An augmented Lagrangian element-free (ALEF) approach for crack discontinuities

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Abstract

A new meshless formulation for numerical analysis in fracture mechanics is presented. The formulation is based on the construction of shape functions by a moving least-squares approximation (MLSA). The peculiarity of the present approach lies in the definition of an augmented Lagrangian total potential energy functional. With this technique, called augmented Lagrangian element-free (ALEF), some drawbacks on imposing boundary and interfaces conditions are worked out. A large number of Lagrangian multipliers can be introduced without increasing the number of primary variables and inducing the strict convexity of the total potential energy functional. A new model for simulating fracture discontinuity based on the imposition of interface conditions on the edges of a virtual crack is defined, which permits to avoid some crack simulation difficulties inherent in the element-free Galerkin method. Some numerical examples are reported to evaluate the accuracy of the formulation. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Meshless methods; Fracture mechanics; Augmented Lagrangian

1. Introduction

The modelling of some problems in solids mechanics, such as moving interfaces, crack propagation, composites and advanced materials, often requires special numerical approaches because of the presence of discontinuities in the data and/or solution.

To deal with these problems, some modifications of the classical finite element method have been implemented, although, as the method relies on the local approximation properties of polynomials, the necessity to follow the discontinuity surfaces implies an iterative and often very complex and costly remeshing of the model [1].

The starting point of some of the currently more advanced methods coping with the mentioned classes of problems is the smooth particle hydrodynamics (SPH) method, originally proposed by Lucy [2] and conceived for dealing with astrophysical phenomena over unbounded domains. The SPH method and the methods developed from its original idea are generally known as “mesh-free” methods, as they are based on a variable coefficients’ linear combination of suitable approximation functions defined over the whole domain. They require only nodal data, no element connectivity is involved and further nodes can be added anytime to locally refine the problem solution.

Recently, a substantial evolution of the mesh-free methods has taken place with the work of several authors. A unifying mathematical approach has been provided by the papers of Duarte and Oden [3] and Melenk and Babuška [4] who recognized that these approaches are particular forms of partitions of unity.

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This allows powerful extensions of these methods and the knowledge of particular properties of the problem solution, if known, can be introduced in the interpolation basis to significantly improve their performances. A typical example is the function \( r^{1/2} \) for the linear elastic fracture mechanics (LEFM) problems [5], \( r \) being the distance from the crack tip. These methods generally have their origin in the data fitting theory and their basic idea is to introduce data fitting bases in a variational formulation.

A very important contribution to the development and disclosure of mesh-free methods is due to the works by Belytschko et al. [5,9] who proposed the element-free Galerkin (EFG) method in a wide range of engineering applications. One of the main difficulties in these methods consists in the direct imposition of essential boundary conditions, as the shape functions from the moving least-squares (MLS) approximation, which will be summarized in the following section, do not have the delta function property. The imposition of these conditions can be performed by various techniques, e.g., Lagrangian multipliers [6], penalty formulation [7,8], modified variational formulations [9].

In the present paper an extension of the augmented Lagrangian element-free (ALEF) method, based on the extremum properties of the total potential energy function and on the augmented Lagrangian (AL) regularization [10], is proposed. It allows a computationally very effective introduction of different kinds of constraints and it is used in this paper to enforce the essential boundary conditions and to introduce a new model for crack discontinuity [11]. The model consists in a virtual extension of the real crack in the direction of the tangent at the tip and the continuity conditions for the displacements and deformations are enforced on a suitable number of interface nodes placed on the two sides of the virtual crack. A cloud of nodes connected to the crack tip follows the tip during the crack propagation. The stress intensity factors evaluated with this model are reported for discussing the global accuracy of the formulation.

2. MLS meshless method

In this section, a brief introduction of the MLS approximation is reported, by using the notation presented by Belytschko et al. [5]. The approximation of a scalar function \( \delta(x) \) in a domain \( \Omega \) is considered. The MLS approximation is a technique which provides an approximation of a function without the use of node connectivity. The technique uses a set of nodal points, a set of weight functions, and a set of basis functions. At each point of the domain, the approximant of a function is a linear combination of basis functions. Within the domain, a set of nodes \( x_i, i = 1, \ldots, N \) (Fig. 1), is considered and the parameter associated with the approximation at node \( I \) is denoted by \( \eta_I \). The coefficients for the basis functions in this

![Fig. 1. A computational model for MLS approximation showing the boundary, the nodes and the weight function supports.](image)
linear combination differ from point to point and are computed with the help of the weight functions and the nodal values of the function under consideration. For this, a system of equations has to be solved at each point of the domain in order to obtain the coefficients for the basis functions.

A weight function \( w_I = w(x - x_I) \) with compact support is associated to each node of the domain. Let \( \Omega_I \) be the support associated to \( w_I \); \( w_I \) reaches the maximum value for \( x = x_I \), is in each point non-negative, monotonically decreasing and such that \( w_I = 0 \ \forall x \in \partial \Omega_I \). The support is generally circular or rectangular and then the weight function assumes the shape of a ball-function, one for each discretization node \( x_I \) (Fig. 1). Generally, a polynomial or exponential function is used [5].

