Efficient evaluation of near-singular integrals of the eXtended Isogeometric Boundary Element Method for three-dimensional fracture mechanics

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Abstract. The Boundary Element Method (BEM) has proven to be a suitable method for the numerical assessment of numerous engineering problems in both two-dimensional and three-dimensional forms. In particular, BEM robustly handles discontinuities in the mechanical response in fracture mechanics. Additionally, its boundary-only nature simplifies the re-meshing process during crack growth modelling. Furthermore, coupling BEM with isogeometric analysis (IgA) is straightforward, as both strategies rely on boundary representation, enabling the direct use of Computer-Aided Design (CAD) geometry as the mesh for the method. IgA basis functions can accurately represent complex surfaces such as spheres and toroids. In this context, the Isogeometric Boundary Element Method (IGABEM) emerges as a reliable tool for solving engineering problems, combining the advantages of BEM with the improved geometric accuracy provided by IgA. In addition, a relevant approach in fracture mechanics is using enrichment functions that incorporate known solution fields, addressing response aspects that standard isogeometric basis functions cannot capture. Combining the enrichment strategy with IGABEM leads to the eXtended IGABEM (XIGABEM) method. Specifically, enriching functions that account for the square-root inverse behaviour on crack surfaces promotes several improvements, such as improved convergence rate and removal of a non-physical jump displacement in the crack front. Another advantage is the direct extraction of Stress Intensity Factors (SIF) as system variables, eliminating the need for costly extraction techniques in three-dimensional problems. However, near-singular integrals require special attention both in BEM, IGABEM and, naturally, in XIGABEM. When the collocation point is close to the integrated patch but does not lie on the patch, the $O(1/r^{\alpha})$ nature of the elastostatics fundamental solution triggers near-singular effects, which require a large number of integration points to its correct assessment. To reduce this amount this study proposes an adaptive scheme for the near-singularities of the three-dimensional XIGABEM in fracture mechanics. Numerical applications demonstrate a reduction in the required integration points for these integrals compared to conventional methods. Therefore, this advancement in the XIGABEM framework reduces the computational cost of this strategy while maintaining accuracy.

Keywords: eXtended Isogeometric Boundary Element Method, Near-singular integration, 3D Fracture Mechanics

1 Introduction

The correct prediction of the mechanical behaviour of solids is a crucial task to prevent the failure of the designed engineering components. Particularly, the collapse induced by crack growth phenomenon requires special attention due to its potential for catastrophic damage, and the difficulty in its prediction. In addition, modern engineering devices normally have complex geometry, loading conditions and mechanical response, which restrains the application of analytical solutions in their analysis. To overcome this issue, numerical methods emerge as a robust approach to determine the mechanical response of these solids, including in the presence of cracks.

Amongst the existing numerical methods for solid mechanics, the Finite Element Method (FEM) and the Boundary Element Method (BEM) are two widespread techniques for cracked bodies. However, the FEM demands a fine mesh to represent the singular behaviour close to the crack front, and once it is a domain mesh, crack growth analysis requires a costly re-meshing task of all cut elements. On the other hand, the BEM handles well the asymptotic behaviour triggered by the cracks, and its boundary-only nature simplifies the numerical framework for the crack propagation assessment.

Another remarkable advantage of the BEM is its direct coupling with isogeometric analysis (IgA). The IgA relies on isogeometric functions, such as B-Splines, NURBS and T-Splines, for the approximation of the geometry and the mechanical fields. The capacity of these functions to represent complex geometries in a precise manner reduces the errors associated to the geometric representation, which poses an advantage of the IgA. In addition, Computer Aided Design (CAD) software normally use these isogeometric curves for representing engineering models, which takes place only in their boundary. In this context, by using the same basis functions from IgA for the interpolation of the mechanical variables in the BEM, the Isogeometric BEM (IGABEM) inherits the advantages of both methods. Moreover, the CAD model is directly the IGABEM mesh, which removes a computationally expensive mesh generation process.

