A well-conditioned and optimally convergent XFEM for 3D linear elastic fracture

Konstantinos Agathos¹, Eleni Chatzi², Stéphane P. A. Bordas³,⁴,*,† and Demosthenes Talaslidis¹

¹Institute of Structural Analysis and Dynamics of Structures, Department of Civil Engineering, Aristotle University of Thessaloniki, Panepistimiopolis Mail Stop 502, 54124 Thessaloniki, Greece
²Institute of Structural Engineering, Department of Civil, Environmental and Geomatic Engineering, ETH Zürich, Stefano-Franscini-Platz 5, CH-8093 Zürich, Switzerland
³Research Unit in Engineering Science, Luxembourg University, 6 rue Richard Coudenhove-Kalergi, L-1359 Luxembourg City, Luxembourg
⁴Institute of Theoretical, Applied and Computational Mechanics, Cardiff University, Cardiff CF24 3AA, UK

SUMMARY

A variation of the extended finite element method for three-dimensional fracture mechanics is proposed. It utilizes a novel form of enrichment and point-wise and integral matching of displacements of the standard and enriched elements in order to achieve higher accuracy, optimal convergence rates, and improved conditioning for two-dimensional and three-dimensional crack problems. A bespoke benchmark problem is introduced to determine the method’s accuracy in the general three-dimensional case where it is demonstrated that the proposed approach improves the accuracy and reduces the number of iterations required for the iterative solution of the resulting system of equations by 40% for moderately refined meshes and topological enrichment. Moreover, when a fixed enrichment volume is used, the number of iterations required grows at a rate which is reduced by a factor of 2 compared with standard extended finite element method, diminishing the number of iterations by almost one order of magnitude. Copyright © 2015 John Wiley & Sons, Ltd.

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1. INTRODUCTION

It is well known that the simulation of three-dimensional (3D) crack propagation problems using the finite element method (FEM) [1] can be problematic. The difficulties emanate from the fact that the finite element (FE) mesh has to conform to the crack surfaces as well as the boundaries of the analyzed domain. One additional requirement, which further complicates the situation, is that the mesh has to be refined in the vicinity of the crack front in order to adequately represent the singularity that occurs in the stress fields. Moreover, for every crack propagation step, local remeshing is necessary, which makes the whole procedure computationally infeasible.

An alternative to the aforementioned procedure, which has produced accurate results, is the boundary element method [2], where only the crack surfaces and domain boundaries have to be meshed. The boundary element method has recently been coupled with isogeometric analysis [3, 4].

Meshless methods, and more specifically the element-free Galerkin (EFG) method [5], have also been applied to crack propagation problems [6], eliminating the need for remeshing and greatly simplifying the process of local refinement. In those methods, the concept of ‘enrichment’ [7] was introduced, which consists of augmenting the EFG basis in order to include asymptotic near-tip
fields or special enrichment functions produced from those near-tip fields. Several other variations have also been proposed [8–11] which extend the applicability of the method.

The concept of enrichment combined with the partition of unity property [12] was also employed in the development of the extended finite element method (XFEM) [13, 14] which, while retaining the basic properties of the finite element method, does not require any remeshing in order to handle crack propagation problems. Additionally, since asymptotic tip enrichment functions are used, the need for local mesh refinement is minimized. The method was successfully extended to 3D problems [15–17] and industrial problems [18–22].

Since the introduction of the method, numerous attempts have been made towards the improvement of some of the initial method’s weaknesses. One of these weaknesses is the lack of optimal convergence, which was remedied by enriching elements in a fixed area around the crack tip [23–25]. The addition of enriched elements, however, leads to poor conditioning of the resulting system matrices which can be solved either by the use of special preconditioners [24, 26] or by using the so-called degree of freedom (dof) gathering [23] technique. Other drawbacks of the method include blending problems between the enriched and the standard part of the approximation for which several solutions have been given [27–32] and problems in numerical integration which can be dealt with by using techniques such as element partitioning and special mappings [23, 24, 31–38]. Some variations of the method have also been proposed which consist in adding higher-order terms of the near-tip asymptotic fields in order to directly obtain stress intensity factors [39–41]. Finally, significant effort has been devoted in the development of special error estimators and methods for derivative recovery specifically designed for XFEM [42–46].

A variation of the method which successfully handles several of the problems discussed earlier, is the one proposed by Laborde et al. [23]. The present work is aimed towards extending the concepts developed in the work of Laborde et al. [23] and other similar works [25, 47] to 3D crack propagation problems, a goal which is not straightforward. The resulting method’s accuracy and convergence properties are tested both for the 2D and the 3D cases; for the latter, a novel benchmark problem is proposed.

2. PROBLEM STATEMENT

The governing equations of the elastostatics problem for a cracked domain will be presented in this section, as well as the weak form of the equilibrium equations.

2.1. Governing equations

Consider the problem of a cracked domain \( \Omega \) bounded by the boundary \( \Gamma \) consisting of the parts \( \Gamma_0 \) and \( \Gamma_u \), where displacements \( \vec{u} \) are imposed as Dirichlet boundary conditions, \( \Gamma_t \) where the surface

![Figure 1. Cracked body and boundary conditions.](image)
tractions $\tilde{t}$ are applied as Neumann conditions and the crack surface $\Gamma_c$ where $\Gamma = \Gamma_0 \cup \Gamma_u \cup \Gamma_f \cup \Gamma_c$ and $\Gamma_c' = \Gamma_c' \cup \Gamma_c''$ as depicted in Figure 1. It should be noted that surface tractions $\tilde{t}_c$ are also applied at a part of the crack surface ($\Gamma_c'$). The equilibrium equations and boundary conditions are:

$$\nabla \cdot \sigma + b = 0 \quad \text{in } \Omega$$  \hspace{1cm} (1a)

$$u = \tilde{u} \quad \text{on } \Gamma_u$$  \hspace{1cm} (1b)

$$\sigma \cdot n = \tilde{t} \quad \text{on } \Gamma_f$$  \hspace{1cm} (1c)

$$\sigma \cdot n = 0 \quad \text{on } \Gamma_c^0$$  \hspace{1cm} (1d)

$$\sigma \cdot n = \tilde{t}_c \quad \text{on } \Gamma_c^f$$  \hspace{1cm} (1e)

where $\sigma$ is the Cauchy stress tensor, $n$ is the unit outward normal, $b$ is the body force per unit volume, $u$ is the displacement field, and $\nabla$ is the gradient operator. The kinematic equations for small deformations define the strain field $\epsilon$ as the symmetric gradient of the displacement field $u$:

$$\epsilon = \nabla_s u$$  \hspace{1cm} (2)

Finally, the constitutive equations are given by Hooke’s law:

$$\sigma = D : \epsilon$$  \hspace{1cm} (3)

where $D$ is the elasticity tensor.

### 2.2. Weak form

For the derivation of the classical finite element formulation, the weak form of the equilibrium equations can be stated as: Find $u \in U$ such that $\forall v \in V$

$$\int_{\Omega} \sigma (u) : \epsilon (v) \, d\Omega = \int_{\Omega} b \cdot v \, d\Omega + \int_{\Gamma_f} \tilde{t} \cdot v \, d\Gamma_f + \int_{\Gamma_c^f} \tilde{t}_c \cdot v \, d\Gamma_c^f$$  \hspace{1cm} (4)

where

$$U = \left\{ u | u \in (H^1 (\Omega))^3, u = \tilde{u} \text{ on } \Gamma_u \right\}$$  \hspace{1cm} (5)

and

$$V = \left\{ v | v \in (H^1 (\Omega))^3, v = 0 \text{ on } \Gamma_u \right\}$$  \hspace{1cm} (6)

Functions of $H^1 (\Omega)$ are implicitly discontinuous along the crack surface.

Using the constitutive equations, the weak form is obtained as:

Find $u \in U$ such that $\forall v \in V$

$$\int_{\Omega} \epsilon (u) : D : \epsilon (v) \, d\Omega = \int_{\Omega} b \cdot v \, d\Omega + \int_{\Gamma_f} \tilde{t} \cdot v \, d\Gamma_f + \int_{\Gamma_c^f} \tilde{t}_c \cdot v \, d\Gamma_c^f$$  \hspace{1cm} (7)

### 3. GLOBAL ENRICHMENT XFEM

The method presented in this work can be viewed as an extension of the method proposed by Laborde et al. [23], since some basic aspects such as point-wise matching, dof gathering, and geometrical enrichment (enrichment in a fixed area around the crack tip/front) are common in both methods. In view of the fact that this work is aimed towards a broader spectrum of applications, including 3D problems, several modifications/extensions are made to the original method. We first recall the general ideas of the work of Laborde et al. [23] before introducing the aforementioned modifications. It should be noted, however, that while in the method of Laborde et al. [23] higher-order elements are considered, in the present work only linear (P1) elements are used.
3.1. The method of Laborde

In the work of Laborde et al., it was observed that by enriching elements in a fixed area around the crack tip, an optimal convergence rate could be achieved. The aforementioned enrichment strategy, in the work of Béchet et al. [24], was referred to as ‘geometrical enrichment’ as opposed to ‘topological enrichment’ where only a layer of elements around the crack tip is enriched.

The addition of layers of tip-enriched elements, however, would lead to a drastic deterioration in the conditioning of the resulting system matrices. As a remedy, dof gathering was proposed, which consists in using a global function to weight the enrichment functions rather than the shape functions of tip-enriched elements. This function is equal to 1 for all nodes lying inside the enrichment area, assumes a value of 0 for all nodes outside the enrichment area, and varies linearly in between. While this technique leads to a decreased number of additional dofs and improved conditioning, it also leads to sub-optimal convergence rates.

