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A POSTERIORI ERROR ESTIMATION FOR SECOND-ORDER OPTIMALLY CONVERGENT G/XFEM

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Summary. This work presents a ZZ-BD a posteriori error estimator tailored for 3-D linear elastic fracture mechanics problems that are approximated by second-order pFEM-GFEM formulations. The proposed error estimator is shown to estimate well discretization errors in the energy norm, with the estimated discretization error converging at the same rate as the exact discretization error. Also, the computed effectivity indexes are close to the optimal value of 1 for a LEFM problem that exhibits 3-D effects.

1 INTRODUCTION

The Generalized/eXtended Finite Element Method (G/XFEM) is well-known as an efficient and accurate methodology for the simulation of problems that generally face difficulties when treated by standard methodologies, such as the Finite Element Method (FEM). These problems appear often within the context of Linear Elastic Fracture Mechanics (LEFM), for example, and because of this, interest in accurately simulating them exists since the G/XFEM initial propositions [1, 2, 3, 4]. LEFM problems present two behaviors that cannot be easily treated by the FEM – the discontinuity that happens across crack surfaces and the singularity that happens at its front. To deal with this, G/XFEM incorporates into the approximation spaces functions that capture well those behaviors. These functions are known as enrichment functions and they (i) allow the mesh to be generated independently of the crack that exists in the problem domain, which comes in handy when dealing with three-dimensional (3-D) simulations, and (ii) enable the numerical method to achieve optimal convergence rates in the energy norm even for problem in which these rates are bounded by the singularity strength when solved by the FEM.

Because of these good approximation properties, extensive research [5, 6, 7, 8, 9, 10] has been done in the past decades aiming at developing first-order optimally convergent approximations to LEFM problems. Despite delivering optimal convergence rates, it has been shown [11], however, that first-order G/XFEM is not competitive with second-order FEM that uses quarter-point elements, especially for 3-D problems. Due to that, second-order optimally convergent G/XFEMs, customized to solve LEFM problems, have been recently proposed [11, 12, 13]. The formulations presented in these works augment both standard lagrangian FEM approximation spaces [13] and p-hierarchical FEM approximation spaces [11, 12] in order to insert into the G/XFEM approximation spaces the discontinuous and singular behaviors of fractures. Nonetheless, in addition to using enrichment functions, it is important to note that G/XFEM still needs local mesh refinement around crack fronts in order to achieve optimal convergence. This must be considered especially for 3-D problems that violate the assumptions of the adopted singular enrichment functions. While this local mesh refinement can be easily performed for simple cases, the level of refinement that must be used with more complicated problems can be difficult to be defined a priori. Adaptive refinement algorithms can address this issue and an important ingredient for the development of such algorithms is an accurate a posteriori error estimator able to estimate well global and local discretization errors associated with these newly developed G/XFEM formulations.

This work presents a Zienkiewicz and Zhu block-diagonal (ZZ-BD) error estimator [14] tailored to estimate discretization errors of second-order G/XFEM formulations for 3-D LEFM problems. The associated recovery procedure involves locally weighted L^2 projections of raw stresses onto approximation spaces including high-order discontinuous and singular stress fields. The basis functions for these improved, or recovered, stress approximations are defined using a low-order partition of unity together with polynomial, discontinuous, and singular recovery enrichment functions. The strategy introduced herein for 3-D problems is based on the one proposed by the same authors in [15] for 2-D analyses. The results presented in this contribution show that the ZZ-BD error estimator proposed to solve 3-D LEFM problems with second-order pFEM-GFEM formulations accurately computes estimated discretization errors in the energy norm, with them converging at the same rate as the exact discretization errors. Also, the computed effectivity index of the proposed error estimator is shown to be close to its optimal value.

2 SECOND-ORDER G/XFEM AND FEM

As introduced in Section 1, a posteriori error estimators are presented in this work for second-order G/XFEM. The methodology is quite general, but here second-order formulations that augment p-hierarchical FEM approximations are adopted. In this section, a very brief overview of so-called pFEM-GFEM formulations [11, 12] used to solve 3-D LEFM problems is presented. Comprehensive details of these formulations for both 2-D and 3-D problems can be found, for instance, in [11, 12].

