An extended finite element optimization method for simulating discrete fracture networks flows

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Abstract. We investigate a new numerical approach for the computation of the 3D flow in a discrete fracture network that does not require the solution of partial differential equations on complex 3D system of planar fractures. The discretization within each fracture is performed independently of the discretization of the other fractures and of their intersections. Independent meshing process within each fracture is a very important issue for practical large scale simulations making easier mesh generation and parallelization. Some numerical simulations are given to show the viability and efficiency of the method.

Key words. Fracture flows, Darcy flows, discrete fracture networks, optimization methods for elliptic problems, uncoupled large scale simulations

AMS subject classifications. 65N30, 65N15, 65N50, 65J15

1. Introduction. Efficient numerical simulations of subsurface fluid flows in fractured rocks are of interest for many applications ranging from water resources management, contaminant transport and dissemination, oil prospecting and enhanced oil/gas recovery. Among the major difficulties are intrinsic heterogeneity, directionality of the medium and multiscale nature of the phenomena, as well as uncertainty in the medium properties. Discrete Fracture Networks (DFNs) models are frequently preferred to more conventional continuum models as basis for simulations; a DFN is an assemblage of resembling fractures. A classical approach to the problem is to model fractures as planar ellipses or polygons and stochastically generate Discrete Fracture Networks with probabilistic distributions of density, aspect ratio, orientation, size, aperture of fractures and hydrologic properties [8] and to simulate the flow through the obtained networks. Intensive numerical simulations with several configurations of DFNs and physical parameters are then performed in order to tackle the issue of uncertainty. The flow pattern strongly depends on density and size of fractures and for large scale simulations different approaches are possible. For dense fracture networks and continuous distribution of size and aspect ratios, flow can be suitably modeled as the flow in an equivalent continuous porous medium where the fracture network pattern leads to the definition of a suitable permeability tensor. For sparse fracture networks with some large fracture that discontinuously increase directionality of the flow in some direction an explicit representation of the fracture network is more reliable. In both cases a stochastic approach to the uncertainty of the parameters is needed and this require many simulations, so that efficiency and large applicability of numerical algorithms are fundamental issues.

Here the steady flow in a given DFN is considered assuming the rock matrix impervious and no longitudinal flow in the intersection between the fractures. These intersections are called traces and are always segments.

DFNs are complex 3D structures obtained intersecting planar fractures. The first classical numerical challenge is to provide a good-quality conforming mesh for this 3D structure to be used for the discretization of the flow equations. Conformity of the mesh requires that the unique discretization of the traces is shared by all the
discretizations of the fractures intersecting along this traces. Conformity of the mesh through the traces for an absolutely arbitrary DFN and good-quality of the mesh can be obtained only with the introduction of a huge number of elements independently of the required accuracy of the numerical solution. In [22], a mixed non-conforming finite element method on a conforming mesh is proposed. In [16], an adaptive approach to the conforming mesh generation requiring adjustments of the trace spatial collocations is proposed. Local modifications of the mesh or of the fracture network in order to preserve conformity of the meshes or alignment of meshes along the traces are considered in several works as [14, 22]. In [10], a method to generate a good-quality conforming mesh on the network system is proposed. In [18], a mixed hybrid mortar method is proposed allowing nonconformities of the meshes on the fractures, but requiring that the traces are contained in the set of the edges of each fracture triangulation. Resorting to mortar methods the discretization of each fracture can lead to a different discretization of the traces.

A different approach to the simulation of the flow in the fracture network is based on its modelization with a system of mono-dimensional pipes that are aligned along the fractures and mutually connect the centers of the fracture intersections with the surrounding fractures. The resulting mesh of pipes still reflects the topological properties of the fracture network [5, 17]. An accurate definition of pipe properties within the fracture system has been obtained by means of a boundary element method in [9]. However, the geometrical simplification implies errors in the assessment of the fluid flow regime, depending on the complexity and geometrical properties of the underlying DFN.

The model of the problem allows discontinuities of fluxes of hydraulic head occurring through the traces when fluxes of hydraulic heads leave a fracture to reach a different fracture at the common trace. In the previous approaches these discontinuities can be modeled if they are localized at edges between elements or at the border of each piece of fracture.

In this article a new approach is proposed; it does not require fracture meshes to match along traces and has high potential for parallel implementation. Discontinuities of fluxes of hydraulic heads can occur on arbitrary traces with respect to the triangulation and the used finite elements allow to catch these discontinuities of the fluxes also inside elements. This can be obtained introducing suitable Extended Finite Elements (XFE).

In Section 2, we recall the physical model and governing equations and the continuous optimization problem that leads to the solution on the network system. In Subsection 3.1, we recall basics on extended finite elements of the type considered herein. In Subsection 3.2, the numerical solution of the discrete problem is described. Finally in Section 4 numerical results are discussed in order to prove the applicability, reliability and efficiency of the method.

2. Description of the problem.

2.1. The continuous problem. The problem of subsurface flows through an open planar polygonal fracture $\omega \subset \mathbb{R}^2$ can be written as:

$$\nabla \cdot (K \nabla h) = q, \quad \text{in } \omega,$$

$$h|_{\Gamma_D} = h_D \quad \text{on } \gamma_D,$$

$$\frac{\partial h}{\partial n} = h_N \quad \text{on } \gamma_N,$$

(2.1)
where $\partial \omega = \gamma_D \cup \gamma_N$ and $\gamma_D \cap \gamma_N = \emptyset$. The scalar function $h = p + \zeta$ is the hydraulic head, $p = p/(g g)$ is the pressure head, $p$ is the fluid pressure, $g$ is the gravitational acceleration constant and $\zeta$ is the fluid density. The variable $\zeta$ is the elevation, and $K$ is the hydraulic conductivity tensor and is a symmetric and uniformly positive definite tensor. The symbol $\frac{\partial h}{\partial \nu}$ is the outward co-normal derivative of the hydraulic head:

$$\frac{\partial h}{\partial \nu} = \hat{n}^t K \nabla h$$

with $\hat{n}$ unit vector outward normal to the boundary $\gamma_N$.

The definition of the hydraulic head in a Discrete Fracture Network $\Omega$ should require the solution of problem (2.1)-(2.3) in a system of intersected polygonal fractures in the space. The solution of this problem requires a definition of a suitable $H^1(\Omega)$ space. In order to define 3D fractures $F_i$, let us consider a set of open planar polygons $\{\omega_i\}_{i \in I}$, with $I$ the set of their indices, and let $F_i \subset \mathbb{R}^3$ be the image of the closure of a polygon $\omega_i \subset \mathbb{R}^2$ through an affine mapping $\Phi_i(\hat{x}) = b_i + Q_i (\hat{x} - \hat{x}_{0,i})$ where $\hat{x}_{0,i}$ is the coordinate of a given vertex of the polygon $\omega_i$ in the planar reference system, and $b_i$ is the position of the same vertex in the 3D space. We assume that $Q_i^t Q_i$ is the identity matrix, such that the differential operators defined on the tangential reference system in $F_i$ are equivalent to the operators defined on the planar fracture $\omega_i$. Let $\Omega$ be the 3D set obtained by the union of the system of polygonal fractures $F_i$ with $i \in I$

$$\Omega = \bigcup_{i \in I} F_i, \quad \partial \Omega = \bigcup_{i \in I} \partial F_i,$$

We assume that $\bar{\Omega}$ is a connected set and that the intersection of the closure of each couple of fractures is either an empty set or a set of non vanishing segments called *trace*, denoted by $S_m$, $m \in M$ with cardinality $M^2$. Let $S$ denote the set of all these traces. Each trace $S_m$ is shared by exactly two polygonal fractures $F_i$ and $F_j$, $i \neq j$, such that $S_m = \bar{F}_i \cap \bar{F}_j$. The set of the two indices $i$ and $j$ of the fractures $F_i$ and $F_j$ sharing trace $S_m$ is denoted by $I_{S_m} = \{i,j\}$. Moreover, for each fracture $F_i$ let us denote by $S_i$ the set of traces shared by $F_i$ and other fractures.

In order to define the problem on the network system of fractures let us assume to have at our disposal a set of subfractures $f_l$, $l \in L$ obtained by a subdivision of each fracture in such a way that each trace is contained in the boundary of some of these subfractures and $\forall m \in M$, $S_m \cap f_l = \emptyset$, $\forall l \in L$, so we have

$$\Omega = \bigcup_{l \in L} f_l \setminus \partial \Omega.$$

Let us split the boundary $\partial \Omega$ in a boundary with Dirichlet boundary conditions $\Gamma_D$ and a boundary with Neumann boundary conditions $\Gamma_N$ with $\partial \Omega = \Gamma_D \cup \Gamma_N$ and $\Gamma_D \cap \Gamma_N = \emptyset$. Let us define the space $V_{f_l} = H^1(f_l)$, $\forall l \in L$.