The lack of optimal convergence was attributed to the problems occurring in the transition layer between enriched and regular elements. These problems were resolved by eliminating the transition layer of elements and matching displacements between enriched and regular elements. The method used to match displacements was point-wise matching.

The aforementioned concepts in addition to an improved numerical integration scheme lead to a method of increased accuracy, which provided optimal convergence rates and improved conditioning. The equations related to the aforementioned ideas, as well as the modifications and extensions made, will be presented in detail in the following sections.

3.2. Crack representation

The proposed method is independent of the crack representation used. Consequently, any of the available possibilities can be used such as level sets [16, 17, 48], vector level sets [49], or a hybrid explicit implicit representation [50].

For the simple examples treated in this work, a level set representation [16, 17, 48] was used and enrichment functions were evaluated using finite element approximation of the level set functions as is commonly performed in XFEM.

In the following sections, the level set functions will be denoted as \( \phi \) and \( \psi \) where, given an arbitrary point \( \mathbf{x} \) in the domain

- \( \phi (\mathbf{x}) \) is the signed distance from the crack surface defined as

  \[
  \phi (\mathbf{x}) = \min_{\mathbf{x} \in \Gamma_c} \| \mathbf{x} - \bar{x} \| \text{sign} (\mathbf{n}^+ \cdot (\mathbf{x} - \bar{x}))
  \]  

  where \( \mathbf{n}^+ \) is the outward normal to the crack surface and \text{sign} () is the sign function.

- \( \psi (\mathbf{x}) \) is a signed distance function such that \( \nabla \phi \cdot \nabla \psi = 0 \) and \( \phi (\mathbf{x}) = 0 \) and \( \psi (\mathbf{x}) = 0 \) defines the crack front.

The polar coordinates used for the definition of the enrichment functions are defined as [16, 17, 48]:

\[
\begin{align*}
  r &= \sqrt{\phi^2 + \psi^2}, \\
  \theta &= \arctan \left( \frac{\phi}{\psi} \right)
\end{align*}
\]

These coordinates refer to a plane normal to the crack front.

3.3. Tip enrichment

The most important extension made to the method of Laborde et al. [23], which enables the application of the idea to 3D problems, is related to the tip-enrichment scheme used and more specifically to dof gathering. In the aforementioned method, tip-enrichment functions were weighted by a global function assuming a value of 1 for all tip-enriched elements in order to decrease the number of additional unknowns and improve the conditioning of the resulting matrices. The aforementioned
approach does not allow any spatial variation of the tip-enrichment functions. Nevertheless, in 3D problems, solution parameters such as stress intensity factors (SIFs) vary along the crack front making the direct extension of the method, as presented in [23], to 3D impossible.

In the present work, a novel approach is introduced for weighting tip-enrichment functions consisting of some global shape functions, which allow spatial variability of the enrichment functions along the crack front but not in any other direction, thus preserving the advantages yielded by dof gathering and enabling the use of geometrical enrichment in 3D problems. The enriched part of the displacement approximation for tip-enriched elements, evaluated at \( \mathbf{x} \in \Omega \), can then be written as

\[
\mathbf{u}_{te} (\mathbf{x}) = \sum_{K} N_K^g (\mathbf{x}) \sum_{j} F_j (\mathbf{x}) \mathbf{c}_{Kj}
\]

(10)

where \( N_K^g \) are the global shape functions which refer to a superimposed mesh of special elements and will be presented in detail in Section 3.8, index \( K \) refers to nodes of the superimposed mesh, \( F_j \) are tip-enrichment functions, and \( \mathbf{c}_{Kj} \) are the corresponding tip dofs. Tip-enrichment functions are defined as in standard XFEM:

\[
F_j (\mathbf{x}) = F_j (r, \theta) = \begin{bmatrix} \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \frac{\theta}{2} \sin \theta, \sqrt{r} \cos \frac{\theta}{2} \sin \theta \end{bmatrix}
\]

(11)

The precise definition of parameters \( r \) and \( \theta \) was given in Section 3.2. For 2D problems, the aforementioned approach coincides with dof gathering.

In order to apply geometrical enrichment, the radius of enrichment \( r_e \) has to be defined. Subsequently, nodal values \( r_i \) of variable \( r \) are computed. If the condition \( r_i < r_e \) is true for every node of a given element, then the element is tip enriched (Figure 2).

3.4. Jump enrichment

Throughout this work, shifted jump-enrichment functions are used [19, 51]. Moreover the jump-enrichment functions are defined as

\[
H(\phi) = \begin{cases} 
1 & \text{for } \phi > 0 \\
-1 & \text{for } \phi < 0 
\end{cases}
\]

(12)

The definition of \( \phi \) was given in Section 3.2.

The nodal set of jump-enriched nodes is defined in a slightly different way than in standard XFEM. In order to justify the proposed approach, some important facts have to be considered. More specifically, the tip-enrichment functions used (Equation (11)) are derived from the first term of the Williams expansion and represent displacements in the vicinity of the crack tip. However, in the general case, displacements around the crack tip consist of higher-order terms as well. This is especially
true for the case where geometrical enrichment with relatively large enrichment radii is used. Such higher-order terms are also essential when computing T-stresses. In standard XFEM, those higher-order terms can be represented by the FE part of the approximation. In addition, the tip-enrichment functions are weighted by the FE shape functions. This provides some additional flexibility and allows the method to approximate higher-order terms by spatially adjusting the coefficients of the enrichment functions. In the proposed method, higher-order terms can only be approximated by the FE part of the approximation, since no spatial variation of the tip-enrichment function coefficients is allowed in the plane normal to the crack front due to the fact that all the coefficients (dofs) pre-multiplying the enrichment functions vary only in the direction of the crack front. As a result, in elements that contain the crack surfaces, displacement jumps caused by higher-order terms cannot be represented. In other words, in elements that are tip-enriched and contain the crack surfaces, crack opening displacements can only assume the form imposed by the tip-enrichment terms.

The aforementioned situation has a negative impact on accuracy, and in order to remedy this issue, we introduce a special enrichment strategy which consists in using both tip-enrichment and jump-enrichment functions for elements that contain the crack and lie inside the area of enrichment (Figure 2). By employing this strategy, crack opening displacements caused by higher-order terms can be represented in tip elements through jump-enrichment functions, whose weights are allowed to vary spatially.

The aforementioned difficulties and associated improvements obtained by the proposed solution will be demonstrated through a numerical example in Section 4.

3.5. Point-wise matching

The basic idea behind point-wise matching, which lies in directly matching displacements between tip-enriched and jump-enriched or tip-enriched and regular elements in order to avoid errors in blending elements, is retained in this work. The implementation, however, is adapted to the specific demands of the proposed approach.

3.5.1. Tip and regular elements. Firstly, displacement approximations of regular and tip-enriched elements are considered:

\[ u_r(x) = \sum_I N_I(x) u_I + \sum_J a_J \]  
\[ u_t(x) = \sum_I N_I(x) u_I + \sum_K \sum_J N_K^g(x) F_j(x) c_{Kj} \]  

where \( N_I \) are FE shape functions, \( u_I \) are standard FE dofs, and \( a_J \) are additional parameters to be determined. Indices \( I \) and \( J \) vary over the set of nodes that are common between tip-enriched and regular elements, while index \( K \) refers to the nodes of the superimposed mesh.

Subsequently, displacements are matched by imposing the condition \(^4\):

\[ u_r(x_I) = u_t(x_I) \]  

at nodal points \( x_I \) that are common between tip-enriched and regular elements. From the aforementioned constraint, the parameters \( a_I \) are determined:

\[ a_I = \sum_K N_K^g(X_I) \sum_j F_j(X_I) c_{Kj} \]  

where \( F_j(X_I) \) are the tip enrichment functions evaluated at nodal point \( X_I \).

The aforementioned procedure is illustrated in Figure 3 where the displacements of a common edge between a tip-enriched and a regular element are depicted.

\(^4\)Note that this procedure also removes completely blending errors [27–32].
From the preceding discussion, it should be clear that parameters $a_I$ do not correspond to any additional dofs, since they are expressed in terms of the tip dofs $c_{Kj}$. Thus, Equation (15) can be reformulated as

$$a_I = \sum_K \sum_j T_I^{r-r} c_{Kj}$$

(16)

where $T_I^{r-r}$ are the components of a matrix correlating the two sets of parameters.

3.5.2. Tip and jump elements. Throughout this work, shifted jump-enrichment functions are used, which assume a value of zero at nodal points. As a result, point-wise patching has to be adapted accordingly. More precisely, displacements for the jump-enriched and tip-enriched elements are (Figure 4):

$$u_J(x) = \sum_I N_I(x) u_I + \sum_J N_J(x) a_J + \sum_L N_L(x) (H(x) - H_L) b_L + \sum_M N_M(x) (H(x) - H_M) b_M^T$$

(17a)

$$u_T(x) = \sum_I N_I(x) u_I + \sum_J N_J(x) (H(x) - H_J) b_J + \sum_K N_K(x) \sum_j F_j(x) c_{Kj}$$

(17b)

where $b_L$ are jump dofs, $b_M^T$ are additional parameters to be determined, $H$ is the Heaviside function, and $H_L$ is the jump-enrichment function evaluated at node $L$. In the preceding discussion, index $L$ refers to the jump-enriched nodes and index $M$ refers to the jump-enriched nodes where point-wise matching is applied. Furthermore, in Equation (17b), index $J$ refers to the nodes that are both jump and tip enriched.
As already mentioned, tip-enriched elements that contain the crack are also jump enriched. Moreover, parameters $b^T_I$ hold a similar role to parameters $a^T_I$ and have to be determined. One possibility would be to treat those parameters as additional dofs and let their values be determined as part of the solution. However, our experience shows that this leads to a reduced accuracy. An alternative procedure is therefore introduced, where those parameters are obtained in terms of the tip dofs by imposing additional constraints at points located at elements edges or faces (for 3D elements).