The moving least-squares interpolant \( \eta(x) \) of the function \( \delta(x) \) in the domain \( \Omega \) is defined from a linear combination of basis functions \( \{p(x)\} \):

\[
\eta(x) = \sum_{i=1}^{m} p_i(x)a_i(x) = \{p(x)\}^T \{a(x)\},
\]

where \( m \) is the number of terms in the basis, \( \{p(x)\} \) is the vector of the basis functions and \( \{a(x)\} \) is the vector of the coefficients which are functions of the spatial coordinates \( x \). The choice of the basis depends on the boundary value problem to be solved. In particular, any function included in the basis can be reproduced exactly by the MLS approximation and therefore the introduction of integrals for a particular boundary value problem enhances the convergence rate. A typical example is constituted by the \( r^{1/2} \) function in the LEFM problem, where \( r \) represents the distance from the crack tip. The most common linear and quadratic bases are reported in Table 1.

The coefficients \( \{a(x)\} \) are obtained, in the MLSA at any point \( x \), by minimizing the square of the difference between the local approximation \( \eta(x) \) and the value \( \delta_I \) of the function \( \delta(x) \) for \( x = x_I \). Therefore, we have to minimize the following functional:

\[
J(x) = \frac{1}{2} \sum_{I=1}^{n} w_I(x - x_I) \left[ \sum_{i=1}^{m} p_i(x_I)a_i(x) - \delta_I \right]^2,
\]

where \( w_I = w(x - x_I) \) is the weight function for the node \( I \) and \( n \) is the number of nodes whose supports contain the point \( x \). In fact it can be noted that, as the weight functions have a compact support, the sum over \( I \) is limited to the nodes for which the associated weight function has the property \( x \in \Omega_I \). Thus the presence of the weight function makes the functional \( J \) defined over a set of neighbour nodes \( n \ll N \) and localizes the moving least-squares interpolation. In practical applications it is generally \( n \ll N \).

Eq. (2) can be rewritten in matrix form:

\[
J(\{a(x)\}) = \frac{1}{2} \left( [P] \{a(x)\} - \{\delta\} \right)^T [W(x)] \left( [P] \{a(x)\} - \{\delta\} \right),
\]

where \( \{\delta\} = \{\delta_1, \delta_2, \ldots, \delta_n\} \), is the vector of function values at the nodal points. \( [P] \) has the following form:

\[
[P]_{(n \times m)} = \begin{bmatrix}
p_1(x_1) & p_2(x_1) & \cdots & p_m(x_1) \\
p_1(x_2) & p_2(x_2) & \cdots & p_m(x_2) \\
\cdots & \cdots & \cdots & \cdots \\
p_1(x_n) & p_2(x_n) & \cdots & p_m(x_n)
\end{bmatrix},
\]

Table 1

<table>
<thead>
<tr>
<th></th>
<th>1D</th>
<th>2D</th>
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</thead>
<tbody>
<tr>
<td>Linear basis</td>
<td>( {p(x)}^T = {1, x} )</td>
<td>( {p(x)}^T = {1, x, y} )</td>
</tr>
<tr>
<td>Quadratic basis</td>
<td>( {p(x)}^T = {1, x, x^2} )</td>
<td>( {p(x)}^T = {1, x, y, xy, x^2, y^2} )</td>
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and \([W(x)]\) is provided by

\[
[W(x)] = \begin{bmatrix}
  w(x - x_1) & 0 & \cdots & 0 \\
  0 & w(x - x_2) & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & w(x - x_n)
\end{bmatrix}.
\]  

(5)

In order to find the coefficients \(\{a(x)\}\), the extremum of \(J\) must be determined:

\[
\begin{bmatrix}
\frac{\partial J}{\partial a} \\
\end{bmatrix} = [A(x)] \{a(x)\} - [B(x)] \{\delta\} = \{0\},
\]

(6)

where \([A(x)]\) and \([B(x)]\) are given by

\[
[A(x)] = [P]^T [W(x)] [P],
\]

(7)

\[
[B(x)] = [P]^T [W(x)].
\]

(8)

Under suitable conditions, the matrix \([A(x)]\) is not singular and the vector of the coefficients \(\{a(x)\}\), from Eq. (6), assumes the expression

\[
\{a(x)\} = [A(x)]^{-1} [B(x)] \{\delta\}.
\]

(9)

By using Eqs. (9) and (1), \(\eta(x)\) can then be expressed as

\[
\eta(x) = \sum_{l=1}^{n} g_l(x) \delta_l \equiv \{g(x)\}^T \{\delta\},
\]

(10)

\(\{g(x)\}\) being the vector of the shape functions for the MLS approximation:

\[
\{g(x)\}^T = [g_1(x) \cdots g_n(x)] = \{p(x)\}^T [A(x)]^{-1} [B(x)],
\]

(11)

where \(\{g(x)\} = \{g_1, g_2, \ldots, g_n\}\) are the MLSA shape functions related to the nodes \(x_1, x_2, \ldots, x_n\). This property preserves the local character of the MLSA. For Eq. (11) to be valid, some hypotheses must be verified. More precisely, the basis \(\{p(x)\}\) must be formed by linearly independent functions and, for every point \(x\) of the domain \(\Omega\), it must be verified that \(m \leq n\), to ensure the matrix \([A] = ([P]^T [W(x)] [P])\) not to be singular. Moreover, very particular nodal arrangements can cause the singularity of \([A]\).