The global hydraulic head $h$ in the whole connected system $\Omega$ is provided by the solution of the following problems $\forall l \in L$:

$$\nabla \cdot (K_{f_l} \nabla h) = q, \quad \text{in } f_l,$$  \hspace{1cm} (2.4)  

$$h_{|f_l \cap \Gamma_D} = h_D, \quad \text{on } \Gamma_D \cap \partial f_l,$$  \hspace{1cm} (2.5)  

$$\frac{\partial h}{\partial \nu_{\partial f_l}} = h_N, \quad \text{on } \Gamma_N \cap \partial f_l,$$  \hspace{1cm} (2.6)
with a 2D local reference system on \( f_i \). Let \( S_m \) be an edge such that there exist subfractures \( f_l, f_k, l \neq k \) sharing this boundary segment and let \( L_{S_m} \subset L \) be the set of indices \( l \) such that \( S_m \subset \partial f_l \). The additional coupling conditions to be added to equations (2.4)-(2.6) are

\[
\begin{align*}
  h_{|f_l} &= h_{|f_k}, \text{ on } S_m, \quad \forall S_m \in \mathcal{S}, \forall l, k \in L_{S_m}, \\
  \sum_{l \in \Lambda_{S_m}} \frac{\partial h_{|f_l}}{\partial \nu_{|f_l}} &= 0, \quad \text{on } S_m, \quad \forall S_m \in \mathcal{S}, \forall l, k \in L_{S_m},
\end{align*}
\]

(2.7)

(2.8)

These two additional conditions correspond to the physical requirement of continuity of the hydraulic head and conservation of hydraulic fluxes in the traces \( S_m \).

In the following we shall focus on the solution in each fracture and not on the subfractures, for this reason let us denote by \( h_i \) the restriction of \( h \) to the fracture \( f_i \), \( \forall i \in I \). Conditions (2.7) and (2.8) imply

\[
\begin{align*}
  h_i|_{S_m} - h_j|_{S_m} &= 0, \quad \text{for } i, j \in I_{S_m}, \forall m \in M, \\
  \left[ \frac{\partial h_i}{\partial \nu_{S_m}} \right]_{S_m} + \left[ \frac{\partial h_j}{\partial \nu_{S_m}} \right]_{S_m} &= 0, \quad \text{for } i, j \in I_{S_m}, \forall m \in M,
\end{align*}
\]

(2.9)

(2.10)

where the symbol \( \left[ \frac{\partial h_i}{\partial \nu_{S_m}} \right]_{S_m} \) denotes the jump of the co-normal derivative along the unique normal \( n_{S_m} \) fixed for the trace \( S_m \) on the fracture \( F_i \). This jump is independent of the orientation of \( n_{S_m} \).

While the trace \( S \) is also a boundary side for the fracture \( F_i \) the symbol \( \left[ \frac{\partial h_i}{\partial \nu_{S_m}} \right]_{S_m} \) becomes the difference between the co-normal derivative \( \frac{\partial h_i}{\partial \nu_{S_m}} \) and the Neumann boundary condition imposed on that side \( (h^N_i)_{S_m} \), assuming that for a boundary segment \( S \) the normal \( n_S \) is always outward. With this assumption we can deal with situations in which the trace \( S \) is also a boundary side for \( F_i \) and an internal side for \( F_j \) or a boundary side for both the fractures \( F_i \) and \( F_j \).

For each fracture \( F_i \) let the boundary \( \Gamma_i \) be the union of the boundary segments and let it is split in \( \Gamma_i^{IN} \), the boundary with Neumann boundary condition \( \frac{\partial h_i}{\partial n} = h_{IN} \), and \( \Gamma_i^{ID} \neq \emptyset \), the boundary with Dirichlet boundary condition \( h_i|_{\Gamma_i^{ID}} = h_{iD} \), satisfying \( \Gamma_i^{IN} \cap \Gamma_i^{ID} = \emptyset \) and \( \Gamma_i^{IN} \cup \Gamma_i^{ID} = \Gamma_i \).

Let us define

\[
V_i = H^1_0(F_i) = \left\{ v \in H^1(F_i) : v|_{\Gamma_i^{ID}} = 0 \right\}
\]

and \( V_i' \) its dual space. The hydraulic head \( h_i \) in each fracture belongs to the space

\[
V_i^{ID} = H^1_0(F_i) = \left\{ v \in H^1(F_i) : v|_{\Gamma_i^{ID}} = h_{iD} \right\}
\]

and the hydraulic head \( h \) on the whole domain \( \Omega \) is obtained by suitably matching via (2.9), (2.10) for \( m \in M \) the solutions \( h_i \in V_i^{ID} \) for each \( i \in I \) and belongs to the space

\[
V^D = H^1_0(\Omega) = \left\{ v \in \prod_{i \in I} V_i^{ID} : (v|_{F_i})_{|\partial S_m} = (v|_{F_i})_{|\partial S_m}, \quad i, j \in I_{S_m}, \forall m \in M \right\}.
\]

(2.11)
For simplicity of notation let us assume that the traces \( S \in \mathcal{S} \) are disjoint. This assumption can be removed at the cost of a more complex and heavy notation. Let us define for each trace \( S \in \mathcal{S} \) a suitable space \( \mathcal{U}^S \) and

\[
\mathcal{U}^S = \prod_{S \in \mathcal{S}} \mathcal{U}^S, \quad \mathcal{U} = \prod_{i \in \mathcal{I}} \mathcal{U}^S.
\]

Moreover, for each side \( S \) common to the fractures \( F_i \) and \( F_j \) we introduce suitable variables \( u_i^S \in \mathcal{U}^S \) and \( u_j^S \in \mathcal{U}^S \) representing the unknown quantities \( \left[ \frac{\partial h_i}{\partial \nu^S} \right]_S \) and \( \left[ \frac{\partial h_j}{\partial \nu^S} \right]_S \) respectively. Moreover, for each fracture \( F_i \) let us denote by

\[
u_i = \prod_{S \in \mathcal{S}_i} u_i^S \in \mathcal{U}^S_i
\]

the tuple of functions \( u_i^S \) with \( S \) spanning \( \mathcal{S}_i \), while for all the fractures of the domain \( \Omega \)

\[
u = \prod_{i \in \mathcal{I}} u_i \in \mathcal{U}
\]

is the tuple of all functions \( u_i^S \) with \( S \in \mathcal{S}_i \) and \( i \in \mathcal{I} \), i.e. it is the \( 2M^2 \)-tuple of control functions \( u_i^S \) on all traces in \( \Omega \).

Let us introduce the following linear bounded operators and their duals:

\[
A_i \in \mathcal{L}(\mathcal{V}_i, \mathcal{V}_i'), \quad (2.12)
\]

\[
A_i^* \in \mathcal{L}(\mathcal{V}_i', \mathcal{V}_i), \quad (2.13)
\]

\[
B_i^S \in \mathcal{L}(\mathcal{U}^S, \mathcal{V}_i'), \quad (2.14)
\]

\[
B_i \in \mathcal{L}(\mathcal{U}^S_i, \mathcal{V}_i') = \prod_{S \in \mathcal{S}_i} B_i^S, \quad (2.15)
\]

\[
B_i^* \in \mathcal{L}(\mathcal{V}_i, \mathcal{U}^{S_i'}), \quad (2.16)
\]

and the Riesz isomorphism:

\[
A_{\mathcal{U}^{S_i}} : \mathcal{U}^{S_i} \rightarrow \mathcal{U}^{S_i'}. \quad (2.17)
\]

The operator \( A_i \) is defined such that

\[
\langle A_i h_i, v \rangle_{\mathcal{V}_i', \mathcal{V}_i} = (K \nabla h_i, \nabla v), \quad h_i \in \mathcal{V}_i, \quad v \in \mathcal{V}_i
\]

and \( B_i \) is defined such that

\[
\langle B_i u_i, v \rangle_{\mathcal{V}_i', \mathcal{V}_i} = \langle u_i, v \rangle_{\mathcal{U}^{S_i}, \mathcal{U}^{S_i'}}.
\]

Let us introduce \( \forall i \in \mathcal{I} \) the problem: find \( h^0_i \in \mathcal{V}_i \) such that:

\[
(K \nabla h^0_i \nabla v) = (q_i, v) + \langle u_i, v \rangle_{\mathcal{H}^{-\frac{1}{2}}(S), \mathcal{H}^{\frac{1}{2}}(S)} + \langle h^0_i, v \rangle_{\mathcal{H}^{-\frac{1}{2}}(\Gamma_{IN}), \mathcal{H}^{\frac{1}{2}}(\Gamma_{IN})} + (K \nabla R h^0_i \nabla v), \quad \forall v \in \mathcal{V}_i \quad (2.18)
\]

where \( B_{\Gamma_{IN}} \in \mathcal{L}(\mathcal{H}^{-\frac{1}{2}}(\Gamma_{IN}), \mathcal{V}_i') \) is defined as

\[
\langle B_{\Gamma_{IN}} h^0_i, v \rangle_{\mathcal{V}_i', \mathcal{V}_i} = \langle h^0_i, v \rangle_{\mathcal{H}^{-\frac{1}{2}}(\Gamma_{IN}), \mathcal{H}^{\frac{1}{2}}(\Gamma_{IN})}
\]
and $\mathcal{R}_i h_{iD} \in H^1_D(\Omega)$ is a lifting of Dirichlet boundary conditions.