The point-wise matching condition assumes the form

$$u_j(x_n) = u_I(x_n)$$

(18)

at selected points $x_n$ in the domain. By evaluating the aforementioned condition at nodal points, parameters $a^T_I$ are obtained as in Equation (15). By evaluating the condition at the additional points, parameters $b^T_I$ are obtained:

$$(H(X_I) - H_I) b^T_I = \sum_K N^e_K(X_I) \sum_j F_j(X_I) e_{Kj} - \sum_I N_I(X_I) a_I$$

(19)

where $F_j(X_I)$ are the tip-enrichment functions evaluated at the additional points $X_I$ and $H(X_I)$ are the jump-enrichment functions evaluated at the additional points $X_I$.

It should be noted that Equation (19) represents a linear system of equations. Nevertheless, due to the properties of shifted jump-enrichment functions, the equations are decoupled in most cases.

In a similar fashion to Equation (15) and by taking into account Equation (16), Equation (19) can be reformulated as

$$b^T_I = \sum_K \sum_j T^{I-j}_{IKj} e_{Kj}$$

(20)

where $T^{I-j}_{IKj}$ are the components of a matrix which comes from the solution of Equation (19).

An important step in the whole procedure is the selection of points where the additional condition is applied. The basic restriction that applies in the selection of those points is imposed by the fact that shifted enrichment functions vanish on one side of the crack, and as a result, the corresponding points have to be selected on the opposite side in order to prevent the coefficient matrix of Equation (19) from being singular.

In this work, the points for the additional constraint are chosen to be the points where the two surfaces of the crack intersect element edges or faces. In order to locate those points, for each edge where the additional condition has to be applied, the point where the first level set assumes a value of zero is initially located. Subsequently, this point is moved by a small increment towards either side of the crack. It should be noted that the size of this increment has negligible effect in the accuracy and/or behavior of the method. In our numerical experiments a value of $10^{-8}$ in the isoparametric coordinate system was used.

This selection procedure is illustrated in Figure 5 for the 2D case, where point-wise matching is taking place in the edge defined by nodes 2 and 5. The points selected are points $a$ and $b$ where parameters $b^T_2$ and $b^T_5$ corresponding to nodes 2 and 5 are defined respectively.

For the 3D case, the selection of points is somewhat more involved due to the complex geometry. For linear hexahedral elements, which are used in this work, point-wise matching can take place at an edge, a face, several faces or edges, and combinations of faces and edges as illustrated in Figure 6. The selection of points, which is also demonstrated in Figure 6 is performed in a similar way as for the 2D case. An additional requirement is that in the case where point-wise matching takes place in several faces (Figure 6(c) and (d)), the selected points must coincide at edges that are common in those faces.

A case of special interest is the one illustrated in Figure 6(d). In particular, at point $f$ which corresponds to node 6, the enrichment functions of nodes 3 and 5 do not vanish, and as a result, the system of Equation (19) is no longer decoupled for face 2–3–6–5, since the coefficient matrix of $b^T_I$ is not diagonal and has to be inverted in order to infer these parameters. The only difference in this
case is that a linear system has to be solved. The added computational cost is of course negligible, since the size of this system is equal to the number of point-wise matching points in a given element.

The situation depicted in Figure 7 is also particularly significant. In this case, point-wise matching would take place at the edges defined by nodes 3, 4 and 4, 7. However, the edge defined by nodes 3 and 4 does not belong to a tip-enriched element, and as a result, evaluating the tip-enrichment functions for a point on that edge would lead to errors. In order to avoid these errors, the values of the parameters $b_t^i$ obtained from edge 4–7 should be also used for edge 3–4. Of course, similar situations occur also in the 3D case.

In order to implement the procedure described earlier, all elements where point-wise matching occurs should be identified and looped over prior to the assembly of the stiffness matrix, and wherever possible, the values of the parameters $b_t^i$ should be computed and stored. This way, the parameters $b_t^i$ can be computed for every node using the correct element edges or faces. Moreover, the whole procedure is computationally inexpensive.
Finally, for cases where the crack passes through a node, the point-wise matching approach is only slightly modified: the node that is intersected by the crack is assigned either a positive or a negative value ($0^+$ or $0^-$) for the first level set so that the jump-enrichment function assumes a value of 1 or $0^+$, respectively. Subsequently, the matching point corresponding to that node is obtained by moving by a small increment along the element edge towards the side of the crack where the first level set assumes a value with a sign opposite to the one given to the intersected node.

3.6. Integral matching

The proposed method is intended to be used both with geometrical and topological enrichment. In the latter case, for the P1 (linear) elements used in the present work, a loss of accuracy is observed, which is more pronounced for mode I loading. This can attributed to the geometry of the deformation and more specifically to the displacement jump between regular and tip-enriched elements (Figure 8). This displacement jump also occurs for mode II crack loading; however, in that case, it can be considered to vanish in a weak (integral) sense, as illustrated in Figure 9, and as a result, the loss of accuracy is smaller.
Figure 9. (a) Displacement jump along element edges for Mode II crack opening. (b) Displacements along an edge of the element depicted in (a). It can be seen that gaps as well as overlaps occur which result in the discontinuity almost vanishing in a weak sense.

One possible solution to the problem is the addition of one layer of enriched elements around the crack tip/front. An alternative solution is proposed here which consists of the addition of hierarchical blending functions. Those functions are added to elements where point-wise matching occurs and serve the purpose of eliminating the displacement jump in a weak sense.

For linear quadrilateral elements, those functions assume the form

\[ N^h(\xi_1, \xi_2) = \frac{(1 - |\xi_1|)(1 + \xi_2)}{2} \]  

where \(\xi_1\) and \(\xi_2\) are the element’s isoparametric coordinates. Variables \(\xi_1\) and \(\xi_2\) in the preceding equation as well as their signs change depending on the side on which the blending functions are added. For 3D brick elements those functions assume a similar form.

Adding to the approximation the blending functions, displacements along the edges of regular and jump-enriched elements take the form

\[ u_r(\xi_1, \xi_2) = \sum_I N_I(\xi_1, \xi_2) u_I + \sum_J N_J(\xi_1, \xi_2) a_J + N^h(\xi_1, \xi_2) a^h \] 

\[ u_t(\xi_1, \xi_2) = \sum_I N_I(\xi_1, \xi_2) u_I + \sum_K N^e_K(x) \sum_J F_J(x) c_{KJ} \]  

where \(a^h\) are the coefficients of the blending functions.

Those coefficients could be obtained by imposing a point-wise matching condition in the midpoints of element edges which is similar to the approach used in previous sections. It was observed, however, that an increased accuracy can be obtained in the general 3D case by applying an integral matching condition of the form

\[ \int_S (u_r - u_t) dS = 0 \]  

where \(S\) is the element edge length.

This approach shares some similarities with the work of Chanine et al. [47]. Nonetheless, in the present case, integral matching is only used for the additional blending functions, and nodal displacements are matched using point-wise matching.

In a similar fashion as in the previous sections, coefficients \(a^h\) can be obtained as functions of the tip dofs:

\[ a^h_I = \sum_K \sum_J T^h_{IKJ} c_{KJ} \]
In the aforementioned relation, index $i$ refers to edges and not nodes (Figure 10).
In the general 3D case, additional functions could be added to match displacements along faces as well. In the present implementation, however, only matching along edges was implemented.

For cases where the crack tip/front is in the close vicinity of element nodes, the method’s accuracy decreases despite the use of those functions. In those cases, neighboring elements should be tip enriched as well in order to prevent this loss of accuracy.

### 3.7. Displacement approximation

Summarizing all the preceding discussions, the displacement approximation for the whole domain can be formulated as

$$u(x) = \sum_{I \in \mathcal{N}} N_I(x) u_I + \sum_{J \in \mathcal{N}^f} N_J(x) (H(x) - H_J) b_J +$$

$$+ \sum_{K \in \mathcal{N}^g} N_K(x) \sum_j T_{Kj}^l c_{Kj} + u_{pm}^l(x) + u_{im}^l(x)$$

$$u_{pm}(x) = \sum_{I \in \mathcal{N}^{t1}} N_I(x) \sum_K \sum_j T_{IKj}^{l-r} c_{Kj} +$$

$$+ \sum_{J \in \mathcal{N}^{t2}} N_J(x) (H(x) - H_J) \sum_K \sum_j T_{IKj}^{l-j} c_{Kj}$$

$$u_{im}(x) = \sum_{I \in \mathcal{N}^{t1}} N_I^h(x) \sum_K \sum_j T_{IKj}^h c_{Kj}$$

The sets mentioned in the preceding equation are defined as follows:

- $\mathcal{N}$ is the set of all nodes in the FE mesh.
- $\mathcal{N}^f$ is the set of jump-enriched nodes. This set includes all nodes whose shape function support is divided in two by the crack. This definition does not change when geometrical enrichment is used as discussed in Section 3.4.
- $\mathcal{N}^g$ is the set of superimposed nodes. This set does not refer to nodes of the FE mesh but to nodes of the superimposed mesh which will be described in the next section.
- $\mathcal{N}^{t1}$ is the set of transition nodes between tip and regular or jump elements.
- $\mathcal{N}^{t2}$ is the set of transition nodes between tip and jump elements.
- $\mathcal{N}^h$ is the set of edges where the blending functions are added.