The MLSA shape functions, \(\{g(x)\}\), can be built such as to have whatever degree of continuity and differentiability, as from Eq. (11), these properties descend from the basis and weight functions.

From Eq. (10) it should be noted that, in general, the approximation \(\eta(x)\) is such that \(\eta(x_l) \neq \delta_l\) (Fig. 2).

In the following, the MLS shape functions will be used to solve the elastic problem so that Eq. (10) will be

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{approximation_function.png}
\caption{The approximation function \(\eta(x)\) as interpolant of the nodal values, such that \(\eta(x_l) \neq \delta_l\).}
\end{figure}
applied to each displacement component. Nevertheless, to avoid unnecessarily involved notation, the displacement field will be denoted by \( \{ \eta \} \).

3. Variational formulation

The shape functions derived in the former section are introduced into a variational formulation for the elastic solid problem. Eq. (11) is referred to the approximation of a scalar variable and the vector \( \{ \delta \} \) has dimension equal to the MLSA node number, \( N \). For an elastic solid in an \( n_d \)-dimensional space, let \( \{ \eta \} \) be the displacement field, with \( n_d \) components and \( N = n_d N \). The MLS approximation can be applied for each component of the displacement field in the form

\[
\{ \eta \} = [G_{\eta}] \{ \delta \},
\]

(12)

where \([G_{\eta}]\) is the matrix of the shape functions and \( \{ \delta \} \) is the vector of all the nodal components of the approximation variables. For simplifying the notation, we introduce the following vector for the deformations:

\[
\{ \epsilon \} = [\partial] [G_{\eta}] \{ \delta \} = [\partial] \{ G_{\eta} \} \{ \delta \} = [G_{\epsilon}] \{ \delta \},
\]

(13)

with \( d = 1 \) for \( n_d = 1 \) and \( d = 3 \times (n_d - 1) \) for \( n_d = 2, 3 \), in which \( \{ \epsilon \} \) is the deformation vector, while the matrix \([\partial][G_{\eta}] = [G_{\epsilon}]\) is determined by ordering and adding appropriately the derivative of the MLSA shape functions.

Let us consider the domain \( \Omega \) of a solid (Fig. 3) subjected to volume forces \( \{ \mathcal{F} \} \), surface forces \( \{ q \} \) and fixed displacements \( \{ \bar{\eta} \} \), acting, respectively, on \( \Omega, \partial\Omega_q \) and \( \partial\Omega_{\bar{\eta}} \) (\( \partial\Omega = \partial\Omega_q \cup \partial\Omega_{\bar{\eta}}, \partial\Omega_q \cap \partial\Omega_{\bar{\eta}} = \emptyset \)).

The minimum of the following total potential energy functional corresponds to the elastic problem solution:

\[
\Pi(\{ \eta \}) = \frac{1}{2} \int_{\Omega} \{ \eta \}^T [\partial] [H] [\partial] \{ \eta \} \, d\Omega - \int_{\Omega} \{ \mathcal{F} \}^T \{ \eta \} \, d\Omega - \int_{\partial\Omega_q} \{ q \}^T \{ \eta \} \, dS
\]

\[
+ \int_{\partial\Omega_{\bar{\eta}}} \text{ind} \left( \begin{array}{c} \{ \eta \} \\ \{ \bar{\eta} \} \end{array} \right) \, dS,
\]

(14)

where \( \{ \eta \} = \{ \eta(x, \delta) \} \) is the displacement vector, whose components are given by Eq. (11), and \( [H] \) is the elastic operator.

---

Fig. 3. Elastic solid subjected to volume forces \( \{ \mathcal{F} \} \), surface forces \( \{ q \} \) and imposed displacements \( \{ \bar{\eta} \} \).
The indicator function is equal to

\[
\ind \left( \{ \eta \} - \{ \eta \} \right) = \begin{cases} 0 & \text{if } \{ \eta \} - \{ \eta \} = \{ 0 \}, \\ +\infty & \text{if } \{ \eta \} - \{ \eta \} \neq \{ 0 \}. \end{cases}
\] (15)

The last part of Eq. (14) is necessary as the MLSA shape functions do not satisfy the essential boundary conditions, being \( \{ \eta(x_1) \} \neq \{ \delta \} \). In fact, the shape functions \( \{ g(x) \} \), defined by Eq. (11), take non-vanishing values for each point included in the influence domain \( \Omega_i \) of the node \( x_i \). The evaluation of the integrals in Eq. (14) is obtained through a Gaussian quadrature on the domain \( \Omega \). For the quadrature, the domain \( \Omega \) is divided into subdomains, by introducing a background mesh, which does not play any role in the approximation and must be chosen so as to ensure an appropriate evaluation of the integrals. A new formulation for avoiding the background mesh is analysed by the authors elsewhere. The total potential energy functional, Eq. (14), is of course not differentiable due to the presence of the indicator function for the kinematically admissible displacements. To transform such a function into a differentiable equivalent one, it will be regularized by the AL technique [10,20].