**Proposition 2.1.** Let

$$u_i^S = \left[ \frac{\partial h_i}{\partial v_S} \right]_S \in H^{-\frac{1}{2}}(S), \ \forall S \in S_i, \ \forall i \in I \quad (2.19)$$

then the following equivalences hold true:

1. equations (2.9), (2.10) are equivalent to (2.7), (2.8), respectively;
2. solving $\forall i \in I$ the problem (2.18) with additional conditions (2.9), (2.10) is equivalent to solve the problems (2.4)-(2.8).

**Proof.** The proof of item 1. is trivial. For the proof of item 2., let us consider the simple case of two fractures intersecting along the internal edge $S$ splitting each fracture $F_i$, $i = 1, 2$ in two subfractures $f^i_1$ and $f^i_2$ (see Figure 2.1 for the shape of $F_i$, $f^i_1$, $f^i_2$ and orientation of $n_S$). Neumann boundary conditions are set for both $F_1$ and $F_2$ on the two opposite edges on which the trace $S$ ends, whereas we set Dirichlet boundary conditions on the other two opposite edges. Let $R_i^\chi$ be the restriction operator of functions in $f^\chi_i$ with $\chi = \sharp, \flat$, and let $R_i$ be the restriction operator of functions in $V_i$ to functions defined in $f^\chi_i$.

Equations (2.18) can be written as: find $h_i \in V_i^D$ such that

$$\int_{F_i} K \nabla h_i \nabla R_i v = \int_{F_i} q_i R_i v + \langle u_i, R_i v|_{\partial S} \rangle_{H^{-\frac{1}{2}}(S), H^{\frac{1}{2}}(S)} + \langle h_i, R_i v|_{\Gamma_i, N} \rangle_{H^{-\frac{1}{2}}(\Gamma_i, N), H^{\frac{1}{2}}(\Gamma_i, N)}, \ \forall v \in V, \ i = 1, 2.$$
Splitting the integrals over the fractures $F_i$ in the integrals over the subfractures $f^X_i$ and resorting to the definition of $\chi$ and $\chi'\chi$ we have

$$
\int_{F_i^X} K \nabla h_i \nabla R_i^X v + \int_{F_i^X} J \nabla h_i \nabla R_i^X v = \int_{F_i^X} q_i R_i^X v + \int_{F_i^X} q_i R_i^X v
$$

$$
+ \left( \frac{\partial h_i}{\partial v^s_{F_i^X}} R_i^X v_{|s} \right)_{H^\frac{1}{2}(\Gamma_s^F), H^\frac{1}{2}(\Gamma_s^F)} + \left( \frac{\partial h_i}{\partial v^s_{F_i^X}} R_i^X v_{|s} \right)_{H^\frac{1}{2}(\Gamma_s^F), H^\frac{1}{2}(\Gamma_s^F)}
$$

$$
+ \langle h_i N, R_i^X v_{|N} \rangle_{H^\frac{1}{2}(\Gamma_i^N), H^\frac{1}{2}(\Gamma_i^N)} \quad \forall v \in V, \quad i = 1, 2
$$

that correspond to the sum of the weak formulations of (2.4)-(2.6) on the sub-fractures $f^X_i$, $\chi = \chi'$.

2.2. The optimal control formulation. Instead of solving the coupled differential problems on the fractures (2.18) or sub-fractures (2.4)-(2.6) with the corresponding matching conditions (2.9), (2.10) or (2.4)-(2.8) we look for the solution as the minimum of a PDE constrained optimal control problem, the variable $u$ being the control variable.

Let us define the spaces

$$
\mathcal{H}^S = \prod_{s \in S} \mathcal{H}_s, \quad \mathcal{H} = \prod_{s \in S} \mathcal{H}_s
$$

and the Riesz isomorphism

$$
\Lambda_{\mathcal{H}_s} : \mathcal{H}_s \rightarrow \mathcal{H}_s'.
$$

The following linear bounded “observation” operators $C^S_i$ and $C_i$ and the dual $C^*_i$

$$
C^S_i \in \mathcal{L}(V_i, \mathcal{H}_s),
$$

$$
C_i \in \mathcal{L}(V_i, \mathcal{H}_s) = \prod_{s \in S} C^S_i,
$$

$$
C^*_i \in \mathcal{L}(\mathcal{H}_s', V'_i),
$$

will be exactly defined later for each choice of the spaces $\mathcal{H}_s$. Let us also define the differentiable functional $J : \mathcal{U} \rightarrow \mathbb{R}$ as

$$
J(u) = \sum_{s \in S} J^S(u)
$$

$$
= \sum_{s \in S} \left( ||C^S_i h_i(u_i) - C^S_j h_j(u_j)||^2_{\mathcal{H}_s} + ||u^S_i + u^S_j||^2_{\mathcal{H}_s} \right)
$$

$$
= \frac{1}{2} \sum_{i \in I} \sum_{s \in S} \left( ||C^S_i h_i(u_i) - C^S_j h_j(u_j)||^2_{\mathcal{H}_s} + ||u^S_i + u^S_j||^2_{\mathcal{H}_s} \right)
$$

$$
= \frac{1}{2} \sum_{i \in I} \left( \prod_{s \in S_i} \left( C^S_i h_i(u_i) - C^S_j h_j(u_j) \right) ||^2_{\mathcal{H}_s} + ||u + \prod_{s \in S_i} u^S_j ||^2_{\mathcal{H}_s} \right)
$$

(2.24)

where, having fixed a fracture $F_i$, we denote by

$$
\prod_{s \in S_i} u^S_j
$$
the tuple of control functions each one defined on the fracture $F_j \neq F_i$ that shares the trace $S \in \mathcal{S}$ with the fracture $F_i$, and by

$$\prod_{S \in \mathcal{S}_i} (C^S_i h_i(u_i) - C^S_j h_j(u_j))$$

the tuple of functions $(C^S_i h_i(u_i) - C^S_j h_j(u_j))$ as $S$ varies in $\mathcal{S}_i$, where $u_i$ is the control variable on $F_i$ and $u_j$ the control variable on fracture $F_j$, with $i, j \in I_S$. Moreover with the symbol $h_i(u_i)$ we denote the solution of (2.18) corresponding to the control variable $u_i$, and similarly for $h_j(u_j)$.

**Proposition 2.2.** Let us define the spaces $\mathcal{U}^S$ and $\mathcal{H}^S$ and the observation operator $C^S_i$ on the trace $S$ as

$$\mathcal{U}^S = H^{-\frac{1}{2}}(S),$$  \hspace{1cm} (2.25)  

$$\mathcal{H}^S = H^{\frac{3}{2}}(S),$$  \hspace{1cm} (2.26)  

$$C^S_i h_i = h_i|_S,$$  \hspace{1cm} (2.27)  

then the hydraulic head $h \in H^1_D(\Omega)$ giving the unique exact solution of (2.4)-(2.8) satisfies the differential problems (2.18) for all $i \in I$ and corresponds to $J(u) = 0$.

**Proof.** The existence and uniqueness of $h \in H^1_D(\Omega)$ satisfying (2.4)-(2.8) is a classical result (see for example [22]). The vanishing of the first term of the functional $J$ ensures the solutions $h_i$ of (2.18) for all $i \in I$ satisfy $h_i = h_i|_{F_i}$ with $h \in H^1_D(\Omega)$ (condition (2.9)), whereas the vanishing of the second term of $J$ ensures condition (2.10).

**Proposition 2.3.** The optimal control $u \in \mathcal{U}$ providing the minimum of the functional $J(u)$ corresponds to the equations (2.18) and

$$(A^*_i)^{-1} B_i^* p_i + u_i + \prod_{S \in \mathcal{S}_i} u^S_j = 0, \quad \forall i \in I$$  \hspace{1cm} (2.28)  

where the functions $p_i \in V_i, \forall i \in I$ is the solution of the equation

$$A^*_i p_i = C^*_i \Lambda_{\mathcal{H}^S_i} \prod_{S \in \mathcal{S}_i} (C^S_i h_i - C^S_j h_j),$$  \hspace{1cm} (2.29)  

(i.e. with boundary conditions $p_i|_{\Gamma_{iD}} = 0$ on $\Gamma_{iD}$, and $\frac{\partial p_i}{\partial n} = 0$ on $\Gamma_{iN}$).

**Proof.** Let us differentiate the cost functional $J(u)$ with respect to the control $u_i$,
This proves that the minimum of the functional corresponds to (2.28).

Instead of solving problems (2.18) coupled with the problems (2.29) and (2.28) \( \forall i \in I \) we aim at setting up a minimization process that requires the decoupled solution of the previous local problems. Here we apply a simple steepest descent method. This approach will require the solution of many simple problems with a small exchange of data between them. The resulting algorithm will be suitable for massively parallel computers and GPU-based computers. More efficient minimization approach will be considered in a future work [4].