### 3.8. Definition of the front elements

In this section, the definition of the superimposed mesh and the corresponding shape functions $N_K^g$ mentioned in Section 3.3 are given.
3.8.1. Approximation along the crack front. The superimposed mesh introduced in this work serves the purpose of providing a basis with which the singular enrichment functions will be weighted. The desired properties for this basis are that it should satisfy the partition of unity property and, additionally, that it should allow spatial variation only along the direction of the crack front. Those requirements can be fulfilled by elements that share properties of both 1D and 3D elements. Those elements are 1D in the sense that their shape functions allow variation only along one dimension and are defined by two nodes (more if higher-order elements are used) and are 3D in the sense that their shape functions are defined in a 3D domain, and as a result, additional information other than their nodal coordinates is required for their definition. An alternative way to view those elements would be as 3D brick elements with their nodes constrained in a way such that variation along only one dimension is allowed.

A concept which is very similar to the superimposed mesh used in this work is the analytical patch and the corresponding nodes and elements used in the work of Langlois et al. [52]. The method also shares some similarities with the s-finite element method [53]; it differs, however, from both methods since, in the present method, the superimposed mesh is only used to provide a basis for weighting the singular enrichment functions. For this reason, the superimposed elements have no particular physical meaning other than that of providing a means to introduce spatial variation of the enrichment functions.

For the definition of the superimposed mesh, a set of points that lie on the crack front have to be identified. The appropriate thickness of the front elements has to be determined depending on the variability of the SIFs along the front. A good starting point for the general case would be a front element thickness equal to the mesh parameter $h$ which should provide a variability along the crack front similar to standard XFEM. As a direction for future work, an error estimator could be used to adaptively refine the crack front discretization.

As far as the identification of the points on the crack front is concerned, the location of such points is usually required also for the calculation of SIFs. Moreover, the use of a hybrid crack representation [50] would further facilitate the whole procedure, since this hybrid approach consists of meshing the crack, and as a result, the location and connectivity of the points required for meshing the crack front would be already available. Of course, a more dense discretization of the crack front might be necessary, in which case some refinement would be needed.

In the present work, only linear elements were implemented for meshing of the crack front. Several alternatives are possible for the definition of front element boundaries. In the next sections, two approaches will be presented that are best suited for open and closed crack fronts, respectively. Moreover, for both approaches, continuous numbering of the front nodes will be assumed.

Figure 11. (a) Crack front discretization for open crack fronts. (b) Vectors associated with front elements.
3.8.1.1. **Open crack fronts.** Elements are defined by two consecutive nodes, and element boundaries are defined in the following way (see also Figure 11):

- For every element a unit vector, $\mathbf{e}_i$ is defined parallel to the direction of the line connecting the two nodes belonging to the element: $\mathbf{e}_i = \frac{x_{i+1} - x_i}{|x_{i+1} - x_i|}$.
- For every nodal point $i$, a unit vector $\mathbf{n}_i$ is defined as the mean of the two vectors corresponding to the elements adjacent to the node: $\mathbf{n}_i = \frac{\mathbf{e}_i + \mathbf{e}_{i-1}}{|\mathbf{e}_i + \mathbf{e}_{i-1}|}$.
- Additionally, a plane is defined that passes through the node and is normal to the vector $\mathbf{n}_i$ corresponding to the node: $\mathbf{n}_i \cdot (x_0 - x_i) = 0$.
- The volume corresponding to the element is defined by the planes corresponding to its nodes and the tip-enriched elements around the crack front. The geometry of front elements is illustrated in Figure 11(a) and in Figure 12, where part of a curved crack front is shown along with the tip-enriched element and the corresponding front element volumes.

In order to deal with cases where the crack intersects with free surfaces, the first and/or last node can be moved in the direction of the crack front so that all finite elements within the radius of interest lie inside the first and/or last superimposed element.

3.8.1.2. **Closed crack fronts.** For closed crack fronts, the aforementioned approach might lead to certain difficulties. More specifically, if the elliptical crack of Figure 13 is considered, the element boundaries defined by the aforementioned approach and depicted in Figure 13(a) overlap, which could cause problems in the definition of front element boundaries if the area used for tip enrichment is large enough to include the point where this overlapping occurs. In order to avoid similar...

![Figure 12](image12.png)

**Figure 12.** Volume corresponding to two consecutive front elements. Different element colors correspond to different front elements.

![Figure 13](image13.png)

**Figure 13.** (a) Application of the method used for open crack fronts to closed crack fronts, it can be seen that front elements overlap. (b) Method used for closed crack fronts, overlaps are avoided.
situations, a different approach is adopted according to which element boundaries are defined by using an additional point \( (x_c) \) in the interior of the closed curve defined by the crack front as in Figure 13(b). For plane cracks, this point lies on the crack surface.

In more detail (see also Figure 14):

- Vectors \( e_i \) are defined for every element.
- A point \( x_c \) in the interior of the crack front is defined as: \( x_c = \frac{\sum_{i=1}^{n} x_i}{n} \).
- For every nodal point \( i \), a vector \( n_{cl} \) joining that point to the internal point \( x_c \) is defined: \( n_{cl} = x_c - x_i \).
- Vectors \( n_{nl} \) normal to the plane defined by vectors \( e_i \) and \( n_{cl} \) are defined as: \( n_{nl} = e_i \times n_{cl} \).
- Vectors \( n_i \) are defined as: \( n_i = \frac{n_{cl} \times n_{nl}}{ \| n_{cl} \times n_{nl} \| } \).
- Planes normal to the vectors \( n_i \) are defined: \( n_i \cdot (x_0 - x_i) = 0 \).
- Element volumes are defined by the planes corresponding to their nodes as for the open crack front case.

In Figure 15, the application of the aforementioned procedure to a closed, non-planar crack front is illustrated.

As already mentioned, superimposed elements have no particular physical meaning; nevertheless, it is important to define their boundaries so as to be able to relate every enriched element to its corresponding superimposed elements.

The problem described for closed cracks can also occur for open cracks or parts of open cracks where the curvature of the crack front is large or if sharp corners are present. In that case, the
closed crack front approach should be used. The definition of point $x_c$, however, will have to be adjusted accordingly.

### 3.8.2. Front element parameter

In order to facilitate the interaction of the XFEM and crack front meshes, one additional function, similar to the level sets, is defined which varies along the direction of the crack front. This parameter takes integer values on the front nodes and the planes defined by front nodes and varies linearly in between (Figure 16). Since front nodes are numbered continuously, the values of the parameter at the nodes should coincide with node numbers.

For a point $x_0$, this parameter is evaluated as follows:

For all front elements, the plane equations corresponding to their nodes are evaluated:

\[
\begin{align*}
f_i(x_0) & = n_i \cdot (x_0 - x_i) \\
\end{align*}
\]

\[
\begin{align*}
f_{i+1}(x_0) & = n_{i+1} \cdot (x_0 - x_{i+1})
\end{align*}
\]  

- If $f_i < 0$ or $f_{i+1} > 0$, the point lies outside the element volume and the next element is checked.
- If $f_i = 0$ or $f_{i+1} = 0$, the point lies on the plane corresponding to node $i$ or $i + 1$, respectively, and it is assigned a front parameter value $\eta = i$ or $\eta = i + 1$.
- If $f_i > 0$ and $f_{i+1} < 0$, the point lies inside the element.

If the point is found to lie inside a certain element (Figure 17), the integer part of the front parameter is equal to the number of the first element node $\eta_i = i$. In order to evaluate the fractional part of the parameter, a line is formed which passes from point $x_0$ and is parallel to vector $e_i$. Points on this line have coordinates:

\[
x = x_0 + t e_i \quad t \in \mathbb{R}
\]  

Figure 16. Iso lines of the front element parameter.

Figure 17. Front element parameter evaluation.
At the point where the line intersects the planes defined by element nodes, parameter \( t \) takes the values

\[
\begin{align*}
t_1 &= \frac{n_i \cdot (x_0 - x_i)}{n_i \cdot e_i} \\
t_2 &= \frac{n_{i+1} \cdot (x_0 - x_{i+1})}{n_{i+1} \cdot e_i}
\end{align*}
\] (28a, 28b)

The coordinates of those points are

\[
\begin{align*}
x_1 &= x_0 + t_1 e_i \\
x_2 &= x_0 + t_2 e_i
\end{align*}
\] (29a, 29b)

The fractional part of the front parameter for point \( x_0 \) is

\[
\eta_f = \frac{|x_{10}|}{|x_{12}|}
\] (30)

where

\[
\begin{align*}
x_{10} &= x_0 - x_1 \\
x_{12} &= x_2 - x_1
\end{align*}
\] (31a, 31b)

Finally, the value of the front parameter is written:

\[
\eta = \eta_i + \eta_f
\] (32)

Parameter \( \eta \) is evaluated for every tip-enriched node.