If we introduce the hypothesis that the assigned displacements \( \{ \eta \} \) are interpolated by a set of Delta Dirac functions placed in correspondence of the node \( x_i \) on \( \partial \Omega_i \) (which is equivalent to enforcing the essential boundary conditions only on a discrete number of points), we obtain the following expression:

\[
\int_{\partial \Omega_i} \ind \left( \{ \eta \} - \{ \eta \} \right) \, dS = \sum_{i=1}^{n_r} \sup_{\{ r \}} \left[ \{ r \}^T \left( \{ \eta \} - \{ \eta \} \right) \right] + \frac{1}{2} \alpha \left( \{ \eta \} - \{ \eta \} \right)^T \left( \{ \eta \} - \{ \eta \} \right),
\] (16)

where \( \{ r \} \) and \( \{ \eta \} \) are, respectively, the reactions (which have the mathematical meaning of Lagrangian multipliers) and the assigned displacements on the \( n_r \) constrained nodes, while \( \alpha \) is a positive constant (penalty parameter).

By introducing Eq. (16) into Eq. (14), and being

\[
[K] = \int_{\Omega} [G_1]^T [H] [G_1] \, d\Omega, \quad \{ F \} = \int_{\Omega} [G_2]^T \{ \mathcal{F} \} \, d\Omega + \int_{\partial \Omega_i} [G_3]^T \{ q \} \, dS,
\] (17)

we obtain the functional

\[
II(\delta, r) = \frac{1}{2} \left\{ \delta \right\}^T \left[ K \right] \left\{ \delta \right\} - \left\{ \delta \right\}^T \left\{ F \right\} + \sum_{i=1}^{n_r} \left[ \{ r \}^T \left( \{ \eta \} - \left\{ G_1 \right\} \left\{ \delta \right\} \right) \\
+ \frac{1}{2} \alpha \left( \{ \eta \} - \left\{ G_1 \right\} \left\{ \delta \right\} \right)^T \left( \{ \eta \} - \left\{ G_1 \right\} \left\{ \delta \right\} \right), \right. \] (18)

Introducing a suitable shape function matrix \( \{ Q \} \), defined as

\[
\begin{align*}
\{ Q \} = \begin{bmatrix}
\{ G_1 \} \\
\{ G_2 \} \\
\vdots \\
\{ G_n \} 
\end{bmatrix},
\end{align*}
\] (19)

the functional in Eq. (18) can be written in the following form:

\[
II(\delta, r) = \frac{1}{2} \left\{ \delta \right\}^T \left[ K \right] \left\{ \delta \right\} - \left\{ \delta \right\}^T \left\{ F \right\} + \sum_{i=1}^{n_r} \left[ \{ r \}^T \left( \{ \eta \} - \left\{ Q \right\} \left\{ \delta \right\} \right) \\
+ \frac{1}{2} \alpha \left( \{ \eta \} - \left\{ Q \right\} \left\{ \delta \right\} \right)^T \left( \{ \eta \} - \left\{ Q \right\} \left\{ \delta \right\} \right), \right. \] (20)
whose saddle-point gives us the problem solution
\[
\min_{\delta} \max_{r} II(\delta, r).
\]
In the last formula, the superior extremum has been substituted by the maximum, in the hypothesis of a well-posed elastic problem, such that the saddle-point exists and is unique and that the reactions \( \{r\} \) are represented by finite real numbers.

The present variational formulation allows to eliminate all the drawbacks related to the use of the Lagrangian and penalty methods and represents a computationally effective approach for the introduction of constraints on direct variables in the MLS approximation [10].

4. Discontinuous approximations

One of the most important properties of the MLS approximation is the ability to produce solutions with the desired degree of continuity. It is immediately noticed in fact that the MLS approximation inherits its continuity and differentiability properties not only from the basis functions, but even from the weight functions. The best approximation properties are therefore obtained from a proper choice of bases and weights.

Although the high continuity is a desirable property, material interfaces and cracks deserve special treatment for the presence of discontinuous quantities in the solution.

Material discontinuities have been studied by Cordes and Moran [12], by cutting the weight supports at the interface line and enforcing the proper conditions through Lagrangian multipliers. This approach suffers the numerical shortcomings pointed out previously in the imposition of the essential boundary conditions [13].

The treatment of crack discontinuities in a solid has been analysed in several ways. The first basic approach, known as visibility criterion [14], considers the crack line as opaque for the weight functions and the support takes the shape illustrated in Fig. 4(a). As a consequence, a discontinuity in the weight and shape functions is introduced, not only on the crack line, but also in the interior of the domain \( \Omega \). Such a discontinuity is introduced for each weight function whose support contains the crack tip, so that the final solution presents the same oscillations near the tip.

A more refined approach, called diffraction method [14], has been applied only to polar-type weight functions (i.e., with circular support) and is based on the evaluation of the distance by a path which passes around the tip, Fig. 4(b). Consequently, the weight and the shape functions are discontinuous across the crack, but continuous and differentiable elsewhere. This approach leads, however, to rather complex shape functions with rapidly varying derivatives, so that the quadrature for the evolution of the GTPE functional or equivalent Galerkin forms can present difficulties [5].