Let us define

\[
\delta u_i = \Lambda_i^{-1} B_i^* p_i + u_i + \prod_{S \in S_i} u_j^S, \quad \forall i \in I, \tag{2.30}
\]

\[
\delta u = \sum_{i \in I} \delta u_i \tag{2.31}
\]

and let \( \delta h_i \in V_i, \, \forall i \in I \) be defined as the solution of the problem

\[
A_i \delta h_i = B_i \delta u_i, \tag{2.32}
\]

(i.e. with boundary conditions \( \delta h_i \rvert_{V_i D} = 0 \) on \( \Gamma_i D \) and \( \frac{\partial \delta h_i}{\partial n} = 0 \) on \( \Gamma_i N \)).
Proposition 2.4. Let us increment the control variable $u$ of a step $\lambda \delta u$, the steepest descent method corresponds to the stepsize

$$
\lambda = - \frac{||\delta u||^2_{\mathcal{H}}}{\sum_{s \in S} (||C_i^S \delta h_i - C_j^S \delta h_j||^2_{\mathcal{H}s} + ||\delta u_i^s + \delta u_j^s||^2_{\mathcal{H}s})}.
$$

(2.33)

Proof.

$$
J(u + \lambda \delta u) = \sum_{s \in S} ||C_i^S h_i(u_i) - C_j^S h_j(u_j) + \lambda (C_i^S \delta h_i - C_j^S \delta h_j)||^2_{\mathcal{H}s} + \sum_{s \in S} ||\delta u_i^s + \delta u_j^s + \lambda (\delta u_i^s + \delta u_j^s)||^2_{\mathcal{H}s}
$$

$$
= J(u) + 2 \sum_{s \in S} (C_i^S h_i(u_i) - C_j^S h_j(u_j), \lambda (C_i^S \delta h_i - C_j^S \delta h_j),)_{\mathcal{H}s}
$$

$$
+ 2 \sum_{s \in S} (u_i^s + u_j^s, \lambda (\delta u_i^s + \delta u_j^s))_{\mathcal{H}s}
$$

$$
+ \lambda^2 \sum_{s \in S} (||C_i^S \delta h_i - C_j^S \delta h_j||^2_{\mathcal{H}s} + ||\delta u_i^s + \delta u_j^s||^2_{\mathcal{H}s})
$$

$$
= J(u) + 2 \sum_{i \in I} \sum_{s \in S_i} (C_i^S h_i(u_i) - C_j^S h_j(u_j), \lambda C_i^S \delta h_i)_{\mathcal{H}s_i}
$$

$$
+ 2 \sum_{i \in I} \left( u_i^s + \frac{\prod_{s \in S_i} (C_i^S h_i(u_i) - C_j^S h_j(u_j))}{C_i^S h_i(u_i) - C_j^S h_j(u_j)}, \lambda C_i^S \delta h_i \right)_{\mathcal{H}s_i}
$$

Moreover,

$$
J(u + \lambda \delta u) - J(u) - \lambda^2 \sum_{s \in S} (||C_i^S \delta h_i - C_j^S \delta h_j||^2_{\mathcal{H}s} - ||\delta u_i^s + \delta u_j^s||^2_{\mathcal{H}s}) =
$$

$$
= 2 \lambda \sum_{i \in I} \left( \left( \prod_{s \in S_i} (C_i^S h_i(u_i) - C_j^S h_j(u_j)), C_i^S \delta h_i \right)_{\mathcal{H}s_i} + \left( u_i + \prod_{s \in S_i} u_j^s, \delta u_i \right)_{\mathcal{H}s_i} \right)
$$

$$
= 2 \lambda \sum_{i \in I} \left( C_i^S \Lambda_{\mathcal{H}s_i} \prod_{s \in S_i} (C_i^S h_i(u_i) - C_j^S h_j(u_j)), \delta h_i \right)_{V_i', V_i}
$$

$$
+ 2 \lambda \sum_{i \in I} \left( A_{\mathcal{H}s_i} (u_i + \prod_{s \in S_i} u_j^s), \delta u_i \right)_{\mathcal{H}s_i, \mathcal{H}s_i}
$$

$$
= 2 \lambda \sum_{i \in I} \left( A_i^{-1} B_i \delta u_i \right)_{V_i', V_i} + 2 \lambda \sum_{i \in I} \left( A_{\mathcal{H}s_i} (u_i + \prod_{s \in S_i} u_j^s), \delta u_i \right)_{\mathcal{H}s_i, \mathcal{H}s_i}
$$

$$
= 2 \lambda \sum_{i \in I} \left( \Lambda_{\mathcal{H}s_i} A_i^{-1} B_i u_i + u_i + \prod_{s \in S_i} u_j^s, \delta u_i \right)_{\mathcal{H}s_i, \mathcal{H}s_i}
$$

$$
= 2 \lambda \sum_{i \in I} ||\delta u_i||^2_{\mathcal{H}s_i}.
$$

10
Then the value of $\lambda$ in (2.33) vanishes the derivative of $J(u + \lambda \delta u)$ with respect to $\lambda$, thus providing the minimum of the function $J(\lambda) = J(u + \lambda \delta u)$. □

The optimal problem can be solved iteratively following the algorithm:
1. Set $k = 0$ and initial guess for control variable $u^0$;
2. find $h^0 = h(u^0)$ solving on each fracture plane the primal problem defined by equation (2.18);
3. evaluate $J(u^0)$ according to equation (2.24)

While $J(u^k) \neq 0$ do:
4. find $p(u^k)$ solving on each fracture plane the dual problem defined by equation (2.29);
5. find $(\delta u)^k$ evaluating equations (2.30), (2.31) and solve problem defined by (2.32) to get $(\delta h_i)^k$ on each plane;
6. evaluate $\lambda^k$ according to equation (2.33) and calculate new value of control variable $u^{k+1} = u^k + \lambda^k (\delta u)^k$;
7. find $h^{k+1} = h(u^{k+1})$ solving the primal problem;
8. evaluate $J(u^{k+1})$;
9. $k = k + 1$;
end do.

3. The discrete fracture network problem with the XFEM.

3.1. XFEM description. The extended finite element method (XFEM) [2, 7, 3] is a mesh-based numerical technique for solving partial differential equations (PDE) in variational form, when non smooth or discontinuous solutions are considered. The XFEM can reproduce irregularities arbitrarily placed in the domain regardless of the underlying numerical triangulation.

The concept at the basis of the XFEM consists in combining the standard finite element (FE) approach with the partition of unity concept, in order to overcome the limitations of FE in dealing with discontinuities, but still remaining in the well established finite element context. Customized enrichment functions are added to the standard finite element approximation space in order to catch the non-smooth character of the solution. An enriching functional space, embedding the enrichment functions and suitable for finite element applications, is obtained with the partition of unity method (PUM) [1] starting from global functions (i.e. defined on the whole problem domain), each carrying a particular discontinuous or non-smooth behaviour of the exact solution into the numerical approximation. The PUM also gives to the enrichments a local character.

In what follows we will limit ourselves to the description of the method in the case of continuous solutions with discontinuous first order derivatives (weak discontinuities). Customizations of the method for various circumstances can be found in [3, 12].

Let us consider a problem in $\omega \in \mathbb{R}^n$, with sharp or weak singularity along the interface described by the manifold $S \subset \omega, S \in \mathbb{R}^{n-1}$. Let also $T_\delta$ be a conforming triangulation set on $\omega$, with $N_{el}$ elements $\tau_e \subset \mathbb{R}^n$:

$$\bar{\omega} = \bigcup_{e=1,...,N_{el}} \tau_e$$

where each element $\tau_e$ is a non degenerate polyhedron. The standard finite dimen-
sional trial and test space $V_{\delta}^{\text{fem}}$ can be defined as

$$V_{\delta}^{\text{fem}} = \{ v_{\delta} \in C^0(\bar{\omega}) : v_{\delta}|_{\partial \omega} \in \mathbb{P}_r, v_{\delta}(\Gamma_D) = 0, \forall \tau_e \in T_\delta \} \subset H^1_0(\omega)$$

where $C^0$ is the functional space of continuous functions and $\mathbb{P}_r$ the space of polynomials of degree less or equal to $r$. Every element $\tau_e \in T_\delta$ has $N_{e}^{\text{ve}}$ vertexes and $N_{e}^{\text{dof}}$ nodes such that functions $v_{\delta}$ are uniquely determined on $\tau_e$. Thus $V_{\delta}^{\text{fem}}$ has dimension $N_{dof} = \sum_{e} N_{e}^{\text{dof}}$ and we choose a Lagrangian base such that:

$$V_{\delta}^{\text{fem}} = \text{span} \left( \{ \phi_\xi(x) \}_{\xi=1,..,N_{dof}} \right). \quad (3.1)$$

Each $\phi_\xi(x)$ is a standard FE shape function uniquely identified by the related degree of freedom (DOF) of index $\xi$. We call the set of local DOF indexes on each triangle as

$$I_e = \{ \xi, \}_{\xi=1,..,N_{e}^{\text{dof}}}$$

and the global set of DOF indexes as

$$I = \bigcup_{e=1,..,N_{el}} I_e,$$

where each $\xi_e$ is one of the $N_{e}^{\text{dof}}$ degrees of freedom indexes. Let further define the support of $\phi_\xi(x)$ as:

$$\Delta_\xi = \bigcup_{e=1,..,N_{el}} \{ \tau_e \in T_\delta : \phi_\xi|_{\tau_e} \neq 0 \}.$$ \quad (3.2)

Provided that the edges of the elements in $T_\delta$ surrounding $S$ exactly match it, the approximate solution with standard finite elements would have the following form:

$$h_{\delta}^{\text{fem}}(x) = \sum_{\xi \in I} h_{\xi}^{\text{fem}} \phi_\xi(x), \quad (3.3)$$

where $h_{\xi}^{\text{fem}}$ is the degree of freedom corresponding to the base function $\phi_\xi(x)$. Functions in $V_{\delta}^{\text{fem}}$ are in fact continuous and can have discontinuities in the first order derivatives across mesh-element edges.