As mentioned before, pFEM-GFEM formulations able to solve LEFM problems augment pFEM spaces in order to insert into them the discontinuous and singular behaviors of fractures. In short, pFEM hierarchically augments linear FEM shape functions, associated with vertex nodes of a mesh, up to functions of the required degree p. The pFEM-GFEM approximation space can then be written as

$$\mathcal{S}_{p\text{FEM-GFEM}} = \mathcal{S}_{p\text{FEM}} + \mathcal{S}_{\text{ENR}}, \tag{1}$$

with $\mathcal{S}_{\text{ENR}}$ a space built based on local approximation spaces glued together by a partition of unity and $\mathcal{S}_{p\text{FEM}}$, in the case of second-order approximations, a space spanned by both 3-D vertex shape functions and edge shape functions that are built from the product between two linear vertex shape functions. For an edge with vertices with indices α and β, for example, the associated edge shape function $\varphi_{\alpha\beta}(\boldsymbol{x})$ is given by the product of vertex shape functions $\varphi_{\alpha}(\boldsymbol{x})$ and $\varphi_{\beta}(\boldsymbol{x})$, i.e., $\varphi_{\beta\alpha}(\boldsymbol{x}) = \varphi_{\alpha}(\boldsymbol{x})\,\varphi_{\beta}(\boldsymbol{x})$.

In Eq. (2), the enriched space $\mathcal{S}_{\text{ENR}}$ is customized to represent the discontinuous and singular behaviors of LEFM problems. Therefore, this space can be split into $\mathcal{S}^{S}_{\text{ENR}}$, which approximates the singularity at the crack front, and $\mathcal{S}^{D}_{\text{ENR}}$, which approximates the discontinuity that happens across the entire crack surface. Based on this, a pFEM-GFEM approximation space used to generate approximate displacement fields for LEFM problems can be defined as

$$\mathcal{S}_{p\text{FEM-GFEM}} = \mathcal{S}_{p\text{FEM}} + \left(\mathcal{S}^{S}_{\text{ENR}} + \mathcal{S}^{D}_{\text{ENR}}\right). \tag{2}$$

In the approximations used in this work, $\mathcal{S}^{S}_{\text{ENR}}$ is built based on Oden-Duarte (OD) singular enrichment functions, modified by their discontinuous interpolant [11], and $\mathcal{S}^{D}_{\text{ENR}}$ is built based on high-order Heaviside enrichment functions. For details about the generation of spaces associated with high-order Heaviside functions and OD singular functions, see [11, 12]. It is important to mention that in the formulations adopted in this work, Heaviside functions are applied at all vertex and edge nodes whose support intersects the crack surface but does not intersect the crack front and that OD functions are applied at all vertex nodes that are at a distance smaller than r_S from the crack front. In this formulation, some nodes are enriched with both Heaviside and OD functions.

3 ZZ-BD ERROR ESTIMATOR

The second-order pFEM-GFEM summarized in Section 2 delivers optimally convergent solutions and well-conditioned stiffness matrices for 2-D and 3-D LEFM problems. Furthermore, it is much more efficient than first-order G/XFEMs and second-order FEMs that use quarter-point elements around the crack tip or front. Besides delivering lower error levels, the second-order pFEM-GFEM provides solutions with errors of the order of $\mathcal{O}(h^{-2})$ in the energy norm. The definition of error estimators that estimate well discretization errors of formulations like those is of interest if one seeks (i) to evaluate the solution accuracy for cases in which no analytical solution is available, which is most (if not all) the situations of practical interest, and (ii) to improve the solution accuracy by utilizing adaptive discretization refinement techniques. As presented in Section 1, the Zienkiewicz and Zhu block-diagonal (ZZ-BD) error estimator [14, 15] is adopted. In summary, the ZZ-BD is an a posteriori, recovery-based error estimator that uses a recovery procedure involving locally weighted L^2 projections of raw stresses onto an approximation space for discontinuous and singular stress fields. Herein, ideas similar to those used in 2-D [15] are applied to second-order pFEM-GFEM formulations used to solve 3-D LEFM problems. The main features related to the error estimator developed herein are that (i) linear partitions of unity, associated with only vertices of tetrahedral finite elements, are used as the weighting ZZ-BD partition of unity, (ii) polynomial recovery enrichment functions of degree $p = 2$ are used to reach the same polynomial degree as the one used to build the approximate displacement field, and (iii) shifted Heaviside functions are used to mimic the discontinuity of the stress field along the crack surface and gradient of OD functions [12] are used to mimic the $1/\sqrt{r}$ singularity that happens at the crack front.