Another feature that improves the IGABEM for fracture mechanics is the enrichment strategy. This proposition allows for the introduction of the a priori known response behaviour in the solution approximation space by augmenting the interpolation of the mechanical fields. In the three-dimensional IGABEM, Rocha et al. [1] proposed an enrichment strategy for the crack front in which the $\sqrt{r}$ behaviour close to the crack front becomes part of the interpolation of the displacements. In addition, this strategy dismisses costly post-processing tasks for the determination of the Stress Intensity Factors (SIFs), since their obtaining becomes part of the solution of the algebraic system, along with the displacement and traction fields. In addition, improved convergence rates are also another advantage of the eXtended IGABEM (XIGABEM).

However, the IGABEM and the XIGABEM also inherit one of the most challenging issues of the BEM: the near-singular integrals. The fundamental solution nature of O($1/r^{\alpha}$), ($\alpha = 1$,2,3) induces a near-singular kernel when the collocation point is close to the integrated region. This integral demands an increased amount of integration points when assessed by standard Gauss Legendre quadrature, especially for the hyper-singular kernel of O($1/r^3$). For the XIGABEM, this excessive amount of integration points promotes a burden in the computational time. This occurs once the enrichment function requires the calculation of the projection of each integration point at the crack front by a Newton-Raphson search procedure.

Based on the issue herein presented, this article presents a strategy to handle near-singular integrals of the XIGABEM to reduce the amount of integration points, and therefore the computational cost. This work proposes an adaptive algorithm, in which the closest elements from the collocation point are subdivided so that the integral determination occurs in a precise manner. This adaptive scheme is inspired on the work of Gong et al. [2], but without using the sinh transformation. The detection of the near-singular elements occurs in two steps, in which the second step calculates the minimum distance from the collocation point and the element in a distinguished manner that Gong et al. [2].

2 Adaptive integration on XIGABEM

The focus of this research is the novelties in the numerical integration of near-singular kernels of the XIGABEM. Further details of the XIGABEM mathematical foundations are present in Rocha et al. [1], while the work of Beer et al. [3] focuses on the IGABEM itself. Consider an integration as:

$$I = \int_{\Lambda} \frac{F(\boldsymbol{x}^s, \boldsymbol{x}^f)}{r^{\alpha}} d\Lambda, \tag{1}$$

in which $\alpha = 1,2,3$ denotes the order of the singularity of the kernel, being 1 for weakly-singular, 2 for strongly-singular and 3 for hyper-singular in IGABEM. $\boldsymbol{x}^s$ and $\boldsymbol{x}^f$ are the source point (also called collocation point) and the field point, respectively, and $r = |\boldsymbol{x}^f - \boldsymbol{x}^s|$. When the surface Λ contains $\boldsymbol{x}^s$, the singularities arise and their treatment requires, among other techniques, the Singularity Subtraction Technique ([4, 5]). When $\boldsymbol{x}^s$ is close to the integrated surface Λ but it is not contained in it, the integrand reaches high values and high gradients, which prevents the standard Gauss Legendre quadrature from promoting an accurate integration.

To reduce the computational cost of near-singular integration, this work proposes a two-step algorithm to detect the knot-spans whose integration is nearly-singular. For a given collocation point $\boldsymbol{x}^s$, the first step is to measure its distance to all other collocation points $\boldsymbol{x}_i^s$ lying on all other patches of the solid. If the distance $d = |\boldsymbol{x}^s - \boldsymbol{x}_c^s| < d_{\text{tol}}$, the patch containing the tested collocation point is set as a candidate patch to receive a near singular integration. This first scan allows the identification of all of the closest patches from the collocation point in a simple manner, since it does not require any derivative on the iterative procedure.

After classifying all candidate patches, the analysis proceeds with finding the smallest distance from a knot-span $[\xi_1^i,\xi_1^{i+1}] \times [\xi_2^j,\xi_2^{j+1}]$ of this patch to the collocation point, as well as the parametric coordinates of the closest point. This work proposes a more robust approach to find this minimum distance when compared to Gong et al. [2], since it is based on the minimisation of the squared distance, as

$$\begin{aligned}&\min f = \frac{1}{2}\sum_{k=1}^{3}[x_k^s - x_k^{\text{ks}}(\xi_1,\xi_2)]^2\\&\text{subject to: } \xi_1^i \leq \xi_1 \leq \xi_1^{i+1}\ , \xi_2^j \leq \xi_2 \leq \xi_2^{j+1},\end{aligned} \tag{2}$$