Let assume $\Phi(x)$ is a continuous bounded function on $\omega$, $\Phi(x) \in H^1(\omega) \cap C^0(\bar{\omega})$ which approximates well the behaviour of $h(x)$ in a neighborhood of $S$. $\Phi(x)$ is chosen to have a defined value on $S$, in most cases equal to zero. It is then desirable to introduce this function and its translations into the FE trial space. In the XFEM the task of building a conforming finite element space that embodies the character of enrichment function is addressed with the partition of unity method, using standard FE shape functions and their support in the definition of a partition of unity.

Let then consider again on $\omega$ our triangulation $T_\delta$. The set $\{ \Delta_\xi \}_{\xi=1,..,N_{e}^{\text{dof}}}$ is a cover for $\omega$, and the FE shape functions $\{ \phi_\xi(x) \}_{\xi=1,..,N_{e}^{\text{dof}}}$ build a partition of unity subordinate to this cover that satisfies the conditions stated in [1]. We now identify with $J \subset I$ the subset of partition of unity function indexes such that $\{ \Delta_\xi \}_{\xi \in J}$ is a cover of a certain neighborhood of $S$. DOF in $J$ are called enriched DOF (and enriched nodes the corresponding nodes). Figure 3.1 depicts one common choice of enriched DOF in
2D with Courant base functions for the standard FE: DOF are enriched only if the support of the corresponding base function is intersected by the interface. Close to the interface $S$ the exact solution $h(x)$ is well approximated by translations of the enrichment function $\Phi(x)$, and therefore we define for each of the $\{\Delta_\xi\}_{\xi \in \mathcal{J}}$ a local approximation space $V_{\xi} \subset H^1(\Delta_\xi)$ which embeds the enrichment function and its translations:

\[ V_{\xi} = \text{span} \{ 1, \Phi(x)|_{\Delta_\xi} \} \quad \forall \xi \in \mathcal{J}. \quad (3.4) \]

The application of the PUM with cover given by the $\{\Delta_\xi\}_{\xi \in \mathcal{J}}$, partition of unity functions $\{\phi_\xi(x)\}_{\xi \in \mathcal{J}}$ and local approximation spaces $\{V_{\xi}\}_{\xi \in \mathcal{J}}$ results in the conforming discrete space

\[ V^{\Phi} = \text{span} \{ \phi_\xi, \phi_\xi(x)\Phi(x) \}_{\xi \in \mathcal{J}} \subset H^1_0(\omega) \quad (3.5) \]

which can be added to the standard FE space in order to obtain the enriched approximation space $V_{\delta}^{\text{xfem}}$ for the XFEM:

\[ V_{\delta}^{\text{xfem}} = \text{span} \left( \{ \phi_\xi(x) \}_{\xi \in \mathcal{I}}, \{ \phi_\xi(x)\Phi(x) \}_{\xi \in \mathcal{J}} \right). \quad (3.6) \]

Consequently the approximate solution $h_{\delta}^{\text{xfem}}(x)$ with the XFEM will be in general:

\[ h_{\delta}^{\text{xfem}}(x) = \sum_{\xi \in \mathcal{I}} h_{\xi}^{\text{xfem}} \phi_\xi(x) + \sum_{\xi \in \mathcal{J}} a_{\xi}^{\text{xfem}} \phi_\xi(x)\Phi(x), \quad (3.7) \]

where $h_{\xi}^{\text{xfem}}$ and $a_{\xi}^{\text{xfem}}$ are the unknowns related to the standard and enriching base functions respectively.

It can be seen that now the singular behaviour of the exact solution can be reproduced by $h_{\xi}^{\text{xfem}}(x)$ independently of the positioning of elements in $T_\delta$ with respect to the interface $S$, since the singularity of the exact solution is now present in the space of approximate solution.

Only a subset of total DOF has been enriched and this is one peculiarity of the XFEM compared to PUM or other similar methods as for example the GFEM ([19, 20]). The criteria for the selection of enriched nodes are related to the specific enrichment function and to the characteristics of the interfaces. This issue will be presented in details in the next Subsection along with a description of the discontinuities and interface behaviours considered in the present application of the method.
Since only a subset of total degrees of freedom is enriched, elements in $\mathcal{T}_\delta$ may have a variable number of enriched nodes. In particular it is possible to group elements in three categories, following classification used in [12] (see Figure 3.2):

i) standard elements: no element node is enriched;

ii) reproducing elements: all nodes are enriched;

iii) blending elements: some nodes are enriched.

The enriching functional space $V^\Phi$ is fully reproduced only in those elements where all nodes are enriched, thus where partition of unity is fully established. In blending elements, on the contrary $V^\Phi$ is not exactly reproduced, since only some of the DOF are in $\mathcal{J}$. This introduces errors and parasitic terms into the XFEM approximation that may affect convergence rate of the method or increase error norms compared to standard FE. Numerous technique are suggested in order to prevent this issue, for example in [6, 21, 11]. We describe the method suggested in [11], termed modified XFEM. The enrichment function $\Phi(x)$ is modified in such a way that it vanishes at boundaries of the enriched domain $\Delta_\Phi$ defined as (see also Figure 3.2):

$$\Delta_\Phi = \bigcup_{\xi \in \mathcal{J}} \Delta_\xi.$$  \hspace{1cm} (3.8)

The new enrichment function $\tilde{\Phi}$ is given by:

$$\tilde{\Phi} = \Phi(x)R(x),$$ \hspace{1cm} (3.9)

being

$$R(x) = \sum_{\xi \in \mathcal{J}} \phi_\xi,$$

and $\tilde{\Phi} = \Phi$ in reproducing elements, where $R = 1$, linearly vanishes in blending elements and $\tilde{\Phi} = 0$ on the boundaries and outside $\Delta_\Phi$, where $R = 0$ (Figure 3.3).

The modified XFEM method also requires a new definition of the set of enriched DOF, in order to include blending element nodes in the enrichment. Let then define the set

$$\tilde{\mathcal{J}} = \{ \xi \in \mathcal{I} : \xi \in N_e^{dof} \land \tau_e \cap \Delta_\Phi \neq \emptyset, \quad \forall e = 1, ..., N_{el} \}$$  \hspace{1cm} (3.10)

of the enriched nodes related to the modified enrichment $\tilde{\Phi}$. Wherever the enrichment function $\Phi$ is non-zero the partition of unity given by functions $\{\phi_\xi\}_{\xi \in \tilde{\mathcal{J}}}$ is fully established and the enrichment space originated starting from $\tilde{\Phi}$ can be correctly reproduced, avoiding problems related to parasitic terms. Given the structure of $\Phi$ continuity of functions in the new XFEM approximating space is not compromised.

The chosen basis of $V^{\text{xfem}}_\delta$ (3.6) is not a Lagrangian basis. This makes the imposition of Dirichlet boundary conditions not as easy as for standard FE applications. To fix this problem, in [3, 11] it is suggested to shift each enrichment function in $V^{\text{xfem}}_\delta$ thus defining the new functions $\tilde{\Phi}_\xi(x) = \Phi(x) - \Phi(x_\xi)/\phi_\xi(x)$ and restoring the Lagrangian property.

Important implementation issues related to the XFEM concern numerical integration and ill-conditioning of the algebraic matrix resulting from the method. Special care is required in order to compute integrals involving enriched basis functions and their derivatives. In fact, only to perform these integrations, a subdivision of the elements into sub-domains that do not cross singularity interface is necessary [15, 3].
The algebraic matrix related to the XFEM method can be ill conditioned or even singular. When discontinuity interface cuts elements of the triangulation close to a face, an edge or a vertex, the ratio of the volumes of the two parts divided by the interface can be very large, thus introducing ill-conditioning in the element matrix related. See [7] for details and methods to avoid the problem. Moreover, for some kind of enrichments, the functions in $V_{\delta}^{\text{xfem}}$ may be linearly dependent or nearly linearly dependent, resulting in a singular or again badly conditioned algebraic system. Details of this can be found in [11] or in [19] in the context of the GFEM.