Based on these three features, a recovered stress field $\sigma^*(\boldsymbol{x})$ can be defined as

$$\sigma^*(\boldsymbol{x}) = \sigma^*_P(\boldsymbol{x}) + \sigma^*_D(\boldsymbol{x}) + \sigma^*_S(\boldsymbol{x}). \tag{3}$$

In this equation, $\sigma^*_P(\boldsymbol{x})$ is devoted to representing the piecewise continuous polynomial part of the recovered stress field and, as mentioned before, is built based on linear partitions of unity and 3-D polynomial recovery enrichment functions. Furthermore, $\sigma^*_D(\boldsymbol{x})$ aims to approximate the discontinuity that also happens in the stress field across the crack surface. This field is herein built based on linear partitions of unity and high-order Heaviside enrichment functions, as presented in [15]. Finally, $\sigma^*_S(\boldsymbol{x})$ aims to approximate the singularity that happens at the crack front and, in this work, terms of the gradients of OD functions are used as recovery enrichment functions to build it. As presented in [15], four linear independent terms of the gradients of all four (2-D) OD functions are used herein when dealing with problems with planar cracks and straight crack fronts.

Finally, for recovery-based a posteriori error estimators, as is the case of the ZZ-BD, this recovered stress field $\sigma^*(\boldsymbol{x})$ substitutes the exact stress field when computing the energy norm of the discretization error. This allows one to define a measure known as estimated discretization error in the energy norm ϵ^*, given by

$$\epsilon^* = \sqrt{B(\boldsymbol{u}^* - \hat{\boldsymbol{u}}, \boldsymbol{u}^* - \hat{\boldsymbol{u}})}, \tag{4}$$

with $B(\cdot, \cdot)$ the bilinear form of the studied variational formulation.

4 NUMERICAL EXPERIMENT AND BRIEF DISCUSSION

As mentioned before, 3-D problems of linear elastostatics that contain strong discontinuities (cracks) are analyzed in this work. The following section presents an example that aims to assess the accuracy of the proposed error estimator for 3-D LEFM problems with planar cracks.

4.1 3-D edge crack problem

This problem consists of a rectangular prism,

$$\bar{\Omega} = [-0.5, 0.5] \times [-0.875, 0.875] \times [-0.75, 0.75],$$

with a through-the-thickness edge crack Γ_C, as shown in Fig. 1. This is the same problem as the one analyzed in [12], in which the second-order pFEM-GFEM summarized in Section 2 has been applied. A linear elastic material, with Young's modulus $E = 1$ and Poisson's ratio $\nu = 0.3$, is adopted and uniform tractions, with magnitude $\sigma_0 = 0.0025$, are applied at the boundaries in which $x_2 = -0.875$ and $x_2 = 0.875$. These tractions are also depicted in Fig. 1. Dirichlet boundary conditions are applied to restrict rigid body motion only.

