{L}^T\boldsymbol{\sigma} + \mathbf{b} = 0 \qquad \text{in } \Omega, \tag{1}$$

$$\mathbf{G}\boldsymbol{\sigma} = \mathbf{t} \qquad \text{on } \Gamma_N, \tag{2}$$

$$\mathbf{G}\boldsymbol{\sigma} = \mathbf{0} \qquad \text{on } \Gamma_C, \tag{3}$$

$$\mathbf{u} = \mathbf{0} \qquad \text{on } \Gamma_D, \tag{4}$$

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \mathbf{L}\mathbf{u} \qquad \text{in } \Omega, \tag{5}$$

$$\boldsymbol{\sigma} = \mathbf{D}(\boldsymbol{\varepsilon}(\mathbf{u}) - \boldsymbol{\varepsilon}_0) + \boldsymbol{\sigma}_0 \qquad \text{in } \Omega, \tag{6}$$

where $\mathbf{L}$ is the differential operator for linear elasticity, and $\mathbf{G}$ is the projection operator that projects the stress field into tractions over any boundary, with $\mathbf{n}$ the outward unit normal to Γ_N, such that

$$\mathbf{L}^T = \begin{bmatrix} \partial/\partial x & 0 & \partial/\partial y \\ 0 & \partial/\partial y & \partial/\partial x \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} n_x & 0 & n_y \\ 0 & n_y & n_x \end{bmatrix}, \tag{7}$$

$\mathbf{D}$ is the matrix of the linear constitutive relation for stress and strain. We consider an homogeneous Dirichlet boundary condition in (4) for simplicity.

The problem expressed in its variational form is written as:

$$\text{Find } \mathbf{u} \in V \text{ such that } \forall \mathbf{v} \in V = \{\mathbf{v} \mid \mathbf{v} \in [H^1(\Omega)]^2, \mathbf{v}|_{\Gamma_D} = \mathbf{0}\}:$$

$$\int_\Omega \boldsymbol{\varepsilon}(\mathbf{u})^T\mathbf{D}\boldsymbol{\varepsilon}(\mathbf{v})\mathrm{d}\Omega = \int_\Omega \mathbf{v}^T\mathbf{b}\mathrm{d}\Omega + \int_{\Gamma_N} \mathbf{v}^T\mathbf{t}\mathrm{d}\Gamma + \int_\Omega \boldsymbol{\varepsilon}(\mathbf{v})^T\mathbf{D}\boldsymbol{\varepsilon}_0\mathrm{d}\Omega - \int_\Omega \boldsymbol{\varepsilon}^T(\mathbf{v})\boldsymbol{\sigma}_0\mathrm{d}\Omega. \tag{8}$$

To evaluate the SIF, noted as K, it is common practice to use the interaction integral in its Equivalent Domain Integral (EDI) form. There are different expressions already available to evaluate EDI integrals for singular problems. In this work, we are going to consider the method based on extraction functions, as shown in [33]:

$$K = -\frac{1}{C}\int_{\Omega_I} \boldsymbol{\sigma}^T \begin{bmatrix} u_x^{\text{aux}} q_{,x} \\ u_y^{\text{aux}} q_{,y} \\ u_y^{\text{aux}} q_{,x} + u_x^{\text{aux}} q_{,y} \end{bmatrix} - \mathbf{u}^T \begin{bmatrix} \sigma_{xx}^{\text{aux}} q_{,x} + \sigma_{xy}^{\text{aux}} q_{,y} \\ \sigma_{xy}^{\text{aux}} q_{,x} + \sigma_{yy}^{\text{aux}} q_{,y} \end{bmatrix} \mathrm{d}\Omega, \tag{9}$$

where $\mathbf{u}^{\text{aux}}$, $\boldsymbol{\sigma}^{\text{aux}}$ are the auxiliary fields used to extract the SIFs in mode I or mode II and C is a constant that is dependent on the geometry and the loading mode. q is an arbitrary C^0 function that defines the extraction zone Ω_I which takes the value of 1 at the singular point and 0 at the boundary Γ. $q_{,x}$ and $q_{,y}$ are the derivatives of the function q with respect to x and y.

2.1. Discrete problem using XFEM

Let us consider a finite element approximation of $\mathbf{u}$ denoted as $\mathbf{u}^h$. In the XFEM formulation [20], the approximation is usually enriched with two types of enrichment functions by means of the partition of unity: (i) a Heaviside function H to describe the discontinuity of the displacement field along the crack, in the set of nodes I^{crack} whose support is intersected by the crack and (ii) a set of branch functions F_ℓ to represent the asymptotic behaviour of the stress field near the crack tip, in the set of nodes I^{tip} whose support contains the singularity. The XFEM displacement interpolation in a 2D model reads:

$$\mathbf{u}^h(\mathbf{x}) = \sum_{i \in I} N_i(\mathbf{x})\mathbf{a}_i + \sum_{i \in I^{crack}} N_i(\mathbf{x})H(\mathbf{x})\mathbf{b}_i + \sum_{i \in I^{tip}} N_i(\mathbf{x})\left(\sum_{\ell=1}^{4} F_\ell(\mathbf{x})\mathbf{c}_i^\ell\right), \tag{10}$$