The approach described is easily generalized to the case of more than one enrichment, let say the solution of physical problem is singular in several parts of the domain, or for a single discontinuous character more than one enrichment function need to be introduced in the approximate solution space to reproduce the discontinuity. Given the set of modified enrichment functions $\tilde{\Phi}_m^m(x)$, $m = 1, ..., M^f$, and corresponding enriched DOF $\tilde{J}_m$ the approximate XFEM solution will be:

$$h^{\text{xfem}}_\delta(x) = \sum_{\xi \in I} h_\xi \phi_\xi(x) + \sum_{m=1}^{M^f} \sum_{\xi \in \tilde{J}_m} a_{\xi}^m \phi_\xi(x) \tilde{\Phi}_m^m(x). \quad (3.11)$$

The generalization to other kind of discontinuities follows the same outline described above, with specific re-definition of functional spaces. A comprehensive review of the XFEM/GFEM method with details of all implementation aspects is available in [12].

### 3.2. The discrete DFN problem

With reference to definitions and nomenclature introduced in section 2 we shall now focus on the specific application of the extended finite elements to the problem concerning the definition of the hydraulic head in a discrete fracture network.

On each fracture plane $F_i$ the exact solutions $h_i$, $p_i$ and $\delta h_i$ may have a jump of fluxes across the traces in $S_i$. The numerical solution of PDEs at steps 2, 4, 5 of the algorithm at the end of Section 2 with the XFEM allows triangulation to be set on each plane independently of the disposition and number of the traces. This is much more relevant as the number of traces increases or when traces intersect with arbitrary orientations.
Let then characterize the application of the XFEM on a fracture plane $F = F_i \subset \mathbb{R}^2$ which has $M^i$ intersections with other planes in $\Omega$ described by the traces $S_m \in \mathcal{S}_i$. The starting point is a standard finite elements setting, defined by a conforming triangulation $\mathcal{T}_h$ and the discrete test space $V_{\text{fem}}^q$ as defined by equation (3.1).

The definition of the enrichment functions is related to the singularity to be reproduced and on the type of interfaces. As mentioned, the physical model only allows for solutions with discontinuous first order derivatives (weak discontinuities), thus different enrichment functions will be employed in relation to the disposition of the traces (our interfaces) in the domain. In particular we can have closed interfaces when traces cut the domain in such a way to separate two sub-domains or open interfaces, with traces ending and/or originating inside the domain, as sketched in Figure 3.4.

The enrichment functions for weak discontinuities here used were introduced in early works with the XFEM mainly in the context of fracture mechanics. A comprehensive description can be found in [3, 21, 7, 12], we will confine to the description of the essential features.

The mathematical description of each trace is performed introducing a signed distance function $f_m(x)$ which is defined in $F$ as the minimum distance with sign from segments $S_m [21, 3]$:

$$f_m(x) = \min_{x \in S_m} \|\bar{x} - x\| \frac{\hat{n}_S \cdot (\bar{x} - x)}{\|\hat{n}_S \cdot (\bar{x} - x)\|},$$

where $\bar{x}$ is the projection of $x$ on $S_m$ and $\hat{n}_S$ the outward unit normal vector to $S_m$, such that $S_m = \{x \in F : f_m(x) = 0\}$. The enrichment functions are built starting from the signed distance functions. In the case of a closed interface we introduce the enrichment function $\Psi^m$ defined as $\Psi^m(x) = |f_m(x)|$. Clearly $\Psi^m$ is a continuous function, but its first order derivatives have a jump across $S_m$, thus introducing the required non-smooth behaviour in the approximation (Figure 3.5).

The enrichment is localized in a neighborhood of $S_m$ defined by the set of DOF $J_{\Psi}^m = \{\xi \in I : \Delta_\xi \cap S_m \neq \emptyset\}$.

If, on the contrary, $S_m$ is an open interface, more than a single enrichment function is needed. In fact it is necessary to reproduce the possibly different character of the exact solution at the extremes of the interface and away from the extremes. Let identify and collect the extreme points of $S_m$ (as depicted in Figure 3.4) in the set $\sigma_m = \{s^\ell \} \in F, \ell \in \{1, 2\}$. Away from the extremes, the non-smooth behaviour of the solution is similar to the case of closed interfaces, and therefore the same function $\Psi^m$ can be used but confining the corresponding DOF to the set $J_{\Psi}^m$ given by:

$$J_{\Psi}^m = \{\xi \in I : \Delta_\xi \cap S_m \neq \emptyset, \Delta_\xi \cap s^\ell = \emptyset\} \quad \forall s^\ell \in \sigma_m.$$

In addition to this, other enrichment functions are needed to describe near-tip behaviour of the solution. We decide to use the functions suggested in [3]:

$$\Theta_{s^\ell j}^m(x) = \begin{bmatrix} r \cos \frac{\theta}{2}, r^2 \cos \frac{\theta}{2}, r \sqrt{\cos \frac{\theta}{2}} \end{bmatrix}, \quad j = 1, \ldots, 3$$

where $r(x) = x - s^\ell$ is the signed distance between the current point and segment tip and

$$\theta(x) = h^{-1} \left( \frac{f_m(x)}{r(x)} \right), \quad -\pi < \theta < \pi$$
calling $h^{-1}$ the four-quadrant inverse tangent function. In order to let the enrichments $\Theta_{s_j}^m(x)$ be defined in a whole neighborhood of discontinuity tip, the segment $S_m$ is virtually extended over its extremes (Figure 3.8).

Functions $\Theta_{s_j}^m(x)$ are continuous and cusp-like on $S_m$. The behaviour around trace tips is proportional to linear combinations of $\{\sqrt{r}, r, r^2\}$ and it is carried in the approximating XFEM space. Figure 3.6 shows one of these functions. The set of DOF for tip enrichments is given by (see also Figure 3.7):

$$J_{\Theta_m}^s = \{\xi \in I : \Delta \xi \cap s^f \neq \emptyset\}, \quad \forall s^f \in \sigma_m.$$  

Traces intersection in a point is allowed. Let then consider two indexes $m, l$ such that $S_m \cap S_l = \pi^{ml} \in F$, being $\pi^{ml}$ the traces intersection point. The non smooth behaviour of the exact solution around the intersecting discontinuities $S_m$ and $S_l$ requires one additional dedicated enrichment function.

For each intersection $\pi^{ml}$ this enrichment is defined as $\chi^\alpha(x) = |f_m(x)||f_l(x)|$ where $\alpha = 1, \ldots, \eta$ counts the number of trace intersections, and uniquely identifies the couple of indexes $(m, l)$. The set of degrees of freedom for these enrichments is

$$J_{\chi}^\alpha = \{\xi \in I : \Delta \xi \cap \pi^{mn} \neq \emptyset\}.$$
This approach can be generalized to the case of more segments intersecting in a single point. This is done by electing a ”principal” trace for each multiple intersection point and introducing one enrichment for each ”secondary segment” crossing it. Let say \( \pi^{mkl} = S_m \cap S_l \cap S_k \), we define \( S_m \) the principal trace and introduce the enrichments \( \chi^{\alpha} \) and \( \chi^{\alpha''} \), with \( \alpha \) representing \((m, l)\) and \( \alpha'' \) \((m, k)\). The value of \( \eta \) should now count the total number of intersections given by this criterion. Further details are again available in [7].

In order to avoid problems with blending elements the modified version of the extended finite element method has been used, as described in the previous Subsection. Also a shift of enrichment function was performed to restore Lagrangian property.

In conclusion the most general shape of the approximated solution on each fracture plane of the discrete fracture network problem can be written in the following way:

\[
h_{P}^{\text{fem}}(x) = \sum_{\xi \in I} \phi_{\xi}(x) \left( h_{\xi} + \sum_{m=1}^{M} \left( a_{\xi}^{m} \Psi_{\xi}^{m}(x) + \sum_{s^{\ell} \in \sigma \in m} b_{\xi s^{\ell}j}^{m} \Theta_{\xi s^{\ell}j}^{m}(x) \right) \right. \\
\left. + \sum_{\alpha=1}^{\eta} c_{\xi}^{\alpha} \chi^{\alpha}(x) \right),
\]

where \( h_{\xi} \) are the nodal values of standard finite element shape functions and the tilde indicates the modified version of enrichments, while for the additional degrees of freedom related to the enrichments we have

\[
a_{\xi}^{m} = 0 \text{ if } \xi \notin  \tilde{\mathcal{J}}_{\Psi} \quad b_{\xi s^{\ell}j}^{m} = 0 \text{ if } \xi \notin  \tilde{\mathcal{J}}_{\Theta}^{s^{\ell}} \quad c_{\xi}^{\alpha} = 0 \text{ if } \xi \notin  \tilde{\mathcal{J}}_{\chi}^{\alpha}.
\]

Figure 3.7 depicts the choice of DOF for the enrichment functions described above when Courant elements are used for standard FE.