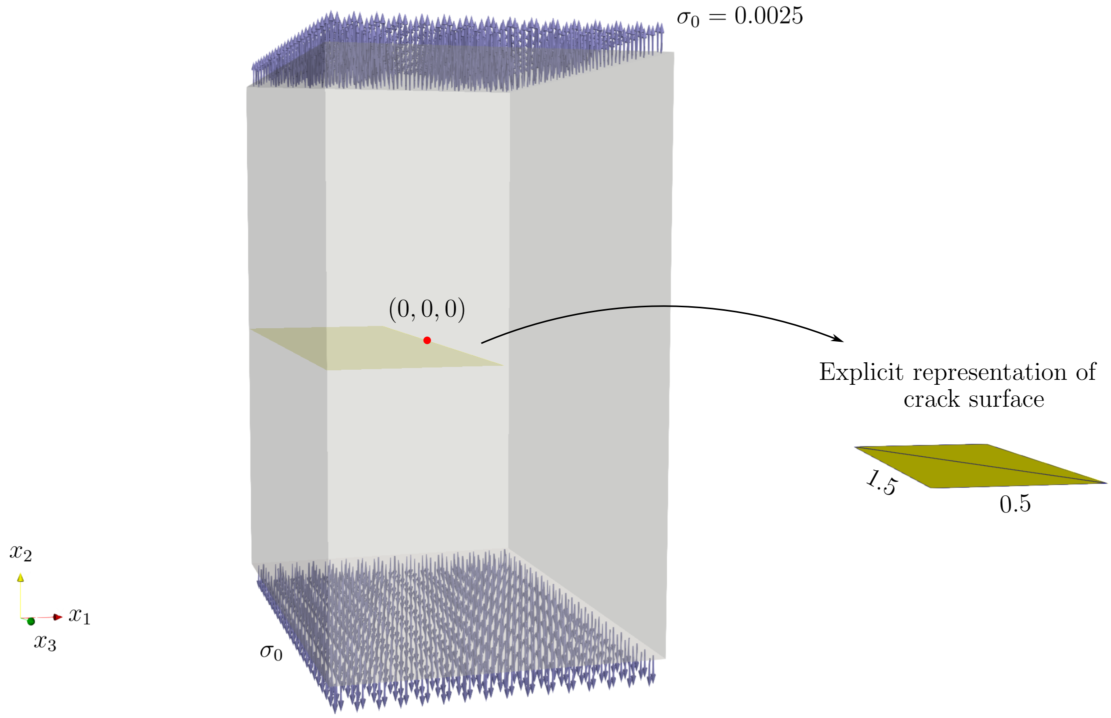

Figure 1: Geometry and boundary conditions of the 3-D edge crack problem.

The main objective of the simulations presented in this section is to assess the accuracy of ZZ-BD estimated errors. This accuracy is measured by the error estimator effectivity index θ, given by

$$\theta = \epsilon^* \big/ \epsilon, \tag{5}$$

with ϵ^* the estimated discretization error in the energy norm (cf. Eq. (4)) and ϵ the exact discretization error in the energy norm. In this example, since the exact solution is not known, values of ϵ are computed as

$$\epsilon = \sqrt{2\left(U_{\text{ref}} - \hat{U}\right)}, \quad \text{with} \quad U_{\text{ref}} = 2.14693601005134 \times 10^{-5} \tag{6}$$

a reference strain energy [12] and $\hat{U}$ the approximated strain energy.

In this section, four structured uniform meshes, obtained by subdividing the sides of $\bar{\Omega}$ by $(8 \times 14 \times 12)$, $(16 \times 28 \times 24)$, $(24 \times 42 \times 36)$, and $(32 \times 56 \times 48)$, are adopted. First, the problem is solved using the second-order pFEM-GFEM presented in Section 2 and then, following what is presented in Section 3, recovered stresses are obtained and the estimated error is computed. To define the recovered stress field, polynomial recovery enrichment functions are adopted at all mesh vertices. High-order Heaviside functions and terms of the gradients of OD functions are also used. Figure 2 depicts these enrichments applied to the mesh $(16 \times 28 \times 24)$.