in which $x_k^{\text{ks}}(\xi_1,\xi_2)$ is the point in the knot-span, defined as

$$x_k^{\text{ks}}(\xi_1,\xi_2) = \sum_{\ell=1}^{n}\phi_\ell x_k^\ell, \tag{3}$$

ϕ_ℓ are the NURBS basis functions, x_k^ℓ are the control point coordinates and n refers to the total of basis functions in the patch. Then, the minimisation seeks the pair (ξ_1,ξ_2) which provides the closest point to the collocation point. To obtain it, an unconstrained optimisation takes place, in which

$$\nabla f = 0 \Rightarrow \left\{ \begin{array}{c} \frac{\partial f}{\partial \xi_1} \\ \frac{\partial f}{\partial \xi_2} \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \end{array} \right\}, \tag{4}$$

and the correspondent derivatives are:

$$\frac{\partial f}{\partial \xi_p} = \sum_{k=1}^{3}\left(x_k^s - x_k^{\text{ks}}(\xi_1,\xi_2)\right)\left(-\sum_{\ell=1}^{n}\phi_{,p}^\ell x_k^\ell\right), \tag{5}$$

in which $\phi_{,p}^\ell$ is the partial derivative of the NURBS function with respect to the parametric coordinate $p = 1,2$. The expansion of eq. (4) in Taylor series and its truncation in the first derivative term lead to an incremental procedure as:

$$\begin{bmatrix} \frac{\partial^2 f}{\partial \xi_1^2} & \frac{\partial^2 f}{\partial \xi_1 \partial \xi_2} \\ \frac{\partial^2 f}{\partial \xi_1 \partial \xi_2} & \frac{\partial^2 f}{\partial \xi_2^2} \end{bmatrix} \left\{ \begin{array}{c} \Delta\xi_1 \\ \Delta\xi_2 \end{array} \right\} = -\left\{ \begin{array}{c} \frac{\partial f}{\partial \xi_1} \\ \frac{\partial f}{\partial \xi_2} \end{array} \right\}, \tag{6}$$

and the second derivatives are:

$$\frac{\partial^2 f}{\partial \xi_p \partial \xi_q} = \sum_{k=1}^{3}\left[\left(\sum_{\ell=1}^{n}\phi_{,p}^\ell x_k^\ell\right)\left(\sum_{\ell=1}^{n}\phi_{,q}^\ell x_k^\ell\right) + \left(x_k^s - x_k^{\text{ks}}(\xi_1,\xi_2)\right)\left(-\sum_{\ell=1}^{n}\phi_{,pq}^\ell x_k^\ell\right)\right], \tag{7}$$

in which $\phi_{,pq}^\ell$ is the second derivative of the NURBS basis function with respect to the parametric coordinates p and q, which can be the same for the diagonal terms of eq. (6). In addition, during the incremental approach the values of ξ_1 and ξ_2 are bounded by the knot-span limits, so that if $\xi_1 + \Delta\xi_1 > \xi_1^{i+1}$, for instance, the algorithm sets $\xi_1 = \xi_1^{i+1}$ and the analysis continues.

After finding the pair (ξ_1^d,ξ_2^d) of the minimum distance of the collocation point, a second distance verification takes place. If $r < r_{\text{tol}}$, the near-singularity is present at this knot-span. To handle this near-singularity, a simple knot-span subdivision shown in Fig. 1 is enough to reduce the required amount of integration points using the conventional Gauss Legendre quadrature.

It is worth mentioning that Gong et al.[2] suggest an equation that associates the characteristic element length with the distance between the element and the collocation point, giving the required amount of integration points for an accurate integration using the Gauss Legendre quadrature. However, preliminary tests have shown that this equation overestimates this quantity for curved patches in IGABEM, and because of this effect, this work has not applied it. It would be of great interest to further investigate this equation. However, this is beyond the scope of this research.