### 3.8.3. Front element shape functions.

Shape functions of the linear front elements used in this work are linear 1D shape functions:

\[
N^f(\xi) = \begin{bmatrix} 1 - \xi & 1 + \xi \\ \frac{2}{2} & \frac{2}{2} \end{bmatrix}
\] (33)

where \( \xi \) is the local coordinate of the superimposed element.

Those functions coincide with the ones used in Equation (10). Index \( K \) used in Equation (10) and throughout Section 3 refers to the nodes of the front elements.

The coordinate \( \xi \) is defined in a similar way to the fractional part of parameter \( \eta \). The only difference being that while \( \eta_f \) assumes values from 0 to 1, \( \xi \) assumes values from -1 to 1 as illustrated in Figure 18.

The evaluation of \( \xi \) is almost identical to the evaluation of \( \eta_f \):

\[
\xi = \frac{2 x_{12} \cdot x_{m0}}{|x_{12}|^2}
\] (34)

where

\[
\begin{align*}
x_{12} &= x_2 - x_1 \\
x_{m0} &= x_0 - x_m \\
x_m &= \frac{x_1 + x_2}{2}
\end{align*}
\] (35a, 35b, 35c)

During the assembly procedure, the exact values of the \( \xi \) coordinate are used rather than their FE approximation. This means that the aforementioned procedure has to be repeated for every Gauss point of every enriched element. In order to simplify the procedure, the nodal values of parameter \( \eta \) can be used to restrict the range of front elements that are checked for each Gauss point.
For the evaluation of shape function derivatives, the derivatives of $\xi$ with respect to the spatial coordinates are also needed. These can be calculated from the derivatives of the expressions given earlier. Further details about the assembly procedure used for the front elements are given in Appendix A.

4. NUMERICAL EXAMPLES

In this section, numerical examples demonstrating the accuracy, convergence properties, and computational cost of the proposed methodology are presented.

4.1. Implementation details

Some details regarding numerical integration and SIF evaluation will be given before presenting the benchmark problems solved.

4.1.1. Numerical integration. In XFEM in general and in the present methodology in particular, integration of enriched elements is of vital importance if optimal convergence and high accuracy are to be achieved. For elements containing the crack front, the approach used herein consists of combining the element-partitioning algorithm proposed in Loehnert et al. [32] with a transformation as the one used in Minnebo [37] in order to integrate the singular tip-enrichment functions as accurately as possible. For tip-enriched elements that do not contain the crack front, a large number of Gauss points ($10 \times 10 \times 10$) was used, and for jump-enriched elements, a simple element partitioning scheme as in Moës et al. [16]. For the 2D examples, a similar approach was used utilizing almost polar integration ([23, 24]) for elements containing the crack tip, a large number of Gauss points ($20 \times 20$) for the rest of the tip elements, and element partitioning for jump elements. Two attractive alternatives for numerical integration would be the methods of Natarajan et al. [36, 54] and Chevaugeon et al. [38]; however, for the 3D case, an extension of both methods would be required.

An additional difficulty that arises in the present work is the treatment of mesh interactions. More specifically, since enriched elements can be intersected by several front elements, those intersections should be appropriately taken into account by the numerical integration scheme in order to accurately integrate the enrichment functions and the front element shape functions. In the present work, the integration scheme described in the previous paragraph was used, and element intersections were ignored. This simplified strategy, which is similar to the one used in the s-finite element method [53], could introduce errors, thus there might be some room for improvement for the results presented in Section 4.
4.1.2. Integration of crack surface tractions. The contribution of the crack surface tractions in the final system of equations is obtained by substituting the displacement approximation of Equation (25) in the third integral of Equation (7). This integral is evaluated in an element-wise fashion by locating the points where the crack faces and front intersect elements. The possible numbers of points are 3, 4, and 5, and the resulting surfaces to be integrated, which are assumed to be flat, are triangles, quadrilaterals, and pentagons which are in turn divided into triangles. Those surfaces are moved by a negative and a positive increment along the direction of the level set gradient that is normal to the crack surface in order to obtain the upper and lower crack faces $\Gamma_{c+}$ and $\Gamma_{c-}$. A large number of Gauss points (20 × 20 for quadrilaterals and 175 for triangles) was used to accurately integrate the surface integral.

4.1.3. Stress intensity factor estimation. For the evaluation of the SIFs, an interaction integral was used. An additional term was added as in Walters et al. [55] in order to account for surface tractions applied at the crack faces:

$$I = -\int_V q_{i,j} \left( \epsilon_{kl}^{aux} \delta_{ij} - \sigma_{kj}^{aux} u_{k,i}^{aux} - \sigma_{ki}^{aux} u_{k,i}^{aux} \right) dV - \int_{\Gamma_{c+} \cup \Gamma_{c-}} (t_j u_j^{aux}) q_i d\Gamma$$ \hspace{1cm} (36)

where $\epsilon^{aux}$, $\sigma^{aux}$, and $u^{aux}$ are the auxiliary stress, strain, and displacement fields, respectively, which are defined as in Moës et al. [16], and $t_j$ are the applied surface tractions. The additional term is integrated over the crack faces $\Gamma_{c+}$ and $\Gamma_{c-}$.

Tensors in the preceding equation refer to a basis defined by the level set gradients as in Moës et al. [16].

4.1.3.1. Three-dimensional domain integral. For the 3D case, the volume integrals of Equation (36) are evaluated in a parallelepiped mesh around each point of interest as in Moës et al. [16] and Sukumar et al. [15]. Function $q$ is also defined as in Sukumar et al. [15].

Special attention has to be given to the evaluation of the third integral of Equation (36). In Walters et al. [55], a procedure is introduced to accurately integrate this term; in the present case however, it is impossible to implement this procedure as the FE mesh does not conform to the crack geometry. The procedure used instead involves the detection of the points where the crack faces and front intersect elements of the parallelepiped mesh used in a similar manner to Section 4.1.2. The crack surfaces obtained this way are an approximation of the FE surfaces in the SIF mesh. In order to make this approximation as accurate as possible, a large number of elements ($8 \times 8 \times 8$) is used for the SIF mesh. Moreover, since the surface integrals are important for the overall accuracy of the SIFs, a large number of integration points, equal to the one used for the evaluation of the contribution of surface tractions, is employed.

The aforementioned procedure is both computationally expensive and of limited accuracy. Nevertheless, it is only used to provide an estimate of the accuracy of the SIFs computed by the proposed method. In the case where no surface tractions were present, a smaller number of elements could be used for the SIF mesh which would make the procedure faster.

4.1.3.2. Two-dimensional domain integral. For the 2D case, the interaction integral is evaluated in a ring of elements around the crack tip, and function $q$ assumes a value of unity for nodes within a predefined distance from the crack tip and a value of zero for the rest of the nodes as in Moës et al. [14].

In addition, no surface tractions were considered so the third integral of Equation (36) vanishes. It should be noted, however, that in the 2D case, a procedure similar to the one proposed by Walters et al. [55] would be possible to implement, making the evaluation of this integral more accurate.
4.2. Benchmark problems

The energy and $L_2$ error norms used throughout this section are defined as follows, where it is noted that vectors and tensors are written in matrix form:

\[
E = \left( \frac{\int_\Omega (\epsilon - \epsilon^h)^T \mathbf{D} (\epsilon - \epsilon^h) \, d\Omega}{\int_\Omega \epsilon^T \mathbf{D} \epsilon \, d\Omega} \right)^{1/2}
\]

(37a)

\[
L_2 = \left( \frac{\int_\Omega (\mathbf{u} - \mathbf{u}^h)^T (\mathbf{u} - \mathbf{u}^h) \, d\Omega}{\int_\Omega \mathbf{u}^T \mathbf{u} \, d\Omega} \right)^{1/2}
\]

(37b)

where $\epsilon$ and $\mathbf{u}$ are the strains and displacements obtained from the analytical solution, and $\epsilon^h$ and $\mathbf{u}^h$ are the corresponding numerically obtained values.

The 2D version of the method was implemented in MATLAB, while for the 3D version, a C++ code was created utilizing the Gmm++ library [56] for linear algebra operations. For the solution of the systems of equations in the 3D examples, the conjugate gradient (CG) solver of the Gmm++ package was employed in combination with a diagonal preconditioner. The convergence tolerance for the solver was set to $10^{-8}$.

4.2.1. Two-dimensional convergence study. The first problem considered in this section is also investigated in several other works and is commonly employed in order to examine the convergence behavior of the numerous variations of the XFEM. It consists of an $L \times L$ square with an edge crack of length $a$, as depicted in Figure 19. The displacements corresponding to the first term of the Williams expansion are imposed to the square as (Dirichlet) boundary conditions. The dimensions of the problem are taken as $L = 1$ unit and $a = 0.5$ units, and the material parameters are $E = 100$ units and $\nu = 0.0$.

By setting Poisson’s ratio to zero and extruding the problem in the normal direction, this may also serve as a 3D benchmark problem. In fact, the problem was also solved using hexahedral elements, and the results were almost identical with some minor (negligible) differences being attributed to numerical integration. As a result, the results given for the energy and $L_2$ norms are also valid for the 3D version of the method, and since the problem does not imply any variation along the crack front, results are also independent of the number of front elements used.

It should be noted that for a different value of the Poisson’s ratio, the behavior of the solution would be almost identical.