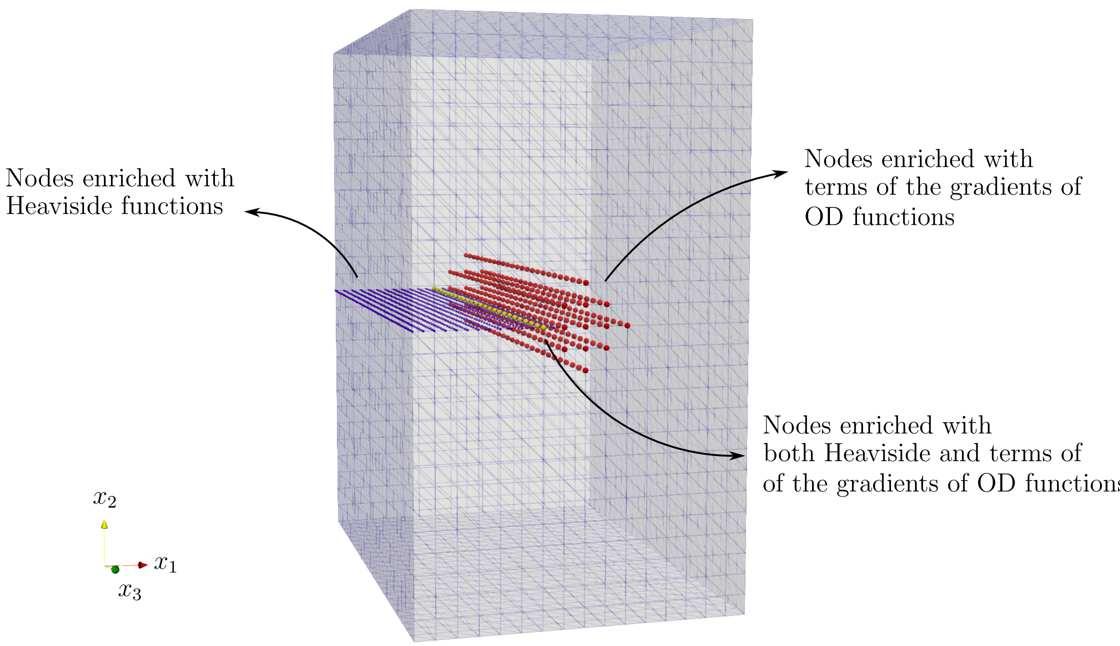

Figure 2: Illustration of the $(16\times28\times24)$ discretization and adopted recovery enrichment functions. Blue spheres • illustrate vertices enriched with Heaviside functions, red spheres • illustrate vertices enriched with terms of the gradient of OD functions, and green spheres • illustrate vertices enriched with both Heaviside and terms of the gradient of OD functions.

The results regarding exact discretization errors in the energy norm ϵ, estimated discretization errors in the energy norm ϵ^*, and effectivity indexes θ are presented in Table 1. A good accuracy for estimated values of the discretization error is obtained for all performed analyses and this is inferred by the closeness between the effectivity indexes and its optimal value of 1. It is noted that [16] recommends $0.8 < \theta < 1.2$, which is the case for all simulations performed herein with results presented in Table 1. Based on simulations not reported here, the same conclusions are obtained when the estimator is applied to non-uniform meshes, as those used in [12]. These meshes lead to optimal convergence rates.

Table 1: Results of exact discretization error in the energy norm ϵ, estimated discretization error in the energy norm ϵ^*, and effectivity index θ for the 3-D edge crack problem.

Mesh	N_{DoFs}	ϵ	ϵ^*	θ
$(8 \times 14 \times 12)$	37 971	3.27×10^{-4}	3.25×10^{-4}	0.99
$(16 \times 28 \times 24)$	280 515	1.56×10^{-4}	1.57×10^{-4}	1.01
$(24 \times 42 \times 36)$	923 391	8.09×10^{-5}	8.62×10^{-5}	1.06
$(32 \times 56 \times 48)$	2 160 531	5.21×10^{-5}	5.79×10^{-5}	1.11

5 CONCLUSIONS

This work presents an initial contribution towards the development of an accurate and computationally efficient a posteriori error estimator for 3-D LEFM problems approximated by second-order G/XFEM formulations. The a posteriori error estimator presented herein consists of an extension to 3-D problems of what is proposed in [15] in a 2-D setting. Based on the results presented herein, the proposed error estimator presents good effectivity indexes also for 3-D LEFM problems. Further propositions, including those related to other singular enrichment functions used in 3-D, mixed mode problems, problems with non-planar crack surfaces or non-straight crack fronts, and adaptivity guided by the ZZ-BD error estimator, will be object of future works.