The necessity of modifying the shape of the supports of the weight functions can be eliminated by the ALEF approach, preserving computational effectiveness and continuity properties as will be shown in the following section.

![Fig. 4. Domains of influence of nodes adjacent to a line of discontinuity: (a) visibility criterion and (b) diffraction method. The shaded regions are removed from the domain of influence.](image-url)
5. Virtual crack model

As pointed out in Section 4, the ALEF approach allows the introduction of Lagrangian multipliers in a computationally effective framework. To take advantage of this property, a new model for the simulation of the crack discontinuity has been developed. This model avoids any modification of the weight functions and is based on the imposition of suitable interface conditions through Lagrangian multipliers.

The crack is virtually extended in the direction of the tangent at the tip (Fig. 5). All the weight functions whose supports intersect the real crack are cut along the crack line (real + virtual), while the weight functions whose supports intersect only the virtual crack are left unchanged. If $D_L$ and $D_R$ are the two sides of the crack, $y_C$ is the real crack tip coordinate and $I$ is a generic point of the discretization whose weight function has radius $r_I$, the model is such that:

- if $|x_I - y_C| > r_I$, the weight function is left unchanged;
- if $I \in D_L$ and $r_I > |x_I - y_C|$, then $w_I = 0 \forall x \in D_R$;
- if $I \in D_R$ and $r_I > |x_I - y_C|$, then $w_I = 0 \forall x \in D_L$.

This model introduces of course a discontinuity along the virtual crack because of the weight function cutting. The discontinuity can be suppressed introducing a suitable number of interface nodes on the two sides of the virtual crack. Each interface node is given by two coincident nodes, one belonging to $D_L$ and the other belonging to $D_R$, subjected to the following interface conditions for the displacements:

$$\{\eta_L\} = \{\eta_R\} \quad \forall I \in \Gamma_{VC}, \quad (21)$$

and for the deformations:

$$\{\epsilon(\eta_L)\} = \{\epsilon(\eta_R)\} \quad \forall I \in \Gamma_{VC} \quad (22)$$

or

$$[\partial] \{\eta_L\} = [\partial] \{\eta_R\} \quad \forall I \in \Gamma_{VC}, \quad (23)$$

where $\Gamma_{VC}$ is the virtual crack.

The length of the virtual crack must be, in general, greater than the maximum diameter of the weight functions in the neighbourhood of the tip, otherwise discontinuities will arise ahead of the virtual crack line. A symmetric arrangement of nodes around the tip is also recommended. The model ensures:

- a well-defined MLS approximation in the whole domain;
- the representation of discontinuous displacements over the crack;

![Fig. 5. The proposed model for simulating the crack discontinuity.](image-url)
• the continuity of the solution in the whole domain;
• the absence of mutual influences for nodes belonging to different sides of the crack.

From the computational point of view, the interface conditions in Eqs. (21) and (22) are introduced into the functional $II(\delta, r)$ by adding the terms

$$
\sum_{i=1}^{n_F} \sup_{\{r_T\} \in \mathcal{R}} \left[ \left( r_T \right)_i^T \{ \eta_L \}_i - \{ \eta_R \}_i \right] + \frac{1}{2} \alpha \left( \{ \eta_L \}_i - \{ \eta_R \}_i \right)^T \left( \{ \eta_L \}_i - \{ \eta_R \}_i \right) + \frac{1}{2} \beta \left( \{ \eta_L \}_i + \{ \eta_R \}_i \right)^T \left( \{ \eta_L \}_i + \{ \eta_R \}_i \right),
$$

where $n_F$ is the number of nodes placed on the virtual crack faces and the vector $\{ \sigma_T \}_i$ represents the multipliers related to the deformations at the $i$th node (having the physical meaning of the stress at the interface nodes), while $\{ r_T \}_i$ represents the relative displacement of the two crack faces at the $i$th node. In the last equation, two penalty parameters, $\alpha$ and $\beta$, have been introduced, the displacements and the deformations being boundary constraints whose relative values differ by more than one order of magnitude. It can be noted that the penalty parameter $\alpha$ can be assumed equal to the one used for the boundary conditions, the quantities being related to the displacements in both cases. By considering the MLS expressions for displacements and deformations, the interface conditions assume the following form:

$$
\left[ \begin{array}{c}
G_{q,i}^L - G_{q,i}^R \\
G_{q,i}^R
\end{array} \right]_{(n_q \times n_d)} \{ \delta \}_i = \{ 0 \}, \quad i = 1, \ldots, n_F,
$$

$$
\left[ \begin{array}{c}
G_{i,i}^L - G_{i,i}^R \\
G_{i,i}^R
\end{array} \right]_{(n_q \times n_d)} \{ \delta \}_i = \{ 0 \}, \quad i = 1, \ldots, n_F.
$$