Figure 19. Edge crack problem geometry and discretization. The boundary conditions are those provided by the Griffith crack problem so as to mimic the infinity of the domain. The dimensions of the problem are $L = 1$ unit and $a = 0.5$ units.
Table I. List of acronyms used for the 2D convergence study.

| Acronym       | Description                                                                 |
|---------------|-----------------------------------------------------------------------------|
| FEM           | The FE part of the approximation                                             |
| XFEM          | Standard XFEM (with shifted enrichment functions)                           |
| XFEMpm1       | XFEM using dof gathering and point-wise matching                             |
| XFEMpm2       | XFEMpm1 with the additional condition of Section 3.5.2                      |
| GE-XFEM       | XFEMpm2 with integral matching (global enrichment XFEM)                     |

XFEM, extended finite element method.

Figure 20. Edge crack problem. $L_2$ and energy ($E$) norms versus the number of elements per side ($n$) for topological enrichment ($r_e = 0.00$ units) for modes I and II. The crack length is $a = 0.5$ units and the size of the domain is $L = 1$ unit. A description of the different methods mentioned in the figure is given in Table I, while the corresponding convergence rates are given in Table II.

The domain is meshed using $n \times n$ linear quadrilateral elements where $n = 11, 21, 41, 61, 81, 101$. The problem is solved using both topological and geometrical enrichment. In the latter case, an enrichment radius $r_e = 0.00$ units is used; this value was chosen so that for the $21 \times 21$ mesh, a full layer of enriched elements is added. For this example, the jump-enrichment strategy of Section 3.4 is not used since displacements only consist of the first term of the Williams expansion.

The problem is solved for several variants of the method which are described in Table I. For the second case (XFEMpm1), the additional condition of Section 3.5.2 is not imposed and the jump dofs of elements in contact to tip elements are treated as additional unknowns.

4.2.1.1. $L_2$ and energy norms. In Figures 20 and 21, the $L_2$ and energy error norms are depicted for Mode I and II fracture, for topological and geometrical enrichment for four cases. In Table II, the convergence rates for all the aforementioned cases are given.
Table II. Edge crack problem.

|                  | $r_e = 0.00$ |                  | $r_e = 0.12$ |
|------------------|--------------|------------------|--------------|
|                  | Mode I       | Mode II          | Mode I       | Mode II          |
| XFEM E           | 0.491        | 0.493            | 1.030        | 0.982            |
| XFEM $L_2$       | 0.908        | 0.928            | 1.980        | 1.955            |
| XFEM pm1 E       | 0.483        | 0.489            | 1.243        | 1.211            |
| XFEM pm1 $L_2$   | 1.044        | 0.984            | 2.355        | 1.773            |
| XFEM pm2 E       | 0.483        | 0.479            | 1.245        | 1.179            |
| XFEM pm2 $L_2$   | 1.022        | 1.414            | 2.311        | 2.151            |
| GE-XFEM E        | **0.477**    | **0.476**        | **1.156**    | **1.140**        |
| GE-XFEM $L_2$    | **1.326**    | **1.446**        | **2.086**    | **2.100**        |

Convergence rates for the curves of Figures 20 and 21 for the energy ($E$) and $L_2$ norms for topological ($r_e = 0.00$ units) and geometrical ($r_e = 0.12$ units) enrichment. Note the superconvergence property of the global enrichment approach in the $L_2$ norm. The method is slightly sub-optimal in the energy norm.

XFEM, extended finite element method; GE, global enrichment.

Figure 22. Edge crack problem. Mode I and II stress intensity factors predicted by XFEM and GE-XFEM versus the number of elements per side ($n$) for topological ($r_e = 0.00$ units) and geometrical ($r_e = 0.12$ units) enrichment. The crack length is $a = 0.5$ units and the size of the domain is $L = 1$ unit. The convergence rates for all cases are given in Table III.

It can be noted from Figures 20 and 21 that the additional point-wise matching condition significantly improves results for Mode II cracks. More specifically, the application of the additional constraint decreases errors by more than 75% for the $L_2$ norm and more than 50% for the energy norm. This improvement may be explained as follows: When point-wise matching is applied, displacements along the common edges between tip-enriched and jump-enriched elements are discontinuous at every point except the nodes where point-wise matching is applied. By applying the additional condition, continuity is imposed in the additional matching points as well. As a result, displacement jumps between those elements are reduced, thus leading to improved accuracy.

Moreover, integral matching mostly influences Mode I cracks when topological enrichment is used, while it improves results only slightly for the rest of the cases. The final curves achieved (GE-XFEM) provide significant improvement compared with standard XFEM, since for all the cases examined, the errors for the proposed method were reduced by more than 50% for the $L_2$ norm and 25% for the energy norm.

Furthermore, it is interesting to note that for all the cases considered, the global enrichment approach provides similar convergence rates and lower errors than standard XFEM while also reducing the number of enriched dofs. We will see in the following that this advantage is compounded by the fact that solution times are reduced considerably thanks to the improved conditioning of the system matrices.

4.2.1.2. Stress intensity factors. Stress intensity factors computed via proposed method and standard XFEM are compared in Figure 22; convergence rates for all cases are given in Table III. A radius $r_d = 0.15$ is used for SIF evaluation.
Table III. Edge crack problem.

|          | $r = 0.00$ |          | $r = 0.12$ |          |
|----------|------------|----------|------------|----------|
|          | Mode I     | Mode II  | Mode I     | Mode II  |
| XFEM     | 1.071      | 1.005    | 2.195      | 2.021    |
| GE-XFEM  | 0.759      | 1.246    | 2.545      | 2.029    |

Convergence rates for the SIFs of Figure 22.
XFEM, extended finite element method; GE, global enrichment.

Figure 23. Edge crack problem. Condition numbers of the system matrices produced by XFEM and GE-XFEM versus the number of elements per side ($n$) for topological ($r_e = 0.00$ units) and geometrical ($r_e = 0.12$ units) enrichment. The crack length is $a = 0.5$ units and the size of the domain is $L = 1$ unit. Condition numbers of the FE part of the approximation are also plotted for reference.

In the results produced by the proposed method, some fluctuations occur which were also observed in Laborde et al. [23]. Nevertheless, despite the fluctuations, the accuracy is substantially improved and the convergence rates are similar to standard XFEM. It should be noted that the convergence rates of the computed SIFs for this example are almost equal to the convergence rates obtained for the displacements ($L_2$ norm).

4.2.1.3. Conditioning. In Figure 23, the condition numbers for standard XFEM and the proposed method are illustrated. The condition numbers of the FE part of the corresponding matrices are also plotted. The proposed method performs significantly better than standard XFEM in every case. When topological enrichment is used, condition numbers corresponding to the global enrichment approach are one order of magnitude lower than standard XFEM and increase in a similar rate, while for the geometrical enrichment case, the rate of increase is reduced by four times, resulting in condition numbers several orders of magnitude lower. Furthermore, when geometrical enrichment is used, condition numbers of the proposed method change only slightly compared with topological enrichment, and for the cases considered are even smaller than the ones corresponding to standard XFEM for the topological enrichment case.

4.2.2. Three-dimensional convergence study. The accuracy and convergence properties of the proposed method for the general 3D case are demonstrated through a novel benchmark problem. This problem is based on the analytical solution for the problem of a penny crack in an infinite solid subjected to uniform normal and shear loading [57]. Full displacement and stress fields are available for this problem [57], which makes possible the evaluation of $L_2$ and energy error norms.

The displacement fields provided by the analytical solution are imposed as constraints along the boundaries of the domain considered as in the 2D convergence study. In addition, a uniform normal or shear load has to be applied on the crack faces.

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The proposed benchmark differs from the one used in 2D convergence studies in several ways:

- Firstly, it includes the full solution for the whole crack, rather than only the first term of the Williams expansion for a small part of the crack around the crack front. Thus, the effects of higher-order terms, and most importantly, of the size of the enriched area in the accuracy of the various methods can be investigated.
- Secondly, the proposed problem involves variation of the solution parameters (e.g., SIFs) across the length of the crack front. This feature is important both for the general case where a 3D behavior is preferable and for the present case where the effectiveness of the superimposed element approach needs to be studied.
- Furthermore, the crack front considered is curved, which is the case in practical applications ([18–22]).

For the aforementioned reasons, the proposed benchmark should provide a reliable means of testing the accuracy of computational fracture methods in general and of the proposed method in particular.

A parallelepiped domain is considered with dimensions $L_x \times L_y \times L_z$ with a penny crack of radius $a$ as in Figure 24. The dimensions of the problem were set to $L_x = L_y = 2L_z = 0.4$ units and $a = 0.1$ unit. A uniform normal and a uniform shear load of magnitude 1 are applied at the crack faces (mixed-mode loading). The material parameters used are $E = 100$ units and $\nu = 0.3$.

The domain is meshed using several meshes consisting of $n_x \times n_y \times n_z$ hexahedral elements where $n_x = n_y = 2n_z = n$ and $n \in \{21, 41, 61, 81, 101\}$.

The acronyms used for the different methods tested are described in Table IV.