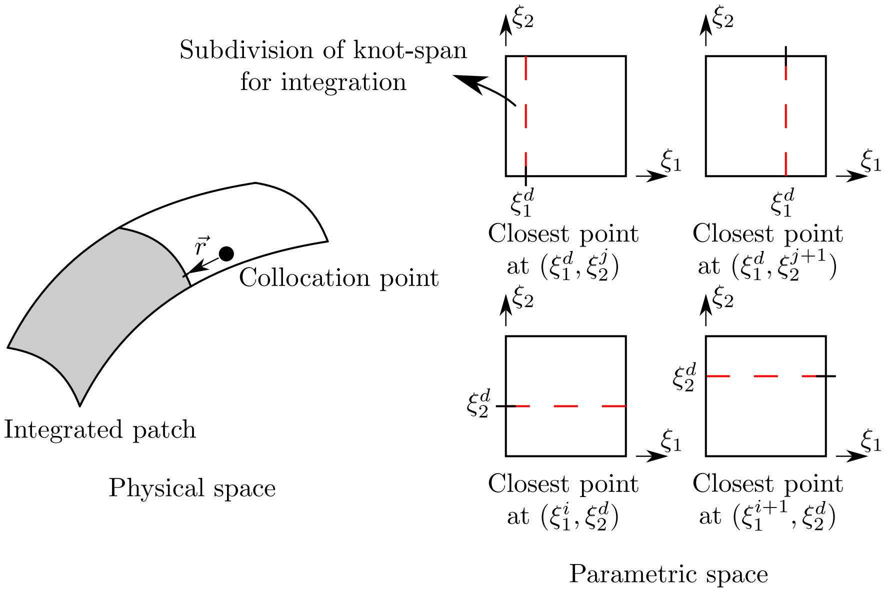

Figure 1. Adaptive subdivision of the closest knot-span to the collocation point.

3 Numerical results

This study presents the improvements associated with the adaptive integration scheme with a numerical application of a penny-shaped crack embedded in an infinite media, similar to the first example of Rocha et al. [1]. The radius is $R = 1.0$ in a cubic box whose side is $a = 200.0$, so that it simulates an infinite media. The boundary conditions are constant traction $\sigma_y = 1.0$ in the upper side, while the bottom side is clamped in all three directions. Fig. 2 presents the crack discretisation with 10 NURBS surfaces, being 5 surfaces for each side. This study utilises two numerical meshes for the analysis, in which the first mesh is in Fig. 2 and the second mesh comes from an uniform knot-insertion in both directions of the first mesh. As provided in the reference, this application has a reference solution, which allows an L_2 norm of error comparison. The numerical analysis takes place in an AMD ® Ryzen 9 7900 12-Core-Processor 64GB RAM, in which the code is built in Fortran-90 language and with the parallel directive OpenMP®.

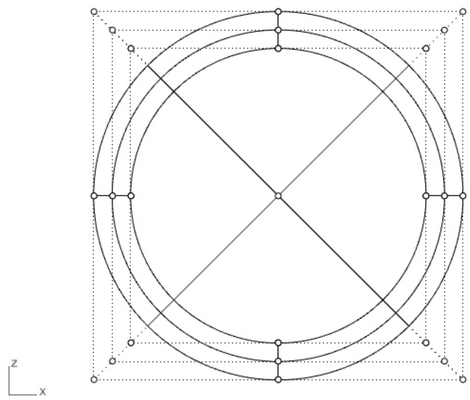

Figure 2. Penny-shaped isogeometric model and control points.

To compare the effects of the adaptive scheme in the displacement field, Fig. 3 presents the deformed shape for both schemes, conventional and adaptive, considering 50 integration points in each direction of each knot-span of the unrefined mesh, namely Mesh 1. It is noticeable a loss in the continuity between patches for the response obtained by the conventional strategy. This is the direct outcome of the inaccurate assessment of near-singularities. Then, the response from the adaptive scheme shows that this behaviour vanishes, once the near-singular integrals are now properly determined.