If the interface conditions for both displacements and deformations are written for all the $n_F$ interface nodes, introducing the following matrices:

$$
\left[ \begin{array}{c}
Q_{q,i}^L - Q_{q,i}^R \\
Q_{q,i}^R
\end{array} \right]_{(n_q \times n_d)} \{ \delta \}_i = \{ 0 \}, \quad i = 1, \ldots, n_F,
$$

$$
\left[ \begin{array}{c}
Q_{i,i}^L - Q_{i,i}^R \\
Q_{i,i}^R
\end{array} \right]_{(n_q \times n_d)} \{ \delta \}_i = \{ 0 \}, \quad i = 1, \ldots, n_F,
$$

they will assume, respectively, the form

$$
\left[ \begin{array}{c}
Q_{q,i}^L \\
Q_{q,i}^R
\end{array} \right]_{(n_q \times n_d)} \{ \delta \}_i = \{ 0 \}, \quad i = 1, \ldots, n_F
$$

$$
\left[ \begin{array}{c}
Q_{i,i}^L \\
Q_{i,i}^R
\end{array} \right]_{(n_q \times n_d)} \{ \delta \}_i = \{ 0 \}, \quad i = 1, \ldots, n_F
$$

where the constraint matrix $[Q_q]$ has dimension $(n_q n_F) \times (N_d)$, for each node displacement vector having $n_d$ components, while $[Q_i]$ has dimension $(dn_F) \times (N_d)$.

The discretized AL functional is extended to the present problem by adding the term

$$
\left[ \begin{array}{c}
\{ r_T \}_i^T \{ Q_q \}_i \{ \delta \} \\
\{ \sigma_T \}_i^T \{ Q_i \}_i \{ \delta \}
\end{array} \right] + \frac{1}{2} \alpha \left( \{ Q_q \}_i \{ \delta \} \right)^T \left( \{ Q_q \}_i \{ \delta \} \right) + \frac{1}{2} \beta \left( \{ Q_i \}_i \{ \delta \} \right)^T \left( \{ Q_i \}_i \{ \delta \} \right),
$$

(29)
where

\[
\{ \sigma_f \} = \begin{bmatrix}
\{ \sigma_f \}_1 \\
\{ \sigma_f \}_2 \\
\vdots \\
\{ \sigma_f \}_n_f
\end{bmatrix},
\]

(30)

\[
\{ r_f \} = \begin{bmatrix}
\{ r_f \}_1 \\
\{ r_f \}_2 \\
\vdots \\
\{ r_f \}_n_f
\end{bmatrix}
\]

(31)

The Hessian with respect to the approximation variables is given by

\[
\nabla^2_{\delta} II(\{ \delta \}, \{ r \}, \{ r_f \}, \{ \sigma_f \}) = \mathbf{K} + \alpha([\mathbf{K}_b] + [\mathbf{K}_0]) + \beta[\mathbf{K}_c],
\]

(32)

where the Hessians $[\mathbf{K}_b] = [\mathbf{Q}_b]^T[\mathbf{Q}_b]$ of the boundary conditions $[\mathbf{K}_0] = [\mathbf{Q}_0]^T[\mathbf{Q}_0]$ and of the material continuity constraints $[\mathbf{K}_c] = [\mathbf{Q}_c]^T[\mathbf{Q}_c]$ have been evidenced. All of them are semi-definite positive because they are evaluated by the dyadic product of the constraint matrices $[\mathbf{Q}]$. The saddle-point of the functional corresponds to the MLS solution of the crack discontinuity problem

\[
\min_{\{ \delta \}} \max_{\{ \omega \}} II(\{ \delta \}, \{ r \}, \{ r_f \}, \{ \sigma_f \}).
\]

(33)

The numerical solution can be determined by using the AL algorithm through the application of the iterative formula by Hestenes and Powell (HP) [15,16] for all the three sets of Lagrangian multipliers: 

**minimization w.r.t. the approximation variables $\{ \delta \}$:**

\[
\{ \delta^{(k+1)} \} = \arg \min_{\{ \delta \}} W(\{ \delta \}, \{ r^{(k)} \}, \{ r_f^{(k)} \}, \{ \sigma_f^{(k)} \}).
\]

(34)

**HP formulas for the Lagrangian multipliers:**

\[
\{ r^{(k+1)} \} = \{ r^{(k)} \} + \alpha([\mathbf{Q}_b] + [\mathbf{Q}_0])\{ \delta^{(k+1)} \},
\]

\[
\{ r_f^{(k+1)} \} = \{ r_f^{(k)} \} + \alpha[\mathbf{Q}_0]\{ \delta^{(k+1)} \},
\]

\[
\{ \sigma_f^{(k+1)} \} = \{ \sigma_f^{(k)} \} + \beta[\mathbf{Q}_0]\{ \delta^{(k+1)} \},
\]

(35)

and the choice of an incremental scheme for both penalty parameters $\alpha$ and $\beta$. The iteration in Eqs. (34) and (35) works alternatively on the variables $\{ \delta \}$ and on the Lagrangian multipliers $\{ r \}, \{ r_f \}, \{ \sigma_f \}$. It should be observed in fact that the functional minimum with respect to $\{ \delta \}$ is calculated by keeping the values of the multipliers fixed, which are updated at the subsequent step.