The numerical integration of discontinuous functions was performed on subdomains where the restriction of basis functions is regular. Gauss quadrature rule was used, adopting the number of integration nodes required by the polynomial degree of the integrands.

Depending on the choices of the discrete subspaces for \( h \) on each fracture \( F_i \) and on the discrete subspace for \( u^S \) for each trace \( S \subset F_i \), possibly different from the discrete subspace for \( u^S \), the minimum of functional \( J(u) \) at step 8 can be different from zero. In the discrete form of the optimization problem the exit condition from iterations is based on the distance between the value of \( J(u^k) \) at two subsequent iterations, typically

\[
|J(u^{k+1}) - J(u^k)| < \Delta_{\text{tol},J}(\sim 10^{-13}.
\]

4. Numerical results. Four test problems are proposed to show the performances of the method. In Problem 1, numerical simulations of the optimization process are performed both with standard finite elements on conforming grids aligned to a trace, and with the XFEM with a trace crossing mesh elements. Numerical results are compared to the known exact solution. In Problem 2 the method is tested against a more complex problem on a similar fractured domain. In Problems 3 and 4 more complex domains are considered.

In the following numerical tests we only consider traces entirely crossing a fracture so we do not need near tip enrichment basis functions and the discrete solution will be in general as in (3.12) where only coefficients \( h_{\xi} \) and \( a_{\xi}^{m} \) are different from zero.
We postpone the application of the method to more complex and realistic fracture configurations to a forthcoming work. Triangular meshes and first order finite elements are used in all the tests. Let further $V_i, \delta$ be the discrete enriched finite element space on the fracture $F_i$, $\forall i \in I$, defined accordingly to (3.6) with the modified and shifted enrichment basis functions introduced in the previous Section. With assumptions (2.25)-(2.27) the minimum of the functional $J(u)$ is characterized by conditions involving a fractional power of the Laplace operator $\triangle_S$ on the traces. For these reasons we opt for developing our numerical method for the approximation of the solution with the following choices

$$U^S = L^2(S), \quad \forall S \in S$$
$$H^S = L^2(S), \quad \forall S \in S.$$  

**Remark 4.1.** A proof of existence and uniqueness of the minimum of the discrete functional $J$ with $U^S = L^2(S)$ and $H^S = L^2(S)$, $\forall S \in S$, can be found in [4]. The proof is based on results of discrete quadratic programming. It is not reported here since it requires the introduction of heavy notation.

Let $U_\delta \subset U$ be the discrete space for the control functions. The space $U_\delta$ is here defined as the space of the piecewise linear functions on the traces $S_m$, $\forall m \in M$, defined on the 1D mesh generated by the nodes given by the intersection of the trace $S_m$ with the edges of mesh elements on the two fractures $F_i$ with $i \in I_{S_m}$. If some edge is contained in the trace, we consider its ending points.

**Remark 4.2.** For each trace $S_m$ the choice of the same discrete space $U^S_{\delta_m}$ for the two controls $u^S_{i,m}$ and $u^S_{j,m}$, $i, j \in I_{S_m}$ is not mandatory and the approach can still be applied if we choose two different finite dimensional subspaces of $U^S_{\delta_m}$. With the discretization choice described above the second term of the functional $J$ can always vanish, whereas the non conformity of the meshes on $F_i$ and $F_j$, $i, j \in I_{S_m}$ implies the non vanishing of the first term of $J$.

**4.1. Problem 1.** The exact solution of the first problem is piecewise linear on the domain, thus it belongs to the finite dimensional subspace both for standard linear finite elements and extended finite elements (3.12). It will be shown that the numerical solution of the optimization process can reproduce the exact solution both with standard FE and extended FE.
Let us define $\Omega = F_1 \cup F_2$ and, being $x = (x, y, z)$, $F_1$ the fracture polygon defined as:

$$F_1 = \{ x \in \mathbb{R}^3 : -1 < x < 1, 0 < y < 1, z = 0 \}$$

and

$$F_2 = \{ x \in \mathbb{R}^3 : x = 0, 0 < y < 1, -1 < z < 1 \}.$$

The resulting domain $\Omega$ is similar to the domain depicted in Figure 2.1. Let be $S = F_1 \cap F_2$, the problem is set as follows:

$$\Delta h = 0 \quad \text{in} \ \Omega \setminus S, \quad (4.3)$$

$$h|_{\Gamma_D} = h_D \quad \text{on} \ \Gamma_D, \quad (4.4)$$

$$\frac{\partial h}{\partial n} = 0 \quad \text{on} \ \Gamma_N, \quad (4.5)$$

where $\Gamma_D = \Gamma_{D_1} \cup \Gamma_{D_2} \cup \Gamma_{D_3}$ is

$$\Gamma_{D_1} = \{ x \in \partial \Omega : x = -1, 0 \leq y \leq 1, z = 0 \}$$

$$\Gamma_{D_2} = \{ x \in \partial \Omega : x = 0, 0 \leq y \leq 1, z = -1 \}$$

$$\Gamma_{D_3} = \{ x \in \partial \Omega : x = 1, 0 \leq y \leq 1, z = 0 \} \cup \{ x \in \partial \Omega : x = 0, 0 \leq y \leq 1, z = 1 \}.$$
and
\[ \Gamma_N = \{ x \in \partial\Omega : -1 < x < 1, y = 0 \text{ or } y = 1, z = 0 \} \cup \{ x \in \partial\Omega : x = 0, y = 0 \text{ or } y = 1, -1 < z < 1 \}, \]

while \( \hat{n} \) is the unit outward vector normal to the boundary \( \Gamma_N \). The function \( h_D(\Gamma_D) \) is defined as:

\[
h_D = \begin{cases} 
1 & \text{on } \Gamma_{D_1} \\
1/2 & \text{on } \Gamma_{D_2} \\
0 & \text{on } \Gamma_{D_3}.
\end{cases}
\]

The exact solution \( h^{exact} \) of the problem is a piecewise linear function on each fracture, constant in the \( y \) direction, with a jump in the first order derivatives along the trace \( S = \{ x = 0, z = 0, 0 \leq y \leq 1 \} \):

\[
h^{\text{exact}}_{F_1} = \begin{cases} 
(3 - 5x)/8 & x \leq 0 \\
(3 - 3x)/8 & x > 0
\end{cases}
\]

\[
h^{\text{exact}}_{F_2} = \begin{cases} 
(3 - z)/8 & z \leq 0 \\
(3 - 3z)/8 & z > 0
\end{cases}
\]

Figure 4.1 shows the initial mesh used for the fractures \( F_1 \) and \( F_2 \) using standard finite elements, whereas Figure 4.2 is the initial mesh used with extended finite elements. The two meshes on \( F_1 \) and \( F_2 \) are not conforming but they induce the same partition on the trace and the minimum of the functional \( J \) computed with the discrete solution is still zero.

Figure 4.5 displays the \( L_2(\Omega) \) and \( H^1(\Omega) \) norm of the error during a uniform refinement process. The stopping criterion for the minimization process is \( J < 10^{-15} \). The target value was reached (and usually largely overcome) in a single iteration. As expected the error norms do not depend on the meshsize. Figures 4.3 and 4.4 display the solutions on \( F_1 \) and \( F_2 \) obtained with XFEM. Near the trace the numerical solution is plot on the sub-elements generated by cutting the XFEM elements along fractures.

**4.2. Problem 2.** The domain is the same as for problem 1. The problem in this case is given by:

\[
\Delta h = f \quad \text{in } \Omega \setminus S, \tag{4.6}
\]
\[
h_{|\Gamma_D} = 0 \quad \text{on } \partial\Omega. \tag{4.7}
\]
\[
(4.8)
\]

The forcing function \( f \) is defined as follows:

\[
f(x) = \begin{cases} 
6(y - y^2)|x| - 2(|x^3| - |x|) & \text{on } F_1 \\
-6(y - y^2)|z| + 2(|z^3| - |z|) & \text{on } F_2
\end{cases}
\]

and the exact solution is given by

\[
h^{\text{exact}}(x) = \begin{cases} 
-y(1 - y)|x|(x^2 - 1) & \text{on } F_1 \\
g(1 - y)|x|(x^2 - 1) & \text{on } F_2
\end{cases}
\]

The following nomenclature is used:
Problem 2: Solution with genXFEM on fracture 1 for intermediate grid

Problem 2: Solution with genXFEM on fracture 2 for intermediate grid

Problem 2: norm $L^2$ trend for different uniform grid refinements

Problem 2: norm $H^1(\Omega)$ trend for different uniform grid refinements
Figure 4.13. Problem 2: Condition number of algebraic system matrix for different uniform grid refinements

Figure 4.14. Problem 2: Degrees of freedom trend for different uniform grid refinements

Figure 4.15. Problem 2: Final functional values for different uniform grid refinements

Figure 4.16. Problem 2: Control variable and exact solution (intermediate grid)

Figure 4.17. Problem 2: Functional trend against iterations with standard FE (intermediate grid)

Figure 4.18. Problem 2: Functional trend against iterations with the XFEM (intermediate grid)
• **FEM**: Discretization with standard FEM: grid elements are aligned to the trace (Figure 4.6). The same grid is used in fractures $F_1$ and $F_2$;
• **XFEM**: Discretization with XFEM: same grid is used in $F_1$ and $F_2$ (Figure 4.7). The two meshes induce the same partition on the trace;
• **genXFEM**: Most general case: XFEM is used and the grids in $F_1$ and $F_2$ do not match on $S$ (Figure 4.8). In this case the minimum of the functional $J$ computed on the discrete solutions cannot vanish.