### 4.2.2.1. $L_2$ and energy norms

In Figure 25, the influence of the crack front mesh on the accuracy of the results is investigated for two different enrichment radii ($r_e = 0.00$ units and $r_e = 0.02$ units) and for a mesh consisting of $31 \times 61 \times 61$ elements. The crack front meshes used consist of $n_f = 4, 8, 16, 32, 64, 128$ elements. Despite the fact that the solution parameters vary significantly along the crack front, the influence of the front mesh density is minimal. More precisely, for all the discretizations except the first two (4 and 8 front elements) the difference is less than 5% in the $L_2$ norm. A possible explanation for the aforementioned situation is the fact that the interactions of the

![Figure 24. Penny crack problem geometry and discretization. The boundary conditions provided by the analytical solution are imposed along the boundaries of the domain. Uniform normal and shear loads are applied to the crack surfaces. The dimensions of the problem are $L_x = L_y = 2L_z = 0.4$ units and $a = 0.1$ unit.](image)

Table IV. List of acronyms used for the 3D convergence study.

| Acronym         | Description                                           |
|-----------------|-------------------------------------------------------|
| XFEM            | Standard XFEM (with shifted enrichment functions)     |
| GE-XFEM         | The proposed method (global enrichment XFEM)          |
| GE-XFEM1        | The proposed method without the enrichment strategy of Section 3.4 |

XFEM, extended finite element method.
Figure 25. Penny crack problem. Influence of the crack front mesh density ($n_f$ is the number of elements along the front) in the energy ($E$) and $L_2$ norms for the proposed method for topological ($r_e = 0.00$ units) and geometrical enrichment with an enrichment radius $r_e = 0.02$ units. The radius of the crack is $a = 0.1$ units and the size of the domain is $L_x = L_y = 2L_z = 0.4$ units. Results refer to a mesh consisting of $31 \times 61 \times 61$ elements.

Figure 26. Penny crack problem. Influence of the enrichment radius ($r_e$) in the energy ($E$) and $L_2$ norms for two variations of the proposed method described in Table IV. The radius of the crack is $a = 0.1$ units and the size of the domain is $L_x = L_y = 2L_z = 0.4$ units. Results refer to a mesh consisting of $31 \times 61 \times 61$ elements. $h$ is the mesh parameter.

two meshes are ignored during numerical integration as mentioned in Section 4.1.1, consequently, for a more accurate numerical integration scheme, a different behavior could occur. For the following examples, 32 elements were used for the $11 \times 21 \times 21$ and $21 \times 41 \times 41$ meshes and 64 elements for the rest.

Next, the influence of the enrichment radius $r_e$ on the accuracy of the results is examined. As already mentioned in Section 3.4, standard XFEM compensates for higher-order terms by allowing spatial variation of the coefficients of the enrichment functions. The proposed method does not allow any variation in the plane normal to the crack front, as a result, when larger enrichment radii are used, a loss of accuracy occurs. The situation is improved by employing the enrichment strategy of Section 3.4; however, as the enrichment radii and the layers of enriched elements around the crack front increase, some loss of accuracy in the displacements is still observed. The situation is illustrated in Figure 26, where $L_2$ and energy norms are plotted against the enrichment radius $r_e$ divided by the mesh parameter $h$, since it was observed that the loss of accuracy occurs when a certain number of layers of enriched elements is added, rather than at some fixed value of the enrichment radius. Figure 26 refers to the $31 \times 61 \times 61$ mesh.

Energy and $L_2$ norms are shown in Figures 27 and 28 for four different cases: topological enrichment ($r_e = 0.00$ units), topological enrichment with a fixed number of layers of enriched elements ($r_e = 2.2h$), and geometrical enrichment with enrichment radii $r_e = 0.02$ units and $r_e = 0.04$ units; the respective convergence rates are given in Table V. For the second case, the enrichment radius was set to the value which yielded the best results in terms of displacements, this value was obtained from Figure 26, where it is observed than when the enrichment radius becomes larger than the aforementioned value, the $L_2$ error norm starts to increase. It may be observed that the proposed method performs better than standard XFEM for almost all cases. Additionally, the proposed enrichment
strategy substantially improves results, especially as the enrichment radius used increases. However, it should be noted that the behavior observed for the larger enrichment radius ($r_e = 0.04$ units) will also occur for the smaller one ($r_e = 0.02$ units) for denser meshes, where the enrichment radius is larger than the ‘optimal’ value observed ($2.2h$), leading to loss of accuracy. This behavior, which affects mostly displacements, can be attributed to the lack of spatial variability of the coefficients of the enrichment functions and can be regarded as a drawback of the dof-gathering approach. A possible solution would be the introduction of some spatial variability to the tip-enrichment functions which would not deteriorate conditioning significantly. Such a solution would be possible within the framework of the proposed method, nevertheless, it will not be considered since it would exceed the scope of the present work, which is mostly to provide a means to extend dof gathering to 3D fracture problems.

4.2.2.2. Stress intensity factors. Stress intensity factors were computed for several of the aforementioned cases. In Figures 29 and 30 errors in the SIFs are illustrated as functions of the angle $\theta$ for two different meshes ($21 \times 41 \times 41$ and $41 \times 81 \times 81$) for topological ($r_e = 0.00$ units) and geometrical ($r_e = 0.02$ units) enrichment. Due to symmetry only the values for $0^\circ \leq \theta \leq 90^\circ$ are presented. A virtual extension domain of dimensions $r_1 = 3h$, $r_2 = 3h$, $r_3 = h$ was used in the calculations.

It is observed that although the errors are quite small, it is not possible to obtain a convergence behavior like that of Section 4.2.1.2 for the 2D case. More specifically, although errors decrease slightly with mesh refinement for most points, this improvement in accuracy is not comparable with...
Table V. Penny crack problem.

|                | \( r_e = 0.00 \) | \( r_e = 2.2h \) | \( r_e = 0.02 \) | \( r_e = 0.04 \) |
|----------------|------------------|------------------|------------------|------------------|
| XFEM E         | 0.492            | 0.686            | 0.911            | 1.015            |
| XFEM \( L_2 \) | 1.009            | 1.405            | 1.824            | 1.976            |
| GE-XFEM1 E     | -                | -                | 1.016            | 0.706            |
| GE-XFEM1 \( L_2 \) | -            | -                | 1.481            | 0.289            |
| GE-XFEM E      | 0.558            | 0.850            | 1.057            | 0.988            |
| GE-XFEM \( L_2 \) | 1.535          | 1.594            | 1.753            | 1.448            |

Convergence rates for the curves of Figures 27 and 28 for the energy \( (E) \) and \( L_2 \) norms for topological \( (r_e = 0.00 \) and \( r_e = 2.2h \) \) and geometrical \( (r_e = 0.02 \) units and \( r_e = 0.04 \) units) enrichment. It is observed that when the proposed enrichment strategy is not used (GE-XFEM1) convergence rates deteriorate significantly.

Figure 29. Penny crack problem. Comparison of the mode I, II, and III stress intensity factors predicted by XFEM and GE-XFEM for topological \( (r_e = 0.00 \) units) and geometrical \( (r_e = 0.02 \) units) enrichment for the \( 21 \times 41 \times 41 \) mesh. The radius of the crack is \( a = 0.1 \) units and the size of the domain is \( L_x = L_y = 2L_z = 0.4 \) units.

that of the 2D case. In addition, for some points along the crack front \( \theta = 80^\circ \) for Mode III, errors increase for finer meshes.

The aforementioned behavior can be associated with the interpolation and integration errors introduced by the use of the SIF mesh, as discussed also in Section 4.1.3.1. An additional cause could be the fact that in the evaluation of the interaction integral, the curvature of the crack front is ignored \[58\]. It should also be noticed that problems in the extraction of SIFs for the 3D case have also been observed for standard finite elements \[59\].

Finally, although it is not possible to attain an accurate estimate, the accuracy of the SIFs predicted by the proposed method is similar to the one provided by standard XFEM. A more accurate SIF evaluation procedure, which is the subject of future work, however, would provide better insight.

4.2.2.3. Conditioning. In this section, the conditioning of the system matrices produced by the proposed method is tested and compared with standard XFEM for the general 3D case. Instead of evaluating the condition numbers of the system matrices, the number of iterations required by the solver to reach the predefined tolerance \( (10^{-8}) \) is used as an estimate; this approach has the additional advantage of providing also a comparison of the time needed to solve the resulting systems of equations for each method, since solution times are dominated by the conjugate gradient iterations.

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Figure 30. Penny crack problem. Comparison of the mode I, II, and III stress intensity factors predicted by XFEM and GE-XFEM for topological \( (r_e = 0.00 \text{ units}) \) and geometrical \( (r_e = 0.02 \text{ units}) \) enrichment for the \( 41 \times 81 \times 81 \) mesh. The radius of the crack is \( a = 0.1 \text{ units} \) and the size of the domain is \( L_x = L_y = 2L_z = 0.4 \text{ units} \).

Figure 31. Penny crack problem. Influence of the crack front mesh density \( (n_f \) is the number of elements along the front) in the number of iterations required to solve the system of equations produced by the proposed method for topological \( (r_e = 0.00 \text{ units}) \) and geometrical enrichment with an enrichment radius \( r_e = 0.02 \text{ units} \). The radius of the crack is \( a = 0.1 \text{ units} \) and the size of the domain is \( L_x = L_y = 2L_z = 0.4 \text{ units} \). Results refer to a mesh consisting of \( 31 \times 61 \times 61 \) elements.

It should be noted that the following figures refer to the number iterations required by a conjugate gradient solver with a diagonal preconditioner.

The number of iterations required for the \( 31 \times 61 \times 61 \) mesh for different numbers of front elements is given in Figure 31 in order to estimate the influence of the front mesh density in conditioning. It can be noted that the number of iterations required increases as the front mesh is refined when geometrical enrichment is used but remains fairly unaffected for topological enrichment.