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REFERENCES

[1] C. A. Duarte, I. Babuška and J. T. Oden, "Generalized finite element methods for three-dimensional structural mechanics problems". *Computers and Structures* **77**, 215–232, (2000).

[2] C. A. Duarte, O. N. Hamzeh, T. J. Liska and W. W. Tworzydlo, "A generalized finite element method for the simulation of three-dimensional dynamic crack propagation". *Computer Methods in Applied Mechanics and Engineering* **190**, 2227–2262, (2001).

[3] T. Belytschko and T. Black, "Elastic crack growth in finite elements with minimal remeshing". *International Journal for Numerical Methods in Engineering* **45**, 601–620, (1999).

[4] N. Moës, J. Dolbow and T. Belytschko, "A finite element method for crack growth without remeshing". *International Journal for Numerical Methods in Engineering* **46**, 131–150, (1999).

[5] I. Babuška and U. Banerjee, "Stable Generalized Finite Element Method (SGFEM)". *Computer Methods in Applied Mechanics and Engineering* **201–204**, 91–111, (2012).

[6] M. Ndeffo, P. Massin, N. Moës, A. Martin and S. Gopalakrishnan, "On the construction of approximation spaces to model discontinuities and cracks with linear and quadratic extended finite elements". *Advanced Modeling and Simulation in Engineering Sciences* **4**, 6, (2017).

[7] K. Agathos, E. Chatzi, S. Bordas and D. Talaslidis, "A well-conditioned and optimally convergent XFEM for 3D linear elastic fracture". *International Journal for Numerical Methods in Engineering* **105**, 643–677, (2016).

[8] A. Sanchez-Rivadeneira and C. A. Duarte, "A simple, first-order, well-conditioned, and optimally convergent Generalized/eXtended FEM for two- and three-dimensional linear elastic fracture mechanics". *Computer Methods in Applied Mechanics and Engineering* **372**, 113388, (2020).

[9] Q. Zhang, I. Babuška and U. Banerjee, "Robustness in stable generalized finite element methods (SGFEM) applied to Poisson problems with crack singularities". *Computer Methods in Applied Mechanics and Engineering* **311**, 476–502, (2016).

[10] C. Cui and Q. Zhang, "Stable generalized finite element method for elasticity crack problems". *International Journal for Numerical Methods in Engineering* **121**, 3066–3082, (2020).

[11] A. Sanchez-Rivadeneira and C. A. Duarte, "A stable generalized/eXtended FEM with discontinuous interpolants for fracture mechanics". *Computer Methods in Applied Mechanics and Engineering* **345**, 876–918, (2019).

[12] A. Sanchez-Rivadeneira, N. Shauer, B. Mazurowski and C. A. Duarte, "A Stable Generalized/eXtended *p*-hierarchical FEM for three-dimensional linear elastic fracture mechanics". *Computer Methods in Applied Mechanics and Engineering* **364**, 112970, (2020).

[13] M. H. C. Bento, S. P. B. Proença and C. A. Duarte, "Well-conditioned and optimally convergent second-order Generalized/eXtended FEM formulations for linear elastic fracture mechanics". *Computer Methods in Applied Mechanics and Engineering* **394**, 114917, (2022).

[14] R. M. Lins, S. P. B. Proença and C. A. Duarte, "Efficient and accurate stress recovery procedure and a posteriori error estimator for the stable generalized/extended finite element method". *International Journal for Numerical Methods in Engineering* **119**, 1279-1306, (2019).

[15] M. H. C. Bento, S. P. B. Proença and C. A. Duarte, "Recovery strategies, a posteriori error estimation, and local error indication for second-order G/XFEM and FEM". *International Journal for Numerical Methods in Engineering* **124**, 3025-3062, (2023).

[16] B. Szabó and I. Babuška, **Finite Element Analysis**. 1st Edition, John Wiley & Sons, Inc., (1991).