Fig. 4 presents the comparison of the L_2 norm of error for the standard integration scheme and the adaptive scheme proposed in this study for the unrefined and refined meshes, being Mesh 1 and Mesh 2, respectively. It is

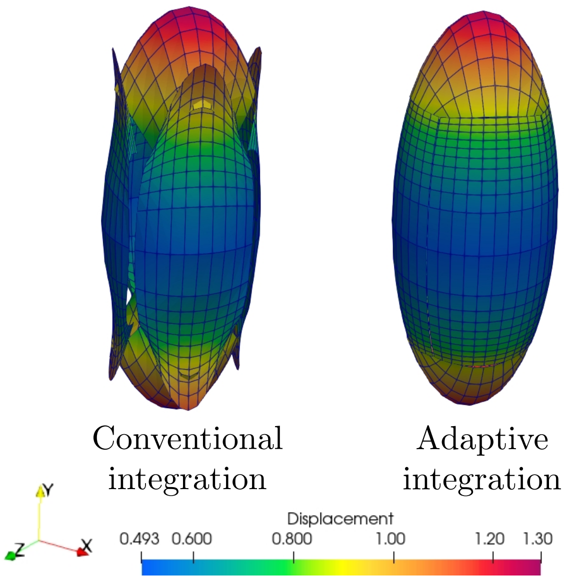

Figure 3. Deformed shape comparison of conventional scheme and adaptive strategy.

noticeable that the adaptive scheme provides a converged error with a reduced amount of integration points, which reflects in a significant reduction in the computational time. This reduction is present in Table 1, in which the error converges with the adaptive scheme using 20% and 15% of the time spent by the conventional scheme, for meshes 1 and 2, respectively. It is also worth mentioning that the L_2 norm of error does not alter significantly when adding one knot at each direction of the unrefined mesh, as also seen in [1]. Therefore, a single subdivision in the parametric direction associated to the closest point from the element to the collocation point allows for speeding up the overall analysis without jeopardising the solution accuracy. When dealing with crack growth analysis, this improvement becomes even more crucial, once for each increment new elements arise, and their integration are required.

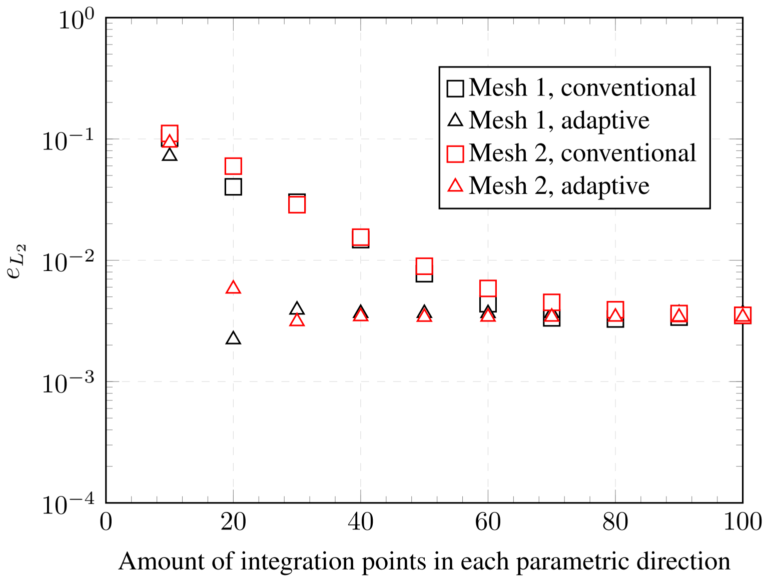

Figure 4. L_2 norm of error in displacements for in-plane penny-shaped crack: conventional vs adaptive integration schemes.

Table 1. Comparison of computational time for both schemes.

	Mesh 1		Mesh 2	
Amount of integration points	Conventional (s)	Adaptive (s)	Conventional (s)	Adaptive (s)
10	2	2	14	16
20	4	4	44	54
30	7	7	95	118
40	12	12	166	208
50	17	19	259	318
60	25	27	371	464
70	35	36	505	628
80	46	47	657	819
90	57	59	827	999
100	71	73	1019	1270

4 Concluding remarks

This study proposed an adaptive scheme to handle near-singular integration of the weakly-singular, strongly-singular and hyper-singular kernels of the XIGABEM. This proposition consists of a single knot-span subdivision in the parametric direction considering the closest point from the patch to the collocation point. A two-stage algorithm detects each knot-span in which near-singularities appear, in which the second step considers a search for the minimum distance between the patch and the collocation point. Numerical results attest a remarkable reduction in computational time, whilst maintaining accuracy. This proposition is even more relevant in the crack growth context, which is the natural extension of this study.

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