6. Optimal selection of the penalty parameters

The importance of the correct selection of the penalty parameters $\alpha$ and $\beta$ in the present formulation is fundamental. From a theoretical point of view [17] the algorithm will converge for any positive value of the penalty parameters $\alpha$ and $\beta$, but in practice the numerical experiments carried out have shown that the selection of appropriate values is not a trivial task. The problems related to an incorrect evaluation of these parameters are recalled in Table 2.

As long as the simple elastic problem is analysed (no crack discontinuity) an easy selection strategy could be that of an initially low value of $\alpha$ that will be automatically incremented measuring the convergence rate [10,17]. This leads to the solution but each increment of the parameter implies, in the computations, a new factorization of the Hessian matrix in Eq. (32) with a consequent numerical inefficiency. The situation becomes critical in the case of the crack discontinuity, where the two parameters $\alpha$ and $\beta$ must be set. The
practical experience has shown that the user selection of these values is often extremely inefficient so that the algorithm does not converge. Therefore, a new automatic penalty selection algorithm has been studied and implemented. Herein it will be described as an empirically very efficient tool. Its theoretical demonstration will be the subject of a forthcoming paper.

The basic idea of the algorithm is simple. Let us recall the Hessian from Eq. (32). The matrices \([K], [K_b], [K_n] and [K_r]\) are summed up, once weighted by the penalty coefficients. To ensure the best numerical conditioning of the problem, the matrices must be properly scaled.

These matrices are all positive semidefinite, and therefore their minimum eigenvalue can be assumed in general to be equal to zero. Before starting with the AL iteration, the following maximum eigenvalues are estimated:

\[
\lambda_K = \max \text{eig}(K),
\]

\[
\lambda_b = \max \text{eig}(K_b),
\]

\[
\lambda_n = \max \text{eig}(K_n),
\]

\[
\lambda_r = \max \text{eig}(K_r),
\]

while the penalty coefficients are set as follows:

\[
\alpha = \begin{cases} 
\frac{\lambda_K}{10 \lambda_b} & \text{simple linear elastic problem,} \\
\frac{\lambda_K}{10 \min(\lambda_b, \lambda_n)} & \text{crack discontinuity problem,}
\end{cases}
\] (36)

\[
\beta = \frac{\lambda_K}{10 \lambda_r}.
\] (37)

Eqs. (36) and (37) fix the augmented parameter values in such a way that the spectral radii of the matrices \([K], [K_b], [K_n], [K_r]\), given by Eq. (32) the total Hessian, are all comparable. As noticed before, \(\alpha\) controls the boundary constraints and virtual crack interface displacements, so that, in general, the eigenvalues \(\lambda_b\) and \(\lambda_n\) will be of the same order of magnitude.

Some results about the convergence behaviour of the AL algorithm for different values of the penalty parameter \(\alpha\) are reported in [10].

7. Numerical examples

In the present section the results produced by the meshless approximation and the virtual crack model are discussed with reference to two classical examples. A flat sheet in tension is examined considering first an orthogonal edge crack (Mode I), and then a slant edge crack (mixed mode). Both examples are modelled in plane stress state using the following enriched basis, where all the integrals of Westergaard’s solution are included:
$$\{p\}^T = \left[ 1, x, y, \sqrt{r} \cos \left( \frac{\theta}{2} \right), \sqrt{r} \sin \left( \frac{\theta}{2} \right), \sqrt{r} \cos \left( \frac{\theta}{2} \right) \sin (\theta), \sqrt{r} \sin \left( \frac{\theta}{2} \right) \sin (\theta) \right],$$

(38)

\(r, \theta\) being the polar coordinates in the crack tip reference system, Fig. 6.

The exponential weight function,

$$w(d) = \begin{cases} 
\frac{e^{-(d/c)^2} - e^{-(d_m/c)^2}}{1 - e^{-(d_m/c)^2}}, & d \leq d_m, \\
0, & d > d_m,
\end{cases}$$

has been used, with \(k = 1, (d_m/c) = 5\) and a radius \(d_m\) of the supports containing a number of MLS nodes equal to seven times the number of basis functions. This radius has been found requiring the maximum accuracy in the execution of patch test problems with irregularly spaced nodes.

The geometry of the first example is illustrated in Fig. 7. Fig. 8 shows the MLS discretization for this geometry, where the nodes surrounded by a circle are the virtual crack interface nodes and the ones surrounded by a square are the real edge crack nodes. Fig. 9 reports the background quadrature cell structure. The stress intensity factor \(K_I\) has been evaluated by the decomposition method, using circular \(J\)-integral evaluation paths centred at the crack tip. The method is described in [18], where a boundary element code is also provided. The BEM code has been used for comparison in the assessment of the results.

![Fig. 6. Local reference system at the crack tip.](image)

![Fig. 7. Orthogonal edge crack example.](image)
The numerical values of the geometrical as well as the mechanical data used in the example are: \( a = 1, \sigma = 1, \ E = 10^5, \nu = 0.3 \). The reference solution of the problem, also reported in [19], is \( K_1/K_0 = 2.105 \), being \( K_0 = \sigma \sqrt{\pi a} \). With reference to Fig. 10, it should be noted that the use of the enhanced basis (38) makes the enforcement of the deformation continuity impossible at the crack tip interface, as infinite values arise. This inconvenience has been circumvented by introducing a couple of interface nodes immediately ahead of the crack tip. At the crack tip only the displacement continuity is therefore constrained.