In Figures 4.9 and 4.10 the numerical solution obtained by the **genXFEM**-method are depicted.

Figures 4.11 and 4.12 display the behaviour of the $L^2$-norm and $H^1$-norm with respect to the meshsize $\delta_{\text{max}}$ during a uniform mesh refinement process. The slopes of the curves, denoted by $m$ in the labels agree with the expected values for $P^1$ elements also in the case of XFEM enrichment on both non-conforming grids considered.

**Remark 4.3.** The exact solution $h^{\text{exact}}(x) \notin H^2(F_i), i = 1, 2, h^{\text{exact}}(x)$ is a function of $H^2(f)$, being $f$ the generic sub-fracture on each of the two sides of trace $S$ in each fracture $F_i$. The convergence orders of Figures 4.11 and 4.12 are the expected ones for $h^{\text{exact}}(x) \in H^2(F_i)$. This is a known behaviour [13, 23].

Figure 4.13 displays the spectral condition number with respect to the mesh-size for each of the two problems on $F_1$ and $F_2$. The slopes of the curves well agree with the theoretical $(\delta_{\text{max}})^{-2}$ behaviour expected for all the considered methods: **FEM, XFEM** and **genXFEM**. Figure 4.14 shows that the enrichment basis functions do not impact on the number of degree of freedom of the problem.

The stopping tolerance in (3.13) for the minimization process is $\Delta \text{tol} < 1.0E^{-13}$. Figure 4.15 displays the final value of the functional when the stopping criterion is satisfied. In the **genXFEM** case the target minimum of the functional strongly depend on the mesh, and the slope of its curve shows a behaviour proportional to $(\delta_{\text{max}})^{3.7}$. In Figure 4.16 the parabolic exact value of $[\frac{\partial h}{\partial \nu}]_S$ is compared with the discrete value of the control variable $u_1$ obtained by the three simulations performed on intermediate grids.

In Figures 4.17-4.19 we see the behaviour of the functional value during the minimization process. We remark that no effort has been spent here for improving con-
4.3. Problem 3. For the third problem a more complex domain composed of three fractures has been considered: \( \Omega = F_1 \cup F_2 \cup F_3 \) (Figure 4.20). Fracture 1 lies on the \( x - y \) plane \((z = 0)\), with

\[
F_1 = \{ x \in \mathbb{R}^3 : 0 < x < 1, \ 0 < y < 2, \ z = 0 \}
\]

while fracture 2 and 3 are parallel to \( x - z \) plane, placed at \( y = 0.5 \) and \( y = 1.5 \) respectively:

\[
F_2 = \{ x \in \mathbb{R}^3 : 0 < x < 1, \ y = \frac{1}{2}, \ -\frac{1}{2} < z < \frac{3}{2} \}, \quad S_1 = F_1 \cap F_2
\]

and

\[
F_3 = \{ x \in \mathbb{R}^3 : 0 < x < 1, \ y = \frac{3}{2}, \ -\frac{3}{2} < z < \frac{1}{2} \}, \quad S_2 = F_1 \cap F_3.
\]

The problem is set as follows:

\[
\Delta h = f \quad \text{in } \Omega \setminus (S_1 \cup S_2) \quad \text{(4.9)}
\]

\[
h_{|\Gamma_D} = 0 \quad \text{on } \Gamma_D, \quad \text{(4.10)}
\]

\[
\frac{\partial h}{\partial \nu} = 0 \quad \text{on } \Gamma_N, \quad \text{(4.11)}
\]
where $\Gamma_N$ is

$$\Gamma_N = \{x \in \partial F_1 : y = 0\}$$

and $\Gamma_D = \partial \Omega \setminus \Gamma_N$, while $\hat{n}$ is as previously defined.

The forcing function $f$ is:

$$f(x) = \begin{cases} 1/2 & \text{on } F_1 \\ 0 & \text{on } F_2 \cup F_3. \end{cases}$$

The exact solution is not known in this case, and therefore we test results obtained with the XFEM on arbitrary matching grids (the case termed genXFEM in the previous problem) against standard FE on conformal matching grids. In Figures 4.21 and 4.24 we plot the solution obtained by XFEM and standard FE for the fracture 1, while in Figures 4.22 and 4.23 also the solution on the fractures 2 and 3 is displayed.

In Figures 4.25 and 4.26 the meshes for the fracture 1 are displayed.

In Figures 4.27-4.28 is shown the behaviour of the functional $J$ in the minimization process. As expected the functional related to the XFEM solution reaches a plateau.
corresponding to a non vanishing value when stopping criterion (3.13) is satisfied, but as shown in Figure 4.27 and 4.29 grid refinement can reduce the functional exit value, thus reducing global error. In particular, in Figure 4.29 the slope of the curve reveals a dependence of functional value at exit from grid parameter as \((\delta_{\text{max}})^{2.6}\). Despite the final value of the functional \(J\) in Figure 4.28 corresponding to standard FE is not vanishing, its value can be reduced up to machine precision for a larger value of the iterations.

4.4. Problem 4. In the last simulation we apply our method to a slightly more complex fracture configuration. We consider a system of seven rectangular fractures, in Figure 4.30 we plot the intersections of the fractures with the plane \(z = 0\). All the fractures have quotes \(z\) ranging from \(z = 0\) to \(z = 1\). In Figure 4.30 we denote by \(P_n, n = 1, \ldots, 14\) the starting and ending points of displayed intersections, by \(F_i, i = 1, \ldots, 7\) the intersection of the fractures with \(z = 0\) and by \(T_m, m = 1, \ldots, 11\) the intersections of the traces \(S_m\) with \(z = 0\).

The problem is set as follows:

\[
\begin{align*}
\Delta h &= 0 \quad \text{in } \Omega \setminus \mathcal{S} \\
h|_{\Gamma_D} &= y + \sqrt{z} \quad \text{on } \Gamma_D, \\
\frac{\partial h}{\partial \nu} &= 0 \quad \text{on } \Gamma_N.
\end{align*}
\]

(4.12)

(4.13)

(4.14)

where \(\mathcal{S} = \bigcup_{m=1, \ldots, 11} S_m\), \(\Gamma_D\) is the set of the edges spanning in the \(z\) direction that intersect \(z = 0\) in the points \(P_{13}, P_9, P_1, P_3, P_6, P_5\) and \(P_7\), whereas \(\Gamma_N\) is the set of all the other boundaries of the fractures.

For these simulations the exit criterion chosen as \(\Delta \text{tol}_J < 10^{-13}\) was not reached in the maximum number of iterations set to 800, being the difference between last two iteration in the range \(10^{-7} > \Delta J > 10^{-8}\) depending on grid refinement. In Fig-
ures 4.31-4.37 we plot the numerical solution on the fractures $F_i, i = 1, \ldots, 7$. All the meshes on the fractures are independently generated without requiring any conformity constraint along the traces. In order to exactly display the enriched numerical solution, it is plotted not on the computing elements but on sub-elements generated by cutting the computing elements along fractures, as in the previous examples. In Figure 4.38 we plot the behaviour of the functional during the minimization process, and in Figure 4.39 the final values. It can be seen that also in this case the minimum of the functional can be reduced by grid refinements.

4.5. Conclusions. In this paper we propose a new approach to the Discrete Fracture Network simulation circumventing all the difficulties related to a mesh generation process that ensures conformity along the system traces. Our approach is based on a PDE constrained optimality approach and is developed in order to be easily parallelized on massively parallel or GPU-based or hybrid parallel computers. The key aspect of this parallel approach are: the solution of many small problems and small exchange of data between the processors at each iteration.

Few simple numerical simulations prove the viability of the approach. A deeper
analysis of the performances of the method on more complex fractures configuration is under investigation, as well as an extension of the method in order to be easily applied to very general fracture configurations. Several improvements of the method can be introduced. In order to speed up the minimization process different descent method can be considered and different choices for the spaces $U^S$ and $H^S$ used in the numerical method as well as mesh dependent norms for the spaces $U^S = H^{-\frac{1}{2}}(S)$ and $H^S = H^\frac{1}{2}(S)$ should be investigated in future works [4].

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