In Figure 32, the number of iterations required by the CG solver for XFEM and the proposed method for topological and geometrical enrichment is presented. Again, the number of iterations required by the proposed method is significantly reduced. In fact, for the smaller enrichment radius used \( (r_e = 0.02 \text{ units}) \), the number of iterations for the proposed method is even smaller than the one required for XFEM with topological enrichment. Another important fact is that even for topological enrichment, the proposed method requires a significantly smaller number of iterations than XFEM. For example, in the \( 51 \times 101 \times 101 \) mesh, where the difference is the smallest, standard XFEM requires 573 iterations versus 330 for the proposed method. In addition, for the larger enrichment radius \( (r_e = 0.04 \text{ units}) \), the systems produced by XFEM are almost unsolvable as they require more than 50,000 iterations for the two denser meshes \( (41 \times 81 \times 81 \text{ and } 51 \times 101 \times 101) \), while...
4.2.2.4. Number of enriched degrees of freedom. For 2D problems, the number of additional unknowns is usually negligible compared to the total number of unknowns. For 3D problems, however, the additional unknowns associated to the enriched part of the approximation could result in significant increase of the total number of degrees of freedom. Motivated by this, the number of enriched dofs added by the proposed method is considered in this section.

In Table VI, a comparison is made between the total number of enriched dofs (both jump and tip) added by standard XFEM and the proposed approach for the cases examined in the previous sections. In contrast to standard XFEM, the number of additional unknowns for the global enrichment approach is completely independent of the enrichment radius. Additionally, the total number of enriched dofs for the proposed method is reduced by at least 45% to more than 98%, depending on the mesh and enrichment radius. Finally, and most importantly, the increase in the total number of unknowns for standard XFEM ranges from less than 1.5% to almost 40%, while for the proposed
Comparison of the total number of enriched dofs added by extended finite element method (XFEM) and the proposed method for topological \((r_e = 0.00)\) units and geometrical enrichment \((r_e = 0.02, 0.04)\) units. FE dofs is the number of regular dofs. Note that for the proposed method the number of additional unknowns is independent of the enrichment radius \((r_e)\).

It should be noted that the dof numbers given in the preceding discussion as well as the numbers of iterations given in the previous sections refer to the specific problem examined and will vary for different problems depending on the size of the crack and/or length of the crack front relative to the domain considered. Nevertheless, although the rate of decrease in the computational cost might change for different problems, the proposed method will always be computationally advantageous when compared with XFEM, since the number of additional unknowns will always be smaller and unaffected by variations in the enrichment radius, and the conditioning of the system matrices will always be improved as a result of dof gathering.

5. CONCLUSIONS

A method was described which enables the use of global enrichment functions for the XFEM. The method is predominantly outweighs the standard XFEM in accuracy while delivering a significantly reduced computational expense. This efficiency is attributed to the use of considerably fewer enriched degrees of freedom and a substantially improved conditioning of the system matrices.

The method relies on the principles introduced in the works of Laborde et al. [23] and Chanine et al. [47] in conjunction with a novel form of enrichment in order to obtain some of the advantages of the 2D method in the general 3D case. Although only plane cracks are treated in the examples presented in this work, the method is also applicable to more general crack geometries.

A benchmark problem was proposed for testing numerical fracture methods which enables the computation of \(L_2\) and energy error norms for the general 3D case. The accuracy of the proposed global enrichment approach was tested and compared with that of standard XFEM through the aforementioned benchmark problem.

From the preceding discussion, it results that the proposed approach provides several advantages. When topological enrichment is used, it produces more accurate results than the standard method requiring smaller solution times. Moreover, it makes possible the application of geometrical enrichment in 3D applications without the use of special preconditioners, because it produces system matrices with significantly improved conditioning compared with standard XFEM. In terms of assembly time, the proposed method is also faster than standard XFEM because of the reduced number of shape functions evaluated for each element.

One possible drawback of the method is that, when the number of enriched elements around the crack front exceeds a certain value, the error in the displacements increases. Also, the method is not straightforward to implement in existing XFEM codes. Finally, the additional point-wise-matching constraints introduced might be quite complex to implement for higher-order elements.

Some directions of future work include the following:

- The improvement of the method in order to minimize the loss of accuracy observed for large enrichment radii.
The use of improved SIF evaluation [58] methods in order to better assess the accuracy of the predicted SIFs.

The combination of the method with goal-oriented a posteriori error estimators [42–46] and local front mesh and FE mesh refinement in order to further improve the accuracy of the method.

The application of the method to crack propagation problems through the use of different crack representation methods [16, 17, 48–50].

APPENDIX A: ASSEMBLY OF THE FRONT ELEMENTS

Due to the fact that the assembly of the stiffness matrices is performed in an element-wise manner and finite elements will be usually intersected by several front elements, the interactions between the two meshes have to be specified. In more detail, for every tip-enriched element the corresponding front elements and dofs, i.e., the front elements that intersect this element and the dof numbers of their nodes, have to be determined. This can be easily achieved by employing the front parameter η.

Once the front parameter has been evaluated for every node of a given element and since the numbering of front elements and nodes is continuous, it is possible to associate elements of the two meshes. The association of the two meshes is performed employing the minimum and maximum values of the front parameter for each element and a mapping between the nodal numbers of the two meshes; these concepts are described next.

A.1 Minimum and maximum values of the front parameter

The minimum and maximum nodal values of the integer part of the front parameter ηi are found (ηmin and ηmax) for a given element. All front elements with numbers in the range between those two values are intersected by the element. For closed cracks, however, there might be cases where the aforementioned statement does not hold. In particular, if a closed crack front discretized with n elements is considered as in Figure A.1, although elements in the vicinity of the first front node will have a minimum value close to unity and a maximum value close to n, front elements within that range will not be intersected.

Elements falling in the case described earlier can be detected by defining a number nt < n and performing the following checks:

\begin{align*}
\eta_{\text{min}} & \leq nt \\
\eta_{\text{max}} & \geq n - nt
\end{align*}

(A.1a)

(A.1b)

Figure A.1. Front element parameter for shape function evaluation.
If those conditions are both true, the minimum and maximum values are interchanged. The range of front element numbers intersected by the element in this case is from $\eta_{\text{max}}$ to $n$ and from 1 to $\eta_{\text{min}}$.

The value of $n_t$ is an estimate of the maximum number of front elements that could intersect any given finite element and should be defined by taking into account the relation between the mesh parameter and the length of the front elements. For curved crack fronts, the value of the enrichment radius should also affect the choice of that value.

For the case of Figure A.1, the preceding discussion would mean that while the initial values for element b would be $\eta_{\text{min}} = 2$ and $\eta_{\text{max}} = n$, those values would have to be interchanged so that $\eta_{\text{min}} = n$ and $\eta_{\text{max}} = 2$.

A.2 Local to global and global to local dof mapping

Using the preceding information, the number of enriched dofs for any tip-enriched element can be computed. In addition, mappings between local and global dof numberings can be defined as

$$i_g = \begin{cases} i_l + \eta_{\text{min}} - 1, & i_l \leq n - \eta_{\text{min}} \\ i_l - n + \eta_{\text{min}} - 1, & i_l > n - \eta_{\text{min}} \end{cases} \quad (A.2a)$$

$$i_l = \begin{cases} i_g - \eta_{\text{min}} + 1, & i_g \geq \eta_{\text{min}} \\ i_g + n - \eta_{\text{min}} + 1, & i_g < \eta_{\text{min}} \end{cases} \quad (A.2b)$$

Applying the aforementioned relations to the case of Figure A.1, it can be easily found that for element b, where $\eta_{\text{min}} = n$ and $\eta_{\text{max}} = 2$, the first associated front node ($i_l = 1$), is node $n$ ($i_g = n$). Conversely, front node 2 ($i_g = 2$) is the third node ($i_l = 3$) associated with element b.

A.3 Shape function evaluation and assembly procedure

Mappings of Equation (A.2) are used in two occasions during the assembly process.

Since every tip element is associated with several front elements, the enriched parts of its shape functions are matrices of corresponding dimensions. Each Gauss point, however, is only associated with one front element, and the enriched shape functions evaluated at that point are matrices with dimensions corresponding to two front nodes. In order to place the enriched shape functions of every Gauss point in the correct position of the matrix corresponding to the whole element, the integer part of the front parameter is evaluated and the global to local mapping is used to obtain the correct location.

During the assembly of element matrices, the global front node numbers associated with every element have to be known. For this purpose, the local to global mapping is employed.

The shape function evaluation and assembly procedure for the enriched part of the stiffness matrix for a given element can be summarized in the following steps:

1. **Minimum and maximum value of front parameter.**
   The minimum and maximum values of the front parameter are found as described in Appendix A.1.

2. **Number of enriched dofs.**
   Using the minimum and maximum values of the front parameter, the number of enriched dofs for the given element is found.

3. **Shape function and stiffness matrix size.**
   Using the number of enriched dofs, the size of the shape functions and of the enriched part of the stiffness matrix are found.

4. **Numerical integration/shape function evaluation.**
   During the numerical integration, the enriched shape functions are evaluated for each Gauss point. The global to local mapping is employed to place individual Gauss point shape functions in the correct location in the element shape function.
5. Assembly.

Once the stiffness of an individual element is computed, the corresponding global dof numbers can be obtained using the local to global mapping.

Finally, as far as computational effort is concerned, since in the majority of cases a tip-enriched finite element should not be associated with more than three or four front nodes and since every integration point is only associated with two nodes, the number of shape function evaluations for each Gauss point is significantly reduced compared to standard XFEM, resulting in reduced assembly times.

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