From the results, it can be noted how the stress intensity factor evaluated by the MLS approximation is more sensible to the \( J \)-integral evaluation path than the BEM method is, but normally more accurate. This is illustrated in Fig. 10, where the ratio \( K_1/K_0 \) vs. the normalized crack tip distance \( r/l \) is plotted, \( l \) being the crack length. The differences, however, are relatively small and it has been verified as they are substantially independent of the number and disposition of the nodes at the virtual crack interface.
The second analysed geometry is illustrated in Fig. 11, with an edge crack of length equal to 0.5a, slanted by π/4 with respect to the lower edge of the model. The MLS nodes and the integration cells are reported, respectively, in Figs. 12 and 13. The dimensionless stress intensity factors for this geometry [17] are $K_1/K_0 = 1.20$, $K_{II}/K_0 = 0.57$.

From the results it emerges again that in particular the Mode II stress intensity factor, computed by the MLS approximation, is sensible to the $J$-integral evaluation path. This is evident in Figs. 14 and 15, where the plots of $K_1/K_0$ and $K_{II}/K_0$ vs. the normalized radius of the $J$ path are reported, respectively. It can be noted how a normalized radius equal to $0.4-0.5a$ should be used in order to obtain results with an error close to 1%. No significant improvement has been obtained by varying the virtual crack interface discretization.

In both numerical examples the AL iteration has performed satisfactorily, although the problem constraints are very differently scaled. Using the automatic optimal penalty parameter selection with a displacement convergence tolerance equal to $10^{-6}$ and a strain convergence tolerance equal to $10^{-8}$, the solution has been found in a few iterations consuming a very small fraction of the total computing time. Table 3 reports the convergence summaries for the above examples. In practical computations it has been observed how the arbitrary selection of the penalty parameters is almost impossible and very in-
efficient. Convergence of the AL iteration has been always observed using the penalty parameters evaluated by the proposed algorithm. Moreover, the total number of iterations is reduced substantially. In the previous examples only one HP iteration has led to the correct evaluation of the Lagrangian multipliers.
Table 3
Convergence summaries for the two examples

<table>
<thead>
<tr>
<th></th>
<th>Newton’s iterations</th>
<th>HP iterations</th>
<th>Hessian factorizations</th>
<th>Penalty parameters evaluation time (%)</th>
<th>Augmented Lagrangian total iteration time (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orthogonal crack</td>
<td>10</td>
<td>1</td>
<td>1</td>
<td>0.98</td>
<td>0.95</td>
</tr>
<tr>
<td>Slant crack</td>
<td>4</td>
<td>1</td>
<td>1</td>
<td>2.60</td>
<td>2.08</td>
</tr>
</tbody>
</table>

8. Conclusions

A meshless method based on the MLS approximation has been proposed. The method considers appropriate AL regularizations of the total potential energy functional and enforces essential boundary conditions and interface constraints through an iterative scheme. While the classical approaches, based on Lagrangian multipliers, produce a set of linear equations with indefinite coefficient matrix, a large number of variables and a loss of banding in the coefficient matrix, the proposed approach has the following advantages:

- The Hessian of the functional is positive definite and banded;
- The constraints are satisfied with high precision in a few iterations;
- A large number of Lagrangian multipliers can be introduced without increasing the size of the direct problem and their evaluation is almost costless, Eq. (34).

The method allows straightforward enforcement of the essential boundary conditions even in the largest problems, strict constraint satisfaction and avoids the shortcomings of the modified variational principles [8]. Moreover, it is numerically stable and further constraints, such as interface conditions, can be introduced in the easiest way.

To develop a new model for the simulation of the crack discontinuity, we took advantage of these properties. The model consists in a virtual extension of the real crack in the direction of the tangent at the tip, and a cloud of nodes rigidly connected to the crack tip, which follow it during crack propagation. The weight functions are cut along the crack (real + virtual) and the continuity conditions for the displacements and for the deformations are enforced on a suitable number of interface nodes placed on the two sides of the crack. This model avoids any modification of the weight functions and is based therefore on the imposition of suitable interface conditions through Lagrangian multipliers.

The model ensures:

- A well-defined MLS approximation in the whole domain;
- The representation of discontinuous displacements over the crack;
• the continuity of the solution in the whole domain;
• the absence of mutual influences between nodes belonging to different sides of the crack.

The stress intensity factors evaluated by this approach show a slight dependence on the $J$-integral evaluation path. A circular contour path around the crack tip of radius approximately equal to 0.4–0.5 times the crack length provides an error close to 1%.

The analysis of crack propagation, which is not the aim of this paper, requires a specific formulation for avoiding or modifying the background mesh. In the former case only a roto-translation of the cloud of nodes connected to the crack tip is requested. This new formulation is actually being studied and is going to be implemented by the authors.

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References